PROPERTIES OF THE $S_N$-EQUIVALENT INTEGRAL TRANSPORT OPERATOR AND THE ITERATIVE ACCELERATION OF NEUTRAL PARTICLE TRANSPORT METHODS

A Thesis in
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by
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ABSTRACT

We have derived expressions for the elements of the matrix representing a certain angular ($S_N$) and spatial discretized form of the neutron integral transport operator. This is the transport operator that if directly inverted on the once-collided fixed particle source produces, without the need for an iterative procedure, the converged limit of the scalar fluxes for the iterative procedure. The asymptotic properties of this operator's elements have then been investigated in homogeneous and periodically heterogeneous limits in one-dimensional and two-dimensional geometries. The thesis covers the results obtained from this asymptotic study of the matrix structure of the discrete integral transport operator and illustrates how they relate to the iterative acceleration of neutral particle transport methods. Specifically, it will be shown that in one-dimensional problems (both homogeneous and periodically heterogeneous) and homogeneous two-dimensional problems, containing optically thick cells, the discrete integral transport operator acquires a sparse matrix structure, implying a strong local coupling of a cell-averaged scalar flux only with its nearest Cartesian neighbors. These results provide further insight into the excellent convergence properties of diffusion-based acceleration schemes for this broad class of transport problems. In contrast, the results of the asymptotic analysis for two-dimensional periodically heterogeneous problems point to a sparse but non-local matrix structure due to long-range coupling of a cell’s average flux with its neighboring cells, independent of the distance between the cells in the spatial mesh. The latter results indicate that cross-derivative coupling, namely coupling of a cell’s average flux to its diagonal neighbors, is of the same order as self-coupling and coupling with its first Cartesian neighbors. Hence they substantiate the conjecture that the loss of robustness of diffusion-based acceleration schemes, in particular of the Adjacent-cell Preconditioner (AP) considered in this work, in the presence of sharp material discontinuities in periodically heterogeneous multi-dimensional problems, is due to a structural deficiency of such low-order operators since they ignore cross-derivative coupling. This conjecture has been successfully verified by amending the AP formalism to account for cross-derivative coupling by the inclusion of matrix elements that account for the coupling of a
cell’s average flux to its first diagonal neighbors. Preliminary results of the Fourier analysis for the novel acceleration scheme indicate that robustness of the accelerated iterations can be recovered by accounting for cross-derivative coupling. The new acceleration scheme has also been implemented in a two-dimensional transport code and numerical results from the code have successfully verified the predictions of the Fourier analysis.
# TABLE OF CONTENTS

List of Figures . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . viii
List of Tables . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . xiii
Acknowledgements . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . xv

Chapter 1  Introduction . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 1
  1.1 Iterative Methods for Solving the Linear Neutron Transport Equation . . . 4
  1.2 Review of Results in One-Dimensional Geometry . . . . . . . . . . . . . 11
  1.3 Review of Results in Two-Dimensional Geometry . . . . . . . . . . . . . 19

Chapter 2  Review of Literature . . . . . . . . . . . . . . . . . . . . . . . . . . . 25

Chapter 3  Integral Transport Matrix in Homogeneous Slabs . . . . . . . . . . . . 37
  3.1 Introduction . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 37
  3.2 Direct Solution of the Transport Equation in Slab Geometry . . . . . . . . 39
  3.3 Expressions for Matrices $A$ and $B$ in Slab Geometry . . . . . . . . . . 46
    3.3.1 Inductive Derivation of the Elements of $A$ . . . . . . . . . . . . . 51
    3.3.2 Constructive Derivation of the Elements of $A$ . . . . . . . . . . . 61
    3.3.3 Numerical Verification . . . . . . . . . . . . . . . . . . . . . . . . 73
  3.4 Asymptotic Analysis for Homogeneous Slabs . . . . . . . . . . . . . . . 77
    3.4.1 Expressions for Matrices $A$ and $B$ in Homogeneous Slabs . . . . 79
    3.4.2 Asymptotic Analysis in the Thick Cell Limit . . . . . . . . . . . . 83
    3.4.3 Asymptotic Analysis in the Thin Cell Limit . . . . . . . . . . . . . 94
    3.4.4 Numerical Verification . . . . . . . . . . . . . . . . . . . . . . . . 102
  3.5 Truncation Strategies for the Integral Transport Matrix in Thick Slabs . . 107
    3.5.1 Neutron Balance . . . . . . . . . . . . . . . . . . . . . . . . . . . . 108
    3.5.2 Numerical Results . . . . . . . . . . . . . . . . . . . . . . . . . . . 118
  3.6 Truncation Strategies for the Integral Transport Matrix in Thin Slabs . . . 164
    3.6.1 Numerical Results . . . . . . . . . . . . . . . . . . . . . . . . . . . 171
  3.7 Conclusion . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 177

Chapter 4  Integral Transport Matrix in Periodically Heterogeneous Slabs . . . . . 179
  4.1 Introduction . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 179
  4.2 Symmetrization of the One-Dimensional Integral Transport Matrix . . . . 182
  4.3 Asymptotic Analysis for the Elements of Matrix $B^S$ . . . . . . . . . . 189
    4.3.1 Derivation of the Asymptotic Results for the Elements of Matrix $B^S$ . 196
    4.3.2 Numerical Verification . . . . . . . . . . . . . . . . . . . . . . . . 204
  4.4 Asymptotic Properties of the Cell-Averaged Scalar Fluxes . . . . . . . . 207
4.4.1 Asymptotic Results for the Elements of Matrix $\bar{A}$ . . . . . . . . . . . . . 211
4.4.2 Shuffling of the Cell-Averaged Scalar Fluxes for the Case $c_K = 1$ . . . 217
4.4.3 Shuffling of the Cell-Averaged Scalar Fluxes for the Case $c_K < 1$ . . 231
4.5 Transformation of $B^S$ into an Asymptotically Tridiagonal Matrix . . . . 236
4.6 Asymptotic Analysis of the Elements of Matrix $\hat{B}$ . . . . . . . . . . . . . 242
4.7 Numerical Results for Periodically Heterogeneous Slabs . . . . . . . . . . . . 246
4.8 Conclusion . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 252

Chapter 5 Integral Transport Matrix and AP Acceleration for Slabs . . . . . . . 256
5.1 Introduction . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 256
5.2 Recipe for the Construction of the AP Matrix . . . . . . . . . . . . . . . . 259
5.3 Asymptotic Analysis in the Thick Cell Limit for Homogeneous Slabs . . . 262
5.4 Asymptotic Analysis for Periodically Heterogeneous Slabs . . . . . . . . . . 274
5.5 Conclusion . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 292

Chapter 6 Integral Transport Matrix in Homogeneous Configurations in Two-
Dimensional Geometry . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 295
6.1 Introduction . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 295
6.2 Direct Solution of the Transport Equation in Two-Dimensional Geometry . 299
6.3 Expressions for Certain Elements of Matrix $B$ in Two-Dimensional
Geometry . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 310
6.4 An Algorithm for Computing the SI Jacobian Matrix in One Mesh-Sweep . 326
6.5 Expressions for Certain Elements of Matrix $B$ in Homogeneous
Configurations . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 334
6.6 Asymptotic Analysis in the Thick Cell Limit for Homogeneous
Configurations . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 337
6.6.1 Asymptotic Estimates for the Strength of Coupling with Far
Neighbors . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 340
6.6.2 Numerical Verification . . . . . . . . . . . . . . . . . . . . . . . . . . . . 352
6.7 Asymptotic Analysis in the Thin Cell Limit for Homogeneous
Configurations . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 355
6.8 Conclusion . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 368

Chapter 7 A Novel Synthetic Acceleration Scheme for the PHI Configuration in
Two-Dimensional Geometry . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 371
7.1 Introduction . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 371
7.2 Loss of Unconditional Robustness of the AP Scheme for the PHI
Configuration . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 377
7.2.1 The AP Formalism in Two-Dimensional Geometry . . . . . . . . . . . . 378
7.2.2 Fourier Analysis of the AP Scheme for the PHI Configuration . . . . . . 384
# LIST OF FIGURES

3.1 Order of sweeping a spatial mesh for $\mu_m > 0$ ........................... 41

3.2 Computational cells involved in the contribution to the $m$th discrete ordinate angular flux in cell $j + k$ from the scalar flux in cell $j$ ($\mu_m > 0$) ........................... 63

3.3 Outline of the procedure for computing the contribution to the $m$th discrete ordinate angular flux in cell $j + k$ from the scalar flux in cell $j$ ($\mu_m > 0$) .... 65

3.4 Sketch of constructive approach with coefficients to be multiplied to determine the influence from the scalar flux in a cell to the $m$th discrete ordinate angular flux in a downstream cell ($\mu_m > 0$) ........................... 68

3.5 Computational cells involved in the contribution to the $m$th discrete ordinate angular flux in cell $j + 1$ from the scalar flux in cell $j$ ($\mu_m > 0$) ........................... 70

3.6 Outline of the procedure for computing the contribution to the $m$th discrete ordinate angular flux in cell $j + 1$ from the scalar flux in cell $j$ ($\mu_m > 0$) .... 70

3.7 Model problem for the comparison between direct solutions from the inversion of matrix $B$ and iterative solutions obtained with SI ........................... 75

3.8 Model problem for the comparison between direct solutions from the inversion of matrix $B$ and iterative solutions obtained with FSM-DSA .... 76

3.9 $A$ matrix elements evaluated at varying cell thicknesses ........................... 103

3.10 $B$ matrix elements evaluated at varying cell thicknesses ........................... 104

3.11 Asymptotic behavior of matrix $A$ elements in the thin cell regime ................. 105

3.12 Asymptotic behavior of matrix $B$ off-diagonal elements in the thin cell regime ............................................. 105

3.13 Asymptotic behavior of matrix $B$ diagonal elements in the thin cell regime 106

3.14 Asymptotic behavior of matrix $B$ elements in the thick cell regime ................. 107

3.15 Procedure for the calculation of $\psi^\mu_{m,j}$ ............................................. 115

3.16 Flux difference for various $c$ for source distribution $1^{10}$ ........................... 122
3.17 Neutron balance difference for various c for source distribution $1^{10}$ . . . . . . 126
3.18 Flux difference for various truncation methods for source distribution $1^{10}$ . . 130
3.19 Neutron balance difference for various truncation methods for $1^{10}$ . . . . . 133
3.20 Flux difference for various c for source distribution $0^21^60^2$ . . . . . . . . 136
3.21 Neutron balance difference for various c for source distribution $0^21^60^2$ . . . 140
3.22 Flux difference for various truncation methods for source distribution $0^21^60^2$. 144
3.23 Neutron balance difference for various truncation methods for $0^21^60^2$. . . 147
3.24 Flux difference for various c for source distribution $0^41^20^4$ . . . . . . . . 150
3.25 Neutron balance difference for various c for source distribution $0^41^20^4$. . . 154
3.26 Flux difference for various truncation methods for source distribution $0^41^20^4$. 158
3.27 Neutron balance difference for various truncation methods for $0^41^20^4$. . . 161
3.28 Flux difference for various c for a thin slab . . . . . . . . . . . . . . . . . . 173
3.29 Neutron balance difference for various c for a thin slab . . . . . . . . . . . . 175

4.1 Configuration of the periodically heterogeneous slab . . . . . . . . . . . . . . . . 179
4.2 Structure of $B^S$ matrix for a periodically heterogeneous slab. . . . . . . . . . 190
4.3 Asymptotic behavior of matrix $B^S$ elements . . . . . . . . . . . . . . . . . . . 205
4.4 Asymptotic behavior of matrix $B^S$ elements (continued) . . . . . . . . . . . 206
4.5 Asymptotic structure of the $\bar{A}$ matrix . . . . . . . . . . . . . . . . . . . . 217
4.6 Asymptotic structure of the $B^S$ matrix . . . . . . . . . . . . . . . . . . . . . 223
4.7 Asymptotic structure of the $\bar{B}^S$ matrix . . . . . . . . . . . . . . . . . . . 225
4.8 Asymptotic structure of the $B'$ matrix . . . . . . . . . . . . . . . . . . . . . 226
4.9 Algebraic transformation for a system of six equations in the $B^S$ matrix. . . 240
4.10 Flux difference for a periodically heterogeneous slab .......................... 248
4.11 Neutron balance difference for a periodically heterogeneous slab ........ 250

5.1 Scalar flux residual at the second AP accelerated iteration for a homogeneous slab with \( c = 1 \) .......................................................... 269
5.2 Scalar flux residual at the second AP accelerated iteration for a homogeneous slab with \( c = 0.8 \) ...................................................... 270
5.3 Scalar flux residual at the second accelerated iteration for modified AP in a homogeneous slab with \( c = 0.8 \) ...................................................... 274

6.1 A three-by-three two-dimensional Cartesian sub-mesh .......................... 296
6.2 Order of sweeping a spatial mesh for \( \mu, \eta > 0 \) ............................... 306
6.3 Transport path for the calculation of \( B_{i,j,i+1,j} \) ............................... 318
6.4 Transport paths for the calculation of \( B_{i,j,i+1,j+1} \) ............................ 322
6.5 Transport paths for the calculation of \( B_{i,j,i+2,j} \) ............................... 323
6.6 Transport paths for the calculation of \( B_{i,j,i+2,j+1} \) ............................ 324
6.7 Transport paths for the calculation of \( B_{i,j,i+2,j+2} \) ............................ 324
6.8 Transport paths for the calculation of \( B_{i,j,i+2,j+2} \) (continued) ......... 325
6.9 Dominant transport path contributing to the leading order of \( B_{i,j,i+2,j+2} \) in the thick cell limit ......................................................... 343
6.10 Dominant transport path contributing to the leading order of \( B_{i,j,i+2,j+1} \) in the thick cell limit ......................................................... 343
6.11 Dominant transport path contributing to the leading order of \( B_{i,j,i+2,j} \) in the thick cell limit ......................................................... 344
6.12 Dominant (solid lines) and weakest paths for a purely diagonal third neighbor in the thick cell limit ........................................ 347

6.13 Dominant paths for the non-purely diagonal third neighbors in the thick cell limit .......................................................... 349

6.14 Summary of asymptotic results for the homogeneous thick cell limit ................................................................. 351

6.15 Numerical verification of $B$ matrix elements asymptotic behavior in the thick cell limit for up to the second neighboring cells ........................................ 353

6.16 Numerically computed values of $B$ matrix elements for the third neighbors in the thick cell limit ........................................ 354

6.17 Numerically computed values of $B$ matrix elements for the fourth neighbors in the thick cell limit ........................................ 355

6.18 Additive order of $\gamma$ coefficients for $B_{i,j=1+2,i+1}$ for rectangular cells in the thin cell limit ........................................ 362

6.19 Asymptotic results in the thin cell limit for a quadrature of order $n > 2$ ........................................ 364

6.20 Dominant paths for a purely diagonal third neighbor in the thin cell limit for the $S_2$ quadrature and a square mesh ........................................ 366

6.21 Dominant paths for the other third neighbors in the thin cell limit for the $S_2$ quadrature and a square mesh ........................................ 367

6.22 Asymptotic results in the thin cell limit for $S_2$ quadrature and a square mesh ........................................ 368

7.1 Periodic Horizontal Interface (PHI) Configuration ........................................ 371

7.2 Two-cell system for the Fourier analysis of the PHI configuration ........................................ 385

7.3 Spectral radius of SI for a PHI configuration with $c_k = c_N = 0.99999999$ ........................................ 391

7.4 Spectral radius of AP for a homogeneous configuration with $c = 0.99999999$ ........................................ 396

7.5 Spectral radius of AP for a PHI configuration with $c_k = c_N = 0.99999999$ ........................................ 399

7.6 A 6×6 PHI configuration with all periodic boundary conditions ........................................ 402
7.7 Maximum eigenvalue of AP for a 6×6 and a 6×2 PHI configurations
\( c_K = c_N = 0.99999999 \) .................................................... 404

7.8 A 2×6 PHI configuration with all periodic boundary conditions .......... 405

7.9 First and second neighboring cells for cell \((i,j)\) in a thick layer ............... 409

7.10 Strength of coupling of a thick cell’s average flux with its neighbors for PHI . 412

7.11 Dominant paths connecting a thick cell to the cells in the next thick layer . . 413

7.12 First and second neighboring cells for cell \((i,j)\) in a thin layer ............... 414

7.13 Strength of coupling of a thin cell’s average flux with its neighbors for PHI . 417

7.14 Spectral radius of APB for a PHI configuration with \( c_K = c_N = 0.99999999 \) . 429

A.1 Spectral radius of AP for the JCP scaling of the PHI configuration with
\( c_K = c_N = 0.9999 \) ................................................................. 457

A.2 Maximum eigenvalue of AP for a 6×6 and a 6×2 PHI configurations with
periodic boundary conditions for the JCP scaling \( (c_K = c_N = 0.9999) \) ....... 458

A.3 Strength of coupling of a thick cell’s average flux with its neighbors for the
JCP scaling of PHI ................................................................. 461

A.4 Numerical verification of B asymptotic behavior predicted in Fig. A.3 ........ 461

A.5 Strength of coupling of a thin cell’s average flux with its neighbors for the
JCP scaling of PHI ................................................................. 462

A.6 Numerical verification of B asymptotic behavior predicted in Fig. A.5 ........ 462

A.7 Error as a function of \( J \) for the case \( \Delta = J^2 \) ................................. 472

A.8 Error as a function of \( J \) for the case \( \Delta = J \) ................................. 473

A.9 Error as a function of \( J \) for the case \( \Delta = J^{1/2} \) ................................. 474
xiii

LIST OF TABLES
3.1

Comparison between solutions from direct inversion of matrix B for the
model problem in Fig. 3.7 and iterative solutions obtained with SI for
decreasing values of the convergence criterion ε . . . . . . . . . . . . . . . . 75

3.2

Comparison between solutions from direct inversion of matrix B for the
model problem in Fig. 3.8 and iterative solutions obtained with FSM-DSA
for decreasing values of the convergence criterion ε . . . . . . . . . . . . . . 76

4.1

Cell-averaged fluxes for a periodically heterogeneous slab with cK = 1 . . . . 209

4.2

Cell-averaged fluxes for a periodically heterogeneous slab with cK = 0.5 . . . 209

5.1

Number of AP accelerated iterations for a homogeneous slab with c = 1 . . . 266

5.2

Number of AP accelerated iterations for a homogeneous slab with c = 0.8 . . 267

5.3

Scalar flux residual at the second AP accelerated iteration for a
homogeneous slab with c = 1 . . . . . . . . . . . . . . . . . . . . . . . . . . 268

5.4

Scalar flux residual at the second AP accelerated iteration for a
homogeneous slab with c = 0.8 . . . . . . . . . . . . . . . . . . . . . . . . . 268

5.5

Number of modified AP accelerated iterations for a homogeneous slab with
c = 0.8 . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 273

5.6

Number of AP accelerated iterations for a periodically heterogeneous slab
for very large Δ . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 285

5.7

Number of modified AP accelerated iterations and scalar flux residual at the
second iteration for the case cK = 1.0 and cN = 1.0 . . . . . . . . . . . . . . . 290

5.8

Number of modified AP accelerated iterations and scalar flux residual at the
second iteration for the case cK = 0.8 and cN = 0.8 . . . . . . . . . . . . . . 290

5.9

Number of modified AP accelerated iterations and scalar flux residual at the
second iteration for the case cK = 0.8 and cN = 0.5 . . . . . . . . . . . . . . 291


xiv
5.10 Number of modified AP accelerated iterations and scalar flux residual at the
second iteration for the case cK = 1.0 and cN = 0.5 . . . . . . . . . . . . . . 291
7.1

Spectral radius of AP for a homogeneous configuration ( c = 0.99999999 ) . . 397

7.2

Number of AP iterations for a homogeneous configuration
( c = 0.99999999 ) . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 398

7.3

Spectral radius of AP for a PHI configuration ( cK = cN = 0.99999999 ) . . . . 400

7.4 Number of AP iterations for a PHI configuration ( cK = cN = 0.99999999 ) . . 401
7.5

Maximum eigenvalue of AP for longitudinal modes of increasing frequency . 406

7.6

Maximum eigenvalue of APB for longitudinal modes of increasing
frequency . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 426

7.7 Spectral radius of APB for a PHI configuration ( cK = cN = 0.99999999 ) . . . 435
7.8 Number of APB iterations for a PHI configuration ( cK = cN = 0.99999999 ) . 436
A.1 Maximum eigenvalue of AP for longitudinal modes of increasing frequency
for the JCP scaling of PHI . . . . . . . . . . . . . . . . . . . . . . . . . . . 459
A.2 Spectral radius of SI for the JCP scaling of PHI (cK = cN = 0.9999) . . . . . . 465
A.3 Number of SI iterations for the JCP scaling of PHI (cK = cN = 0.9999) . . . . . 466


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Chapter 1

Introduction

One of the goals of nuclear computational science is to simulate, accurately and efficiently, the particle and radiation transport processes involved in the interaction of radiation with matter. In numerous applications in Nuclear Engineering, e.g. reactor core design and shielding, it is necessary to obtain a detailed quantitative description of transport processes in which neutral particles (typically neutrons and photons) interact directly with the dense atoms and nuclei of a host material. From a mathematical point of view such transport processes are usually described in terms of a linear integro-differential equation, unless non-linear phenomena are explicitly taken into account in the transport model. One of these non-linear phenomena is represented, for example, by the temperature dependence of the material’s cross-sections, quantities that express the probabilities of various interactions a particle may undergo with the host material.

The solution of the equation describing a general-geometry radiation transport problem is a function of seven independent scalar variables: three spatial variables ($x$, $y$ and $z$ in Cartesian geometry), two angular or direction-of-flight variables ($\mu = \cos \theta$ and $\gamma = \phi$, the polar angle, $\gamma$ = azimuthal angle), one energy or speed variable ($E$ or $v$), and the time variable ($t$). To introduce the basic concepts a steady-state, one-speed, non-multiplying (no fission) neutron transport problem characterized by isotropic scattering
and with isotropic fixed neutron source is considered in planar (or infinite slab) geometry:

\[ \mu \frac{\partial \psi}{\partial x}(x, \mu) + \sigma(x)\psi(x, \mu) = \frac{\sigma_s(x)}{2} \int_{-1}^{+1} \psi(x, \mu') d\mu' + \frac{Q(x)}{2}, \]  

(1.1)

\[ 0 < x < X, \quad -1 \leq \mu \leq +1 \]

Vacuum boundary conditions, i.e. no incoming particles, are assumed on both edges of the slab that extends from 0 to \( X \):

\[ \begin{cases} 
\psi(0, \mu) = 0, & 0 < \mu \leq +1 \\
\psi(X, \mu) = 0, & -1 \leq \mu < 0 
\end{cases} \]  

(1.2)

The notation in Eq.s (1.1) and (1.2) is standard: \( x \) denotes the spatial variable, \( \mu = \cos \theta \) is the cosine of the neutron angle-of-flight \( \theta \) relative to the positive \( x \) axis, \( \sigma(x) \) and \( \sigma_s(x) \) represent the macroscopic total cross-section and macroscopic scattering cross-section, respectively, and \( Q(x) \) is the isotropic fixed source distribution. The unknown function of two variables \( \psi(x, \mu) \) represents the to-be-determined neutron angular flux.

Despite the simplifications that have been introduced in writing Eq. (1.1), the solution of the neutron transport equation, even when carried out by numerical means, represents a formidable task. While the numeric algorithms that have been developed to date may be broadly classified as either stochastic (Monte Carlo) or deterministic, the focus in this work is on deterministic methods.
In deterministic algorithms the linear neutron transport equation is discretized into a typically large system of linear algebraic equations. The resulting discrete system of equations is then solved numerically. Since the system is typically large in size, direct solution methods are impractical and the recourse to iterative methods is therefore necessary. Desirable properties sought in the development of efficient iterative algorithms are: unconditional stability, robustness and rapid convergence.

The development of efficient iterative methods for solving deterministic transport problems presents different mathematical requirements and difficulties depending on the discretization method that is employed for the angular (direction-of-flight) variable. In the development of this effort, the angular variable will be discretized using the discrete ordinates (SN) approximation. This approximation consists of requiring Eq. (1.1) to hold only for a number \( M \) of distinct angles \( \mu_m \) and then applying a compatible approximation (quadrature with specified weights \( w_m \)) to the integral term appearing on the right hand side. The iterative methods discussed in the following have been specifically developed for this angular discretization and do not apply to other angular discretizations, such as the spherical harmonics or \( P_N \) approximation, which possess different mathematical properties and inherent difficulties.

The development of efficient iteration schemes for \( S_N \) problems has been carried out by many researchers since the early 1960’s and has led to dramatic theoretical and practical successes. In the present day, it is almost unthinkable to compose a large-scale \( S_N \) particle transport code that does not employ a reasonably efficient iterative method.
Nevertheless, the development of such methods is not easy and significant difficulties and open issues remain.

1.1 Iterative Methods for Solving the Linear Neutron Transport Equation

The most basic iteration scheme originally proposed for the solution of the linear neutron transport equation is Source Iteration (SI). The essential features of this iterative scheme can be discussed in the simpler setting of the continuous equations previously introduced, avoiding the details and complications involved in their angular and spatial discretizations. To further simplify notation, it is convenient to write Eq. (1.1) in compact operator form by defining:

\[ L = \mu \frac{\partial}{\partial x} + \sigma(x) = \text{“streaming plus collision” operator}, \tag{1.3} \]

\[ P = \frac{1}{2} \int_{-1}^{+1} (\cdot) d\mu' = \text{“angular-averaging” operator}, \tag{1.4} \]

\[ q(x) = \frac{Q(x)}{2} \tag{1.5} \]

In view of the assumption of isotropic scattering it is also convenient to recall the definition of the scalar flux:

\[ \phi(x) = \frac{1}{2} \int_{-1}^{+1} \psi(x, \mu') d\mu' = P \psi \tag{1.6} \]
Consequently, Eq. (1.1) may be expressed in the following form:

\[ \mathbf{L} \psi = \sigma_s \phi + q \]  

(1.7)

The SI iterative scheme is then defined mathematically by:

\[ \mathbf{L} \psi^{(\ell+1)} = \sigma_s \phi^{(\ell)} + q, \quad \ell \geq 0 \]  

(1.8)

where \( \phi^{(0)} \) is an initial guess specified by the user.

From an algorithmic point of view, the SI scheme is implemented in the following way. At the beginning of each iteration step, an “old” estimate of the neutron scalar flux is introduced on the right hand side of Eq. (1.8). Using this estimate, Eq. (1.8) is solved with appropriate boundary conditions to obtain an estimate for \( \psi^{(\ell+1)} \), which is then employed to obtain the “new” estimate \( \phi^{(\ell+1)} \) via Eq. (1.6). The composition of these two steps leads to the following expression for \( \phi^{(\ell+1)} \):

\[ \phi^{(\ell+1)} = \mathbf{A} \left( \sigma_s \phi^{(\ell)} + q \right), \quad \ell \geq 0 \]  

(1.9)

In this way the SI scheme is finally formulated in terms of scalar flux only, a consequence of the original assumption of isotropic scattering that will be maintained throughout this work. The operator \( \mathbf{A} = \mathbf{P} \mathbf{L}^{-1} \), introduced on the right hand side of Eq. (1.9), resulting from the integration over all angular directions of the inverse of the “streaming plus collision” operator:

\[ \mathbf{A} \left( \sigma_s \phi^{(\ell)} + q \right) = \frac{1}{2} \int_{-1}^{+1} \left[ \mu' \frac{\partial}{\partial \mu} + \sigma \right]^{-1} \left( \sigma_s \phi^{(\ell)} + q \right) d\mu', \]  

(1.10)

may be interpreted as an “iteration” operator for the SI scheme.
The iterative process defined by Eq. (1.9), starting with the initial guess \( \phi^{(0)} \), is repeated until the difference between two successive scalar flux estimates is less than a pre-assigned convergence criterion, or an upper limit on the number of iterations is reached. If the initial SI guess for the scalar flux is \( \phi^{(0)} = 0 \), then for \( \ell \geq 1 \) it can be shown that [1]:

\[
\phi^{(\ell)}(x) = \text{the scalar flux due to particles that have scattered at most } (\ell - 1) \text{ times.}
\]

Thus, for problems in which particles undergo few collisions before dissipating, the SI scheme converges rapidly. Such conditions are encountered in small systems dominated by leakage (where particles are likely to exit through the outer boundary after a few collisions), or in systems of arbitrary size dominated by absorption (where particles are likely to be captured after a few collisions).

However, for systems containing “diffusive” spatial regions that are optically thick (the probability of leakage is small) and scattering dominated (the probability of capture is small), a significant number of particles undergoes many collisions before being captured or leaking out. For such systems, the SI algorithm converges slowly, hence is inefficient and expensive, and may potentially lead to the phenomenon of false convergence. Namely the magnitude of the difference between the final iterate, satisfying a pre-assigned convergence criterion, and the iteration limit of the solution, \( \phi \equiv \phi^\infty \), can far exceed that convergence criterion [1]. Since many important applied problems are indeed characterized by “diffusive” regions that are optically thick, it has long been desired to speed up, or accelerate, the iterative convergence of SI.
In an effort to develop more efficient iteration strategies, transport researchers in the 1960’s explored two basic paths. One path has traditionally become known as synthetic acceleration. The other is instead constituted by a class of rapidly convergent methods that are not true acceleration methods, because they do not necessarily produce the same discrete solution as the SI scheme [1]. For this reason, this latter class of methods is not relevant for the motivation of this work and will not be considered further.

In synthetic acceleration schemes, one single source iteration, Eq. (1.9), is considered as the first stage of (at least) a two-stage iteration process. In this connection, $\phi^{(\ell+1/2)}$ is defined as the result of this single source iteration:

$$\phi^{(\ell+1/2)} = A\left(\sigma_s \phi^{(\ell)} + q\right), \quad \ell \geq 0$$  \hspace{1cm} (1.12)

It is then necessary to formulate an equation for $\phi^{(\ell+1)}$. The goal is for $\phi^{(\ell+1)}$ to be a significantly more accurate approximation to $\phi$ than is $\phi^{(\ell+1/2)}$. This is accomplished in the synthetic method by at first subtracting from Eq. (1.7) the following:

$$L\psi^{(\ell+1/2)} = \sigma_s \phi^{(\ell)} + q$$  \hspace{1cm} (1.13)

The resulting equation is:

$$L\left(\psi - \psi^{(\ell+1/2)}\right) = \sigma_s \left(\phi - \phi^{(\ell)}\right)$$  \hspace{1cm} (1.14)

The latter equation may be used as a starting point for obtaining an exact equation for the additive correction $\left(\phi - \phi^{(\ell+1/2)}\right)$. First, $\phi^{(\ell+1/2)}$ is added and subtracted inside the parentheses on the right hand side of Eq. (1.14) and the “streaming plus collision” operator is inverted on the right hand side:
\[
\left( \psi - \psi^{(t+1/2)} \right) = L^{-1} \sigma_s \left( \phi - \phi^{(t+1/2)} \right) + L^{-1} \sigma_s \left( \phi^{(t+1/2)} - \phi^{(t)} \right)
\]

(1.15)

Applying the “angular-averaging” operator to both sides of this equation and using the definition of the “iteration” operator \( A \), the following exact equation is obtained for the additive correction \( \phi - \phi^{(t+1/2)} \):

\[
(I - A \sigma_s) \left( \phi - \phi^{(t+1/2)} \right) = A \sigma_s \left( \phi^{(t+1/2)} - \phi^{(t)} \right),
\]

(1.16)

where \( I \) is the identity operator.

The operator appearing on the left hand side of Eq. (1.16) is the integral transport operator \([2]\) and will be denoted in the following using the symbol:

\[
B = I - A \sigma_s
\]

(1.17)

The integral transport operator is then inverted on the right hand side of Eq. (1.16) and the equation solved for \( \phi \):

\[
\phi = \phi^{(t+1/2)} + B^{-1} A \sigma_s \left( \phi^{(t+1/2)} - \phi^{(t)} \right)
\]

(1.18)

In this way the exact solution \( \phi \) is defined in terms of the iterate \( \phi^{(t+1/2)} \) and the additive correction \( \left( \phi^{(t+1/2)} - \phi^{(t)} \right) = \Delta \phi^{(t+1/2)} \). Unfortunately, Eq. (1.18) requires the inversion of the full integral transport operator \( B \), a task that is as complicated as solving for \( \phi \) the original transport problem defined by Eq. (1.7) that may be formulated in the following equivalent integral form known as the integral transport equation \([2]\):

\[
B \phi = A q
\]

(1.19)
Hence, if the inversion of the full integral transport operator could be done efficiently then one would more directly solve Eq. (1.19) for the scalar flux in the first place. The idea behind synthetic acceleration is to replace $B$ by a “low-order” approximation:

$$M = B,$$  \hspace{1cm} (1.20)

for which $M^{-1}A\sigma_s \Delta \phi^{(r+1/2)}$ is easier to evaluate than $B^{-1}A\sigma_s \Delta \phi^{(r+1/2)}$. The equation for the additive correction, Eq. (1.18), is therefore approximated by:

$$\phi^{(r+1)} = \phi^{(r+1/2)} + M^{-1}A\sigma_s \left( \phi^{(r+1/2)} - \phi^{(r)} \right)$$  \hspace{1cm} (1.21)

The synthetic acceleration scheme is now defined by Eq. (1.12) and Eq. (1.21). The former equation represents the high-order equation; the latter uses a low-order approximation for the exact additive correction to $\phi^{(r+1/2)}$. It is straightforward to show that no matter how the low-order operator $M$ is defined, if the synthetic scheme converges then the converged solution must satisfy the original transport equation [1].

Different choices of the low-order operator $M$ yield different synthetic acceleration schemes. If Eq. (1.20) holds, then Eq. (1.21) is nearly the same as Eq. (1.18), so $\phi^{(r+1)}$ is very “close” to $\phi$, and convergence should be rapid. However, a practical requirement that conflicts with Eq. (1.20) is that $M^{-1}A\sigma_s \Delta \phi^{(r+1/2)}$ should be much less costly to evaluate than $B^{-1}A\sigma_s \Delta \phi^{(r+1/2)}$. Thus, the low-order approximation $M$ should be “close” to the high-order operator $B$, but far simpler to invert.

While on the subject, it is worthwhile noting that the mathematical structure of SI and synthetic acceleration schemes can be further clarified by showing that they can be
formulated as Richardson and Preconditioned Richardson matrix iteration schemes. In other words, the concept of synthetic acceleration is mathematically equivalent to the concept of preconditioning, a term more commonly employed in the mathematical community to designate this technique for the acceleration of iterative methods for the solution of large linear algebraic systems.

The low-order operators considered in the vast majority of iterative methods implemented to date, notably in Diffusion Synthetic Acceleration (DSA) schemes and in the more recently developed schemes based on Adjacent-Cell Preconditioners (AP), are of a diffusive-type. These methods have yielded extremely good results, in terms of rate of convergence, in problems characterized by a high degree of homogeneity and low neutron absorption, both in one-dimensional and multi-dimensional problems. Historically, the development of DSA schemes has actually marked the difference between being able to solve the neutron transport equation within a reasonable computational time and not being able to solve it at all.

Nonetheless, currently open issues have arisen when these preconditioning schemes are employed in the treatment of heterogeneous problems characterized by the presence of sharp material discontinuities. These problems may, for example, be encountered in periodically heterogeneous structures in which optically thick computational cells are alternated with optically thin cells in a repeated pattern, the optical thickness of a cell being proportional to the number of neutron mean free paths (MFP = 1/\(\sigma\)) contained in the cell width.

Of course periodically heterogeneous structures represent only a particular instance of heterogeneity. Nonetheless, and given the impossibility of treating all kinds of
heterogeneity in a general way, a particular emphasis is given in this effort to this kind of structures. For one thing, they well model situations of interest from an applied standpoint (e.g., fuel-moderator arrangement in reactor cores). Also, many previous results are available on the behavior of acceleration methods for periodically heterogeneous model problems. Therefore, even when not explicitly stated, the discussion and results presented in the following will refer to periodically heterogeneous structures. It is hoped that the obtained results may eventually lead to a more complete understanding and resolution of issues arising in the presence of other kinds of heterogeneities. At the same time, we are aware that much caution will have to be exercised in extending results that are true for periodically heterogeneous structures to other kinds of heterogeneity.

1.2 Review of Results in One-Dimensional Geometry

Distinctly different issues are raised according to the dimensionality of the problem considered. In particular, the features observed in one-dimensional geometry are different than those found in multi-dimensional geometry and need a separate discussion.

In the case of one-dimensional geometry, both DSA schemes and AP schemes have proved to be successful in reducing the number of iterations necessary to achieve convergence even in treating problems characterized by the presence of sharp material discontinuities. In other words, no significant deterioration in the convergence rate of these acceleration schemes has been observed in numerical tests conducted on
heterogeneous structures, even in the presence of unbounded discontinuities in the optical properties of adjacent cells.

This positive result appears to be somehow puzzling in terms of mathematical-physics intuition. This may be understood observing, on one hand, that the spatially-discretized low-order diffusive operators that are employed in DSA and AP schemes are characterized by a tridiagonal matrix structure. This mathematical property translates, on physical grounds, into the fact that only the coupling between two adjacent cells is important in determining the (suitably averaged) neutron scalar fluxes for the computational cells in the slab spatial grid.

On the other hand, in the case of a periodically heterogeneous slab, in which optically thick cells are alternated with thin cells in a repeated pattern, physical intuition suggests that the coupling between two optically thick cells, separated by an interposed thin cell, should be strong. This physical intuition translates, on mathematical grounds, in the expectation that a suitable matrix structure for the low-order operator employed in the acceleration scheme should actually be pentadiagonal. How can this expectation be reconciled with the successful results of acceleration schemes that are based on low-order operators characterized by a tridiagonal diffusion-like coupling stencil? Finding an answer to the previous question has led to the motivation for the preliminary work carried out as part of this research effort, namely obtaining a basic understanding of the success of tridiagonal low-order operators traditionally employed in acceleration schemes in one-dimensional problems.

The fundamental result obtained in this work is that the tridiagonal structure of these low-order operators represents a good approximation of the full transport operator
not only for optically thick homogeneous slabs but also in the case of periodically heterogeneous slabs, comprised of optically thick and thin computational cells. The methodological approach followed to obtain this result is based on the construction and study of the asymptotic properties of the matrix elements of the one-dimensional $S_N$-equivalent integral transport operator. As evident from Eq. (1.19), this is the transport operator that, if directly inverted on the once-collided fixed sources, would directly produce, without the need for an iterative procedure, the limit of the iterative procedure for the scalar fluxes.

The construction of the matrix elements of the integral transport operator can be carried out using as a starting point the SI formulation. The governing equations comprise the two sets of equations constituting the Weighted Diamond Difference (WDD) spatially-discretized form of the one-group, steady-state, discrete ordinates approximation of the neutron transport equation in slab geometry. Again, a non-multiplying system with isotropic scattering and isotropic fixed source is assumed.

The first set of equations represents a per cell statement of the balance of sources and sinks of neutrons that, in the most basic iterative approach to the solution of the transport equation, namely SI, may be expressed in the following form:

$$
\kappa_{m,j} \left[ \phi_{m,j}^{o,(+1)} - \phi_{m,j}^{i,(+1)} \right] + \phi_{m,j}^{l,(+1)} = c_j \tilde{\phi}_j^{(f)} + s_j, \quad m = 1, \ldots, M; \quad j = 1, \ldots, J
$$

(1.22)

In these equations, $\phi_{m,j}^{l,(+1)}$ is the present iterate of the $m^{th}$ discrete ordinate angular flux averaged over cell $j$; $\phi_{m,j}^{o,(+1)}$ and $\phi_{m,j}^{i,(+1)}$ are the present iterates of the $m^{th}$ discrete ordinate angular flux evaluated at the outgoing and incoming edges of cell $j$, respectively.
respectively; \( \bar{\phi}_j^{(t)} \) is the previous iterate of the scalar flux averaged over cell \( j \); 
\( s_j = q_j / \sigma_j \) is the ratio of the fixed neutron source density averaged over cell \( j \) to the macroscopic total cross-section in cell \( j \); \( \kappa_{m,j} \) has been introduced to denote the reciprocal of the optical thickness of cell \( j \):

\[
\kappa_{m,j} = \left( \frac{\sigma_j \Delta x_j}{\mu_m} \right)^{-1}, \quad m = 1, \ldots, M; \quad j = 1, \ldots, J \tag{1.23}
\]

In the previous relation \( \mu_m \) is the cosine of the \( m \)th discrete ordinate direction; \( \Delta x_j \) is the size of computational cell \( j \). The macroscopic scattering cross-section for cell \( j \) will be indicated by the symbol \( \sigma_{S_j} \) and the coefficient \( c_j \) in Eq. (1.22) represents the scattering ratio, \( \sigma_{S_j} / \sigma_j \), for cell \( j \).

Equation (1.22) is exact in the sense that it is obtained by direct integration of the continuous transport equation and using standard definitions of the cell-averaged flux and source. The terms on the left hand side of Eq. (1.22) represent the loss of neutrons from cell \( j \) by streaming and collisions, while the terms on the right hand side represent the sources from isotropic scattering, and external fixed sources, respectively.

The second set of equations in a generic WDD form of the discrete-variable transport equation provides an additional weighted-difference relation between the cell-averaged and cell-edge flux variables:

\[
\hat{\psi}_m^{(+1)} = \left( \frac{1 + \alpha_{m,j}}{2} \right) \hat{\psi}_m^{(+1)} + \left( \frac{1 - \alpha_{m,j}}{2} \right) \hat{\psi}_m^{(-1)} \quad m = 1, \ldots, M; \quad j = 1, \ldots, J \tag{1.24}
\]
The dependence of the spatial weights \( \alpha_{m,j} \in [0,1] \) on the problem parameters is determined by the formalism of the underlying numerical spatial discretization method or simplifying assumptions applied directly to Eq. (1.24). For example, Eq. (1.24) readily incorporates the thin cell Diamond Difference (DD) approximation corresponding to \( \alpha_{m,j} = 0 \), equivalent to expanding the flux within cell \( j \) in a Taylor series expansion truncated at order two. The Step method assumes, instead, a thick cell where the exponential decay of the incoming cell-edge flux is such that the outgoing flux may be identified with the cell-averaged flux, hence \( \alpha_{m,j} = 1 \).

The results that will be presented in the following have been obtained using the Arbitrarily High Order Transport method of the Nodal type and 0-order spatial approximation (AHOT-N0). It is the lowest spatial expansion order member of a class of spatial discretization methods whose order denotes the truncation order of the Legendre spatial-expansion of the flux within each cell, and in multi-dimensional cases on cell edges also [3]. The spatial weights for the AHOT-N0 are given by [3]:

\[
\alpha_{m,j} = \text{coth} \left( \frac{1}{2 \kappa_{m,j}^r} \right) - 2 \kappa_{m,j}^r, \quad m = 1,\ldots,M; j = 1,\ldots,J \quad (1.25)
\]

In Eq. (1.25) the spatial weights are a function of the cell width \( \Delta x_j \), via Eq. (1.23). It can be shown that the spatial weights in the AHOT-N0 formulation approach 0 in the limit as \( \Delta x_j \to 0 \), giving the same weights in the thin cell limit as the DD method. Also, they approach 1 in the limit as \( \Delta x_j \to \infty \), so that in the thick cell limit the same weights are obtained as in the Step method.
The solution of the two sets of equations, Eqs. (1.22) and (1.24), for a given cell-averaged scalar flux, i.e., initial guess or previous iterate, along one discrete ordinate over the entire spatial mesh is conducted via the classical “mesh-sweep” algorithm, the discrete implementation of a transport sweep (see Sec. 3.2).

The composition of the mesh-sweep operator with the summation over angles operator that yields the cell-averaged scalar fluxes can be viewed as a linear mapping of the scalar fluxes from the previous iteration to the present iteration. This can be expressed using the following compact matrix notation:

\[
\begin{align*}
\phi^{(f+1)} &= A\left(\sigma_s\phi^{(f)} + q\right) \\
&= A\phi^{(f)} + Aq
\end{align*}
\]  

(1.26)

In Eq. (1.26), \( \phi^{(f)} \) and \( \phi^{(f+1)} \) are vectors containing the old and new iterates of the cell-averaged scalar fluxes, respectively, each of length \( J \), the number of computational cells in slab geometry; \( \sigma_s \) is a diagonal matrix whose non-zero elements are the \( J \) macroscopic scattering cross-sections; \( q \) is a \( J \)-dimensional vector of the cell-averaged fixed neutron source density. Matrix \( A \) is the iteration matrix originating from the angular and spatial discretization of the continuous iteration operator \( A \) previously defined in Sec. 1.1. Of particular interest is considering the form assumed by Eq. (1.26) when the iterative scheme converges. Indicating with \( \phi^{\infty} \) the limit of the iterates of the scalar flux vector, the following result is obtained:

\[
B\phi^{\infty} = Aq,
\]

(1.27)

where matrix \( B \), representing the discretized one-dimensional integral transport operator, has been defined as:
In Eq. (1.28), $\mathbf{I}$ is the $J$–dimensional identity matrix. Thus Eq. (1.27) is the discrete approximation to the integral transport equation, Eq. (1.19), that we seek.

A comparison of the matrix structure of the low-order operators traditionally employed in acceleration schemes with the asymptotic structure acquired by the integral transport operator in limits of interest, is expected to shed light on the effectiveness of these algorithms in reducing the number of iterations necessary to achieve convergence for one-dimensional problems. This structural comparison may be intended as a direct comparison, particularly in the presence of optically thick computational cells, with reference to the AP preconditioner. As it will be explained in the following chapter, the expressions for the matrix elements of this low-order operator are asymptotically related to the diagonal and first off-diagonal elements of the discrete integral transport operator. In the case of DSA, though, no such direct relationship exists since this low-order operator is based on a consistent diffusion prescription. Any conclusion valid for the AP preconditioner may eventually be extended to DSA but only if properly mediated through the relationship between integral transport theory and diffusion theory. The investigation of this relationship is itself still an area of current active research [4].

The comparative structural approach appears to be promising, as witnessed by the results of this work obtained in slab geometry. In the case of homogeneous slabs, it will be shown that the integral transport operator matrix, that has in general a dense structure, acquires asymptotically, in a diffusive limit obtained as the thick limit of computational
size for a highly scattering medium, a tridiagonal structure characterized by a diffusion-like coupling stencil.

The asymptotic analysis has also been extended to heterogeneous slab configurations characterized by a periodic material discontinuity wherein an optically thick cell is surrounded by two optically thin cells in a repeated pattern. The two cell types’ optical thicknesses are pushed apart, i.e. the thick is made thicker while the thin is made thinner at a prescribed rate and the asymptotic expressions for the matrix elements are obtained and investigated in this limit.

The results obtained have confirmed the intuitive expectation that the $S_N$-equivalent integral transport operator acquires a sparse pentadiagonally dominated matrix structure in this limit. In fact, elements on the second off-diagonal coupling the cell-averaged scalar fluxes in two optically thick cells, separated by a single interposed optically thin cell, are of the same order as the corresponding elements on the diagonal in the specified limit. In this connection, the existence of algebraically equivalent transformations that, while preserving the exact cell-averaged scalar fluxes, map the discrete integral transport operator matrix into a matrix asymptotically characterized by a tridiagonal structure, has been successfully obtained. These conclusions possibly reconcile the puzzling result of an asymptotically pentadiagonally dominated matrix with the success of acceleration schemes based on tridiagonal low-order operators.

Finally the results of the comparative structural approach have been employed in slab geometry to provide insight into the excellent convergence properties of diffusion-based acceleration schemes in one-dimensional transport problems. More specifically, the acceleration scheme analyzed in this work is that based on the Adjacent-cell
Preconditioner (AP). The AP formalism provides a recipe for the construction of a diffusive cell-centered tridiagonal preconditioner that has proved to work extremely well for acceleration purposes, especially for purely scattering media, both in homogeneous and heterogeneous cases. For cases in which non-purely scattering media are present, the results of the structural analysis of the integral transport matrix have been used to improve the convergence properties of the AP acceleration scheme.

1.3 Review of Results in Two-Dimensional Geometry

One of the main objectives of this work is an exploration of the asymptotic properties of the $S_\nu$-equivalent integral transport operator in two-dimensional configurations, with a particular interest in two-dimensional Cartesian computational meshes characterized by increasing material discontinuities in adjacent cells.

The interest in this kind of problems is motivated by the fact that deterioration in the performance of acceleration methods based on diffusive-type low-order operators has been widely observed in multi-dimensional problems characterized by the presence of sharp material discontinuities [5-9]. Even strictly consistent DSA schemes, that are unconditionally stable and robust in homogeneous configurations, have been found in such cases to consume a number of iterations that is far too large to explain with the results of a Fourier error mode analysis for the iteration scheme.

Recent research [10] has proved that for a broad class of Weighted Diamond Difference spatial discretization methods, that include Diamond Difference (DD) and Nodal methods, there exists no diffusive-type cell-centered operator that yields a robust
and unconditionally stable iterative procedure. In this connection, it should be noted that the AP operator belongs to this class of operators. Numerical evidence suggests the validity of this conclusion for cell edge-based schemes also.

The overall objective of the asymptotic analysis of the matrix elements of the discrete integral transport operator is, therefore, to obtain a basic understanding of the causes that lead to deterioration in the performance of acceleration methods that possess a diffusion-like coupling stencil in the presence of sharp material discontinuities in multi-dimensional problems.

The fundamental conjecture that has been explored in this work is that the matrix structure of these low-order operators may no longer present a good approximation of the full transport operator in the case of periodically heterogeneous multi-dimensional problems. To fix ideas, with reference to two-dimensional geometry and to a cell-centered diffusion-like operator (like the AP preconditioner), the five-band sparse structure of the diffusion-like operator stencil ignores cross-derivative coupling. In other words, the operator stencil accounts for the coupling of a cell-averaged scalar flux with itself (self-coupling) and with its right-left and bottom-top neighbors (the first Cartesian neighbors) but ignores the coupling with all the other neighbors, in particular with the first diagonal neighbors (cross-derivative coupling).

The results obtained have confirmed that cross-derivative coupling, while negligible in the case of homogeneous problems, can become important in the presence of unbounded discontinuities in the nuclear properties of adjacent cells. The methodological approach that has been followed to investigate this conjecture is again
based on the construction and study of the asymptotic properties of the matrix elements of the two-dimensional $S_N$ - equivalent integral transport operator.

This study has been carried out considering initially a three-by-three computational cell mesh in two-dimensions that allows concentrating on the effect of the couplings with the different kinds of neighbors in a simple, yet significant, setting. A comparison of the matrix structure of the low order operators traditionally employed in acceleration schemes with the asymptotic structure acquired by the integral transport operator in limits of interest, is expected to shed light on potential deficiencies of these algorithms in multi-dimensional problems. Once again, this structural comparative study may give direct indications for the AP preconditioner, while only indirect indications may be obtained for DSA.

The procedure followed in slab geometry has been repeated in two-dimensional Cartesian geometry, in the same sequence: derivation of the expressions for elements of the discrete $S_N$ - equivalent integral transport operator matrix, asymptotic analysis for homogeneous configurations with a particular emphasis on the thick cell limit, then asymptotic analysis for heterogeneous configurations characterized by a periodically increasing material discontinuity.

In the case of homogeneous configurations, it will be shown that the integral transport operator matrix, that has in general a dense structure, acquires asymptotically, in a diffusive limit obtained as the thick limit of computational size for a highly scattering medium, a five-banded block structure characterized by a diffusion-like coupling stencil. The existence of this low-order banded approximation, pointing to a strong local coupling
of a cell with its first Cartesian neighbors, provides further insight into the excellent convergence properties of diffusion based acceleration schemes in two-dimensional homogeneous configurations with low absorption.

The asymptotic analysis has then been extended to heterogeneous two-dimensional configurations characterized by a periodic material discontinuity wherein an optically thick horizontal layer of cells is sandwiched by two optically thin layers of cells in a repeated pattern. This periodically heterogeneous configuration is therefore referred to in the literature as the Periodic Horizontal Interface (PHI) configuration. The layers’ optical thicknesses are pushed apart, i.e. the thick is made thicker while the thin is made thinner at a prescribed rate by varying the problem’s properties via a scaling parameter.

The asymptotic expressions for the transport matrix elements have been investigated in the limit defined by a scaling of the PHI configuration in which the total cross-section vanishes like $\Delta^{-1}$ in one layer and diverges like $\Delta$ in the other layer, as $\Delta \to \infty$. The results of the asymptotic analysis conducted for the matrix elements of the discrete integral transport operator show that elements outside the five-banded block of the integral transport matrix are indeed no longer negligible in the proposed limit. In particular cross-derivative coupling of a cell in a thin layer with its diagonal neighbors is of the same order as self-coupling and coupling with the bottom-top neighbors. Another distinctive feature of the asymptotic limit for the PHI configuration is that the integral transport matrix acquires a sparse matrix structure that is non-local. In other words, a cell-averaged scalar flux in the PHI configuration can be coupled with the same strength to other fluxes in the spatial mesh independent from the distance of the respective cells in the mesh. These findings have been used to gain a basic understanding of the
mechanisms involved in the degradation of the spectral properties of the AP acceleration scheme in the asymptotic limit for the PHI configuration. Specifically, the results of the asymptotic analysis sustain the conjecture that the crisis of the AP formalism is indeed due to a structural deficiency of the AP preconditioner in accounting for the strong cross-derivative coupling of two adjacent layers in the PHI configuration. Finally, the validity of the conjecture has been tested by amending the structure of the AP preconditioner to account for cross-derivative coupling of a cell’s average flux with its first diagonal neighbors. A Fourier analysis has been performed for the amended acceleration scheme. Preliminary results of the latter analysis for a model problem based on the PHI configuration confirm that a significant improvement is obtained in the spectral properties of the novel acceleration scheme thanks to the inclusion of cross-derivative coupling. The novel acceleration scheme has also been implemented in a simple test code designed to verify the results of the analysis. The numerical results obtained for the model problem, in terms of estimates of the spectral radius and of the number of iterations consumed to achieve convergence to within a specified convergence criterion, have successfully confirmed the predictions of the Fourier analysis. These preliminary findings appear encouraging and constitute the foundation for future work aimed at devising extended (non-diffusive) low order operators that are more resilient to adverse material discontinuity effects in multi-dimensional transport problems.

In conclusion, an outline of the remainder of the thesis follows. In Ch. 2 a review of the literature closely related to the research presented in this work is given. The results obtained in slab geometry are discussed in the subsequent three chapters. In particular, the asymptotic properties of the elements of the integral transport matrix are presented in
Ch. 3 for homogeneous slabs and in Ch. 4 for periodically heterogeneous slabs. The results of this asymptotic study are applied to obtain further insight into the success of the AP formalism for the iterative acceleration of one-dimensional transport problems in Ch. 5. The study of the asymptotic properties of the elements of the integral transport matrix is then extended to two-dimensional geometry in the next two chapters of the thesis. The results obtained for homogeneous configurations are presented in Ch. 6 while Ch. 7 contains a discussion of the results obtained for the PHI configuration. These results are used to gain a basic understanding of the mechanisms of failure of the AP preconditioner in the PHI configuration and to devise a novel acceleration scheme that is more resilient to material discontinuities’ adverse effect on the effectiveness of AP in accelerating iterative convergence of transport methods. Finally, Ch. 8 contains a summary of the main findings of this research and some suggestions for future work.
Chapter 2

Review of Literature

Though this work is not, at least initially, directly dedicated to the development of iterative strategies for the deterministic solution of the neutron transport equation, the motivation for this research is nonetheless deeply rooted in the realm of iterative methods. The overall objective of this work is in fact obtaining a basic understanding of the causes that lead to deterioration in the performance of acceleration methods for discrete ordinates ($S_N$) particle transport calculations that possess a diffusion-like coupling stencil in the presence of sharp material discontinuities in multi-dimensional problems. Specifically, it is desired to test the conjecture that amending the structure of diffusive low-order operators to account for cross-derivative coupling can lead to the development of novel acceleration schemes that are more resilient to adverse material discontinuities in multi-dimensional geometry. In order to investigate the latter conjecture the elements of the matrix representing a certain angular ($S_N$) and spatially-discretized form of the neutron integral transport operator are derived, and the asymptotic properties of these elements are studied in various limits of interest, in one-dimensional and two-dimensional geometries.

The conceptual foundations for this work may be found in the theory of the integro-differential and integral forms of the neutron transport equation, covered in great detail in the now classic manuscript on Nuclear Reactor Theory by Bell and Glasstone
Fundamental background information is also represented by the developments in the field of Computational Methods for the numerical solution of neutron or, more generally, neutral particle (neutrons and photons) transport problems. A clear and comprehensive introduction to the computational techniques of neutron transport can be found in the more recent textbook by Lewis and Miller, Jr. [11]. This text is especially valuable in the way the exposition of computational techniques is developed starting from the theoretical foundations of neutral particle transport.

As mentioned earlier, the focus in this project is on iterative methods for discrete ordinates transport calculations. In this respect an invaluable source of information and guidance into the more technical area of fast iterative methods for the solution of the discrete ordinates formulation of the neutron transport equation is represented by the extensive review paper by Adams and Larsen [1].

The paper by Adams and Larsen opens with an overview section which also contains an interesting historical perspective on the development of iterative techniques. The foundations for the understanding of iterative methods are introduced, referring to planar geometry and isotropic scattering, in the following two sections. These sections have a tutorial nature and are intended to give an introduction to iterative schemes for continuous transport problems and a discussion of the effects of spatial and angular discretizations, respectively. The remaining sections cover more technical or advanced topics such as the extension to other one-dimensional and multi-dimensional geometries, the more recent developments in non-linear and algebraic iterative methods, the acceleration of other scattering iterations (e.g., highly forward-peaked scattering) and finally the acceleration of $k$-eigenvalue problems for multiplicative systems. Elements of
great interest in this paper are represented by the gradual exposition of topics, the extensive coverage of previous works on the subject (more than 250 references) and a thorough and accurate review not only of the work done in the Western community but also in the Former Soviet Union.

As pointed out by Adams and Larsen in their historical review, it was the slow convergence displayed by the most basic iterative method traditionally employed in solving neutral particle transport problems, namely Source Iteration (SI), in the diffusive regime (highly scattering medium with low leakage of particles) that prompted the search for efficient acceleration schemes. Among these, and of great importance in relation to the motivation behind this work, the Diffusion Synthetic Acceleration (DSA) method was initially attractive because it was believed that standard, highly efficient, cell-centered codes based on diffusion theory could be simply linked as an acceleration module to any transport code.

Synthetic methods for accelerating the iterative convergence of transport problems were firstly introduced in the mid 1960s both in the Western literature [12,13] and, independently and almost simultaneously, in the Eastern literature by Lebedev [14]. A review of the Western literature follows. The idea of utilizing the diffusion operator as a low-order approximation to the transport operator was initially proposed by Kopp [12]. In his original paper, Kopp described and applied a general residue iteration method (the synthetic method) to the solution of the neutron transport equation. Gelbard and Hageman [13] were then the first authors to apply the synthetic method for the acceleration of $S_N$ iterations in two-dimensional Cartesian geometry. Two different
options were explored for the low-order operator: diffusion and $S_2$ (discrete ordinates transport operator with order 2 quadrature set), using these to accelerate $S_N$ iterations. For the analytic equations, with a diffusion preconditioner, the convergence rates obtained performing a Fourier analysis of the iterative algorithm appeared to be much faster than for unaccelerated Source Iteration. For the discretized equations, though, such fast rates were observed only for problems with fine spatial grids.

Later work by Reed [15] showed, by testing and analysis, that while the “diffusion” synthetic method employed by Gelbard and Hageman is rapidly convergent for sufficiently fine grids, it is ineffective and sometimes divergent for problems with coarse spatial grids, actually the problems most in need of acceleration in the first place. The conditional stability of the method for accelerating the Diamond Difference (DD) method, the dominant numerical solution method of the time, was proved through the analysis by Reed of a model configuration, i.e., an infinite row of identical computational cells.

This behavior was later articulated in Alcouffe’s Consistency Principle [16] stating that a necessary condition for stability and efficiency of the synthetic algorithm, which he called Diffusion Synthetic Acceleration (DSA), is the consistency between the discrete-variable forms of the diffusion and transport operators involved. However, the nature of this consistency, and a systematic approach to deriving the discrete-variable DSA equations remained unspecified until Larsen interpreted consistency in the derivational sense and prescribed the Four Step Method (FSM) as a means of deriving an unconditionally stable and efficient DSA. He successfully derived unconditionally stable
DSA using FSM for several spatial approximations in slab geometry [17]. Subsequently McCoy and Larsen verified the predicted spectral properties for model, as well as non-model, problems [18]. Even though the test problems were more complicated (finite, heterogeneous) than the model problem, the observed iterative performance was always at least as good as that predicted by the model-problem analysis. These papers conclusively demonstrated that there are indeed cell-edge centered diffusion discretizations that yield rapidly convergent DSA methods for a wide variety of transport discretizations, and moreover presented a simple prescription for generating them, at least in one-dimensional or Cartesian configurations.

More recently, another class of synthetic acceleration schemes based on diffusive-type low-order operators has been introduced through the work done by Azmy on Adjacent-Cell Preconditioners (APs), both in one-dimensional geometry [19] and in two-dimensional geometry [20]. The first paper, in particular, is also of great importance since it represented a fundamental starting point and reference for the work on the $S_x$-equivalent integral transport operator in one-dimensional geometry presented in Ch. 3 of this dissertation. In fact, the definitions and formalism, previously presented in Ch. 1, relating to the iteration Jacobian matrix $A$ and to the discrete integral transport matrix $B$, have been introduced in the paper by Azmy and utilized there to build the general expressions for the diagonal and first off-diagonal elements of the $B$ matrix in one-dimensional geometry.

With reference to the more particular case of a homogeneous slab, results have also been presented, in reference [19], for an asymptotic analysis to the $B$ matrix
elements up to the second off-diagonal elements. The focus in that paper, though, was not on the discrete integral transport operator matrix and a study of its structure and asymptotic properties per se. A mix of asymptotic analysis of the tridiagonal elements of the $B$ matrix and of Fourier analysis was instead utilized, as a guiding tool, for the development of a new preconditioner, the AP. The AP is still characterized by the same coupling stencil as traditional diffusion schemes, but possesses two attractive features: (1) its cell-centered coupling stencil, more adequate for extension to multi-dimensional, higher order situations than the standard edge-centered or point-centered DSA methods; and (2) its decreasing spectral radius with increasing cell thickness to the extent that immediate point-wise convergence, i.e., in one iteration, can be achieved for problems with sufficiently thick cells even in heterogeneous configurations characterized by the presence of sharp material discontinuities. The latter quality is due to the “engineering” of the AP operator in a way that is reminiscent of the thick cell asymptotic properties of the discrete integral transport operator.

Despite the great success obtained in the treatment of one-dimensional problems and in the extension to the treatment of homogeneous multi-dimensional problems, both DSA and AP acceleration schemes are known to be flawed for multi-dimensional problems having large spatial discontinuities in cross-section data. In particular, even strictly-consistent DSA schemes that are unconditionally effective for homogeneous problems become increasingly ineffective in reducing the number of iterations necessary to achieve convergence as the magnitude of the cross-section discontinuity is increased.

Early results on the crisis of AP in multi-dimensional problems characterized by the presence of increasing discontinuities in material properties have been reported by
Azmy in his analysis of the performance of Adjacent-cell Preconditioners for accelerating generic fixed-weight, Weighted Diamond Difference (WDD) neutron transport methods in multi-dimensional Cartesian geometry [5,6]. Azmy, Wareing and Morel [7] have shown, using a Fourier error mode analysis along with numerical results, that the performance of DSA, even Larsen’s four-step consistent DSA, in accelerating Even Parity Methods (EPM) discrete-variable equations, degrades significantly in two-dimensional problems with very strong periodic heterogeneities. Warsa, Wareing and Morel have later used a similar analysis to show analogous, or even more severe degradation, on tetrahedral grids in three-dimensional problems with a variety of DSA methods (fully consistent and partially consistent) [8,9]. The spatial discretization considered in these papers was a Linear Discontinuous Finite Element Method (LDFEM) [21]. Later research by Azmy [10] has proved for a broad class of Weighted Diamond Difference (WDD) methods, including Diamond Difference and Nodal methods, in two-dimensional geometry that there exists no diffusive-type cell-centered operator that yields a robust and unconditionally stable iterative procedure. Numerical evidence suggests validity of this conclusion for edge-centered schemes also.

Independently from the spatial discretization considered, as pointed out in [9], the intrinsic limitation of acceleration schemes such as DSA and AP ultimately lies in the very structure of preconditioners characterized by a block-diffusion coupling stencil. In this connection, as indicated in Ch. 1, it is desired in the work reported here, to gain a more complete understanding of the inadequacy of this type of low-order operators by contrasting their structure to that attained by the $S_N$—equivalent integral transport operator in asymptotic limits of interest. In particular, when mention is made in this work
of a “diffusive limit” in the asymptotic analysis of the matrix elements, this will be intended as the thick limit of computational cell size for a highly scattering medium (scattering ratio \( c \) very close or equal to a unit value). In this case, actually, the fixed source strength is also scaled in order to avoid dealing with divergent fluxes as the cell width tends to infinity, due to the absence of sinks for neutrons when \( c \) is exactly equal to unity.

A necessary distinction has to be made, in this connection, with respect to the fundamental and consolidated notion of Diffusion Limit that has been introduced in the field of transport theory by the pioneering work of Larsen and collaborators [22-26] and also extended to other fields of related interest, as radiative transfer [27,28]. The work by Larsen, Morel and Miller in relation to various spatial discretization schemes [24], in particular, has defined the Diffusion Limit as the limit obtained by scaling the scattering and absorption cross-sections in terms of a small parameter \( \varepsilon \), representing the ratio of a typical mean free path and a representative geometric dimension for the considered system, as to asymptotically effect a value of \( c \rightarrow 1 \) as \( \varepsilon \rightarrow 0 \). Though not incorporated as part of the work conducted for homogeneous slab geometry and presented in Ch. 3, the determination of the asymptotic behavior of the elements of the \( B \) matrix in the Thick Diffusion Limit would also be of great conceptual interest. This interest is, in particular, motivated by the results obtained from studying the pure thick cell limit previously defined.

Some preliminary work has been conducted by Morel [4] on the relationship between the integral transport operator and the diffusion operator that confirms the different nature of \( B \) and the standard discretized diffusion operator \( D \) in the Diffusion
The results of this preliminary work seem to point to the potential existence of a hybrid transport-diffusion approximation to transport theory that may prove to be superior to traditional diffusion theory.

In this connection, a further element of interest is constituted by the fact that, at least for the vacuum boundary conditions considered in this dissertation, the $B$ matrix automatically incorporates the effect of the boundary conditions in the equations pertaining to the boundary cells. Of course additional and thorough research is needed in this direction and is considered outside the scope of this dissertation.

The last part of this literature review will be dedicated to the potential relations of this work with the “linear algebraic” approach recently introduced in the mathematical community to prove the effectiveness of DSA in various asymptotic regimes, on one hand, and with the approach of Fourier error mode analysis for the study of the stability and convergence properties of acceleration schemes traditionally used in the transport community, on the other. Finally, it will be discussed how this effort may fit into the more general theory of preconditioning, leading to potential extensions of related results to unstructured spatial meshes.

The “operator” or “structural” approach adopted in the research presented in this thesis, namely examining the properties of the full transport operator that is to be approximated by a low-order operator in the acceleration step, has been pursued as a possible alternative to the traditional approach of Fourier error mode analysis. The necessity for this alternative approach has been prompted by the difficulties of extending the Fourier analysis from the traditional infinite homogeneous or periodically heterogeneous medium model-problem configuration to non-periodic heterogeneous
problems in finite domains. The philosophy behind this practical approach is akin to the theoretical viewpoint originally introduced by Faber and Manteuffel [29] in their linear algebraic treatment of the DSA formalism to the continuous steady-state, one-speed, linear transport equation with isotropic scattering in slab geometry. In particular, the authors showed that the continuous formulation of the DSA algorithm is the Neumann series solution of the integral formulation of the transport equation preconditioned by an operator involving the Green’s function of a diffusion operator. The treatment introduced in [29] has then been extended by Ashby, Brown, Dorr and Hindmarsh by incorporating the angular and spatial discretization of the continuous steady-state, one-speed, linear transport equation with isotropic scattering in slab geometry [30]. In particular, they assumed a discrete ordinates collocation of the angular variable and a diamond difference approximation of the spatial variable. A matrix formulation of the resulting discretization is then presented in order to obtain an algebraic derivation and representation of the DSA preconditioner. This formulation allows an asymptotic analysis of the system matrix and DSA preconditioned system matrix in various limits that comprise the Diffusion Limit, a thick cell limit for problems containing absorption that is bounded away from zero (the thick limit) and a thin cell limit (the thin regime). The latter two limits are equivalent to the thick cell limit and the thin cell limit considered in Ch. 3 of this dissertation, under the assumption of a homogeneous, uniform-mesh slab. In Ch. 1 it was noted that the AHOT-N0 spatial approximation limits to diamond difference in the case of optically thin cells. In this respect, the theoretical results presented in [30] relative to the asymptotic properties of the integral transport discrete operator matrix (A₀ in their paper) in the thin regime have been positively contrasted with the results of the asymptotic analysis to the
elements of the \( \mathbf{B} \) matrix carried out in the thin cell limit in Ch. 3. In closing, it is noted that the linear algebraic analysis of DSA has recently been extended to three-dimensional geometry and finite element spatial discretizations \([31,32]\). It is also important to mention that the linear algebraic approach has played an important role in the development of Krylov subspace iterative methods \([33]\) preconditioned by DSA used to replace the traditional acceleration schemes for SI. In particular, Warsa, Wareing and Morel have shown \([34,9]\) that recourse to the more powerful Krylov iterative method can significantly improve convergence for heterogeneous multi-dimensional configurations in which the convergence of accelerated SI degraded in the presence of material discontinuities, allowing the treatment of problems that are virtually intractable with accelerated SI. In this connection it is pointed out that, while the results presented in this thesis aim at restoring robustness of acceleration techniques for traditional SI by accounting for cross-derivative coupling in multi-dimensional problems, we believe that the same results can also contribute to the development of more efficient preconditioners for Krylov iterative methods.

As mentioned earlier, the constructive nature of the operator analysis appears particularly useful to analyze the behavior of acceleration schemes in the case of non-periodic heterogeneous problems on finite domains. Notwithstanding, we believe this approach is not expected to replace the tool of Fourier analysis in iterative stability studies. Ultimately, the stability and convergence properties of any novel acceleration scheme, eventually based on the indications emerging from the asymptotic study of the discrete \( S_N \) – equivalent integral transport operator, will have to be confirmed through a Fourier analysis of the resulting algorithm. It is therefore interesting to note that some
recent work has been done, on the front of Fourier analysis in slab geometry, in order to extend the tool of error mode analysis to consider periodically heterogeneous slabs (Zika and Larsen) [35] and finite problems (Sanchez) [36]. The results for periodically heterogeneous slabs, in particular, have confirmed that DSA converges more slowly in a heterogeneous medium than in a homogeneous medium composed of the same volume-averaged scattering ratio. This is due to the presence of “resonant” wave numbers such that, in the presence of material heterogeneities, error modes corresponding to these resonant wave numbers are “excited” more than other error modes.

Finally, the work developed for one-dimensional geometry on the construction of matrices $A$ and $B$, and more importantly the work undertaken in the same direction in two-dimensional problems, may have some interesting connections with the more general mathematical theory of preconditioning techniques for the iterative solution of large linear systems [37,38].

In particular the way $A$ and $B$ are currently constructed seems to bear some similarity with a technique known as $Incomplete LU Factorization$ [37]. It is of great interest to investigate whether or not the construction of $B$ may be interpreted, $a posteriori$, as an incomplete LU factorization of order 1 for the discrete integral transport operator. If this turns out to be true, it will open the way to a more systematic algorithmic approach for the construction of preconditioners based on the $B$ matrix, independent of the particular spatial discretization and spatial mesh considered. This last aspect would be useful in the computational realm since it would permit potential extension of the results from this work, exclusively dealing with structured spatial meshes, into the currently active research area of transport computational methods on unstructured spatial meshes.
Chapter 3

Integral Transport Matrix in Homogeneous Slabs

3.1 Introduction

Exact analytic expressions for the elements of the $B$ matrix introduced in Sec. 1.2 have been derived in one-dimensional or slab geometry and the asymptotic properties of these elements as a function of computational-cell size have then been investigated for homogeneous and periodically heterogeneous slabs. The results of these asymptotic analyses for homogeneous slabs are presented in this chapter while those referring to periodically heterogeneous slabs are discussed in the next chapter.

The asymptotic limits of interest for homogeneous slabs are a thick cell diffusive limit and a thin cell limit. The thick cell limit is obtained by scaling the width of a computational cell $\Delta x$ as a dimensionless parameter $\Delta$ times the appropriate length units and forming the limit of the matrix elements as $\Delta \to \infty$. Similarly the thin cell limit is obtained by scaling $\Delta x$ through a dimensionless parameter $\delta$ and forming the limit of the matrix elements as $\delta \to 0$. As it will become apparent in the following, the elements of matrix $B$ are, in general, dependent on the product of a computational cell’s width and macroscopic total cross-section. In other words the elements of matrix $B$ depend on the optical thickness of the cell expressed in mean free paths (MFPs). Therefore scaling the geometric cell width is equivalent to scaling the total cross-section alone or both parameters simultaneously.
The choice of these asymptotic limits has also been motivated by the desire to maintain a unified approach in progressing from the homogeneous structure to periodically heterogeneous structures where optically thick and optically thin cells are alternated in a repeated pattern. Hence, in addition to their intrinsic value, the asymptotic analyses carried out in the two notable limits for homogeneous configurations have been developed to serve as a preliminary tool and to guide the development of the asymptotic analysis for periodically heterogeneous slabs.

As shown in this chapter, the results obtained in the thick cell diffusive limit prove that the $B$ matrix acquires a tridiagonally dominated structure characterized by a diffusion-like coupling stencil. Interestingly enough, in slab geometry the $B$ matrix displays this asymptotic behavior at a fast exponential rate, manifested by the exponential vanishing of the elements beyond the first off-diagonal with increasing cell thickness. The exponential nature of this convergence is strictly related to the AHOT-N0 spatial discretization utilized in the analysis and does not extend to other WDD discretization schemes. In contrast, in the thin cell limit $B$ acquires a diagonally dominated structure that is approached at a slower linear rate. Notwithstanding, it will be shown that it is possible to identify an exact algebraic manipulation that transforms $B$ into a matrix that acquires a diagonally dominated structure at a faster quadratic rate in the thin cell limit.

An outline of the chapter follows. The direct solution of the transport equation in its integral form for slab geometry is illustrated in Sec. 3.2. General expressions for the elements of the $A$ and $B$ matrices are derived in Sec. 3.3, both using an inductive derivation (Sec. 3.3.1) and separately a constructive approach (Sec. 3.3.2), and the cell-averaged scalar fluxes obtained by inverting matrix $B$ are verified against the results
obtained from an iterative solution of the transport problem (Sec. 3.3.3). Expressions for the elements of matrices \( A \) and \( B \) for the homogeneous, uniform-mesh case are derived in the first part of Sec. 3.4, that also contains the results of the asymptotic analysis in the thick cell limit (Sec. 3.4.2) and in the thin cell limit (Sec. 3.4.3) and their numerical verification (Sec. 3.4.4). Finally, the results of the asymptotic analysis are employed in Secs. 3.5 and 3.6 to devise truncation strategies for the integral transport matrix in optically thick and thin slabs, respectively.

3.2 Direct Solution of the Transport Equation in Slab Geometry

The construction of the matrix elements of the integral transport operator has been carried out using as a starting point the Source Iteration (SI) formulation. The governing equations comprise the two sets of equations [see Eqs. (1.22) and (1.24)] constituting the Weighted Diamond Difference (WDD) spatially-discretized form of the one-group, steady-state, discrete ordinates approximation of the neutron transport equation in slab geometry. Also, a non-multiplying system with isotropic scattering and isotropic fixed source is assumed.

Since ordinarily right and left particle flows are of equal importance, a symmetric quadrature set \( \{\mu_m, w_m\}, \quad m = 1, \ldots, M \), where \( M \) is coincident with the order \( N \) of the \( S_N \) quadrature, defined on an even number of ordinates that are symmetric about \( \mu = 0 \), will be used in the following. This set may be defined by the following relations:
The quadrature weights are usually normalized to 2 [11], but in the following, largely as a matter of convenience, they will be assumed to be renormalized to unity so that the following normalization condition holds

\[
\sum_{m=1}^{M} w_m = 1
\]  

The solution of Eqs. (1.22) and (1.24) for a single discrete ordinate over a given problem domain is conducted via the classical “mesh-sweep” algorithm. Closure of the iterative process is accomplished, in the SI scheme, by setting the values for the cell-averaged scalar flux distribution employed in computing the scattering source in the next iteration equal to the values obtained at the end of the present one.

The mesh-sweep algorithm amounts to the following procedure. The starting cell for each angle \( \mu_m \) is one with an external boundary condition where the incoming flux is explicitly (e.g., vacuum boundary condition) or implicitly specified in terms of the outgoing flux at the same, or another boundary (reflective, albedo, or periodic boundary conditions). The incoming flux in Eqs. (1.22) and (1.24) is set equal to the prescribed value in case an explicit boundary condition is specified, as it will be assumed in the following referring to vacuum boundary conditions on both edges of the slab. In case of a reflective boundary condition, the incoming flux is set to a previously computed outgoing flux, i.e. resulting from the mesh sweep along \(-\mu_m\) or the previous flux iterate when both boundary conditions are implicit thus requiring iterations on the boundary conditions. The
mesh-sweep algorithm then proceeds by recursively solving Eqs. (1.22) and (1.24) simultaneously for the cell-averaged flux and the outgoing cell-edge flux, assigning the latter to the incoming cell-edge flux of the adjacent down-stream cell (angular flux continuity across cell edges) and repeating the process for all cells of the mesh. To fix these ideas, the equation expressing angular flux continuity for $\mu_m > 0$ is:

$$\tilde{\psi}^{i,(+)}_{m,j+1} = \tilde{\psi}^{o,(+)}_{m,j}, \quad m = 1,\ldots,M/2; \ j = 1,\ldots,(J-1)$$

(3.3)

A sketch illustrating the mesh-sweep algorithm for $\mu_m > 0$ is depicted in Fig. 3.1.

Fig. 3.1: Order of sweeping a spatial mesh for $\mu_m > 0$.

Upon completion of the mesh-sweep for all discrete ordinates the scalar flux is updated, as described shortly, and convergence of the iterations is tested, thus completing a single inner iteration. As indicated previously, closure of the iterative process is
accomplished, in the SI scheme, by setting the values of the cell-averaged scalar fluxes in the next iteration equal to the values obtained at the end of the present one.

To illustrate mathematically how the mesh-sweep algorithm is used to solve the two sets of equations constituting the most general WDD form of the discrete ordinates approximation to the transport equation it is convenient to express Eqs. (1.22) and (1.24) in the following compact matrix form:

\[
\begin{bmatrix}
\psi_{m,j}^{(t+1)} \\
\psi_{m,j}^{o,(t+1)}
\end{bmatrix}
= \begin{bmatrix}
A
\end{bmatrix}
\begin{bmatrix}
0
\end{bmatrix}
+ \begin{bmatrix}
S
\end{bmatrix}
\begin{bmatrix}
1
\end{bmatrix}
\]

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\end{bmatrix}
= \begin{bmatrix}
A
\end{bmatrix}
\begin{bmatrix}
0
\end{bmatrix}
+ \begin{bmatrix}
S
\end{bmatrix}
\begin{bmatrix}
1
\end{bmatrix}
\]

Matrices \( L_{m,j}^0 \) and \( S_{m,j}^0 \) in Eq. (3.4) represent the discretized form of the “streaming plus collision” operator and of the “self-scattering” operator in the original continuous transport equation, respectively. The superscript on the matrices in Eq. (3.4) denotes the AHOT-N0 method that is utilized in all of the following developments. The expressions for the two matrices are readily obtained from Eqs. (1.22) and (1.24):

\[
L_{m,j}^0 = \begin{bmatrix}
1 & \kappa_{m,j} \\
1 & 1 + \alpha_{m,j}
\end{bmatrix}, \quad m = 1, \ldots, M; \quad j = 1, \ldots, J
\]

\[
S_{m,j}^0 = \begin{bmatrix}
1 & \kappa_{m,j} \\
0 & 1 - \alpha_{m,j}
\end{bmatrix}, \quad m = 1, \ldots, M; \quad j = 1, \ldots, J
\]

where \( \kappa_{m,j} \), the reciprocal of the optical thickness of cell \( j \), has been defined in Eq. (1.23).
Inversion of matrix $L_{m,j}^0$ is readily accomplished and allows to explicitly express $\tilde{\psi}_{m,j}^{(t)}$ and $\tilde{\psi}_{m,j}^{o,(t)}$ in terms of $\tilde{\phi}_j^{(t)}$, $\tilde{\psi}_{m,j}^{i,(t)}$ and $s_j$:

$$\begin{align*}
\tilde{\psi}_{m,j}^{(t+1)} &= \left(1 + \frac{1 + \alpha_{m,j}}{1 + 2\kappa_{m,j} + \alpha_{m,j}}\right)\left(c_j \tilde{\phi}_j^{(t)} + s_j\right) + \frac{2\kappa_{m,j}}{1 + 2\kappa_{m,j} + \alpha_{m,j}} \tilde{\psi}_{m,j}^{i,(t+1)} \\
\tilde{\psi}_{m,j}^{o,(t+1)} &= \left(\frac{2}{1 + 2\kappa_{m,j} + \alpha_{m,j}}\right)\left(c_j \tilde{\phi}_j^{(t)} + s_j\right) + \frac{2\kappa_{m,j} + \alpha_{m,j} - 1}{2\kappa_{m,j} + \alpha_{m,j} + 1} \tilde{\psi}_{m,j}^{i,(t+1)} \quad \text{ (3.7)}
\end{align*}$$

$m = 1,...,M; j = 1,...,J$

Closure of the iterative process is accomplished in the SI scheme by setting:

$$\tilde{\phi}_j^{(t+1)} = \sum_{m=1}^{M} w_m \tilde{\psi}_{m,j}^{o,(t+1)}, \quad j = 1,...,J, \quad \text{ (3.8)}$$

where $w_m$ are the weights associated with the angular quadrature.

Equation (3.7) along with the continuity condition expressed by Eq. (3.3), for $\mu_m > 0$, represent the standard mesh-sweep algorithm commonly used to solve the discretized integro-differential form of the discrete ordinates approximation of the neutron transport equation. Notice therefore that this algorithm is focused on the discrete-variable angular flux. In view of the linearity of these equations the operator performing the mesh-sweep is a linear operator. The weighted sum over angles of the discrete ordinate cell-averaged angular fluxes, performed in Eq. (3.8) to obtain the update of the cell-averaged scalar flux in the present iteration, is also a linear operation.

As indicated in Ch. 1, the composition of the mesh-sweep operator with the summation over angles operator that yields the cell-averaged scalar fluxes can therefore
be viewed as a linear mapping of the scalar fluxes from the previous to the present iteration. This mapping has been expressed, using compact matrix notation, in Eq. (1.26).

Under the assumption that the iterative scheme converges, it has also been shown that the vector $\tilde{\phi}^\infty$, containing the limit of the iterates of the scalar fluxes, may be computed as the solution of the linear system in Eq. (1.27). As a matter of fact, the latter represents a discrete approximation to the integral transport equation, Eq. (1.19). Was it possible to construct the two matrices $A$ and $B$, and to invert (or factor) matrix $B$, the transport problem would be immediately solvable without iterations in a direct approach.

However, for most practical applications, especially in multi-dimensional problems, this approach would be inadequate in view of its computational cost, i.e. memory and time consumption. Therefore, a splitting of matrix $B$ is generally sought in order to set up a possibly fast convergent robust iterative procedure through the introduction of a suitable preconditioner [19]. In this connection though, the construction of the full transport operator in its $A$ and $B$ matrices representation would still prove to be highly valuable as a reference for preconditioners building strategies. This follows from the fact that the preconditioner is usually chosen to be a more easily invertible approximation of the full operator through some kind of truncation of the number of diagonal stripes comprising the full matrix $B$. This raises the important issue of how many diagonal elements ought to be included in a suitably truncated replica of the original transport operator. Also, it is necessary to devise quantitative means to understand the possible strengths and flaws of a certain preconditioner as applied to a specific problem. In this respect the determination of the expressions for the elements
belonging to the diagonal and first two off-diagonal stripes of \( B \) has been previously carried out [19] with particular reference to the case of homogeneous cell properties.

Another important consequence of the availability of the most general expressions for the full \( A \) and \( B \) matrices would be the possibility to directly solve Eq. (1.27), at least for some interesting reference problem (benchmarking). This would allow determining without any iterative residual the limit cell-averaged fluxes that a suitable iterative algorithm should converge to. Such direct solution could then be used to quantitatively evaluate and compare the performance of iterative procedures based on different preconditioners. In particular, this approach will be followed in Sec. 3.5 to evaluate the impact of different truncation strategies on the solution of Eq. (1.27) that might eventually lead to the choice of a particular preconditioner.

Since matrices \( A \) and \( B \) correspond to a certain angular and spatial discretization of the integral transport operator, they also represent an important tool for the investigation of the impact of these discretizations on the accuracy of the solution to the original continuous transport problem. In particular, they may be employed in the development of spatial discretizations that possess a high order of accuracy and preserve the correct asymptotic solution to the transport equation in notable limits, such as the \textit{Thick Diffusion Limit} [24].

In view of the previous observations, the construction of the full \( A \) and \( B \) matrices has been carried out finding closed analytic expressions for their elements in the most general heterogeneous and non-uniform mesh configurations, as illustrated in the next section.
3.3 Expressions for Matrices A and B in Slab Geometry

In view of Eq. (1.28) the expressions for the elements of matrix $B$ may be readily obtained once matrix $A$ has been constructed. To this end it is convenient to rewrite the two sets of equations for the general WDD form of the discrete ordinates approximation to the transport equation, Eqs. (1.22) and (1.24), in homogeneous form. This is accomplished by subtracting the sets of equations in two consecutive iterations, thus eliminating the fixed source, $s_j$, and replacing the dependent discrete variables by their iterative residual counterparts. Accordingly the equations for the residual quantities may be derived from Eq. (3.4) in the following compact matrix form:

$$
L^0_{m,j} \left[ \psi^{(+)}_{m,j}, \psi^{o,(+)}_{m,j} \right]^T = S^0_{m,j} \left[ c_j \phi^{(l)}, \psi^{i,(+)}_{m,j} \right]^T, \quad m = 1, \ldots, M; \quad j = 1, \ldots, J
$$

where, for example, $\psi^{(+)}_{m,j} = \psi_{m,j}^{(+)} - \tilde{\psi}_{m,j}^{(l)}$ is the mesh-sweep residual in the $m$th discrete ordinate angular flux averaged over cell $j$, and so on. Inversion of matrix $L^0_{m,j}$ may be readily accomplished producing the homogeneous form of Eq. (3.7) expressing the residuals $\psi^{(+)}_{m,j}$ and $\psi^{o,(+)}_{m,j}$ in terms of $\phi^{(l)}_{j}$ and $\psi^{i,(+)}_{m,j}$:

$$
\begin{align*}
\psi^{(+)}_{m,j} &= \left( \frac{1 + \alpha_{m,j}}{1 + 2 \kappa_{m,j} + \alpha_{m,j}} \right) c_j \phi^{(l)}_{j} + \left( \frac{2 \kappa_{m,j}}{1 + 2 \kappa_{m,j} + \alpha_{m,j}} \right) \psi^{i,(+)}_{m,j}, \\
\psi^{o,(+)}_{m,j} &= \left( \frac{2}{1 + 2 \kappa_{m,j} + \alpha_{m,j}} \right) c_j \phi^{(l)}_{j} + \left( \frac{2 \kappa_{m,j} + \alpha_{m,j} - 1}{2 \kappa_{m,j} + \alpha_{m,j} + 1} \right) \psi^{i,(+)}_{m,j}
\end{align*}
$$

m = 1, \ldots, M; \quad j = 1, \ldots, J
For the residual quantities too, the mesh-sweep algorithm proceeds by recursively solving Eq. (3.10) simultaneously for the residual cell-averaged flux and the residual outgoing cell-edge flux. The latter is equated to the residual incoming cell-edge flux of the adjacent down-stream cell; residual angular flux continuity across cell edges is a direct consequence of angular flux continuity across cell edges. In particular, for $\mu_m > 0$:

$$\psi_{m,j}^{i,(\ell+1)} = \psi_{m,j}^{o,(\ell+1)}, \; m = 1, \ldots, M / 2; \; j = 1, \ldots, (J - 1)$$

(3.11)

As stated previously, explicit vacuum boundary conditions will be assumed at both ends of the slab. Under this assumption, the starting point in the mesh-sweep algorithm for the positive cosine angles in the quadrature is represented, in view of Eq. (3.1), by the condition:

$$\psi_{m,1}^{i,(\ell+1)} = 0, \; m = 1, \ldots, M / 2,$$

(3.12)

applied to the residual of the incoming flux for the first computational cell $(j = 1)$ in the present iteration step, $(\ell + 1)$. The starting point in the mesh-sweep algorithm for the negative cosine angles in the quadrature is represented by the analogous condition:

$$\psi_{m,J}^{i,(\ell+1)} = 0, \; m = M / 2 + 1, \ldots, M,$$

(3.13)

applied to the residual of the incoming flux for the last computational cell $(j = J)$ in the present iteration step. Both boundary conditions, Eqs. (3.12) and (3.13), are a direct consequence of the vacuum boundary conditions for the actual quantities and of the definition of their residual.

Closure of the iterative process is once again accomplished in the SI scheme for the residual quantities by setting:
\[ \phi_j^{(n+1)} = \sum_{m=1}^{M} w_m \psi_{m,j}^{(n+1)}, \quad j = 1, \ldots, J \]  

(3.14)

The composition of the mesh-sweep operator with the summation over angles operator can be viewed as a mapping of the residuals of the scalar fluxes from the previous iteration to the present iteration that represents the homogeneous form of Eq. (1.26). It is convenient to write this equation in terms of its components:

\[ \phi_i^{(n+1)} = \sum_{j=1}^{J} A_{i,j} \sigma_{S_j} \phi_j^{(n)}, \quad i = 1, \ldots, J \]  

(3.15)

Equation (3.15) provides a recipe for constructing the elements of the iteration matrix \( A \) by differentiating both sides of the equation with respect to the cell-averaged scalar fluxes (for brevity the term residuals will be implied from here on when referring to quantities without a tilde) in the previous iteration:

\[ A_{i,j} = \frac{1}{\sigma_{S_j}} \frac{\partial \phi_i^{(n+1)}}{\partial \phi_j^{(n)}}, \quad i, j = 1, \ldots, J \]  

(3.16)

Note that, to within a factor \( 1/\sigma_{S_j} \), the elements of the SI iteration matrix \( A \) may be identified with the elements of the Jacobian matrix \( J \) for the linear transformation defined by Eq. (3.15):

\[ J_{i,j} = \frac{\partial \phi_i^{(n+1)}}{\partial \phi_j^{(n)}}, \quad i, j = 1, \ldots, J \]  

(3.17)

For this reason, matrix \( A \) is at times also referred to as the Jacobian matrix [19].

Using Eq. (3.16) recursively in the mesh-sweep algorithm and applying angular flux continuity across cell-boundaries, see Eq. (3.11), yields expressions for the elements of matrix \( A \). Employing the inductive derivation, and separately a constructive procedure,
presented in Secs. 3.3.1 and 3.3.2, respectively, we obtain the following analytic formulas for the elements of matrix $A$.

**Diagonal elements:**

$$A_{j,j} = \frac{1}{\sigma} \sum_{m=1}^{M} W_m \frac{1 + \alpha_{m,j}}{1 + 2 \kappa_{m,j} + \alpha_{m,j}}, \quad j = 1, ..., J$$

(3.18)

**$k^{th}$ off-diagonal elements with $k \geq 1$ coupling cells $j \xrightarrow{\mu_m > 0} j + k :$**

$$
A_{j+k,j} = \frac{1}{\sigma} \sum_{m=1}^{M/12} W_m \frac{2}{1 + 2 \kappa_{m,j} + \alpha_{m,j}} \left( \prod_{i=j+1}^{j+k} 2 \kappa_{m,i} + \alpha_{m,i} - 1 \right) \frac{2 \kappa_{m,j+k}}{1 + 2 \kappa_{m,j+k} + \alpha_{m,j+k}},
$$

(3.19)

$$j = 1, ..., (J-1); \quad k = 1, ..., (J-j)$$

**$k^{th}$ off-diagonal elements with $k \geq 1$ coupling cells $j \xleftarrow{\mu_m < 0} j + k :$**

$$
A_{j,j+k} = \sum_{m=1}^{M} W_m \frac{2 \kappa_{m,j}}{1 + 2 \kappa_{m,j} + \alpha_{m,j}} \left( \prod_{i=j}^{j+k-1} 2 \kappa_{m,i} + \alpha_{m,i} - 1 \right) \frac{2}{1 + 2 \kappa_{m,j+k} + \alpha_{m,j+k}} \frac{1}{\sigma_{j+k}},
$$

(3.20)

$$j = 1, ..., (J-1); \quad k = 1, ..., (J-j)$$

Notice that in the case of the first off-diagonal elements, $k=1$, the product terms in Eqs. (3.19) and (3.20) reduce to unity.

Inserting these expressions in Eq. (1.28) produces the elements of matrix $B$.

**Diagonal elements:**

$$B_{j,j} = 1 - c \sum_{m=1}^{M} W_m \frac{1 + \alpha_{m,j}}{1 + 2 \kappa_{m,j} + \alpha_{m,j}}, \quad j = 1, ..., J$$

(3.21)

**$k^{th}$ off-diagonal elements with $k \geq 1$ coupling cells $j \xrightarrow{\mu_m > 0} j + k :$**
\[ B_{j+k,j} = -c_j \sum_{m=1}^{M/2} w_m \frac{2}{1 + 2\kappa_{m,j} + \alpha_{m,j}} \left( \prod_{i=j+1}^{j+k-1} \frac{2\kappa_{m,i} + \alpha_{m,i} - 1}{1 + 2\kappa_{m,i} + \alpha_{m,i}} \right) \frac{2\kappa_{m,j+k}}{1 + 2\kappa_{m,j+k} + \alpha_{m,j+k}}, \]

\[ j = 1, \ldots, (J - 1); \quad k = 1, \ldots, (J - j) \]

**k\textsuperscript{th} off-diagonal elements with** \( k \geq 1 \)** coupling cells**

\[ B_{j,j+k} = -\sum_{m=M/2}^{M} w_m \frac{2\kappa_{m,j}}{1 + 2\kappa_{m,j} + \alpha_{m,j}} \left( \prod_{i=j+1}^{j+k-1} \frac{2\kappa_{m,i} + \alpha_{m,i} - 1}{1 + 2\kappa_{m,i} + \alpha_{m,i}} \right) \frac{2}{1 + 2\kappa_{m,j+k} + \alpha_{m,j+k}} c_{j+k}, \]

\[ j = 1, \ldots, (J - 1); \quad k = 1, \ldots, (J - j) \]

Notice that, even under the assumption of a symmetric quadrature, both matrices \( \mathbf{A} \) and \( \mathbf{B} \) could be non-symmetric depending on the material properties in the various computational cells; compare, for example, Eqs. (3.22) and (3.23) for a configuration where two adjacent cells have different sizes so that \( \kappa_{m,j} \neq \kappa_{m,j+1} \). That’s why separate expressions have been given for the super-diagonal and sub-diagonal elements. Of course, as it will be shown in Sec. 3.4, both matrices are indeed symmetric in configurations characterized with homogeneous material composition and a uniform mesh. Therefore, the topic concerned with the symmetrization of matrix \( \mathbf{B} \) is deferred to Sec. 4.2.

Two different approaches are now presented in order to demonstrate that the expressions for the elements of matrices \( \mathbf{A} \) and \( \mathbf{B} \) are indeed given by the previous equations. The first approach is based on an inductive proof and is presented in Sec. 3.3.1 while the second approach is based on a constructive proof and is outlined in Sec. 3.3.2.
3.3.1 Inductive Derivation of the Elements of A

The starting point is represented by the system of linear equations in Eq. (3.10) expressing \( \psi_{m,j}^{(\ell+1)} \) and \( \psi_{m,j}^{(\ell+1)} \) as linear functions of \( \phi_{j}^{(\ell)} \) and \( \psi_{m,j}^{(\ell+1)} \). Notice that this system of equations holds for a generic cell since it was derived for a generic \( j \) and for the purpose of the current derivation may be more conveniently rewritten in the following form:

\[
\begin{align*}
\psi_{m,j}^{(\ell+1)} &= o_{m,j} c_{j} \phi_{j}^{(\ell)} + p_{m,j} \psi_{m,j}^{(\ell+1)} , \quad m = 1, \ldots, M; \ j = 1, \ldots, J \\
\psi_{m,j}^{\alpha,(\ell+1)} &= r_{m,j} c_{j} \phi_{j}^{(\ell)} + q_{m,j} \psi_{m,j}^{(\ell+1)}
\end{align*}
\] (3.24)

The coefficients \( o_{m,j} \), \( p_{m,j} \), \( r_{m,j} \) and \( q_{m,j} \) in Eq. (3.24) have the following definitions:

\[
o_{m,j} \equiv \frac{\partial \psi_{m,j}^{(\ell+1)}}{\partial (c_{j} \phi_{j}^{(\ell)})} = \left( \frac{1 + \alpha_{m,j}}{1 + 2\kappa_{m,j} + \alpha_{m,j}} \right), \quad m = 1, \ldots, M; \ j = 1, \ldots, J; \quad (3.25)
\]

\[
p_{m,j} \equiv \frac{\partial \psi_{m,j}^{(\ell+1)}}{\partial \psi_{m,j}^{(\ell+1)}} = \left( \frac{2\kappa_{m,j}}{1 + 2\kappa_{m,j} + \alpha_{m,j}} \right), \quad m = 1, \ldots, M; \ j = 1, \ldots, J; \quad (3.26)
\]

\[
r_{m,j} \equiv \frac{\partial \psi_{m,j}^{\alpha,(\ell+1)}}{\partial (c_{j} \phi_{j}^{(\ell)})} = \left( \frac{2}{1 + 2\kappa_{m,j} + \alpha_{m,j}} \right), \quad m = 1, \ldots, M; \ j = 1, \ldots, J; \quad (3.27)
\]

\[
q_{m,j} \equiv \frac{\partial \psi_{m,j}^{\alpha,(\ell+1)}}{\partial \psi_{m,j}^{(\ell+1)}} = \left( \frac{2\kappa_{m,j} + \alpha_{m,j} - 1}{2\kappa_{m,j} + \alpha_{m,j} + 1} \right), \quad m = 1, \ldots, M; \ j = 1, \ldots, J (3.28)
\]
Notice that $\psi_{m,j}^{(e+1)}$ contains the information on how previously swept cells influence the flux in cell $j$ and depends (linearly) on the previous iterate of the scalar fluxes (assuming vacuum boundary conditions) up to cell $j-1$ for $\mu_m > 0$, or up to cell $j+1$ for $\mu_m < 0$, but not on $\phi_j^{(e)}$.

The expressions for the diagonal and the first off-diagonal elements of matrix $A$ represent a special case and will be treated separately in the derivation.

**Diagonal elements**

The calculation of the diagonal elements $A_{j,j}$ may be performed by applying Eq. (3.16) to the case $i = j$:

$$A_{j,j} = \frac{1}{\sigma_{S_j}} \frac{\partial \phi_j^{(e+1)}}{\partial \phi_j^{(e)}}, \quad j = 1, \ldots, J$$  \hspace{1cm} (3.29)

The partial derivative in Eq. (3.29) may be evaluated using the following result obtained simply by differentiating both sides of Eq. (3.14) with respect to $\phi_j^{(e)}$:

$$\frac{\partial \phi_j^{(e+1)}}{\partial \phi_j^{(e)}} = \sum_{m=1}^{M} W_m \left( \frac{\partial \psi_{m,j}^{(e+1)}}{\partial \phi_j^{(e)}} \right), \quad j = 1, \ldots, J,$$  \hspace{1cm} (3.30)

along with the following result deriving from the definition of $o_{m,j}$ in Eq. (3.25):

$$\frac{\partial \psi_{m,j}^{(e+1)}}{\partial \phi_j^{(e)}} = c_j o_{m,j}, \quad m = 1, \ldots, M; \quad j = 1, \ldots, J$$  \hspace{1cm} (3.31)
Substitution of Eq. (3.30) and Eq. (3.31) into Eq. (3.29) and use of the expression for \( a_{m,j} \) given in Eq. (3.25) prove that the expression for the diagonal elements of matrix \( A \) is indeed given by Eq. (3.18).

**First off-diagonal elements coupling cells** \( j \xrightarrow{\mu_m > 0} j + 1 \)

The calculation of the first off-diagonal elements \( A_{j+1,j} \) may be performed by applying Eq. (3.16) to the case \( i = j + 1 \):

\[
A_{j+1,j} = \frac{1}{\sigma_{S_j}} \frac{\partial \phi^{(i+1)}_{j+1}}{\partial \phi^{(i)}_j}, \quad j = 1, \ldots, (J-1) \tag{3.32}
\]

In evaluating the partial derivative on the right hand side of Eq. (3.32) it must be noticed that the previous iterate of the scalar flux in cell \( j \) contributes, or is coupled to the to-be-determined (in the present iterate) scalar flux in cell \( j + 1 \) only through the discrete ordinates characterized by \( \mu_m > 0 \). Cell \( j \) influences cell \( j + 1 \) when the one-dimensional structure is swept from left to right along \( \mu_m > 0 \), while cell \( j + 1 \) influences cell \( j \) when the structure is swept from right to left along \( \mu_m < 0 \). Keeping in mind this observation, the partial derivative on the right hand side of Eq. (3.32) may be evaluated by differentiating with respect to \( \phi^{(i)}_j \) both sides of Eq. (3.14) written for cell \( j + 1 \), taking the sum only over the first \( M/2 \) angles, \( \mu_m > 0 \), since all remaining partial derivatives are equal to zero.

\[
\frac{\partial \phi^{(i+1)}_{j+1}}{\partial \phi^{(i)}_j} = \sum_{m=1}^{M/2} W_m \left( \frac{\partial \psi^{(i+1)}_{m,j+1}}{\partial \phi^{(i)}_j} \right), \quad j = 1, \ldots, (J-1) \tag{3.33}
\]
The system of equations in Eq. (3.24), along with the continuity condition Eq. (3.11) may be used to express $\psi_{m,j+1}'^{(f+1)}$ as a function of $\phi_j^{(f)}$. The first equation in the system is first written for cell $j+1$:

$$
\psi_{m,j+1}'^{(f+1)} = o_{m,j+1} c_{j+1} \phi_j^{(f)} + p_{m,j+1} \psi_{m,j+1}'^{(f+2)} \quad m = 1, \ldots, M / 2 \tag{3.34}
$$

The continuity condition is used in Eq. (3.34) to express $\psi_{m,j+1}'^{(f+1)}$ in terms of the angular flux exiting cell $j$:

$$
\psi_{m,j+1}'^{(f+1)} = \psi_{m,j}'^{(f+1)} \quad m = 1, \ldots, M / 2 \tag{3.35}
$$

The latter angular flux may in turn be expressed in terms of $\phi_j^{(f)}$ and of the incoming angular flux for cell $j$, $\psi_{m,j}'^{(f+1)}$, simply using the second system equation in Eq. (3.24) written for cell $j$:

$$
\psi_{m,j}'^{(f+1)} = r_{m,j} c_j \phi_j^{(f)} + q_{m,j} \psi_{m,j}'^{(f+1)} \quad m = 1, \ldots, M / 2 \tag{3.36}
$$

Substitution of Eq. (3.36) into Eq. (3.35) and of the resulting equation into Eq. (3.34) leads to the following expression for $\psi_{m,j+1}'^{(f+1)}$:

$$
\psi_{m,j+1}'^{(f+1)} = o_{m,j+1} c_{j+1} \phi_j^{(f+1)} + p_{m,j+1} r_{m,j+1} c_j \phi_j^{(f+1)} + p_{m,j+1} q_{m,j+1} \psi_{m,j}'^{(f+1)} \quad m = 1, \ldots, M / 2 \tag{3.37}
$$

Notice that $\psi_{m,j}'^{(f+1)}$ contains the information on how previously swept cells influence cell $j$ and depends (linearly) only on the previous iterate of the scalar fluxes (assuming vacuum boundary conditions) up to cell $j-1$ but not on $\phi_j^{(f)}$.

The partial derivatives on the right hand side of Eq. (3.33) may be directly calculated using Eq. (3.37):
Substitution of Eq. (3.38) and Eq. (3.33) into Eq. (3.32) and use of the expressions for \( p_{m,j+1} \) and \( r_{m,j} \) given in Eq. (3.26) and Eq. (3.27) respectively, prove that the expression for the first off-diagonal elements of matrix \( A \) coupling cell \( j+1 \) to cell \( j \) is indeed given by Eq. (3.19) for \( k = 1 \).

**First off-diagonal elements coupling cells** \( j \leftarrow \mu_m < 0 \rightarrow j + 1 \)

The calculation of the first off-diagonal elements \( A_{j,j+1} \) may be performed by applying Eq. (3.16) for this choice of indices:

\[
A_{j,j+1} = \frac{1}{\sigma_{S_{j+1}}} \frac{\partial \phi_j^{(l+1)}}{\partial \phi_{j+1}^{(l)}} , \quad j=1,\ldots,(J-1)
\]  

(3.39)

Similar considerations to those applied in the derivation of the expressions for the first sub-diagonal elements apply to Eq. (3.39). In evaluating the partial derivative on the right hand side of Eq. (3.39) it must be noticed that the previous iterate scalar flux in cell \( j+1 \) contributes or is coupled to the to-be-determined (in the present iterate) scalar flux in cell \( j \) only through the discrete ordinates characterized by \( \mu_m < 0 \). Keeping in mind this observation and in view of the assumption of a symmetric angular quadrature, Eq. (3.1), the partial derivative on the right hand side of Eq. (3.39) may be evaluated using the expression obtained exchanging the indices \( j \) and \( j+1 \) in Eq. (3.33):
\[
\left. \frac{\partial \psi^{(r+1)}_{m,j}}{\partial \phi^{(r)}_{j+1}} \right|_{m} = \sum_{m=2}^{M} w_m \left( \frac{\partial \psi^{(r+1)}_{m,j}}{\partial \phi^{(r)}_{j+1}} \right), \quad j = 1, \ldots, (J-1)
\]  
(3.40)

The partial derivatives on the right hand side of Eq. (3.40) may be readily evaluated by exchanging the subscripts \(j\) and \(j + 1\) everywhere in Eq. (3.38). This is a consequence of the fact that the original system consisting of Eqs. (1.22) and (1.24) has been cast in an incoming- and outgoing-edge form and may be used indistinguishably both for positive and negative \(\mu_m\). The following expression is obtained:

\[
\left. \frac{\partial \psi^{(r+1)}_{m,j}}{\partial \phi^{(r)}_{j+1}} \right|_{m} = p_{m,j} r_{m,j+1} e_{j+1}, \quad m = \frac{M}{2} + 1, \ldots, M
\]  
(3.41)

Substitution of Eqs. (3.41) and (3.40) into Eq. (3.39) and use of the expressions for \(p_{m,j}\) and \(r_{m,j+1}\) given in Eqs. (3.26) and (3.27), respectively, proves that the expression for the first off-diagonal elements of matrix \(\mathbf{A}\) coupling cell \(j\) to cell \(j + 1\) is indeed given by Eq. (3.20) for \(k = 1\).

**\(k^{th}\) off-diagonal elements with \(k \geq 2\) coupling cells** \(j \xrightarrow{\mu_m > 0} j + k\)

First of all an expression for \(\psi^{(r+1)}_{m,j+k}\) in terms of the previous iterate scalar fluxes in cells \(j + 3, j + 2, j + 1\) and \(j\) and of the incoming angular flux for cell \(j\) is constructed starting from the first equation in Eq. (3.24) written for cell \(j + 3\). Then the continuity relation in Eq. (3.11) is used along with the second equation in Eq. (3.24) to express explicitly the dependence of the incoming angular flux for one cell in terms of the previous iterate of the scalar flux and the incoming angular flux for the previously swept
cell from cell $j+3$ down to cell $j$. The resulting expression obtained following the outlined procedure is:

$$\psi_{m,j+3}^{(i+1)} = o_{m,j+3}c_{j+3}^{(i)} \phi_{j+3}^{(i)} + p_{m,j+3}r_{m,j+2}c_{j+2}^{(i)} \phi_{j+2}^{(i)} + p_{m,j+3}q_{m,j+2}r_{m,j+1}c_{j+1}^{(i)} \phi_{j+1}^{(i)} +$$

$$+ p_{m,j+3}q_{m,j+2}q_{m,j+1}r_{m,j}^{(i)} \phi_{j}^{(i)} + p_{m,j+3}q_{m,j+2}q_{m,j}^{(i)} \psi_{m,j}^{(i)} \psi_{m,j}^{(i+1)}$$

(3.42)

Notice that the first two terms on the right hand side of Eq. (3.42) have already been encountered in the derivation of the expressions for the diagonal and first off-diagonal matrix elements. The expressions for the third and fourth terms on the right hand side of Eq. (3.42) may be readily used to determine the expressions for the second and third off-diagonal matrix elements respectively, by taking the partial derivative of $\psi_{m,j+3}^{(i+1)}$ with respect to $\phi_{j+1}^{(i)}$ and $\phi_{j}^{(i)}$ respectively. Most importantly, though, they suggest the following inductive hypothesis (IH) that we employ below to determine expressions for the matrix elements lying on the $k^{th}$ off-diagonal band of matrix $A$, for generic $k \geq 2$.

$$\text{(IH)} \quad \frac{\partial \psi_{m,j+k}^{(i+1)}}{\partial (c_{j}\phi_{j}^{(i)})} = p_{m,j+k} \left( \prod_{i=j+1}^{j+k-1} q_{m,i} \right) r_{m,j}$$

(3.43)

In view of the ensuing demonstration that (IH) is valid for all $k \geq 2$, it is useful to notice that Eq. (3.43) implies the following relation that will be designated as (IH'):

$$\text{(IH')} \quad \frac{\partial \psi_{m,j+k}^{(i+1)}}{\partial (c_{j}\phi_{j}^{(i)})} = \left( \prod_{i=j+1}^{j+k-1} q_{m,i} \right) r_{m,j}$$

(3.44)

As a matter of fact, the following equality is readily obtained by applying the well known derivative chain rule and recalling the definition given in Eq. (3.26):
The validity of the inductive hypothesis (IH) is hereby verified. In particular, proof is given that if (IH) holds then it is also true that:

\[
\frac{\partial \psi^{(i+1)}_{m,j+k}}{\partial (c_j \phi_j^{(i)})} = \left( \frac{\partial \psi^{(i+1)}_{m,j+k}}{\partial \psi^{(i+1)}_{m,j+k}} \right) \left( \frac{\partial \psi^{(i+1)}_{m,j+k}}{\partial (c_j \phi_j^{(i)})} \right) = p_{m,j+k} \left( \frac{\partial \psi^{(i+1)}_{m,j+k}}{\partial (c_j \phi_j^{(i)})} \right)
\]  

\((3.45)\)

\((\text{IH'}) \) directly follows comparing the right hand sides of Eqs. (3.43) and (3.45).

To this end, an explicit expression is given for \(\psi^{(i+1)}_{m,j+k+1}\) using the first equation in Eq. (3.24) written for cell \(j+k+1\):

\[
\psi^{(i+1)}_{m,j+k+1} = o_{m,j+k+1} c_{j+k+1} \phi_{j+k+1}^{(i)} + p_{m,j+k+1} \psi^{(i+1)}_{m,j+k+1}
\]  

\((3.47)\)

Substituting the continuity condition, Eq. (3.11), written for \(j+k+1\) and using the second equation in Eq. (3.24) to explicitly express \(\psi^{(i+1)}_{m,j+k}\), the following result is obtained:

\[
\psi^{(i+1)}_{m,j+k+1} = o_{m,j+k+1} c_{j+k+1} \phi_{j+k+1}^{(i)} + p_{m,j+k+1} r_{m,j+k} c_{j+k} \phi_{j+k}^{(i)} + p_{m,j+k+1} q_{m,j+k} \psi^{(i+1)}_{m,j+k}
\]  

\((3.48)\)

The partial derivative of \(\psi^{(i+1)}_{m,j+k+1}\) with respect to \(c_j \phi_j^{(i)}\) may be calculated using Eq. (3.48) and noting that \(\psi^{(i+1)}_{m,j+k+1}\) depends on \(c_j \phi_j^{(i)}\) only through the last term on the right hand side of Eq. (3.48):

\[
\frac{\partial \psi^{(i+1)}_{m,j+k+1}}{\partial (c_j \phi_j^{(i)})} = p_{m,j+k+1} q_{m,j+k} \frac{\partial \psi^{(i+1)}_{m,j+k}}{\partial (c_j \phi_j^{(i)})}
\]  

\((3.49)\)
Using (IH') in Eq. (3.49) the following result is finally obtained:

\[
\frac{\partial \psi_{m,j+k+1}^{(i+1)}}{\partial \left( c_j \phi_j^{(i)} \right)} = p_{m,j+k+1}q_{m,j+k} \left( \prod_{j=j+1}^{j+k} q_{m,i} \right) r_{m,j} = p_{m,j+k+1} \left( \prod_{j=j+1}^{j+k} q_{m,i} \right) r_{m,j} 
\]

This result verifies Eq. (3.46) and permits the use of mathematical induction in the ensuing derivation.

The \( k \)th off-diagonal elements of matrix \( A \) are now derived in a straightforward way using (IH), Eq. (3.43). The calculation of the \( k \)th off-diagonal elements \( A_{j+k,j} \) is performed by applying Eq. (3.16) to the case \( i = j+k \):

\[
A_{j+k,j} = \frac{1}{\sigma_{S_j}} \frac{\partial \phi_{j+k}^{(i+1)}}{\partial \phi_j^{(i)}} , \quad j = 1,\ldots,(J-2) ; k = 2,\ldots,(J-j) 
\]

The same considerations that led to Eq. (3.33) may be applied in this case and yield the following expression for the partial derivative on the right hand side of Eq. (3.51):

\[
\frac{\partial \phi_{j+k}^{(i+1)}}{\partial \phi_j^{(i)}} = \sum_{m=1}^{M/2} w_m \left( \frac{\partial \psi_{m,j+k}^{(i+1)}}{\partial \phi_j^{(i)}} \right) 
\]

The partial derivatives on the right hand side of the previous equation may be evaluated using mathematical induction embodied in the inductive hypothesis (IH), Eq. (3.43), yielding:

\[
\frac{\partial \psi_{m,j+k}^{(i+1)}}{\partial \phi_j^{(i)}} = c_j p_{m,j+k} \left( \prod_{j=j+1}^{j+k} q_{m,i} \right) r_{m,j} 
\]
Substitution of Eqs. (3.53) and (3.52) into Eq. (3.51) and use of the expressions for \( p_{m,j+k} \), \( r_{m,j} \) and \( q_{m,j} \) given in Eqs. (3.26), (3.27) and (3.28) respectively, proves that the expression for the \( k \)th off-diagonal elements of matrix \( A \) coupling cell \( j+k \) to cell \( j \) is indeed given by Eq. (3.19).

**\( k \)th off-diagonal elements with \( k \geq 2 \) coupling cells** \( j \leftarrow \frac{\mu_{m} < 0}{j+k} \)

The calculation of the \( k \)th off-diagonal elements \( A_{j,j+k} \) may be performed applying Eq. (3.16) for this choice of indices:

\[
A_{j,j+k} = \frac{1}{\sigma_{S_{j+k}}} \frac{\partial \phi_{j}^{(\epsilon+1)}}{\partial \phi_{j+k}^{(\epsilon)}} \quad j = 1, \ldots, (J-2); k = 2, \ldots, (J-j).
\]  

(3.54)

The same considerations that led to Eq. (3.40) may be applied to this case and yield the following expression for the partial derivative on the right hand side of Eq. (3.54):

\[
\frac{\partial \phi_{j}^{(\epsilon+1)}}{\partial \phi_{j+k}^{(\epsilon)}} = \sum_{m=\frac{M}{2}+1}^{M} w_{m} \left( \frac{\partial \psi_{m,j}^{(\epsilon+1)}}{\partial \phi_{j+k}^{(\epsilon)}} \right)
\]

(3.55)

The partial derivative in the previous equation may be evaluated by applying to the inductive hypothesis (IH), Eq. (3.43), the same considerations that led to Eq. (3.41). The subscripts \( j \) and \( j+k \) are interchanged in Eq. (3.43) and the indices reordered in the product according to the natural spatial ordering of the cells (increasing from left to right). Exploiting the fact that the product is commutative, the following expression is finally obtained:
Substitution of Eqs. (3.56) and (3.55) into Eq. (3.54) and use of the expressions for $p_{m,j}$, $r_{m,j+k}$ and $q_{m,i}$ given in Eqs. (3.26), (3.27) and (3.28), respectively, proves that the expression for the $k$th off-diagonal elements of matrix $A$ coupling cell $j$ to cell $j+k$ is indeed given by Eq. (3.20).

This completes the inductive derivation of Eqs. (3.18) - (3.20).

### 3.3.2 Constructive Derivation of the Elements of $A$

The starting point for the constructive approach is still represented by Eq. (3.24) along with the definitions for the coefficients $a_{m,i}$, $p_{m,i}$, $r_{m,i}$ and $q_{m,i}$ given in Eqs. (3.25), (3.26), (3.27) and (3.28), respectively. As noted previously, $\psi^{(i+1)}_{m,j}$ contains the information on how previously swept cells influence the flux in cell $j$ and depends linearly only on the previous iterate of the scalar fluxes (assuming vacuum boundary conditions) up to cell $j-1$, for $\mu_m > 0$, or up to cell $j+1$, for $\mu_m < 0$, but not on $\phi^{(i)}_j$. In this respect and for the purpose of the current demonstration, it is convenient to rewrite the system of linear equations in Eq. (3.24) in yet another form. In particular, a subscript $i$ is used to refer to a generic computational cell in the mesh for reasons that will become apparent in the following derivation (no confusion should arise with the use of the superscript $i$ to designate incoming angular fluxes).
\[
\begin{align*}
\psi_{m,i}^{(s+1)} &= \psi_{m,i}^{(s+1)} \phi_i^{(s)} + \psi_{m,i}^{(s+1)} \phi_j^{(s+1)} \quad , \quad m = 1, \ldots, M; i = 1, \ldots, J \\
\psi_{m,i}^{\alpha,(s+1)} &= \psi_{m,i}^{\alpha,(s+1)} \phi_i^{(s)} + \psi_{m,i}^{\alpha,(s+1)} \phi_j^{(s+1)} 
\end{align*}
\] (3.57)

The following notation has been introduced in Eq. (3.57):

\[
\psi_{m,i}^{(s+1)} \bigg|_{\phi_i^{(s)}} = o_{m,i} \phi_i^{(s)}, \quad m = 1, \ldots, M; i = 1, \ldots, J
\] (3.58)

is the (linear) contribution to \(\psi_{m,i}^{(s+1)}\) due to \(\phi_i^{(s)}\);

\[
\psi_{m,i}^{(s+1)} \bigg|_{\psi_j^{(s+1)}} = p_{m,i} \psi_j^{(s+1)}, \quad m = 1, \ldots, M; i = 1, \ldots, J
\] (3.59)

is the contribution to \(\psi_{m,i}^{(s+1)}\) due to \(\psi_j^{(s+1)}\);

\[
\psi_{m,i}^{\alpha,(s+1)} \bigg|_{\phi_j^{(s)}} = r_{m,i} \phi_j^{(s)}, \quad m = 1, \ldots, M; i = 1, \ldots, J
\] (3.60)

is the contribution to \(\psi_{m,i}^{\alpha,(s+1)}\) due to \(\phi_j^{(s)}\);

\[
\psi_{m,i}^{\alpha,(s+1)} \bigg|_{\psi_j^{(s+1)}} = q_{m,i} \psi_j^{(s+1)}, \quad m = 1, \ldots, M; i = 1, \ldots, J
\] (3.61)

is the contribution to \(\psi_{m,i}^{\alpha,(s+1)}\) due to \(\psi_j^{(s+1)}\).

The expressions for the elements of matrix \(A\) may be constructed using the previous equations. The most general situation, leading to the determination of the expressions for the \(k\)th off-diagonal elements with \(k \geq 2\), will be considered first. The peculiarities of the construction of the diagonal and first off-diagonal elements will then be treated and become more evident in view of the more general derivation.
\( k^{th} \) off-diagonal elements with \( k \geq 2 \) coupling cells

\[
j \xrightarrow{\mu_m > 0} j + k
\]

As in the inductive proof, the starting point for the calculation of the \( k^{th} \) off-diagonal elements \( A_{j+k,j} \) is Eq. (3.51). This equation suggests that matrix element \( A_{j+k,j} \) is intimately related to the contribution to the scalar flux in cell \( j+k \), to-be-determined in the present iteration, from the scalar flux in cell \( j \), determined in the previous iteration. In view of Eq. (3.14), this contribution is evaluated once the contribution to the cell-averaged angular flux \( \psi_{m,j+k}^{(\ell+1)} (k \geq 2) \) due to \( \phi_j^{(\ell)} \) has been determined. The latter contribution will be indicated as \( \psi_{m,j+k}^{(\ell+1)} \bigg|_{\phi_j^{(\ell)}} \), consistent with the previously introduced notation. This quantity is determined noting that going from cell \( j \) to cell \( j+k \), see Fig. 3.2, by performing the mesh-sweep along \( \mu_m > 0 \), is equivalent to applying a cascade of linear discrete dynamical systems each governed by the system of equations in Eq. (3.57). Recall that the angular flux continuity condition, Eq. (3.11), holds at each interface between adjacent cells.

![Fig. 3.2: Computational cells involved in the contribution to the \( m^{th} \) discrete ordinate angular flux in cell \( j+k \) from the scalar flux in cell \( j \) (\( \mu_m > 0 \)).](image-url)
Due to the linearity of the system the contribution of $\phi_j^{(i)}$ to $\psi_{m,j+k}^{(i+1)}$ may be calculated independently from contributions by all other cells’ scalar flux. This is accomplished by considering the system in Eq. (3.57) with $i$ set to the cell index $j+k$ and focusing on the partial contributions to the angular flux in that cell, as indicated in the procedure outlined in Fig. 3.3. Notice the use of the short-hand notation:

$$
\psi_{m,j+1}^{\alpha,i}(\phi_j^{(i)}) = \psi_{m,j+1}^{\alpha,i}(\phi_j^{(i)})
$$

introduced to avoid the more cumbersome notation that would derive from a consistent application of the definitions given previously. In general $\phi_j^{(i)}$ is used to designate the contribution to $\psi_{m,j+1}^{\alpha,i}$ due to $\phi_j^{(i)}$.

The arrows in Fig. 3.3 indicate the operation that must be performed on the term on the left hand side in order to obtain the desired contribution from $\phi_j^{(i)}$ to the term on the right hand side. The indicated operation follows from the system in Eq. (3.57) applied to the cell under consideration along with the definitions in Eqs. (3.58) through (3.61).
Fig. 3.3: Outline of the procedure for computing the contribution to the $m^{th}$ discrete ordinate angular flux in cell $j+k$ from the scalar flux in cell $j$ ($\mu_m > 0$).
In view of the previous sequence the ratio obtained from dividing \( \psi^{(t+1)}_{m,j+k} \bigg/ \phi_j \) by \( \phi_j \) may be formed in the following way:

\[
\psi^{(t+1)}_{m,j+k} \bigg/ \phi_j = \left( \frac{\psi^{o,(t+1)}_{m,j}}{\phi_j} \right) \times \left( \frac{\psi^{o,(t+1)}_{m,j+1}}{\phi_j} \right) \times \left( \frac{\psi^{i,(t+1)}_{m,j+2}}{\phi_j} \right) \times \ldots \times \left( \frac{\psi^{i,(t+1)}_{m,j+k}}{\phi_j} \right)
\]

(3.63)

The ratios on the right hand side of Eq. (3.63) may be written explicitly considering the multiplicative operations attached to the arrows in the sequence reported in Fig. 3.3:

\[
\psi^{(t+1)}_{m,j+k} \bigg/ \phi_j = c_j r_{m,j} \times q_{m,j+1} \times q_{m,j+2} \times \ldots \times q_{m,j} \times \ldots \times q_{m,j+k-1} \times p_{m,j+k}
\]

(3.64)

Equation (3.64) may finally be written in the following more compact form:

\[
\psi^{(t+1)}_{m,j+k} \bigg/ \phi_j = c_j r_{m,j} \left( \prod_{i=j+1}^{j+k-1} q_{m,i} \right) p_{m,j+k}
\]

(3.65)

The latter result may be used to evaluate the partial derivative on the right hand side of Eq. (3.51) by virtue of the expression contained in Eq. (3.52). In fact, in view of
the linearity of the mesh-sweep algorithm, \( \psi_{m,j+k}^{(f+1)} \) is determined by a linear combination of the previous iterate average scalar fluxes in the cells previously swept starting from the vacuum boundary condition. Therefore Eq. (3.52) may equivalently be written in the following form:

\[
\frac{\partial \psi_{m,j+k}^{(f+1)}}{\partial \phi_j^{(f)}} = \sum_{m=1}^{M/2} w_m \frac{\psi_{m,j+k}^{(f+1)}}{\phi_j^{(f)}} \quad (3.66)
\]

Substitution of Eq. (3.65) in Eq. (3.66) yields:

\[
\frac{\partial \psi_{m,j+k}^{(f+1)}}{\partial \phi_j^{(f)}} = c_j \sum_{m=1}^{M/2} w_m r_{m,j} \left( \prod_{i=j+1}^{j+k-1} q_{m,i} \right) p_{m,j+k} \quad (3.67)
\]

Substitution of Eq. (3.67) into Eq. (3.51) and use of the expressions for \( r_{m,j} \) and \( q_{m,i} \) given in Eqs. (3.26), (3.27) and (3.28), respectively, proves that the expression for the \( k \)th off-diagonal elements of matrix \( A \) coupling cell \( j+k \) to cell \( j \) is indeed given by Eq. (3.19).

It is noted that, in view of the residual angular flux continuity across cell edges, the expression in Eq. (3.63) may be readily interpreted as a differentiation chain rule:

\[
\frac{\partial \psi_{m,j+k}^{(f+1)}}{\partial \phi_j^{(f)}} = \left( \frac{\partial \psi_{m,j+k}^{(f+1)}}{\partial \psi_{m,j+k}^{(f)}} \right) \left( \frac{\partial \psi_{m,j+k}^{(f+1)}}{\partial \psi_{m,j}^{(f+1)}} \right) \left( \frac{\partial \psi_{m,j}^{(f+1)}}{\partial \psi_{m,j}^{(f)}} \right) \left( \frac{\partial \psi_{m,j}^{(f+1)}}{\partial \phi_j^{(f)}} \right) \quad (3.68)
\]

Keeping in mind this observation, the comparison of Eq. (3.65) with Eq. (3.53) may offer a constructive more physical interpretation of the mathematical inductive hypothesis, Eq. (3.43), formulated in the inductive proof. A sketch of the constructive approach is presented in Fig. 3.4, for a case in which \( k = 6 \).
Fig. 3.4: Sketch of constructive approach with coefficients to be multiplied to determine the influence from the scalar flux in a cell to the $m^{th}$ discrete ordinate angular flux in a downstream cell ($\mu_m > 0$).

$k^{th}$ off-diagonal elements with $k \geq 2$ coupling cells $j \leftarrow \mu_m < 0 \rightarrow j + k$

The starting point for the calculation of the $k^{th}$ off-diagonal elements $A_{j,j+k}$ is again represented by Eqs. (3.54) and (3.55). Derivation of these elements is straightforward, once it is recognized that now cell $j+k$ is the starting cell while cell $j$ is the arrival cell. The result for $\mu_m < 0$ equivalent to Eq. (3.64) may be obtained by simply interchanging the subscripts $j$ and $j+k$ and traversing intervening cells in reverse order yielding:

$$
\psi_m^{(f)}_{j,k} \bigg|_{\phi^{(f)}_{j+k}} = c_{j+k} r_{m,j+k} \times q_{m,j+k-1} \times q_{m,j+k-2} \times \cdots \times q_{m,j} \times \cdots \times q_{m,j+k+1} \times p_m
$$

(3.69)

Rearranging terms in the usual fashion the following result is obtained:

$$
\psi_m^{(f+1)}_{m,j} \bigg|_{\phi^{(f)}_{j+k}} = p_m \left( \prod_{i=j+1}^{j+k} q_{m,i} \right) r_{m,j+k} c_{j+k}
$$

(3.70)
Equation (3.70) may be used to evaluate the partial derivatives on the right hand side of Eq. (3.55). Considerations similar to those leading to Eq. (3.66) allow making the following identification:

\[
\frac{\partial \phi_{j}^{(r+1)}}{\partial \phi_{j+k}^{(r)}} = \sum_{m=M/2+1}^{M} w_{m} \frac{\psi_{m,j}^{(r+1)}}{\phi_{j+k}^{(r)}}
\]  

Substitution of Eq. (3.70) into Eq. (3.71) yields:

\[
\frac{\partial \phi_{j}^{(r+1)}}{\partial \phi_{j+k}^{(r)}} = c_{j+k} \sum_{m=M/2+1}^{M} w_{m} r_{m,j+k} \left( \prod_{i=j+1}^{j+k-1} q_{m,i} \right) p_{m,j}
\]  

Substitution of Eq. (3.72) into Eq. (3.54) and use of the expressions for \( p_{m,j} \), \( r_{m,j+k} \) and \( q_{m,i} \) given in Eqs. (3.26), (3.27) and (3.28) respectively, proves that the expression for the \( k \)th off-diagonal elements of matrix \( A \) coupling cell \( j \) to cell \( j+k \) is indeed given by Eq. (3.20).

**First off-diagonal elements coupling cells** \( j \xrightarrow{\mu_{m}>0} j+1 \)

As in the inductive derivation, the starting point for the calculation of the first off-diagonal elements \( A_{j+1,j} \) is represented by Eq. (3.32). The determination of the contribution to \( \psi_{m,j+1}^{(r+1)} \) from \( \phi_{j}^{(r)} \) can be carried out following much the same steps used in the previous derivation of the \( k \)th off-diagonal elements (\( k > 1 \)).
Fig. 3.5: Computational cells involved in the contribution to the $m^{th}$ discrete ordinate angular flux in cell $j + 1$ from the scalar flux in cell $j$ ($\mu_m > 0$).

In this case the calculation is more straightforward because two adjacent cells are considered and no effect due to intermediate cells interposed between the starting cell and the arrival cell has to be considered (see Fig. 3.5). Consequently the $q_{m,j}$ coefficients will be absent from the final expression for the matrix elements on the first off-diagonal band. The two step sequence for this case is depicted in Fig. 3.6.

In view of the previous sequence the ratio obtained from dividing $\psi_{m,j+1}^{l+1}$ by $\phi_j^{(l)}$ may be formed in the following way:

Fig. 3.6: Outline of the procedure for computing the contribution to the $m^{th}$ discrete ordinate angular flux in cell $j + 1$ from the scalar flux in cell $j$ ($\mu_m > 0$).
The ratios on the right hand side of Eq. (3.73) may be written explicitly considering the multiplicative operations attached to the arrows in the sequence:

\[
\frac{\psi_{m,j+1}^{(r+1)}}{\phi_j^{(r)}} = \left(\frac{\psi_{m,j}^{(r)}}{\phi_j^{(r)}}\right) \left(\frac{\psi_{m,j+1}^{(r+1)}}{\phi_j^{(r)}}\right)
\]  
(3.73)

It must be noticed that both Eq. (3.52) and its equivalent Eq. (3.66) are actually valid for any \( k > 0 \), and in particular for \( k = 1 \). Substitution of Eq. (3.74) into Eq. (3.66), written for \( k = 1 \), yields the following result:

\[
\frac{\partial \phi_j^{(r+1)}}{\partial \phi_j^{(r)}} = c_j r_{m,j} \times p_{m,j}
\]  
(3.74)

Substitution of Eq. (3.75) into Eq. (3.32) and use of the expressions for \( p_{m,j+1} \) and \( r_{m,j} \) given in Eqs. (3.26) and Eq. (3.27) respectively, prove that the expression for the first off-diagonal elements of matrix \( \mathbf{A} \), coupling cell \( j + 1 \) to cell \( j \), is indeed given by Eq. (3.19) for \( k = 1 \).

**First off-diagonal elements coupling cells**  
\( j \leftarrow_{\mu_m < 0} j + 1 \)

In view of the discussion presented for the case \( j \leftarrow_{\mu_m < 0} j + k \), the expression for \( A_{j,j+1} \) is readily obtained by exchanging \( j \) and \( j + 1 \) in Eq. (3.75) and consequently
in Eq. (3.32). The result obtained from substituting the expressions for \( p_{m,j} \) and \( r_{m,j+1} \) given in Eqs. (3.26) and (3.27) respectively, proves that the expression for the first off-diagonal elements of matrix \( A \) coupling cell \( j \) to cell \( j+1 \) is indeed given by Eq. (3.20) for \( k = 1 \).

**Diagonal elements**

The derivation is the same as that given in the inductive proof since the single cell case is very peculiar and is already contained in the first of the cell equations in Eq. (3.57). Notice that, consistent with the use of Eq. (3.57), in this case Eq. (3.31) may be obtained as a consequence of Eq. (3.58) and Eq. (3.25) leading to the identification:

\[
\frac{\partial \psi_{m,j}^{(t+1)}}{\partial \phi_j^{(t)}} = \psi_{m,j}^{(t+1)} \frac{\partial \phi_j^{(t)}}{\phi_j^{(t)}} = c_j o_{m,j}
\]

Substitution of Eqs. (3.30) and (3.76) into Eq. (3.29) and use of the expression for \( o_{m,j} \) given in Eq. (3.25) proves that the expression for the diagonal elements of matrix \( A \) is indeed given by Eq. (3.18).

This completes the constructive derivation of Eqs. (3.18) - (3.20).

Notice that the constructive derivation gives a direct recipe to build a matrix element, once the starting and arriving cells whose average scalar fluxes are coupled by that matrix element are given, hence the attribute ‘constructive’ given to this proof: see Fig. 3.4.
3.3.3 Numerical Verification

The expressions for the elements of matrices $A$ and $B$ have been implemented in a computer code that builds and stores the matrices and directly solves Eq. (1.27). The correctness of the numerical calculation of the matrix elements has been progressively verified following two different approaches.

The first approach is presented in the current section. It is based on the comparison of the iterative limit of the cell-averaged fluxes, obtained through direct inversion of matrix $B$, with the solutions obtained iteratively, via a progressively more stringent requirement on the imposed convergence criterion. Two different iterative algorithms are employed to obtain the latter solution, namely Source Iteration (SI) and Larsen’s Four Step Method Diffusion Synthetic Acceleration (FSM-DSA).

The iterative algorithms are implemented in the AP1 code [19] for solving one-dimensional transport problems. Both the AP1 code and the code developed for the construction of the $A$ and $B$ matrices are written in FORTRAN 90 and execute under the Windows and Linux operating systems in 32 or 64-bit arithmetic. Standard routines from the LINPACK library [39] are used to solve the linear system in Eq. (1.27) in double precision arithmetic.

The second approach, presented in Sec. 3.4.4, is based on a comparison of the computed numerical values for the matrices elements with values computed via an asymptotic analysis of the analytic expressions obtained in the previous section. This comparison will be performed both in the thin and in the thick cell limits under the assumption of homogeneous cell properties and uniform mesh.
In view of the slow convergence of the standard Source Iteration algorithm for highly neutron-preserving configurations, the comparison of the results obtained for different choices of the relative convergence criterion $\varepsilon$ with the exact solution from direct matrix inversion, has been made with reference to the model problem presented in Fig. 3.7. A heterogeneous computational cell structure containing neutron-absorbing cells and a fixed source distribution localized at the center of the slab has been considered in this model problem.

The verification of the correctness of the calculation of the $B$ matrix elements is based on the observation that the inversion of the matrix on the once-collided fixed source should give as solution the limit that the SI method should converge to. The smaller the convergence criterion used in the convergence test of the iterative algorithm, the better the agreement to be expected between the direct and iterative solutions.

The results obtained for the cell-averaged fluxes in the first five computational cells of the symmetric model problem depicted in Fig. 3.7 are reported in Table 3.1 for comparison. The trend in the values reported in Table 3.1 confirms that the iterative solution approaches the solution given by the direct inversion of matrix $B$. This verifies the numerical calculation of the matrix elements based on the analytic expressions derived above.

The FSM-DSA has been applied to the homogeneous highly neutron-preserving system represented by the model problem shown in Fig. 3.8. The results obtained for the cell-averaged fluxes in the first five computational cells of the symmetric model problem presented in Fig. 3.8 are reported in Table 3.2 for comparison.
Problem Parameters: Vacuum Boundary Conditions
$S_6$ Angular Quadrature
AHOT-N0 Spatial Weights

Geometric Properties: $\Delta x_1 = 0.1$ $\Delta x_2 = 1$

Nuclear properties: $q_1 = 1$ $q_2 = 0$
$\sigma_1 = 1$ $\sigma_2 = 1$
$c_1 = 0.3$ $c_2 = 0.7$

Fig. 3.7: Model problem for the comparison between direct solutions from the inversion of matrix $B$ and iterative solutions obtained with SI.

Table 3.1: Comparison between solutions from direct inversion of matrix $B$ for the model problem in Fig. 3.7 and iterative solutions obtained with SI for decreasing values of the convergence criterion $\varepsilon$.

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<th>$\varepsilon$</th>
<th>$\tilde{\phi}_1$</th>
<th>$\tilde{\phi}_2$</th>
<th>$\tilde{\phi}_3$</th>
<th>$\tilde{\phi}_4$</th>
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<td>2.427×10^{-2}</td>
<td>5.773×10^{-2}</td>
<td>1.574×10^{-1}</td>
<td>3.147×10^{-1}</td>
</tr>
<tr>
<td>Direct</td>
<td>9.763×10^{-3}</td>
<td>2.427×10^{-2}</td>
<td>5.773×10^{-2}</td>
<td>1.574×10^{-1}</td>
<td>3.147×10^{-1}</td>
</tr>
</tbody>
</table>
Problem Parameters: Vacuum Boundary Conditions  
$S_6$ Angular Quadrature  
AHOT-N0 Spatial Weights

Geometric Properties: $\Delta x_i = 1$

Nuclear properties: $q_i = 1$  $\sigma_i = 1$  $c_i = 1$

**Fig. 3.8:** Model problem for the comparison between direct solutions from the inversion of matrix $B$ and iterative solutions obtained with FSM-DSA.

**Table 3.2:** Comparison between solutions from direct inversion of matrix $B$ for the model problem in Fig. 3.8 and iterative solutions obtained with FSM-DSA for decreasing values of the convergence criterion $\varepsilon$.

<table>
<thead>
<tr>
<th>$\varepsilon$</th>
<th>$\tilde{\phi}_1$</th>
<th>$\tilde{\phi}_2$</th>
<th>$\tilde{\phi}_3$</th>
<th>$\tilde{\phi}_4$</th>
<th>$\tilde{\phi}_5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^{-1}$</td>
<td>15.62</td>
<td>25.40</td>
<td>32.75</td>
<td>37.66</td>
<td>40.11</td>
</tr>
<tr>
<td>$10^{-2}$</td>
<td>15.90</td>
<td>26.03</td>
<td>33.46</td>
<td>38.40</td>
<td>40.86</td>
</tr>
<tr>
<td>$10^{-3}$</td>
<td>15.90</td>
<td>26.06</td>
<td>33.49</td>
<td>38.41</td>
<td>40.87</td>
</tr>
<tr>
<td>$10^{-4}$</td>
<td>15.90</td>
<td>26.07</td>
<td>33.49</td>
<td>38.41</td>
<td>40.87</td>
</tr>
<tr>
<td>$10^{-5}$</td>
<td>15.90</td>
<td>26.07</td>
<td>33.49</td>
<td>38.41</td>
<td>40.87</td>
</tr>
<tr>
<td>Direct</td>
<td><strong>15.90</strong></td>
<td><strong>26.07</strong></td>
<td><strong>33.49</strong></td>
<td><strong>38.41</strong></td>
<td><strong>40.87</strong></td>
</tr>
</tbody>
</table>
Again, the trend in the values reported in Table 3.2 confirms that the iterative solution eventually coincides with the solution given by the direct inversion of matrix $B$ further verifying the numerical calculation of the matrix elements based on the analytic expressions derived above.

### 3.4 Asymptotic Analysis for Homogeneous Slabs

In the homogeneous, uniform-mesh case all the computational cells in which the slab is subdivided are characterized by the same geometric and physical properties so that the spatial index $j$ may be dropped in the expressions referring to parameters characterizing a generic computational cell. More specifically, the symbol $\Delta x$ will be used to indicate the size of each computational cell, $\sigma$ and $\sigma_s$ will represent the macroscopic total and scattering cross-sections, respectively, and $c$ is the scattering ratio. The reciprocal of the optical thickness for a generic cell along the $m^{th}$ discrete ordinate is denoted by $\kappa_m$ and $\kappa_m = \left| \mu_m \right| / (\sigma \Delta x)$.

For the purposes of the ensuing asymptotic analysis, that will be performed both in the thick and in the thin cell limit, the WDD spatial weights corresponding to the AHOT-N0 method have been utilized both in the theoretical analysis and in the numerical experiments. As pointed out in Ch. 1, the AHOT-N0 spatial weights acquire the step method value of 1 in the thick cell limit, and the Diamond Difference value of 0 in the thin cell limit, and are better suited to cover any intermediate thickness regime [3].

In terms of the parameters introduced for the homogeneous, uniform-mesh case, the expression for the spatial weights contained in Eq. (1.25) becomes:
\[
\alpha_m = \coth\left(\frac{1}{2\kappa_m}\right) - 2\kappa_m, \quad m = 1, \ldots, M
\]  

(3.77)

As far as the matrices \( \mathbf{A} \) and \( \mathbf{B} \) are concerned, having assumed a symmetric quadrature, they both become symmetric in the homogeneous, uniform-mesh case and all the elements on the diagonal and a given off-diagonal stripe become equal. Consequently the following symbols will be introduced to identify the matrix \( \mathbf{A} \) elements:

\[
A_{j,j} = A_j, \quad j = 1, \ldots, J
\]

(3.78)

\[
A_{j+k,j} = A_{j,j+k} = A_k, \quad j = 1, \ldots, (J-1); k = 1, \ldots, (J-j)
\]

(3.79)

In the same fashion the following symbols will be used to reference the elements of matrix \( \mathbf{B} \):

\[
B_{j,j} = B_j, \quad j = 1, \ldots, J
\]

(3.80)

\[
B_{j+k,j} = B_{j,j+k} = B_k, \quad j = 1, \ldots, (J-1); k = 1, \ldots, (J-j)
\]

(3.81)

The first off-diagonal elements are treated separately from the general \( k^{th} \) off-diagonal case in the ensuing asymptotic analysis. Also, for the purpose of the asymptotic analysis, the expressions for the matrices elements in the homogeneous, uniform-mesh case are determined by substituting Eq. (3.77) in Eqs. (3.18) through (3.23) and writing the resulting expressions explicitly in terms of the homogeneous parameters.
3.4.1 Expressions for Matrices A and B in Homogeneous Slabs

The matrix elements acquire the following form in the homogeneous, uniform-mesh case:

\[ A_d = \frac{1}{\sigma} - \frac{1}{\sigma} \sum_{m=1}^{M} w_m |\mu_m| \left( 1 - e^{-\sigma \Delta x |\mu_m|} \right) \frac{1}{\sigma \Delta x} \] (3.82)

\[ A_i = \frac{1}{\sigma} \sum_{m=1}^{M/2} w_m |\mu_m| \left( 1 - e^{-\sigma \Delta x |\mu_m|} \right)^2 \frac{1}{\sigma \Delta x} \] (3.83)

\[ A_k = \frac{1}{\sigma} \sum_{m=1}^{M/2} w_m |\mu_m| \left( 1 - e^{-\sigma \Delta x |\mu_m|} \right)^2 \frac{1}{\sigma \Delta x}, \quad k \geq 2 \] (3.84)

The expressions for the matrix elements in the homogeneous, uniform-mesh case become:

\[ B_d = (1 - c) + c \sum_{m=1}^{M} w_m |\mu_m| \left( 1 - e^{-\sigma \Delta x |\mu_m|} \right) \] (3.85)

\[ B_i = -c \sum_{m=1}^{M/2} w_m |\mu_m| \left( 1 - e^{-\sigma \Delta x |\mu_m|} \right)^2 \] (3.86)
The verification of the above expressions, Eqs. (3.82) through (3.87), will now be conducted considering a detailed direct derivation of the $B$ matrix elements. The expressions for the elements of matrix $A$ may then be easily derived using the relationship with the corresponding elements of matrix $B$, given by the definition in Eq. (1.28), specialized to the homogeneous, uniform-mesh case (in which $\sigma_s = \sigma_s I$). Of course, the reverse procedure starting from matrix $A$ might as well be used and would lead to the same results.

**Diagonal elements**

In the homogeneous case Eq. (3.21) for the diagonal elements belonging to matrix $B$ acquires the following form:

$$B_d = 1 - c \sum_{m=1}^{M/2} w_m \left( e^{-(k-1)|\sigma\Delta|/|\mu_m|} \right) \left( 1 - e^{-\sigma\Delta|/|\mu_m|} \right)^2 / \sigma\Delta x, \quad k \geq 2$$ (3.87)

Using Eq. (3.77), the numerators in the previous equation may be expressed in terms of the cell parameters and of the quadrature angles:

$$1 + \alpha_m = 1 + \coth \left( \frac{\sigma \Delta x}{2 |\mu_m|} \right) - \frac{2 |\mu_m|}{\sigma \Delta x}$$ (3.89)

The denominators in Eq. (3.88) are treated in the same way. After the due simplifications the following result is obtained:
Substituting Eqs. (3.89) and (3.90) into Eq. (3.88) the following expression is obtained for the diagonal elements in terms of the homogeneous cell parameters:

\[ B_d = 1 - c \sum_{m=1}^{M} w_m \left[ 1 + \coth \left( \frac{\sigma_{\Delta x}}{2|\mu_m|} \right) \right] \]

For the benefit of the ensuing asymptotic analysis it is preferred to express the hyperbolic cotangent, appearing in both the numerator and the denominator of the previous equation, in terms of exponential functions using the well-known relation:

\[ \coth \left( \frac{\sigma_{\Delta x}}{2|\mu_m|} \right) = \frac{e^{\sigma_{\Delta x}/|\mu_m|} + e^{-\sigma_{\Delta x}/|\mu_m|}}{e^{\sigma_{\Delta x}/|\mu_m|} - e^{-\sigma_{\Delta x}/|\mu_m|}} \]

In order to perform the asymptotic analysis, especially in the thick cell limit, it is actually more convenient to substitute Eq. (3.92) into Eq. (3.91) expressing the hyperbolic cotangent in terms of only negative exponentials:

\[ B_d = 1 - c \sum_{m=1}^{M} w_m \left[ \frac{1 + e^{-\sigma_{\Delta x}/|\mu_m|}}{1 - e^{-\sigma_{\Delta x}/|\mu_m|}} \right] \]

A few algebraic manipulations are in order to simplify the expressions contained in Eq. (3.93) and once performed they reduce the diagonal elements into the more compact form:
The latter expression simplifies further to Eq. (3.85) in view of the normalization condition for the quadrature weights, Eq. (3.2).

First off-diagonal elements

In the homogeneous case both Eq. (3.22) and Eq. (3.23), considered for the special case \( k = 1 \) corresponding to the first off-diagonal elements of matrix \( \mathbf{B} \), acquire the following form:

\[
B_1 = -c \sum_{m=1}^{M/2} w_m \frac{2 (2 \kappa_m)}{(1 + 2 \kappa_m + \alpha_m)^2} \tag{3.95}
\]

Use of Eq. (3.77) in the previous equation reduces the expression for \( B_1 \) in terms of the cell parameters and of the quadrature angles to:

\[
B_1 = -c \sum_{m=1}^{M/2} w_m \frac{2 \left( \frac{2 |\mu_m|}{\sigma \Delta x} \right)}{\left[ \coth \left( \frac{\sigma \Delta x}{2 |\mu_m|} \right) + 1 \right]^2} \tag{3.96}
\]

Substituting the explicit form of the hyperbolic cotangent, Eq. (3.92), in terms of only negative exponentials into Eq. (3.96) and performing the due simplifications the final result obtained is coincident with Eq. (3.86).
**$k^{th}$ off-diagonal elements with $k \geq 2$**

In the homogeneous, uniform-mesh case both Eq. (3.22) and Eq. (3.23), considered for $k \geq 2$, acquire the following form:

$$B_k = -c \sum_{m=1}^{M/2} \frac{2(2\kappa_m^2)(2\kappa_m + \alpha_m - 1)^{k-1}}{(1 + 2\kappa_m + \alpha_m)^{k+1}}$$

(3.97)

Use of Eq. (3.77) in the previous equation reduces the expression for $B_k$ in terms of the cell parameters and of the quadrature angles to:

$$B_k = -c \sum_{m=1}^{M/2} \frac{2|\mu_m|}{\sigma \Delta x} \left( \coth \left( \frac{\sigma \Delta x}{2|\mu_m|} \right) - 1 \right)^{k-1}$$

$$\left[ \coth \left( \frac{\sigma \Delta x}{2|\mu_m|} \right) + 1 \right]^{k+1}$$

(3.98)

Substituting the explicit form of the hyperbolic cotangent, Eq. (3.92), in terms of only negative exponentials into Eq. (3.98) and performing the due simplifications the final result obtained is coincident with Eq. (3.87).

**3.4.2 Asymptotic Analysis in the Thick Cell Limit**

Conducting an asymptotic analysis to the $A$ and $B$ matrix elements for a homogeneous slab with a uniform mesh yields the following asymptotic behavior of the symmetric matrix $B$ elements in the thick cell limit. This is the limit in which the cell width $\Delta x$ is scaled as a dimensionless parameter $\Delta$ times the appropriate length units and $\Delta \to \infty$. 
\[ B_d = (1-c) + \frac{c}{(\sigma \Delta)} \sum_{m=1}^{M} w_m |\mu_m| + O \left( \frac{e^{-\sigma \Delta |\mu_{\max}|}}{(\sigma \Delta)} \right) \]  

(3.99)

\[ B_i = -\frac{c}{(\sigma \Delta)} \sum_{m=1}^{M/2} w_m |\mu_m| + O \left( \frac{e^{-\sigma \Delta |\mu_{\max}|}}{(\sigma \Delta)} \right) \]  

(3.100)

\[ B_k = -c w_{\max} |\mu_{\max}| \frac{e^{-(k-1)\sigma \Delta |\mu_{\max}|}}{(\sigma \Delta)} + O \left( \frac{e^{-k \sigma \Delta |\mu_{\max}|}}{(\sigma \Delta)} \right), \quad k \geq 2 \]  

(3.101)

where the following notation has been introduced for the maximum angle and its associated weight in the quadrature:

\[
\begin{align*}
\mu_{M/2} &= \mu_{\max} \\
w_{M/2} &= w_{\max}
\end{align*}
\]  

(3.102)

Note that in Eq. (3.99) and Eq. (3.100), for \( B_i \) the quadrature sum runs over half the angles in the symmetric quadrature while for \( B_d \) it runs over all the angles. Substitution of Eq. (3.99) into Eq. (3.100) yields, to leading order, the following result:

\[ B_i \sim \frac{1}{2} [(1-c) - B_d] \]  

(3.103)

This relation is familiar from Diffusion Theory. Since in the limit \( \Delta \to \infty \) the elements in the \( B \) matrix from the second off-diagonal on are rapidly (exponentially) vanishing, as indicated by Eq. (3.101), it is apparent from Eq. (3.103) that in the thick cell limit for the homogeneous case the full transport operator represented by matrix \( B \) acquires a tridiagonal diffusion-like coupling stencil. This result provides further insight
into the superior convergence properties of diffusion-based acceleration schemes in slab geometry, in the homogeneous case.

The asymptotic expressions for the symmetric matrix \( A \) elements in the thick cell limit for the homogeneous slab and uniform mesh are the following:

\[
A_d = \frac{1}{\sigma} \left[ 1 - \frac{1}{(\sigma\Delta)} \sum_{m=1}^{M} w_m |\mu_m| \right] + O\left( \frac{e^{-\sigma\Delta |\mu_{\text{max}}|}}{(\sigma\Delta)} \right)
\]  

(3.104)

\[
A_i = \frac{1}{\sigma} \left( \frac{1}{\sigma\Delta} \right) \sum_{m=1}^{M/2} w_m |\mu_m| + O\left( \frac{e^{-\sigma\Delta |\mu_{\text{max}}|}}{(\sigma\Delta)} \right)
\]  

(3.105)

\[
A_k = \frac{1}{\sigma} w_{\text{max}} |\mu_{\text{max}}| e^{-(k-1)\sigma\Delta |\mu_{\text{max}}|} + O\left( \frac{e^{-k\sigma\Delta |\mu_{\text{max}}|}}{(\sigma\Delta)} \right), \quad k \geq 2
\]  

(3.106)

Substitution of Eq. (3.104) into Eq. (3.105) immediately gives the following result:

\[
A_d \sim \frac{1}{\sigma} - 2A_i
\]  

(3.107)

Equation (3.107) may also be solved for \( A_i \) and then cast in the equivalent form:

\[
A_i \sim \frac{1}{2} \left[ \frac{1}{\sigma} - A_d \right]
\]  

(3.108)

The last two results are quite interesting. A similar relation may be obtained by imposing a diffusive coupling stencil for the \( B \) matrix diagonal and first off-diagonal elements, for example in the form provided by Eq. (3.103). Substituting in this latter
equation the relationship between the $B$ matrix elements and the $A$ matrix elements given by Eq. (1.28), the following result is obtained:

$$-\sigma_s A_i \sim \frac{1}{2}\left[(1-c)-(1-\sigma_s A_d)\right]$$

(3.109)

Dividing both sides of Eq. (3.109) by the macroscopic scattering cross-section, explicitly expressing the scattering ratio and performing the due simplifications, the same result given by Eq. (3.108) is finally obtained. Solving Eq. (3.109) for $A_d$ the same result given by Eq. (3.107) is also recovered.

Since in the limit $\Delta \rightarrow \infty$ the elements in the $A$ matrix from the second off-diagonal on are rapidly vanishing, as indicated by Eq. (3.106), it is apparent from either Eq. (3.107) or Eq. (3.108) that in the thick cell limit for the homogeneous, uniform-mesh case the full iteration matrix $A$ also becomes tridiagonally dominated with a diffusion-like coupling stencil. In view of the previous observations, this coupling stencil is also consistent with the diffusion-like coupling stencil acquired by matrix $B$ in the same limit.

Finally, proof of the validity of the previous asymptotic expressions for the matrix elements will be provided considering at first the $A$ matrix elements and then moving to the $B$ matrix elements. The defining relationship between the elements of the two matrices, i.e. Eq. (1.28), is expected to hold also in the asymptotic limit, as is confirmed by the former discussion based on Eq. (3.109). Nonetheless, in this case the defining relationship has been used as a tool to check the results independently obtained for matrix $A$ and for matrix $B$ rather than as a means to determine the expressions for one matrix once the corresponding results have been obtained for the other matrix.
Thick-cell asymptotic limit of the diagonal elements of matrix $A$

In view of the $(\sigma \Delta)^{-1}$ dependence in Eq. (3.82), the asymptotic behavior of the diagonal elements as $\Delta \to \infty$ may be conveniently investigated via the following expression:

$$
\lim_{\Delta \to \infty} \left\{ A_d - \frac{1}{\sigma} \right\}(\sigma \Delta) e^{\sigma \Delta |\mu_{\text{max}}|}
$$

(3.110)

Substitution of Eq. (3.82) into Eq. (3.110) leads to the following equality:

$$
\lim_{\Delta \to \infty} \left\{ A_d - \frac{1}{\sigma} \right\}(\sigma \Delta) e^{\sigma \Delta |\mu_{\text{max}}|} = \\
= \lim_{\Delta \to \infty} \left\{ -\frac{1}{\sigma} \sum_{m=1}^{M} w_m |\mu_m| (1 - e^{-\sigma \Delta |\mu_m|}) e^{\sigma \Delta |\mu_{\text{max}}|} \right\}
$$

(3.111)

It is convenient to rewrite the latter equation in the following equivalent form benefiting from the assumption of a symmetric quadrature:

$$
\lim_{\Delta \to \infty} \left\{ A_d - \frac{1}{\sigma} \right\}(\sigma \Delta) + \frac{1}{\sigma} \sum_{m=1}^{M} w_m |\mu_m| e^{\sigma \Delta |\mu_{\text{max}}|} = \\
= \lim_{\Delta \to \infty} \left\{ 2 \frac{1}{\sigma} \sum_{m=1}^{M} w_m |\mu_m| e^{-\sigma |\mu_m| - 1/|\mu_{\text{max}}|} \right\}
$$

(3.112)

The sum on the right hand side of the previous expression is then rewritten isolating the contribution to the sum from $|\mu_{\text{max}}|$, and the limit of the sum is split into the sum of the respective limits. The following result is obtained:
The limit on the right hand side of Eq. (3.113) can be shown to be equal to zero. In fact, the ordering relations existing between the angles in the quadrature lead to the following result:

\[
|\mu_{\text{max}}| \equiv \mu_M > \mu_{M-1} > \ldots > |\mu_1| \Rightarrow \left( \frac{1}{|\mu_m|} - \frac{1}{|\mu_{\text{max}}|} \right) > 0, \quad m = 1, \ldots, \frac{M}{2} - 1
\]  

(3.114)

All the exponentials appearing in the limit on the right hand side of Eq. (3.113) are therefore characterized by a negative exponent and tend to 0 in the limit as \( \Delta \to \infty \).

Solving Eq. (3.113) for \( A_d \) in the limit confirms the result for the diagonal elements asymptotic behavior in the thick cell limit reported in Eq. (3.104).

**Thick-cell asymptotic limit of the first off-diagonal elements of matrix A**

The asymptotic behavior of the first off-diagonal elements as \( \Delta \to \infty \) may be investigated by forming the following limit:

\[
\lim_{\Delta \to \infty} \left\{ A_d (\sigma \Delta) e^{\sigma \Delta |\mu_{\text{max}}|} \right\}
\]

(3.115)

Substitution of Eq. (3.83) into the previous expression leads to the following equality:
\[
\lim_{\Delta \to \infty} \left\{ A_i (\sigma \Delta) e^{\sigma \Delta |\mu_{\text{max}}|} \right\} = \\
\lim_{\Delta \to \infty} \left\{ \frac{1}{\sigma} \sum_{m=1}^{M/2} w_m |\mu_m| \left(1 - e^{-\sigma \Delta |\mu_m|}\right)^2 e^{\sigma \Delta |\mu_{\text{max}}|} \right\}
\]

(3.116)

It is convenient to expand the square term on the right hand side and rewrite the latter equation in the following equivalent form:

\[
\lim_{\Delta \to \infty} \left\{ A_i (\sigma \Delta) - \frac{1}{\sigma} \sum_{m=1}^{M/2} w_m |\mu_m| e^{\sigma \Delta |\mu_{\text{max}}|} \right\} = L_1 + L_2
\]

(3.117)

The two limits on the right hand side of Eq. (3.117) are defined by:

\[
L_1 = - \lim_{\Delta \to \infty} \left\{ \frac{2}{\sigma} \sum_{m=1}^{M/2} w_m |\mu_m| e^{-\sigma \Delta |\mu_m| - 1/|\mu_{\text{max}}|} \right\}
\]

(3.118)

\[
L_2 = \lim_{\Delta \to \infty} \left\{ \frac{1}{\sigma} \sum_{m=1}^{M/2} w_m |\mu_m| e^{-\sigma \Delta (|\mu_m| - 1/|\mu_{\text{max}}|)} \right\}
\]

(3.119)

The first limit has already been encountered on the right hand side of Eq. (3.112) and is equal to:

\[
L_1 = - \frac{2}{\sigma} w_{\text{max}} |\mu_{\text{max}}|
\]

(3.120)

The second limit can be shown to be equal to zero. In fact, the ordering relations existing between the angles in the quadrature lead to the following result:

\[
|\mu_{\text{max}}| \equiv |\mu_{M/2}| > |\mu_{M/4}| > ... > |\mu_1| \Rightarrow \left( \frac{1}{|\mu_m|} - \frac{1}{2 |\mu_{\text{max}}|} \right) > 0, \ m = 1, ..., M/2
\]

(3.121)

All the exponentials appearing in the limit in Eq. (3.119) are therefore characterized by a negative exponent and tend to 0 in the limit as \( \Delta \to \infty \).
Solving Eq. (3.117) for \( A_i \) in the limit confirms the result for the first off-diagonal elements asymptotic behavior in the thick cell limit reported in Eq. (3.105).

**Thick-cell asymptotic limit of the \( k^{th} \) off-diagonal elements of matrix \( A \)**

The asymptotic behavior of the \( k^{th} \) off-diagonal elements as \( \Delta \to \infty \) may be investigated by forming the following limit:

\[
\lim_{\Delta \to \infty} \left\{ A_k (\sigma \Delta) e^{(k-1)\sigma \Delta |\mu_{\max}|} \right\}
\]

(3.122)

Substitution of Eq. (3.84) into the previous expression leads to the following equality:

\[
\lim_{\Delta \to \infty} \left\{ A_k (\sigma \Delta) e^{(k-1)\sigma \Delta |\mu_{\max}|} \right\} =
\]

(3.123)

It is convenient to rewrite the sum on the right hand side of the previous expression isolating the contribution due to the \( M/2 \) angle, that is to say, the contribution coming from \( |\mu_{\max}| \), and break up the limit of the sum into the sum of the respective limits. The following result is obtained:

\[
\lim_{\Delta \to \infty} \left\{ A_k (\sigma \Delta) e^{(k-1)\sigma \Delta |\mu_{\max}|} \right\} = L_1 + L_2
\]

(3.124)

The two limits on the right hand side of Eq. (3.124) are:

\[
L_1 = \lim_{\Delta \to \infty} \left\{ \frac{1}{\sigma} w_{\max} |\mu_{\max}| \left(1 - e^{-\sigma \Delta |\mu_{\max}|}\right)^2 \right\}
\]

(3.125)
\[ L_2 = \lim_{\Delta \to \infty} \left\{ \frac{1}{\sigma} \sum_{m=1}^{M} w_m |\mu_m| \left( e^{-(k-1)|\sigma\Delta|/|\mu_m|-1/|\mu_{\text{max}}|} \right) \left( 1 - e^{-\sigma \Delta/|\mu_m|} \right) \right\} \quad (3.126) \]

The limit in Eq. (3.126) is equal to zero by the same argument that yields Eq. (3.114). The limit in Eq. (3.125) may be readily evaluated leading to the following result valid in the asymptotic limit:

\[ A_k (\sigma \Delta) e^{(k-1)|\sigma\Delta|/|\mu_{\text{max}}|} = \frac{1}{\sigma} w_{\text{max}} |\mu_{\text{max}}| + O\left( e^{-\sigma \Delta/|\mu_{\text{max}}|} \right) \quad (3.127) \]

Solving Eq. (3.127) for \( A_k \) in the asymptotic limit leads to the result reported in Eq. (3.106) for the \( k^{th} \) off-diagonal elements asymptotic behavior in the thick cell limit.

**Thick-cell asymptotic limit of the diagonal elements of matrix B**

The asymptotic behavior of the diagonal elements as \( \Delta \to \infty \) may be investigated considering the following limit:

\[ \lim_{\Delta \to \infty} \left\{ \left[ B_d - (1-c) \right] (\sigma \Delta) e^{\sigma \Delta/|\mu_{\text{max}}|} \right\} \quad (3.128) \]

Substitution of Eq. (3.85) into the previous equation leads to the following equality:

\[ \lim_{\Delta \to \infty} \left\{ \left[ B_d - (1-c) \right] (\sigma \Delta) e^{\sigma \Delta/|\mu_{\text{max}}|} \right\} = \]

\[ \lim_{\Delta \to \infty} \left\{ c \sum_{m=1}^{M} w_m |\mu_m| \left( 1 - e^{-\sigma \Delta/|\mu_m|} \right) e^{\sigma \Delta/|\mu_{\text{max}}|} \right\} \quad (3.129) \]
The limit on the right hand side of Eq. (3.129) is the same as the limit already encountered on the right hand side of Eq. (3.111), when the factor \( c \) is replaced by \( 1/\sigma \), both \( O(1) \), and may be computed following the same procedure. The following result immediately follows:

\[
\lim_{\Delta \to \infty} \left\{ \left[ B_d - (1-c) \right] (\sigma \Delta) + \frac{1}{\sigma} \sum_{m=1}^{M} w_m |\mu_m| \right\} e^{\sigma \Delta |\mu_{\text{max}}|} = \]

\[
= 2c w_{\text{max}} |\mu_{\text{max}}| \]

(3.130)

Solving Eq. (3.130) for \( B_d \) in the limit confirms the result for the diagonal elements asymptotic behavior in the thick cell limit reported in Eq. (3.99).

**Thick-cell asymptotic limit of the first off-diagonal elements of matrix B**

The asymptotic behavior of the first off-diagonal elements as \( \Delta \to \infty \) may be investigated by forming the following limit:

\[
\lim_{\Delta \to \infty} \left\{ |B_i| (\sigma \Delta) e^{\sigma \Delta |\mu_{\text{max}}|} \right\} \]

(3.131)

The absolute value of the negative definite \( B_i \) elements is considered in Eq. (3.131) to simplify the treatment and the presentation of the results, and also in view of the future discussions on numerical results in Sec. 3.4.4. The treatment of Eq. (3.131) follows much the same steps indicated for Eq. (3.115) and comparison of the absolute value of Eq. (3.83) with Eq. (3.86) shows that the equations obtained for \( |B_i| \) would be the same as Eqs. (3.116) and (3.117) for \( A_i \) when the factor \( 1/\sigma \) is replaced by \( c \).
Following the same procedure outlined for Eq. (3.117) the following relation is obtained for $|B_1|$ in the thick cell asymptotic limit:

$$\lim_{\Delta \to \infty} \left\{ |B_1| (\sigma \Delta) - c \sum_{m=1}^{M/2} w_m |\mu_m| \right\} e^{\sigma \Delta/|\mu_{\max}|} = -2c w_{\max} |\mu_{\max}|$$  \hspace{1cm} (3.132)

Solving Eq. (3.132) for $|B_1|$ in the limit confirms the result for the first off-diagonal elements asymptotic behavior in the thick cell limit reported in Eq. (3.100), once the absolute value is removed.

**Thick-cell asymptotic limit of the $k^{th}$ off-diagonal elements of matrix $B$**

Similar to the treatment discussed for the correspondent elements of the $A$ matrix, the asymptotic behavior of the $k^{th}$ off-diagonal elements as $\Delta \to \infty$ may be conveniently investigated by forming the following limit:

$$\lim_{\Delta \to \infty} \left\{ B_k (\sigma \Delta) e^{(k-1)\sigma \Delta/|\mu_{\max}|} \right\}$$  \hspace{1cm} (3.133)

The treatment of Eq. (3.133) follows much the same steps indicated for Eq. (3.122) and comparison of the absolute value of Eq. (3.87) with Eq. (3.84) shows that the equations obtained for $|B_k|$ would be the same as Eqs. (3.123) through (3.126) for $A_k$ when the factor $1/\sigma$ is substituted by $c$. Therefore $|B_k|$ satisfies the following relation in the thick-cell asymptotic limit:

$$|B_k| (\sigma \Delta) e^{(k-1)\sigma \Delta/|\mu_{\max}|} = c w_{\max} |\mu_{\max}| + O \left( e^{-\sigma \Delta/|\mu_{\max}|} \right)$$  \hspace{1cm} (3.134)
Solving Eq. (3.134) for $|B_k|$ in the limit confirms the result for the $k^{th}$ off-diagonal elements asymptotic behavior in the thick cell limit reported in Eq. (3.101), once the absolute value is removed.

### 3.4.3 Asymptotic Analysis in the Thin Cell Limit

Conducting an asymptotic analysis to the $B$ matrix elements for a homogeneous slab yields the following asymptotic behavior for $B_d$, $B_i$ and $B_k$ in the thin cell limit. This is the limit in which the cell width $\Delta x$ is scaled as a dimensionless parameter $\delta$ times the appropriate length units and $\delta \to 0$.

\[
B_d = 1 - c \left( \sum_{m=1}^{M/2} \frac{W_m}{|\mu_m|} \right) (\sigma \delta) + O\left((\sigma \delta)^2\right) \quad (3.135)
\]

\[
B_i = -c \left( \sum_{m=1}^{M/2} \frac{W_m}{|\mu_m|} \right) (\sigma \delta) + O\left((\sigma \delta)^2\right) \quad (3.136)
\]

\[
B_k = -c \left( \sum_{m=1}^{M/2} \frac{W_m}{|\mu_m|} \right) (\sigma \delta) + O\left((\sigma \delta)^2\right), \quad k \geq 2 \quad (3.137)
\]

It is noted that the result in Eq. (3.137) implies that, to leading order, all the $k^{th}$ off-diagonal elements have the same asymptotic behavior, independent of $k \geq 2$. Comparison of Eq. (3.137) with Eq. (3.136) actually suggests that, to leading order, all the off-diagonal elements of matrix $B$ have the same asymptotic behavior, converging to
zero like \((\sigma \delta)\), for a given scattering ratio, in the limit as \(\delta \to 0\). The result in Eq. (3.135) indicates that the diagonal elements are instead converging, at the same rate, to a unit value. Therefore, under the assumption made in this chapter that the number \(J\) of cells in the spatial mesh is a fixed (non-scaled) parameter, the results contained in Eqs. (3.135) through (3.137) show that the corresponding \((J \times J)\) \(B\) matrix approaches the identity matrix \(I\), in the thin cell limit. The latter result appears in agreement with the conclusion obtained in Theorem 6.11 of [30], with reference to the *thin regime* for the case of the Diamond Difference spatial discretization. In this connection it is recalled that, as stressed in Ch. 1, the AHOT-N0 spatial weights limit to the Diamond Difference weights in the thin cell limit. A discussion of the implications of a diagonally dominated \(B\) matrix with respect to the synthetic acceleration of iterative methods for the solution of the transport equation is deferred until Appendix A. The reader is also referred to Sec. A.5 for a discussion of the case in which both parameters \(\delta\) and \(J\) are simultaneously scaled.

The asymptotic expressions for \(A_d\), \(A_t\) and \(A_k\) obtained in the same limit are hereby summarized:

\[
A_d = \frac{1}{\sigma} \sum_{m=1}^{M/2} \left( \frac{w_m}{\mu_m} \right) (\sigma \delta) + O\left((\sigma \delta)^2\right) \tag{3.138}
\]

\[
A_t = \frac{1}{\sigma} \sum_{m=1}^{M/2} \left( \frac{w_m}{\mu_m} \right) (\sigma \delta) + O\left((\sigma \delta)^2\right) \tag{3.139}
\]
\[ A_k = \frac{1}{\sigma} \sum_{m=2}^{M+2} \left( \frac{w_m}{\mu_m} \right) (\sigma \delta) + O\left((\sigma \delta)^2\right), \quad k \geq 2 \]  

(3.140)

It is noted that the result in Eq. (3.140) implies that, to leading order, all the \( k \)th off-diagonal elements have the same asymptotic behavior, independent of \( k \geq 2 \). Comparison of Eq. (3.140) with Eqs. (3.139) and (3.138) actually reveals that, to leading order, all the elements of matrix \( A \) have the same asymptotic behavior, converging to zero like \( (\sigma \delta) \), for a given total cross-section, in the limit as \( \delta \to 0 \). Therefore, under the assumption made in this chapter that the number \( J \) of cells in the spatial mesh is a fixed (non-scaled) parameter, the results contained in Eqs. (3.138) through (3.140) show that the corresponding \( (J \times J) \) \( A \) matrix approaches the zero matrix \( 0 \), in the thin cell limit. As a matter of fact, since for a fixed \( J \) the thickness of the slab as a whole is going to shrink to zero in the thin cell limit, the cell-averaged fluxes are also expected to vanish in the same limit. Therefore, the vanishing of the \( A \) matrix elements in the thin cell limit reflects the vanishing of the slab structure and grants the vanishing of the cell-averaged fluxes, no matter what the value of the fixed source density is (provided the source density is bounded, as it usually is in practical applications).

Finally, proof of the validity of the previous expressions will now be given, considering at first the \( A \) matrix elements and then moving to the \( B \) matrix elements.
Thin-cell asymptotic limit of the diagonal elements of matrix A

In view of the \((\sigma \delta)^{-1}\) dependence in Eq. (3.82), the asymptotic behavior of the diagonal elements in the limit \(\delta \to 0\) may conveniently be investigated considering the asymptotic behavior of the following expression:

\[
\begin{bmatrix}
A_d - \frac{1}{\sigma}
\end{bmatrix}(\sigma \delta)
\]

(3.141)

Substitution of Eq. (3.82) into the previous expression leads to the following equality:

\[
\begin{bmatrix}
A_d - \frac{1}{\sigma}
\end{bmatrix}(\sigma \delta) = -\frac{1}{\sigma} \sum_{m=1}^{M} w_m |\mu_m| \left(1 - e^{-\frac{\sigma \delta |\mu_m|}{\mu_m}}\right)
\]

(3.142)

In the thin cell limit, the exponential term appearing on the right hand side of Eq. (3.142) is conveniently approximated by its Taylor series expansion truncated at the second order term:

\[
e^{-\frac{\sigma \delta |\mu_m|}{\mu_m}} = 1 - \frac{\sigma \delta}{|\mu_m|} + \frac{1}{2} \left(\frac{\sigma \delta}{|\mu_m|}\right)^2 + O\left(\left(\frac{\sigma \delta}{|\mu_m|}\right)^3\right)
\]

(3.143)

Substitution of this expansion truncated to second order into Eq. (3.142) leads to the following result:

\[
\begin{bmatrix}
A_d - \frac{1}{\sigma}
\end{bmatrix}(\sigma \delta) = -\frac{1}{\sigma} \sum_{m=1}^{M} w_m |\mu_m| \left[1 - 1 + \frac{\sigma \delta}{|\mu_m|} - \frac{1}{2} \left(\frac{\sigma \delta}{|\mu_m|}\right)^2 + O\left(\left(\frac{\sigma \delta}{|\mu_m|}\right)^3\right)\right]
\]

(3.144)

Rearranging terms, solving for \(A_d\) and performing the due simplifications the following expression is obtained for the diagonal elements:
\[ A_y = \frac{1}{\sigma} - \frac{1}{\sigma} \left( \sum_{m=1}^{M} w_m \right) + \frac{1}{\sigma} \left( \sum_{m=1}^{M} \frac{w_m}{\mu_m} \right) (\sigma \delta) + O((\sigma \delta)^2) \] (3.145)

The latter equation simplifies further to Eq. (3.138) in view of the normalization condition for the quadrature weights in Eq. (3.2) and benefiting from the assumption of a symmetric quadrature.

**Thin-cell asymptotic limit of the first off-diagonal elements of matrix A**

The asymptotic behavior of the first off-diagonal elements may be investigated considering the asymptotic behavior of the following expression:

\[ A_i (\sigma \delta) \] (3.146)

Substitution of Eq. (3.83) into the previous expression leads to the following equality:

\[ A_i (\sigma \delta) = \frac{1}{\sigma} \sum_{m=1}^{M/2} w_m |\mu_m| \left( 1 - e^{-\sigma \delta |\mu_m|} \right)^2 \] (3.147)

In the thin cell limit the exponential term appearing on the right hand side of Eq. (3.147) is conveniently approximated by its Taylor series expansion, Eq. (3.143), truncated at its first order term obtaining:

\[ A_i (\sigma \delta) = \frac{1}{\sigma} \sum_{m=1}^{M/2} w_m |\mu_m| \left( 1 - \frac{\sigma \delta |\mu_m|}{1+O\left( \frac{|\sigma \delta|}{|\mu_m|} \right)^2} \right)^2 \] (3.148)

Solving for \( A_i \) and performing the due simplifications the result presented in Eq. (3.139) is finally obtained.
Thin-cell asymptotic limit of the \(k^{th}\) off-diagonal elements of matrix \(A\)

The asymptotic behavior of the \(k^{th}\) off-diagonal elements may be investigated considering the asymptotic behavior of the following expression:

\[
A_k (\sigma \delta)
\]  
(3.149)

Substitution of Eq. (3.84) into the previous expression leads to the following equality:

\[
A_k (\sigma \delta) = \frac{1}{\sigma} \sum_{m=1}^{M/2} w_m |\mu_m| \left( e^{-(k-1)\sigma \delta |\mu_m|} \right) \left(1 - e^{-\sigma \delta |\mu_m|} \right)^2
\]  
(3.150)

In the thin cell limit the exponential terms appearing on the right hand side of Eq. (3.150) is conveniently approximated by their Taylor series expansion, Eq. (3.143), truncated at its first order term obtaining:

\[
A_k (\sigma \delta) = \frac{1}{\sigma} \sum_{m=1}^{M/2} w_m |\mu_m| \left\{ 1 - \frac{(k-1)\sigma \delta}{|\mu_m|} + O \left( \frac{(\sigma \delta)^2}{|\mu_m|^2} \right) \right\}.
\]  
(3.151)

Expansion of the product of the terms in parenthesis leads to

\[
A_k (\sigma \delta) = \frac{1}{\sigma} \sum_{m=1}^{M/2} w_m |\mu_m| \left[ \left( \frac{(\sigma \delta)^2}{|\mu_m|^2} \right) + O \left( \frac{(\sigma \delta)^3}{|\mu_m|^3} \right) \right]
\]  
(3.152)

Solving for \(A_k\) and performing the due simplifications the result presented in Eq. (3.140) is finally obtained. In particular, it is proved that to leading order all the \(k^{th}\) off-diagonal elements of matrix \(A\) have the same behavior, independent of \(k \geq 2\).
**Thin-cell asymptotic limit of the diagonal elements of matrix B**

The asymptotic behavior of the diagonal elements in the limit $\delta \to 0$ may be investigated considering the asymptotic behavior of the following expression:

$$\left[ B_d - (1 - c) \right](\sigma \delta)$$  \hspace{1cm} (3.153)

The treatment of Eq. (3.153) follows much the same steps indicated for Eq. (3.141) and is based on the Taylor expansion truncated at the second order term reported in Eq. (3.143). Comparison of Eq. (3.82) and Eq. (3.85) shows that the equations for $B_d$ would be the same as Eq. (3.142) and Eq. (3.144) for $A_d$, once the factor $-1/\sigma$ on the right hand side is replaced by $c$. The following relation, corresponding to Eq. (3.145) for $A_d$, is obtained for the diagonal elements of matrix B:

$$B_d = (1 - c) + c \left( \sum_{m=1}^{M} w_m \right) - \frac{c}{2} \left( \sum_{m=1}^{M} \frac{w_m}{\mu_m} \right)(\sigma \delta) + O\left( (\sigma \delta)^2 \right)$$  \hspace{1cm} (3.154)

The latter equation simplifies further to Eq. (3.135) in view of the normalization condition for the quadrature weights in Eq. (3.2) and using the assumption of a symmetric quadrature.

**Thin-cell asymptotic limit of the first off-diagonal elements of matrix B**

The asymptotic behavior of the first off-diagonal elements may be investigated considering the asymptotic behavior of the following expression:

$$|B_{ij}|(\sigma \delta)$$  \hspace{1cm} (3.155)
The treatment of Eq. (3.155) follows much the same steps indicated for Eq. (3.146) and is based on the Taylor expansion reported in Eq. (3.143), in this case truncated at the first order term. Comparison of Eq. (3.83) and Eq. (3.86) shows that the equations for $|B_i|$ would be the same as Eq. (3.147) and Eq. (3.148) for $A_i$, once the factor $1/\sigma$ on the right hand side is replaced by $c$. The following relation, corresponding to Eq. (3.148) for $A_i$, is obtained for $|B_i|$:  

$$|B_i|(\sigma\delta) = c \sum_{m=1}^{M/2} w_m \mu_m \left( \frac{\sigma\delta}{\mu_m} \right)^2 + O\left( \left( \frac{\sigma\delta}{\mu_m} \right)^2 \right)^2$$  

(3.156)

Solving for $|B_i|$ and performing the due simplifications the result presented in Eq. (3.136) is finally obtained, once the absolute value is removed.

**Thin-cell asymptotic limit of the $k^{th}$ off-diagonal elements of matrix B**

The asymptotic behavior of the $k^{th}$ off-diagonal elements may be investigated considering the asymptotic behavior of the following expression:

$$|B_k|(\sigma\delta)$$  

(3.157)

The treatment of Eq. (3.157) follows much the same steps indicated for Eq. (3.149) and is based on the Taylor expansion reported in Eq. (3.143), in this case truncated at the first order term. Comparison of Eq. (3.84) and Eq. (3.87) shows that the equations for $|B_k|$ would be the same as Eq. (3.150) and Eq. (3.151) for $A_k$, once the factor $1/\sigma$ on the right hand side is replaced by $c$. The following relation, corresponding to Eq. (3.152) for $A_k$, is obtained for $|B_k|$:  

...
\[ |B_k| (\sigma \delta) = c \sum_{m=1}^{M/2} w_m |\mu_m| \left[ \frac{(\sigma \delta)^2}{|\mu_m|^2} + O\left(\frac{\sigma \delta}{|\mu_m|}\right)^3 \right] \]  

(3.158)

Solving for \(|B_k|\) and performing the due simplifications the result presented in Eq. (3.137) is finally obtained. In particular, it is proved that to leading order all the \(k^{th}\) off-diagonal elements of matrix \(B\) have the same behavior, independent of \(k \geq 2\).

### 3.4.4 Numerical Verification

The theoretical results from the asymptotic analysis have been used to verify the correctness of the numerical construction of the elements of matrices \(A\) and \(B\). Of particular interest is the form acquired, especially by the \(B\) matrix, in the thick cell limit for a homogeneous system characterized by a scattering ratio value close to unity. In fact, it is known that iterative methods based on a preconditioner characterized by a tridiagonal diffusion-like coupling stencil are rapidly and efficiently convergent in this diffusive regime.

In this connection, the elements of the two matrices have been calculated for a reference homogeneous configuration comprised of ten computational cells \((J=10)\). The cell thickness, expressed in terms of number of mean free paths (MFPs), has been varied over the interval from \(10^{-6}\) and \(10^2\) assuming \(c=1\), \(\sigma = 1\), \(S_6\) Angular Quadrature and AHOT-N0 Spatial Weights. The results obtained are reported up to the third off-diagonal element in Figs. 3.9 and 3.10 for matrix \(A\) and \(B\), respectively.
The lower bound of $10^{-16}$ introduced on the ordinates axis corresponds to the epsilon machine limit. Below this threshold the matrix elements may be considered equal to zero for all purposes of their numerical representation.

The behavior of the elements of matrix $A$ in the thin cell limit has been exploded in Fig. 3.11 considering more conveniently the results of their product with the reciprocal of the corresponding value of cell thickness they are evaluated at. The expressions for the elements of matrix $A$, from the asymptotic analysis presented in Eqs. (3.138), (3.139) and (3.140), suggest that the results of these products should correspond, to leading order, to a constant asymptotic value. This value depends on the quadrature choice and is equal to 1.345 for the $S_6$ Quadrature. The numerical results approach the predicted theoretical value, as evident from Fig. 3.11.
Fig. 3.10: B matrix elements evaluated at varying cell thicknesses.

The same conclusion holds true for the off-diagonal elements of matrix B as predicted by Eqs. (3.136) and (3.137) for \( c=1 \) and verified by the numerical results presented in Fig. 3.12.

The result of the asymptotic analysis for the diagonal elements of matrix B reported in Eq. (3.135), namely that these elements should approach a value of unity in the thin cell limit is verified by the numerical results reported both in Fig. 3.10 and in greater detail in Fig. 3.13. Notice that in this latter figure the values of the matrix elements, not the absolute value, are reported on the ordinates axis. The diagonal elements are in fact positive.
Fig. 3.11: Asymptotic behavior of matrix $A$ elements in the thin cell regime.

Fig. 3.12: Asymptotic behavior of matrix $B$ off-diagonal elements in the thin cell regime.
As far as the behavior of the matrices elements in the thick cell limit is concerned Fig. 3.9 already confirms the expectation evident from Eq. (3.104) that the diagonal elements of matrix $A$ should tend to a unit value for the case $\sigma = 1$.

Both Figs. 3.9 and 3.10 also point to the fast exponential (in a log-log plot) decaying behavior of the off-diagonal elements from the second off-diagonal elements on. A particular emphasis on the theoretical provision that the diagonal and first off-diagonal elements of matrix $B$ should acquire a diffusion-like coupling stencil in the thick cell limit is presented in Fig. 3.14.

Figure 3.14 shows that the ratio of the numerically evaluated first off-diagonal to the diagonal elements of matrix $B$ tends to the corresponding value of 0.5. The exponential dominated decay for the ratio of the second off-diagonal elements to the
diagonal elements that is obtained from Eq. (3.101) and Eq. (3.99) under the assumption of $c=1$ and use of $S_6$ quadrature is well captured in Fig. 3.14. In this case too the numerically evaluated elements follow the theoretically predicted asymptotic behavior.

![Graph](image)

Fig. 3.14: Asymptotic behavior of matrix B elements in the thick cell regime.

### 3.5 Truncation Strategies for the Integral Transport Matrix in Thick Slabs

The availability of the full form of matrices $A$ and $B$ permits evaluating different strategies for their truncation into a tridiagonal structure at finite $\Delta x$, for a homogeneous, uniform-mesh slab. The interest in these strategies is twofold: (i) obtaining an accurate solution to Eq. (1.27) without the computational burden of inverting a full matrix; (ii) evaluating potential candidates for non-traditional preconditioners to be used in iterative algorithms in future research.
The quantitative evaluation of various truncation strategies is based on two different measures. The first measure is of point-wise nature: it is the maximum (over all cells) absolute value of the relative difference between the cell-averaged scalar fluxes obtained by inversion of the truncated matrix and those obtained by inversion of the full \( \mathbf{B} \) matrix. The second measure is of integral nature and is based on the observation that any truncation in the coefficients coupling fluxes in different cells results in violating the global conservation of neutrons in the slab. In order to devise the latter measure it is first necessary to formulate the neutron balance for the slab problem in terms of the discrete cell-averaged scalar fluxes.

### 3.5.1 Neutron Balance

The neutron balance for the slab problem is first written in the following form:

\[
\sum_{m=1}^{M/2} w_m |\mu_m| \tilde{\psi}_{m,J}^o + \sum_{m=M/2+1}^M w_m |\mu_m| \tilde{\psi}_{m,1}^o + \sum_{j=1}^J (1-c_j) \sigma_j \tilde{\phi}_j \Delta x_j = \sum_{j=1}^J q_j \Delta x_j, \tag{3.159}
\]

for \( j = 1, \ldots, J \).

As will be shown in the following, the neutron balance in Eq. (3.159) can be derived from the continuous transport equation, Eq. (1.1), written for slab geometry. Of course the same neutron balance can also be interpreted as a straightforward consequence of the discrete cell balance equations, Eq. (1.22), for the \( J \) computational cells.

Notice that the neutron balance expressed in Eq. (3.159) has been derived for the case of vacuum boundary conditions on both sides of the slab, consistent with the assumption made throughout this effort. It is also noted that the balance in Eq. (3.159) is
written for a generic slab configuration in the sense that it allows for different material composition and cell widths in the spatial mesh, as signaled by the index \( j \) on the nuclear and geometric properties of the computational cells.

The continuous steady-state, one-speed neutron transport equation for slab geometry that was introduced in operator notation in Eq. (1.7) for a fixed isotropic source (non-multiplying) system with isotropic scattering is explicitly written as:

\[
\mu \frac{\partial \psi}{\partial x} + \sigma \psi(x, \mu) = \sigma_s \phi(x) + q(x)
\]  

(3.160)

The previous equation is considered along with the vacuum boundary conditions reported in Eq. (1.2). It is noted that Eq. (3.160) represents a local statement of neutron balance \( \textit{per se} \) [2].

In order to derive an integral balance relation for the slab in terms of cell-averaged scalar fluxes Eq. (3.160) is integrated over the angular variable:

\[
\frac{1}{2} \int_{-1}^{1} d\mu \left\{ \mu \frac{\partial \psi}{\partial x} + \sigma \psi = \sigma_s \phi + q \right\}
\]  

(3.161)

Notice that the factor of 1/2 in front of the integral has been introduced consistently with the treatment of the angular variable as a normalized angle [11] implied in the writing of Eq. (3.160).

In view of the linearity of the integral operator, the contributions from the various terms in Eq. (3.161) will be considered separately starting from the streaming term. As a consequence of the independence of the spatial and angular variables the following equality holds:
\begin{equation}
\frac{1}{2} \int_{-1}^{+1} d\mu \left( \mu \frac{\partial \psi}{\partial x} \right) = \frac{d}{dx} \left( \frac{1}{2} \int_{-1}^{+1} \mu \psi \, d\mu \right)
\end{equation} \tag{3.162}

It is convenient to recall the definition of neutron current density:

\[ J(x) = \frac{1}{2} \int_{-1}^{+1} \mu \psi(x,\mu) \, d\mu, \tag{3.163} \]

that permits writing Eq. (3.162) in the following more compact form:

\begin{equation}
\frac{1}{2} \int_{-1}^{+1} d\mu \left( \mu \frac{\partial \psi}{\partial x} \right) = \frac{dJ}{dx}
\end{equation} \tag{3.164}

The integration of the total interaction and of the scattering source terms is conducted in a straightforward way in view of the postulated independence of the macroscopic cross-sections from the angular variable. The integration of the fixed source term is also straightforward under the assumption of an isotropic fixed source. Using the definition of scalar flux, Eq. (1.6), the following spatially dependent ordinary differential equation is finally obtained:

\begin{equation}
\frac{dJ}{dx} + \sigma_a \phi = q \tag{3.165}
\end{equation}

In the latter equation it has been recognized that, for the system under consideration, the macroscopic total cross-section \( \sigma \) is the sum of the macroscopic scattering cross-section \( \sigma_s \) and of the macroscopic absorption cross-section:

\[ \sigma_a = \sigma - \sigma_s \tag{3.166} \]

Integrating Eq. (3.165) over the slab’s extent \((0, L)\):

\begin{equation}
[J]_0^L + \int_0^L dx \sigma_a \phi = \int_0^L dx q \tag{3.167}
\end{equation}
The slab is then subdivided into $J$ computational cells ($j = 1, ..., J$) characterized by widths $\Delta x_j$ and by homogeneous physical properties ($\sigma_j$, etc.), consistent with the formulation of Eq. (1.22). Consequently Eq. (3.167) may be written in the following equivalent form:

$$[J]_0^L + \sum_{j=1}^{J} \sigma_j \tilde{\phi}_j \Delta x_j = \sum_{j=1}^{J} q_j \Delta x_j \quad (3.168)$$

The cell-averaged scalar flux for cell $j$ appearing in Eq. (3.168) is defined as:

$$\tilde{\phi}_j = \frac{1}{\Delta x_j} \int_{\Delta x_j} dx \phi (x) \quad (3.169)$$

The cell-averaged neutron fixed source for cell $j$ appearing in Eq. (3.168) is similarly defined as:

$$q_j = \frac{1}{\Delta x_j} \int_{\Delta x_j} dx q(x) \quad (3.170)$$

Introducing the cell scattering ratio $c_j$ and using Eq. (3.166), the cell macroscopic absorption cross-section may be written in the following form:

$$\sigma_{aj} = \sigma_j - \sigma_{sj} = \sigma_j - c_j \sigma_j = (1 - c_j) \sigma_j \quad (3.171)$$

Substituting this result into Eq. (3.168) the following expression for the neutron balance is obtained:

$$J|_L - J|_0 + \sum_{j=1}^{J} (1 - c_j) \sigma_j \tilde{\phi}_j \Delta x_j = \sum_{j=1}^{J} q_j \Delta x_j \quad (3.172)$$
The evaluation of the contribution due to the leakage of neutrons from the right edge of the slab, at $x = L$, is carried out starting from the neutron current definition in Eq. (3.163):

\[
J|_L = \frac{1}{2} \int_{-1}^{+1} d\mu \mu \psi(L, \mu) = \frac{1}{2} \int_{-1}^{0} d\mu \mu \psi(L, \mu) + \frac{1}{2} \int_{0}^{+1} d\mu \mu \psi(L, \mu)
\]  

(3.173)

The first integral on the right hand side of Eq. (3.173) vanishes in view of the vacuum boundary condition at $x = L$. The second integral is discretized referring to a discrete ordinates symmetric angular quadrature $\{\mu_m, w_m\}$ ($m = 1, ..., M$) to be consistent with the assumptions made in the previous sections:

\[
J|_L = \sum_{m=1}^{M/2} w_m |\mu_m| \tilde{\psi}_{m,J}
\]  

(3.174)

In the last expression the usual notation for the angular flux exiting from cell $J$ is used. Also, the quadrature weights $w_m$ have been renormalized to 1 consistently with Eq. (3.2).

Analogously, the contribution due to the leakage of neutrons from the left edge of the slab, at $x = 0$, is:

\[
-J|_0 = -\frac{1}{2} \int_{-1}^{+1} d\mu \mu \psi(0, \mu) = -\frac{1}{2} \int_{-1}^{0} d\mu \mu \psi(0, \mu) - \frac{1}{2} \int_{0}^{+1} d\mu \mu \psi(0, \mu),
\]  

(3.175)

and:

\[
-J|_0 = \sum_{m=-M/2}^{M/2} w_m |\mu_m| \tilde{\psi}_{m,1}
\]  

(3.176)
Substituting Eq. (3.174) and Eq. (3.176) into Eq. (3.172) the final expression for the neutron balance over the entire slab reported in Eq. (3.159) is obtained.

In order to formulate the neutron balance for the slab in terms of discrete cell-averaged scalar fluxes only, it is then necessary to obtain expressions for the first two contributions in Eq. (3.159), due to leakage of neutrons from the right and left edges of the slab respectively, in terms of the cell-averaged scalar fluxes.

**Contribution of leakage from the right edge of the slab**

The starting point is represented by the equations for the \( m \)th discrete ordinate relating the scattering and fixed sources and the incoming angular flux to the average angular flux and the outgoing angular flux for a generic cell \( j \):

\[
\begin{align*}
\Psi_{m,j} &= o_{m,j} \left( c_j \phi_j + s_j \right) + p_{m,j} \Psi_{m,j}^\prime, \\
\Psi_{m,j}^\prime &= r_{m,j} \left( c_j \phi_j + s_j \right) + q_{m,j} \Psi_{m,j}^{j},
\end{align*}
\]

\( m = 1, \ldots, M; j = 1, \ldots, J \) (3.177)

The coefficients \( o_{m,j}, p_{m,j}, r_{m,j} \) and \( q_{m,j} \) have the same definitions given in Eqs. (3.25) through (3.28). Notice that in Eq. (3.177) the iteration indices \((\ell)\) and \((\ell + 1)\) originally present in Eq. (3.7) have been dropped. The variables in Eq. (3.177) refer to “converged” physical quantities.

Actually only the second equation of the system in Eq. (3.177) along with the continuity condition, Eq. (3.3), is needed in order to determine the expression for \( \Psi_{m,J}^\prime \).

For \( \mu_m > 0 \) this equation is used recursively starting from cell \( J \) and then considering the contiguous cells in the slab, for decreasing values of the \( j \) index, until the external side of
cell 1 (where the zero vacuum boundary condition incoming flux is known) is reached, as illustrated in Fig. 3.15.

The expression for $\tilde{\psi}_{m,j}^\alpha$, obtained from the procedure outlined in Fig. 3.15, is used to evaluate the first leakage contribution in Eq. (3.159) by simply applying the operator $\sum_{m=1}^{M/2} w_m |\mu_m|$ to the resulting expression. The result obtained may be written using the following compact notation:

$$\sum_{m=1}^{M/2} w_m |\mu_m| \tilde{\psi}_{m,j}^\alpha = \sum_{j=1}^{J-2} \left( \sum_{m=1}^{M/2} w_m |\mu_m| \prod_{i=j+1}^{J} q_{m,i} \right) r_{m,j} \left( c_j \tilde{\phi}_j + s_j \right) +$$

$$+ \left( \sum_{m=1}^{M/2} w_m |\mu_m| q_{m,J-1} r_{m,J-1} \right) \left( c_{J-1} \tilde{\phi}_{J-1} + s_{J-1} \right) +$$

$$+ \left( \sum_{m=1}^{M/2} w_m |\mu_m| r_{m,J} \right) \left( c_j \tilde{\phi}_j + s_j \right)$$

(3.178)

For the purpose of the numerical evaluation of the right hand side of Eq. (3.178) it is convenient to introduce the following matrix notation:

$$\sum_{m=1}^{M/2} w_m |\mu_m| \tilde{\psi}_{m,j}^\alpha = \mathbf{v} \cdot \mathbf{s}^T$$

(3.179)

In Eq. (3.179), vector $\mathbf{v}$ contains the coefficients coupling the cell sources to the leakage at the right boundary of the slab:

$$\mathbf{v} = \left[ \sum_{m=1}^{M/2} w_m |\mu_m| \prod_{i=j+1}^{J} q_{m,i} \right] r_{m,j}, \left( \sum_{m=1}^{M/2} w_m |\mu_m| q_{m,J-1} r_{m,J-1} \right), \left( \sum_{m=1}^{M/2} w_m |\mu_m| r_{m,J} \right), j = 1, \ldots, (J - 2)$$

(3.180)
Fig. 3.15: Procedure for the calculation of $\tilde{\psi}_{m,j}^\mu$.

Finally, vector $\mathbf{s}$ represents a generalized, i.e. scattering plus external, source vector:

$$\mathbf{s} = \left[ (c_j \tilde{\phi}_j + s_j), \ldots, (c_i \tilde{\phi}_i + s_i), \ldots, (c_j \tilde{\phi}_j + s_j) \right]$$ (3.181)
Contribution of leakage from the left edge of the slab

Since the system of equations in Eq. (3.177) are written in an incoming- and outgoing-edge formulation and the quadrature is assumed to be symmetric, the expression for the second leakage contribution in Eq. (3.159) may be directly derived starting from Eq. (3.178) and traversing the computational cells in reverse order for \( \mu_m < 0 \). The following expression is obtained:

\[
\sum_{m=M+1}^{M} w_m |\mu_m| \psi_{m,1}^{\beta} = \left( \sum_{m=M+1}^{M} w_m |\mu_m| r_{m,1} \right) \left( c_1 \phi_1 + s_1 \right) +
\]

\[
+ \left( \sum_{m=M+1}^{M} w_m |\mu_m| q_{m,1} r_{m,2} \right) \left( c_2 \phi_2 + s_2 \right) +
\]

\[
+ \sum_{j=3}^{J} \left( \sum_{m=M+1}^{M} w_m |\mu_m| \prod_{i=1}^{j-1} q_{m,i} r_{m,j} \right) \left( c_j \phi_j + s_j \right)
\]

For the purpose of the numerical evaluation of the right hand side of Eq. (3.182) it is convenient to introduce the following matrix notation:

\[
\sum_{m=M+1}^{M} w_m |\mu_m| \psi_{m,1}^{\beta} = \mathbf{w} \cdot \mathbf{s}^T
\]

In Eq. (3.183), \( \mathbf{s} \) is the generalized source vector introduced in Eq. (3.181) while vector \( \mathbf{w} \) contains the coefficients coupling the cell sources to the leakage at the left boundary of the slab:
Notice that the expression for the coefficient pertaining to the penultimate cell in the sweeping direction, both in Eq. (3.180) and in Eq. (3.184), might be included in the general formulation given for the other coefficients (the product would reduce to a single factor). The reason why it has been written separately is that the last two terms in vector $v$ and the first two terms in vector $w$ are expected to dominate over all other terms in the thick cell limit. This conclusion is based on the results obtained from the asymptotic analysis performed for matrices $A$ and $B$ and on the similarity in structure between the coefficients in vectors $v$ and $w$ and the matrices elements. Anyway, in view of the utilization of the neutron balance as a tool for the evaluation of the impact of the truncation of matrices $A$ and $B$ on the calculated cell-averaged fluxes, the full $v$ and $w$ vectors are retained in the evaluation of the neutron balance. This way avoids the introduction of further, unnecessary, approximations along with the effect of the truncated coupling stencil. In other words, the neutron balance is meant to be exactly implemented and the difference between the fixed, exact source term and the sink terms (absorption and leakage) computed via the non-exact fluxes produced by the use of truncated versions of the matrices is used to evaluate the impact of the truncation procedure itself on solution accuracy. The relative error, i.e. the ratio of the difference
between the sinks contribution and the fixed source contribution to the fixed source contribution itself, in Eq. (3.159) has actually been considered in the following numerical results.

### 3.5.2 Numerical Results

Three different kinds of tridiagonal approximations have been considered for matrix $\mathbf{B}$: (i) abrupt truncation of the matrix elements, where for any value of $\Delta x$ only the original elements of the diagonal and first off-diagonals are retained, all other elements are set to zero; (ii) then considering the effect of imposing a diffusive-like coupling stencil on the elements of the matrix, retaining the original diagonal elements and deriving the expression for the first off-diagonal elements from Eq. (3.103); (iii) or vice versa.

The interest in (i) is of a theoretical nature, namely determining the cell thickness beyond which the full matrix becomes asymptotically tridiagonal for numerical purposes. This would hopefully introduce a cut-off thickness above which even this abrupt truncation might actually give the exact solutions by solving only a tridiagonal system. Of course this abrupt truncation is expected to give errors both in the fluxes and in the neutron balance in the intermediate thickness range. The quantitative evaluation of this error is particularly interesting in view of the search for other truncation patterns that may work as effectively as the abrupt one in the very thick limit but also give a lower error in the intermediate thickness range. Strategies (ii) and (iii) are considered having in mind this objective and are based on the conclusions of the thick cell limit asymptotic analysis.
From a preconditioner’s point of view these diffusion-like low-order approximations of the full integral transport operator are of interest for the role they play in synthetic acceleration methods. From a diffusion neutron balance point of view this form of tridiagonal approximation may introduce a smaller error in the neutron balance in the intermediate cell thickness range.

In all three cases matrix $A$ can either be used in its full form, since unlike $B$, $A$ does not need to be inverted, or approximated consistently with $B$, leading to the six combinations examined in the plots presented in this section, using the following acronyms:

- **TBFA**: abruptly Truncated $B$ and Full $A$;
- **TBTA**: abruptly Truncated $B$ and $A$;
- **DBFA**: Neutron conserving Diagonal elements based truncated $B$ and Full $A$;
- **DBDA**: Neutron conserving Diagonal elements based truncated $B$ and $A$;
- **OBFA**: Neutron conserving Off-diagonal elements based truncated $B$ and Full $A$;
- **OBOA**: Neutron conserving Off-diagonal elements based truncated $B$ and $A$.

The attribute “neutron conserving” is intended in the diffusion neutron balance sense. Any truncation of the full matrix elements introduces an error in the slab neutron balance based on the original continuous transport problem. The tridiagonal approximations based on the diffusion-like stencil in Eq. (3.103) attempt to better conserve the slab neutron balance form in terms of a diffusion approximation.
The six methods have been evaluated for three different homogeneous structures comprised of ten computational cells. The three structures differ in their fixed source distribution. It is in fact desired to evaluate the impact of the fixed source term on the system in Eq. (1.27). Notice in particular that, apart from the case of a pure scattering medium \((c=1)\), no scaling of the source is implied in determining the solution to Eq. (1.27). Each of the three structures has been considered for different values of the scattering ratio \(c\) to determine the impact of more or less neutron preserving situations on the various truncation strategies, since matrix \(B\) is \(c\) dependent. In the cases in which the scattering ratio has a unit value, the fixed source in the computational cells has been scaled as the inverse of the cell thickness, in order to prevent the numerical evaluation of increasingly growing cell-averaged fluxes as the cell width is increased. All the other parameters have been retained constant for the three structures, using the \(S_6\) quadrature and a unit value for the macroscopic total cross-section \((\sigma = 1)\). For brevity the three source distributions will be indicated as \(1^{10}\), \(0^21^60^2\) and \(0^41^20^4\) in the following figures where 1 represents a unit fixed density source, for \(c < 1\), or scaled as the inverse of the cell thickness, for \(c = 1\), and 0 indicates no fixed source.

The relative difference in the cell-averaged fluxes determined by the various approximate methods for the \(1^{10}\) source distribution is presented in Fig. 3.16 sorted by the different values of the scattering ratio attempted: \(c = 1\) in A, \(c = 0.99\) in B, \(c = 0.9\) in C, \(c = 0.7\) in D, \(c = 0.5\) in E, \(c = 0.3\) in F, \(c = 0.1\) in G and \(c = 0.01\) in H. The relative difference in the neutron balance for the \(1^{10}\) source distribution is presented in Fig. 3.17 sorted by the different values of the scattering ratio that are arranged in the same order as
Fig. 3.16. The relative difference in the cell-averaged fluxes for the $^{10}$ source distribution is presented in Fig. 3.18 this time sorted by the different approximate methods applied: TBFA in A, TBTA in B, DBFA in C, DBDA in D, OBFA in E, OBOA in F. The relative difference in the neutron balance for the $^{10}$ source distribution is presented in Fig. 3.19 this time sorted by the different approximation methods arranged in the same order as Fig. 3.18. Figures 3.20 through 3.23 have the same meaning for structure 021^602, while Fig. 3.24 through 3.27 have the same meaning for structure 0^{41^20^4}, respectively.

The presented figures convey much information and might be considered under various points of view. Some distinct conclusions emerge especially from an operational point of view and are hereby stressed.

A threshold of ~1 MFP divides the regime in which the truncation strategies yield an acceptably low difference (cells thicker than ~1 MFP) and the regime in which the solutions are highly inaccurate (cells thinner than 1 MFP). In any case, even in the thin cell limit, where the results are very poor, retaining the full $A$ matrix gives better results than truncating it, even if the truncation is consistent with that for $B$.

Above the ~1 MFP threshold all methods’ accuracies appear comparable since the full transport matrix approaches a tridiagonal structure anyway; this is signaled by a sharp drop in the error around 30 MFPs. Between 1 MFP and 30 MFPs the DBFA method effectively gives lower differences both in the flux values and in the neutron balance. The fact that in the thin cell limit the truncation methods based on forcing a diffusion-like coupling stencil tend to give divergent differences is consistent with the results of the asymptotic analysis of the full transport operator in the thin cell limit. The
differences above 30 MFPs exhibit finite arithmetic random noise around the machine epsilon value.

Fig. 3.16: Flux difference for various $c$ for source distribution $1^{st}$ (see text).
$c = 0.90$

Fig. 3.16: (Continued).
Fig. 3.16: (Continued).
Fig. 3.16: (Continued).
Fig. 3.17: Neutron balance difference for various c for source distribution $1^{10}$. 
Fig. 3.17: (Continued).
Fig. 3.17: (Continued).
Fig. 3.17: (Continued).
Fig. 3.18: Flux difference for various truncation methods for source distribution $1^{10}$. 
Fig. 3.18: (Continued).
Fig. 3.18: (Continued).
Fig. 3.19: Neutron balance difference for various truncation methods for $I^{10}$. 
Fig. 3.19: (Continued).
Fig. 3.19: (Continued).
Fig. 3.20: Flux difference for various $c$ for source distribution $0^2T^00^2$ (see text).
Fig. 3.20: (Continued).
Fig. 3.20: (Continued).
Fig. 3.20: (Continued).
Fig. 3.21: Neutron balance difference for various $c$ for source distribution $\theta^3 I^0 \theta^3$. 
Fig. 3.21: (Continued).
Fig. 3.21: (Continued).
Fig. 3.21: (Continued).
Fig. 3.22: Flux difference for various truncation methods for source distribution $0^2 T^0_0^2$. 

A

B
Fig. 3.22: (Continued).
Fig. 3.22: (Continued).
Fig. 3.23: Neutron balance difference for various truncation methods for $0^2 l^4 0^2$. 
Fig. 3.23: (Continued).
Fig. 3.23: (Continued).
Fig. 3.24: Flux difference for various $c$ for source distribution $0^d1^20^d$ (see text).
Fig. 3.24: (Continued).
Fig. 3.24: (Continued).
Fig. 3.24: (Continued).
Fig. 3.25: Neutron balance difference for various $c$ for source distribution $\theta^1 I^2 0^4$. 
Fig. 3.25: (Continued).
Fig. 3.25: (Continued).
Fig. 3.25: (Continued).
Fig. 3.26: Flux difference for various truncation methods for source distribution $0^4T^20^4$. 
Fig. 3.26: (Continued).
Fig. 3.26: (Continued).
Fig. 3.27: Neutron balance difference for various truncation methods for $0^4t^20^4$. 

A

B
Fig. 3.27: (Continued).
Fig. 3.27: (Continued).
3.6 Truncation Strategies for the Integral Transport Matrix in Thin Slabs

As evident from the results presented in the previous section, the truncation strategies based on the asymptotic results valid in the thick cell regime do in general fail when extended to the thin cell regime. In particular, the failure of the DB and OB strategies can be understood in view of the asymptotic results obtained for the thin cell limit in Sec. 3.4.3. In the thin cell limit $\mathbf{B}$ is approaching the identity matrix $\mathbf{I}$ possessing a diagonal matrix structure. When applied in the thin cell regime, the DB strategies result in imposing finite, instead of asymptotically small, first off-diagonal elements on the $\mathbf{M}$ matrix approximating $\mathbf{B}$. On the other hand, the OB strategies impose vanishing instead of finite elements on the diagonal of the matrix approximating $\mathbf{B}$. In both cases, the very structure of the original integral transport matrix is being poorly approximated in the thin cell limit.

The only strategy that doesn’t fail is TBFA in which the full $\mathbf{A}$ matrix is used on the right hand side while the original tridiagonal block of the $\mathbf{B}$ matrix is retained in the $\mathbf{M}$ approximation and has therefore the correct asymptotic behavior. It may be noticed that the rate of decrease of the error in the cell-averaged scalar fluxes for the TBFA strategy is at most only first order in the cell optical thickness in the thin cell regime. This may also be understood in view of the asymptotic behavior of matrix $\mathbf{B}$ in the thin cell limit. In Sec. 3.4.3 it was shown that all the off-diagonal elements of matrix $\mathbf{B}$ are $O(\delta)$ in the limit as $\delta \to 0$. This is therefore the expected order in $\delta$ for the error that is introduced by inverting a matrix $\mathbf{M}$ that is a truncated version of $\mathbf{B}$, with a truncation error that is $O(\delta)$. 
In the remainder of this section it will be shown that it is possible to improve on the order of the truncation error, from $O(\delta)$ to $O(\delta^2)$, by exploiting the peculiar diagonally dominant structure acquired by matrix $B$ in the thin cell limit. In order to expose this structure it is convenient to make the following identification:

$$ b = c \sum_{m=1}^{M/2} \left( \frac{w_m}{|\mu_m|} \right) (\sigma \delta) $$

(3.185)

The expression for $b$ introduced in Eq. (3.185) represents the $O(\delta)$ term that appears in Eqs. (3.135) through (3.137). With reference to a spatial mesh comprised of $J$ computational cells, the corresponding ($J \times J$) matrix $B$ has to leading order, ignoring terms that are $O(\delta^2)$, the following asymptotic structure in the thin cell limit:

$$ B \sim \begin{bmatrix}
(1-b) & -b & \ldots & -b & -b & \ldots & -b & -b \\
-b & (1-b) & \ldots & -b & -b & \ldots & -b & -b \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
-b & -b & \ldots & (1-b) & -b & \ldots & -b & -b \\
-b & -b & \ldots & -b & (1-b) & \ldots & -b & -b \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
-b & -b & \ldots & -b & -b & \ldots & (1-b) & -b \\
-b & -b & \ldots & -b & -b & \ldots & -b & (1-b)
\end{bmatrix} $$

(3.186)

It is convenient to follow a similar approach for writing the structure acquired by the $A$ matrix in the same limit by introducing the quantity:

$$ a = \frac{1}{\sigma} \sum_{m=1}^{M/2} \left( \frac{w_m}{|\mu_m|} \right) (\sigma \delta) $$

(3.187)
The expression for $a$ introduced in Eq. (3.187) represents the $O(\delta)$ term that appears in Eqs. (3.138) through (3.140). With reference to a spatial mesh comprised of $J$ computational cells, the corresponding $(J \times J)$ matrix $A$ has to leading order, ignoring terms that are $O(\delta^2)$, the following asymptotic structure in the thin cell limit:

\[
A \sim \begin{bmatrix}
a & a & \ldots & a & a & a & a \\
a & a & \ldots & a & a & a & a \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
a & a & \ldots & a & a & a & a \\
a & a & \ldots & a & a & a & a \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
a & a & \ldots & a & a & a & a \\
a & a & \ldots & a & a & a & a
\end{bmatrix}
\]

(3.188)

It is possible to exploit the peculiar asymptotic structure of matrix $B$ to devise an algebraic transformation that eliminates terms that are $O(\delta)$ from outside the matrix diagonal and retain terms that are only at most $O(\delta^2)$, thereby improving the accuracy of the solution obtained from the truncated matrix as $\delta \rightarrow 0$. First of all, in the thin cell limit it is possible to show that the $B$ matrix is either equivalent to a matrix $B_L$ that is lower-triangular dominated or an equivalent matrix $B_U$ that is upper-triangular dominated. Indicating terms that are $O(\delta^2)$, or higher-order, with 0 for simplicity, the asymptotic triangular structures acquired by matrices $B_L$ and $B_U$ are:
The sum of matrices $B_L$ and $B_U$ would of course yield a matrix that is dominated by its tridiagonal block in the same asymptotic limit and is characterized by a diffusive stencil. More importantly though, it is possible to use either $B_L$ or $B_U$ as a starting point for a further transformation that leads to a matrix $B_D$ that is diagonally dominated in the thin cell limit:
\[ B_D \sim \]

\[
\begin{bmatrix}
(1-Jb) & 0 & \ldots & 0 & 0 & \ldots & 0 & 0 \\
0 & (1-Jb) & \ldots & 0 & 0 & \ldots & 0 & 0 \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
0 & 0 & \ldots & (1-Jb) & 0 & \ldots & 0 & 0 \\
0 & 0 & \ldots & 0 & (1-Jb) & \ldots & 0 & 0 \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
0 & 0 & \ldots & 0 & 0 & \ldots & (1-Jb) & 0 \\
0 & 0 & \ldots & 0 & 0 & \ldots & 0 & (1-Jb)
\end{bmatrix}
\]

(3.191)

The previous transformations are exact from an algebraic point of view and have been applied on both sides of the original system in Eq. (1.27). When applied to the right hand side of Eq. (1.27), the various transformations lead from matrix \( A \) to matrices \( A_L \), \( A_U \) and \( A_D \) corresponding to matrices \( B_L \), \( B_U \) and \( B_D \), respectively. To leading order, the asymptotic structures these matrices limit to in the thin cell limit are the following:

\[ A_L \sim \]

\[
\begin{bmatrix}
a & a & a & \ldots & a & a & \ldots & a & a \\
0 & 0 & 0 & \ldots & 0 & 0 & \ldots & 0 & 0 \\
0 & 0 & 0 & \ldots & 0 & 0 & \ldots & 0 & 0 \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
0 & 0 & 0 & \ldots & 0 & 0 & \ldots & 0 & 0 \\
0 & 0 & 0 & \ldots & 0 & 0 & \ldots & 0 & 0 \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
0 & 0 & 0 & \ldots & 0 & 0 & \ldots & 0 & 0 \\
0 & 0 & 0 & \ldots & 0 & 0 & \ldots & 0 & 0 \\
0 & 0 & 0 & \ldots & 0 & 0 & \ldots & 0 & 0 \\
0 & 0 & 0 & \ldots & 0 & 0 & \ldots & 0 & 0
\end{bmatrix}
\]

(3.192)
A comparison of Eqs. (3.188) and (3.194) shows that, to leading order, the asymptotic structure acquired by the original matrix $A$ is the same as that acquired by matrix $A_D$.

The algebraic system in the $B_D$ and $A_D$ matrix representation, like the original system in the $B$ and $A$ matrix representation in Eq. (1.27), preserves the original fluxes and satisfies:

$$B_D \tilde{\phi}^\infty = A_D q$$  \hspace{1cm} (3.195)
Assuming a uniform, fixed, unit source $q$, the system in Eq. (3.195) may be readily solved, in the thin-cell asymptotic limit, leading to the conclusion that all cell-averaged fluxes tend to the same value $\tilde{\phi}$ to within $O(\delta^2)$ terms:

$$\tilde{\phi} \sim \frac{Ja}{(1-Jb)} \quad (3.196)$$

It should be noted that this result has been obtained and is valid under the assumption that $J$ is a fixed (non-scaled) parameter, so that the thin cell limit is also a thin slab limit. The existence of the diagonal system in Eq. (3.195) is a direct consequence of Eq. (1.27) in the thin cell limit, in which matrices $B$ and $A$ acquire the structures in Eqs. (3.186) and (3.188). Therefore, the system of $J$ equations in Eq. (1.27) becomes:

\[
\begin{bmatrix}
(1-b) & -b & \ldots & -b & -b & \ldots & -b & \ldots & -b \\
-b & (1-b) & \ldots & -b & -b & \ldots & -b & \ldots & -b \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
-b & -b & \ldots & (1-b) & -b & \ldots & -b & \ldots & -b \\
-b & -b & \ldots & -b & (1-b) & \ldots & -b & \ldots & -b \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
-b & -b & \ldots & -b & -b & \ldots & (1-b) & \ldots & -b \\
-b & -b & \ldots & -b & -b & \ldots & (1-b) & \ldots & -b
\end{bmatrix}
\begin{bmatrix}
\tilde{\phi}_1 \\
\tilde{\phi}_2 \\
\vdots \\
\tilde{\phi}_{(j-1)} \\
\tilde{\phi}_j \\
\vdots \\
\tilde{\phi}_{(j-1)} \\
\tilde{\phi}_j
\end{bmatrix} = \begin{bmatrix}
q_1 \\
q_2 \\
\vdots \\
q_{(j-1)} \\
q_j \\
\vdots \\
q_{(j-1)} \\
q_j
\end{bmatrix}
\quad (3.197)
The system equations in rows (2) to (J) of Eq. (3.197) readily imply that the cell-averaged scalar fluxes from $\tilde{\phi}_2$ to $\tilde{\phi}_J$ are all equal to each other and to the scalar flux in the first cell, $\tilde{\phi}_1$. Indicating the latter scalar flux as $\tilde{\phi}$ in the equation in row (1) of Eq. (3.197), the following result follows:

$$\tilde{\phi} \sim \frac{a}{(1-Jb)} \sum_{j=1}^{J} q_j$$

(3.198)

This same solution is obtained from Eq. (3.195) solved with the expressions for matrices $B_D$ and $A_D$ given in Eqs. (3.191) and (3.194), respectively. This proves the equivalence of Eq. (3.195) to the original Eq. (1.27) in the thin-cell asymptotic limit. The systems of equations obtained by replacing $B$ and $A$ with $(B_U)$ and $(A_U)$ respectively in the original Eq. (1.27) are of course also equivalent in the thin-cell asymptotic limit.

The numerical results obtained devising a truncation strategy based on the existence of an equivalent diagonally dominated matrix with elements that are $O(\delta^2)$ on the off-diagonals are presented in Sec. 3.6.1.

### 3.6.1 Numerical Results

A truncation strategy based on the equivalence of the $B$ matrix with a diagonal matrix $B_D$ exposed in the previous section, referred to as DIAG in the following, has been implemented for the thin cell regime. This strategy is based on truncating the $B_D$ matrix retaining only the diagonal elements. The full $A_D$ matrix is instead retained on the
right hand side of Eq. (3.195). Since the elements truncated are $O(\delta^2)$ for $B_D$, it is expected that the maximum relative difference in the cell-averaged scalar fluxes be $O(\delta^2)$ for DIAG, as opposed to the $O(\delta)$ behavior observed in Sec. 3.5.2 for the TBFA strategy. In the latter $B$ is truncated at its tridiagonal band and the elements ignored are in fact $O(\delta)$. An improvement is also expected in the order displayed by the relative difference in the neutron balance.

These expectations are verified by the results presented in this section in Figs. 3.28 and 3.29 for the relative errors in the cell-averaged fluxes and in the neutron balance respectively. These figures are obtained using the $S_6$ quadrature and a unit value for the macroscopic total cross-section ($\sigma = 1$) for source structure 1\textsuperscript{10}. The uniform source is scaled as usual, in the purely scattering case, for optically thick cells between 1 MFP and 100 MFPs.

The relative difference in the cell-averaged fluxes determined by the DIAG method is contrasted with that obtained by TBFA in Fig. 3.28 sorted by the different values of the scattering ratio: $c = 1$ in A, $c = 0.9$ in B, $c = 0.5$ in C and $c = 0.1$ in D. The improvement in the order, from $O(\delta)$ for TBFA to $O(\delta^2)$ for DIAG, is evident in all cases.

The relative difference in the neutron balance is presented in Fig. 3.29 sorted by the different values of the scattering ratio that are arranged in the same order as Fig. 3.28. Even for this measure an improvement is gained in the order of the error in all cases.
It is evident, from both Figs. 3.28 and 3.29, that the DIAG strategy based on the asymptotic results in the thin cell limit fails when extrapolated to the thick cell regime.

Fig. 3.28: Flux difference for various $c$ for a thin slab.
Fig. 3.28: (Continued).
Fig. 3.29: Neutron balance difference for various $c$ for a thin slab.
Fig. 3.29: (Continued).
3.7 Conclusion

Exact analytic expressions for the elements of the \( A \) and \( B \) matrices introduced in Sec. 1.2 have been derived in slab geometry and the asymptotic properties of these elements, as a function of computational-cell size, have been investigated for homogeneous slabs in a thick cell diffusive limit and in a thin cell limit.

The results obtained in the thick cell limit prove that the \( B \) matrix acquires a tridiagonally dominated structure, characterized by a diffusion-like coupling stencil, at a fast exponential rate, manifested by the exponential vanishing of the elements beyond the first off-diagonal with increasing cell thickness. Therefore, these results provide further insight into the convergence properties of diffusion-based acceleration schemes in optically thick homogeneous configurations with low absorption. In contrast, in the thin cell limit matrix \( B \) acquires a diagonally dominated structure that is approached at a much slower linear rate. Notwithstanding, it is possible to identify an exact algebraic manipulation that transforms \( B \) into a matrix that acquires a diagonally dominated structure at a faster quadratic rate in the thin cell limit.

Availability of the integral transport discrete operator matrix has also permitted evaluation of different truncation strategies of the full matrix, suggested by the results of the asymptotic analysis. This evaluation has been carried out comparing the solution from the truncated matrices to that obtained from the direct solution of the system of linear equations resulting from the angular and spatial discretization of the transport equation, Eq. (1.27). The results of these accuracy studies point to the existence of three distinct regimes for the solution to Eq. (1.27): 1) a thick cell regime, for cells that have a
thickness greater than 30 MFPs, where strategies based on a tridiagonal approximation of \( B \) yield the correct solution to Eq. (1.27); 2) an intermediate regime, from a cell thickness of 1 MFP to 30 MFPs, in which the solution transitions to the thick cell regime and the errors of the tridiagonal approximations rapidly decay at an exponential rate; 3) a thin cell regime, below 1 MFP, where the solution to Eq. (1.27) is better approximated by a strategy that exploits the diagonal dominance of matrix \( B \).

These results point to the difficulty of devising a single truncation strategy that can yield satisfactory results for the approximate solution of Eq. (1.27) for all cell thicknesses. At the same time, it is explicitly noted that these results do not necessarily imply the impossibility of devising a preconditioner that may effectively accelerate the iterative solution of the transport problem over the entire cell thickness spectrum. As a matter of fact, while the accuracy of a preconditioner can guarantee pointwise convergence in limits of interest, the lack of accuracy doesn’t necessarily imply ineffectiveness of the preconditioner in improving the rate of convergence of standard Source Iteration. In other words, as stressed in Ch. 2, both the structural and spectral properties of a preconditioner, and in particular how the structural properties may influence the spectral properties, are instrumental in devising a successful acceleration scheme. An investigation of this relationship for homogeneous (and periodically heterogeneous) slabs will be conducted in Ch. 5.
Chapter 4

Integral Transport Matrix in Periodically Heterogeneous Slabs

4.1 Introduction

The study of the asymptotic properties of the integral transport matrix initiated in Ch. 3 for the case of a homogeneous slab on a uniform mesh is extended in this chapter to an important class of heterogeneous slabs, namely periodically heterogeneous slabs. In particular, the asymptotic limit considered for these periodic structures is one in which the heterogeneity in the optical properties of adjacent computational cells is progressively pushed apart, i.e. the thick cells are made thicker while the thin are made thinner at a prescribed rate. To fix ideas, the configuration considered in this chapter to treat the periodically heterogeneous case is depicted in Fig. 4.1.

![Fig. 4.1: Configuration of the periodically heterogeneous slab.](image)

As indicated in Fig. 4.1, in the following it will be assumed that the left-most computational cell is optically thick while the right-most one is optically thin, considering an even number of computational cells in the spatial discretization of the slab. This assumption in no way limits the generality of the results that will be presented.
The following choice has been made for the geometrical and material properties of a thick cell and of a thin cell, denoted by K and N, respectively:

K cell: \( \Delta x_K = \delta_K \Delta, \quad \sigma_K, \quad c_K \)

N cell: \( \Delta x_N = \delta_N / \Delta, \quad \sigma_N, \quad c_N \)

The scattering ratios and the total macroscopic cross-sections are taken as fixed parameters. The cell widths are scaled according to the dimensionless parameter \( \Delta \). In the limit as \( \Delta \to \infty \), the thick cells become thicker while the thin cells become thinner according to this prescribed rate. Notice that since the expressions for the \( B \) matrix elements are only dependent on the product \( \sigma_j \Delta x_j \), namely the number of neutron MFPs in a computational cell \( j \), the choice of scaling the cell’s geometrical width is equivalent to scaling the total cross-sections.

As it will be shown in this chapter, the discrete integral transport operator is approximated by a sparse matrix characterized by a pentadiagonal structure in the asymptotic limit considered for a periodically heterogeneous slab. This result confirms physical intuition, suggesting that the coupling between two optically thick cells, separated by an interposed thin cell, should be strong. It will also be used to obtain an analytical derivation of some notable asymptotic properties displayed by the numerically computed cell-averaged scalar fluxes for periodically heterogeneous slabs. However, as it will be shown in the last part of the chapter, the matrix representing the integral transport operator is also amenable to algebraic transformations that lead to a matrix representation that asymptotically approaches a tridiagonal structure in the limit of interest. Also, the algebraic transformations considered ensure that, like for the case of a homogeneous slab,
the tridiagonal structure is approached at a fast exponential rate even for the periodically heterogeneous configuration considered. Once again, availability of the integral transport operator matrix permits evaluation of the impact of truncating the full matrix into a sparse structure retaining the original diagonal and first off-diagonal stripes of the transformed matrix in the periodically heterogeneous case. The resulting solutions from the truncated operator and the full transport operator are compared to determine their difference in the limit as $\Delta \to \infty$.

The obtained results contribute to the basic understanding of the excellent convergence properties of acceleration methods for the neutron transport equation based on cell-centered preconditioners characterized by a diffusion-like coupling stencil even for the case of heterogeneous slabs. In fact, deterioration of the convergence properties of these acceleration schemes has been widely observed in the presence of sharp material discontinuities in multi-dimensional problems but not in one-dimensional problems. In this connection, the results presented in this chapter point to the existence of a low-order approximation to the full discrete integral transport operator characterized by a tridiagonal structure even in the case of a periodically heterogeneous slab.

An outline of the chapter follows. As it was pointed out in Sec. 3.3, the $\mathbf{B}$ matrix can in general be non-symmetric, depending on the material properties in the various computational cells. This is particularly true for periodically heterogeneous slabs. In Sec. 4.2 it is shown that the $\mathbf{B}$ matrix can be symmetrized in a general and rather straightforward way by means of an algebraic transformation that leads to a symmetric $\mathbf{B}^s$ matrix. The results of the asymptotic analysis for the elements of the $\mathbf{B}^s$ matrix, for a periodically heterogeneous slab in the limit as $\Delta \to \infty$, are derived in Sec. 4.3. These
results are employed in Sec. 4.4 to explain some interesting asymptotic properties possessed by the cell-averaged scalar fluxes for periodically heterogeneous slabs. The algebraic transformation that brings matrix $B$ into a $\tilde{B}$ matrix that possesses a tridiagonal dominant matrix structure, in the asymptotic limit as $\Delta \to \infty$, is introduced in Sec. 4.5. The results of the asymptotic analysis for the elements of the $\tilde{B}$ matrix are presented in Sec. 4.6. Numerical results for periodically heterogeneous slabs that confirm the findings of the asymptotic analysis are finally presented in Sec. 4.7.

### 4.2 Symmetrization of the One-Dimensional Integral Transport Matrix

Before setting up the asymptotic analysis for the periodically heterogeneous case, the fundamental issue of the symmetrization of the discrete integral transport operator matrix is solved. A close comparison of Eqs. (3.22) and (3.23) reveals that the originally constructed matrix $B$ possesses this property for homogeneous slabs on uniform meshes. Nonetheless, $B$ may in general be non-symmetric for heterogeneous configurations and/or non-uniform meshes, including the periodically heterogeneous case, whenever $\kappa_{n,j} \neq \kappa_{n,j+k}$ for cell $j$ and its $k^{th}$ neighboring cell $j+k$.

The availability of a generally symmetric matrix is highly desirable not only due to the convenience of working with a symmetric matrix, but especially for the availability of numerous theoretical and numerical results on the convergence properties of methods for the solution of linear systems characterized by a symmetric matrix.

As it will be presently shown, the $B$ matrix can be symmetrized in a rather straightforward way by applying the following transformation:
The symmetrized matrix will be referred to in the following as $B^S$. Provided the same algebraic transformation is also performed on the right hand side of Eq. (1.27), the transformed system yields the same cell-averaged scalar fluxes $\bar{\phi}^\infty$.

In order to prove that Eq. (4.1) indeed produces a symmetric matrix, first it is convenient to rewrite the original expressions for the elements of matrix $A$, Eqs. (3.18) through (3.20), in terms of the positional index $j$ and of the off-diagonal index $k$, returning to the standard matrix notation where $i$ is the row index while $j$ serves also as the column index. The double use of $j$ is unambiguous due to the natural ordering of cell variables on the spatial mesh that matches a cell’s spatial index with its location in the flux vector in Eq. (1.27), the latter identifying the column index of matrix elements multiplying that particular flux.

**Diagonal elements:**

$$A_{i,i} = \frac{1}{\sigma_i} \sum_{m=1}^{M} W_m \left( \frac{1 + \alpha_{m,i}}{1 + 2\kappa_{m,i} + \alpha_{m,j}} \right), \quad i = 1, ..., J$$

(4.2)

**Off-diagonal elements:**

$$A_{i,j} = \frac{1}{\sigma_j} \sum_{m=1}^{M/2} W_m \frac{2}{1 + 2\kappa_{m,j} + \alpha_{m,j}} \left( \prod_{k=\min(i,j)+1}^{\max(i,j)-1} \frac{2\kappa_{m,k} + \alpha_{m,k} - 1}{1 + 2\kappa_{m,k} + \alpha_{m,k}} \right) \frac{2\kappa_{m,i}}{1 + 2\kappa_{m,i} + \alpha_{m,i}}$$

$$i, j = 1, ..., J; \quad i \neq j$$

(4.3)

Analogously, the original expressions for the elements of matrix $B$, Eqs. (3.21) through (3.23), can be equivalently written in the following form using Eq. (1.28):
Diagonal elements:

\[ B_{i,i} = 1 - c_i \sum_{m=1}^{M} w_m \left( \frac{1 + \alpha_{m,i}}{1 + 2 \kappa_{m,i} + \alpha_{m,i}} \right), \quad i = 1, \ldots, J \]  

(4.4)

Off-diagonal elements:

\[ B_{i,j} = -c_i \sum_{m=1}^{M/2} w_m \frac{2}{1 + 2 \kappa_{m,i} + \alpha_{m,j}} \left( \prod_{k=\min(i,j)+1}^{\max(i,j)-1} \frac{2 \kappa_{m,k} + \alpha_{m,k} - 1}{1 + 2 \kappa_{m,k} + \alpha_{m,k}} \right) \frac{2 \kappa_{m,j} - 1}{1 + 2 \kappa_{m,i} + \alpha_{m,i}}, \quad i, j = 1, \ldots, J; \quad i \neq j \]  

(4.5)

For the purposes of the ensuing proof it is also convenient to define the following matrix:

\[ S_{i,j} = \sum_{m=1}^{M/2} w_m |\mu_m| \frac{2}{1 + 2 \kappa_{m,i} + \alpha_{m,j}} \left( \prod_{k=\min(i,j)+1}^{\max(i,j)-1} \frac{2 \kappa_{m,k} + \alpha_{m,k} - 1}{1 + 2 \kappa_{m,k} + \alpha_{m,k}} \right) \frac{2}{1 + 2 \kappa_{m,j} + \alpha_{m,i}}, \quad i, j = 1, \ldots, J; \quad i \neq j \]  

(4.6)

The elements on the diagonal of matrix \( S \) are not relevant for the discussion that follows and are left unspecified. Since Eq. (4.6) is invariant upon transposing its indices \( i \) and \( j \), it may be concluded that:

\[ S_{i,j} = S_{j,i}, \quad i, j = 1, \ldots, J; \quad i \neq j \]  

(4.7)

Hence, matrix \( S \) is symmetric. Using the definition of \( \kappa_{m,j} \), Eq. (1.23), and Eq. (4.6) into Eq. (4.3), the off-diagonal elements of matrix \( A \) may be obtained as:

\[ A_{i,j} = \frac{1}{\sigma_j \sigma_i \Delta x_i} S_{i,j}, \quad i, j = 1, \ldots, J; \quad i \neq j \]  

(4.8)

Similarly, the off-diagonal elements of matrix \( B \) may be derived from:
\[ B_{i,j} = -\frac{c_j}{\sigma_i \Delta x_i} S_{i,j}, \quad i, j = 1, \ldots, J; \quad i \neq j \]  

(4.9)

It is evident that both Eqs. (4.8) and (4.9) are not invariant upon transposing their indices \( i \) and \( j \). Therefore, neither \( \mathbf{A} \) nor \( \mathbf{B} \) are in general symmetric matrices. The proof of the symmetry of \( \mathbf{B}^S \) is rather straightforward. Substitution of Eq. (4.9) into Eq. (4.1), for \( i \neq j \), yields:

\[
B_{i,j}^S = \left( c_i \sigma_j \Delta x_i \right) \left( -\frac{c_j}{\sigma_j \Delta x_j} \right) S_{i,j} = -c_i c_j S_{i,j},
\]

(4.10)

\[
i, j = 1, \ldots, J, \quad i \neq j
\]

This concludes the proof of the symmetry of matrix \( \mathbf{B}^S \).

In order to preserve the exact scalar fluxes \( \bar{\phi}^\infty \) that are obtained from the linear system in Eq. (1.27) it is, of course, necessary to apply the same transformation to both sides of the equations in the system. To this end the system in Eq. (1.27) is written in scalar form:

\[
\sum_{j=1}^{J} B_{i,j} \bar{\phi}_j = \sum_{j=1}^{J} A_{i,j} q_j, \quad i = 1, \ldots, J
\]

(4.11)

Applying the transformation in Eq. (4.1) amounts to considering the algebraically equivalent system:

\[
\left( c_i \sigma_i \Delta x_i \right) \sum_{j=1}^{J} B_{i,j} \bar{\phi}_j = \left( c_i \sigma_i \Delta x_i \right) \sum_{j=1}^{J} A_{i,j} q_j, \quad i = 1, \ldots, J
\]

(4.12)

The multiplying coefficient can be carried under the summation operator on both sides of Eq. (4.12) leading to:
\[
\sum_{j=1}^{J} \left[ (c_i \sigma_i \Delta x_i) B_{i,j} \right] \tilde{q}_j = \sum_{j=1}^{J} \left[ (c_i \sigma_i \Delta x_i) A_{i,j} \right] q_j, \quad i = 1, \ldots, J
\]  
(4.13)

The matrix contained in the square brackets on the left hand side is readily identified as the symmetrized integral transport matrix \( \mathbf{B}^S \) defined in Eq. (4.1). The matrix resulting from applying the same transformation to the \( \mathbf{A} \) matrix on the right hand side will be indicated in the following as \( \mathbf{\bar{A}} \). As evident from Eq. (4.13), the elements of matrix \( \mathbf{\bar{A}} \) have the following expression:

\[
\bar{A}_{i,j} = (c_i \sigma_i \Delta x_i) A_{i,j}, \quad i, j = 1, \ldots, J
\]  
(4.14)

By way of the previous matrix definitions, the cell-averaged flux preserving system in Eq. (4.14) is finally expressed using the following compact matrix notation:

\[
\mathbf{B}^S \tilde{\phi}^\infty = \mathbf{\bar{A}} q
\]  
(4.15)

It is noted that matrix \( \mathbf{\bar{A}} \) is not in general symmetric. Substitution of Eq. (4.8) into Eq. (4.14), for \( i \neq j \), yields:

\[
\bar{A}_{i,j} = (c_i \sigma_i \Delta x_i) \left( \frac{1}{\sigma_j \sigma_i \Delta x_i} \right) S_{i,j} = \frac{c_i}{\sigma_j} S_{i,j},
\]  
(4.16)

\[i, j = 1, \ldots, J, \quad i \neq j\]

Transposing indices \( i \) and \( j \) in Eq. (4.16) gives the following expression:

\[
\bar{A}_{j,i} = (c_j \sigma_j \Delta x_j) \left( \frac{1}{\sigma_i \sigma_j \Delta x_j} \right) S_{j,i} = \frac{c_j}{\sigma_i} S_{j,i},
\]  
(4.17)

\[i, j = 1, \ldots, J, \quad i \neq j\]
Therefore, the expressions in Eqs. (4.16) and (4.17) may be equal if and only if:

\[ \frac{c_i}{\sigma_i} = \frac{c_j}{\sigma_j}, \quad i, j = 1, \ldots, J, \quad i \neq j \]  

(4.18)

Notice that the condition expressed by Eq. (4.18) is also equivalent to requiring that the scattering cross-sections for cells \( i \) and \( j \) be equal \( (\sigma_{si} = \sigma_{sj}) \). The fact that \( \mathbf{A} \) is not in general symmetric is not considered to be a critical issue since this matrix is needed to give the correct right hand side vector for Eq. (4.15) and does not need to be inverted or iterated.

We conclude this section by writing expressions for the elements of both matrices \( \mathbf{B^s} \) and \( \mathbf{A} \) employing the same notation, in terms of the off-diagonal index \( k \), originally used to introduce the elements of \( \mathbf{A} \) and \( \mathbf{B} \), Eqs. (3.18) through (3.23). These expressions are useful in view of the ensuing asymptotic analysis and as a “recipe” for the numerical evaluation of matrices \( \mathbf{B^s} \) and \( \mathbf{A} \) in the code developed to test the results of the linear algebraic analysis.

The expressions for the elements of matrix \( \mathbf{B^s} \) are hereby reported.

**Diagonal elements:**

\[ B_{s,j,j} = (c_j \sigma_j \Delta x_j) B_{j,j} = (c_j \sigma_j \Delta x_j) - (c_j^2 \sigma_j \Delta x_j) \sum_{m \neq l} w_m \frac{1 + \alpha_{m,j}}{1 + 2 \kappa_{m,j} + \alpha_{m,j}}, \]  

(4.19)

\[ j = 1, \ldots, J \]
\( k \)th off-diagonal elements with \( k \geq 1 \) coupling cells \( j \xrightarrow{\mu_m > 0} j + k \):

\[
B_{j+k,j}^S = \left( c_{j+k} \sigma_j \Delta x_{j+k} \right) B_{j+k,j} = -c_{j+k} c_j.
\]

\[
\frac{M/2}{\sum_{m=1}^{M/2} w_m |\mu_m|} \frac{2}{1 + 2 \kappa_{m,j} + \alpha_{m,j}} \left( \prod_{i=j+1}^{j+k-1} \frac{2 \kappa_{m,i} + \alpha_{m,i} - 1}{1 + 2 \kappa_{m,i} + \alpha_{m,i}} \right) \frac{2}{1 + 2 \kappa_{m,j+k} + \alpha_{m,j+k}},
\]

\( j = 1, \ldots, (J-1); \ k = 1, \ldots, (J-j) \)

\( k \)th off-diagonal elements with \( k \geq 1 \) coupling cells \( j \xleftarrow{\mu_m < 0} j + k \):

\[
B_{j,j+k}^S = \left( c_j \sigma_j \Delta x_j \right) B_{j,j+k} = -c_j c_{j+k}.
\]

\[
\frac{M/2}{\sum_{m=1}^{M/2} w_m |\mu_m|} \frac{2}{1 + 2 \kappa_{m,j} + \alpha_{m,j}} \left( \prod_{i=j+1}^{j+k-1} \frac{2 \kappa_{m,i} + \alpha_{m,i} - 1}{1 + 2 \kappa_{m,i} + \alpha_{m,i}} \right) \frac{2}{1 + 2 \kappa_{m,j+k} + \alpha_{m,j+k}},
\]

\( j = 1, \ldots, (J-1); \ k = 1, \ldots, (J-j) \)

Inspection of the last two equations confirms that \( B^S \) is indeed a symmetric matrix. Finally, the expressions for the elements of matrix \( \overline{A} \) are the following.

**Diagonal elements:**

\[
\overline{A}_{j,j} = \left( c_j \sigma_j \Delta x_j \right) A_{j,j} = \left( c_j \Delta x_j \right) \sum_{m=1}^{M} w_m \frac{1 + \alpha_{m,j}}{1 + 2 \kappa_{m,j} + \alpha_{m,j}},
\]

\( j = 1, \ldots, J. \)
4.3 Asymptotic Analysis for the Elements of Matrix $B^S$

Due to the periodic nature of the structure considered, the matrix elements populating the diagonal and the even off-diagonal stripes of $B^S$ will be of two different kinds pertaining to the coupling of two thick cells or the coupling of two thin cells. In contrast, only a single kind of element is found on an odd off-diagonal stripe, expressing the coupling of a thick and a thin cell. This pattern is exemplified in Fig. 4.2.
It is therefore convenient to refer to a material index \( l = K, N \) for the two materials in the periodically heterogeneous structure and to introduce the following notation to refer to the reciprocal of the optical thickness, see Eq. (1.23), of a cell hosting a material with index \( l \):

\[
K_{m,l} = \frac{|\mu_m|}{\sigma_l \Delta x_i}, \quad l = K, N \tag{4.25}
\]

Similarly, the following notation is used to refer to the AHOT-N0 spatial weights, see Eq. (1.25), of a cell hosting a material with index \( l \):

\[
\alpha_{m,l} = \coth \left( \frac{\sigma_l \Delta x_i}{2 |\mu_m|} \right) - \frac{2|\mu_m|}{\sigma_l \Delta x_i}, \quad l = K, N \tag{4.26}
\]

The expressions for the matrix elements of matrix \( B^S \), pertaining to the periodically heterogeneous structure in Fig. 4.1, are hereby reported in terms of the quantities introduced in Eqs. (4.25) and (4.26). The first off-diagonal elements are treated as a separate case in view of the results of the ensuing asymptotic analysis.

**Diagonal elements:**

\[
B_{g,l}^S = (c_i \sigma_i \Delta x_i) - (c_i^2 \sigma_i \Delta x_i) \sum_{m=1}^{M} w_m \frac{1 + \alpha_{m,l}}{1 + 2K_{m,l} + \alpha_{m,l}}, \quad l = K, N \tag{4.27}
\]
First off-diagonal elements:

\[
B_{1,K\rightarrow N}^S = -c_K c_N \sum_{m=1}^{M/2} w_m \mu_m \frac{2}{1 + 2\kappa_{m,K} + \alpha_{m,K}} \frac{2}{1 + 2\kappa_{m,N} + \alpha_{m,N}}
\]  \hspace{1cm} (4.28)

\[k^\text{th}\] off-diagonal elements with \(k > 1\) and \(k\) even:

\[
B_{k,K\rightarrow K}^S = -4c_K^2 \sum_{m=1}^{M/2} w_m \mu_m \left[ \frac{2\kappa_{m,K} + \alpha_{m,K} - 1}{2} \right]^{k-1} \left[ \frac{2\kappa_{m,N} + \alpha_{m,N} - 1}{2} \right]^k
\] \hspace{1cm} (4.29)

\[
B_{k,N\rightarrow N}^S = -4c_N^2 \sum_{m=1}^{M/2} w_m \mu_m \left[ \frac{2\kappa_{m,N} + \alpha_{m,N} - 1}{2} \right]^{k-1} \left[ \frac{2\kappa_{m,K} + \alpha_{m,K} - 1}{2} \right]^k
\] \hspace{1cm} (4.30)

\[k^\text{th}\] off-diagonal elements with \(k > 1\) and \(k\) odd:

\[
B_{k,K\rightarrow N}^S = -4c_K c_N \sum_{m=1}^{M/2} w_m \mu_m \left[ \frac{2\kappa_{m,K} + \alpha_{m,K} - 1}{2} \right]^{k-1} \left[ \frac{2\kappa_{m,N} + \alpha_{m,N} - 1}{2} \right]^k
\] \hspace{1cm} (4.31)

The expression for the diagonal elements in Eq. (4.27) is immediately derived from Eq. (4.19) switching from the cell index \(j\) to the material index \(l\) for a cell. The expression in Eq. (4.29) is derived in a straightforward fashion from Eq. (4.20), or the equivalent Eq. (4.21), observing that an odd number \((k-1)\) of cells is interposed between two K cells, and of these \((k/2-1)\) are K cells while \((k/2)\) are N cells. The expression in Eq. (4.30) is the equivalent of Eq. (4.29) with switched K and N indices. Similarly, the expression in Eq. (4.31) is obtained from Eq. (4.20) noting that an even number \((k-1)\) of cells is interposed between a K cell and an N cell. Half of these are K cells while the other half is made of N cells.
The elements of matrix $B^s$ are functions of the dimensionless scaling parameter $\Delta$ in view of the dependence of both $\kappa_{m,l}$ and $\alpha_{m,l}$ on the cell width $\Delta x_i$. The different dependence on $\Delta$ characteristic of a K cell and of an N cell can be more conveniently exposed by introducing the following $\Delta$–independent quantities:

$$\epsilon_{m,l} = \frac{2|\mu_m|}{\sigma_l \delta_l}, \quad l = K, N \quad (4.32)$$

The dependence on $\Delta$ of the reciprocal of the optical thickness for a K cell is obtained by using Eq. (4.32) in Eq. (4.25), for $l = K$, and recalling that $\Delta x_K = \delta_K \Delta$:

$$\kappa_{m,K} = \frac{\epsilon_{m,K}}{2} \frac{1}{\Delta} \quad (4.33)$$

Repeating the same reasoning for $l = N$ and recalling that $\Delta x_N = \delta_N / \Delta$, the expression pertaining to an N cell is also obtained:

$$\kappa_{m,N} = \frac{\epsilon_{m,N}}{2} \Delta \quad (4.34)$$

Substitution of Eqs. (4.32) and (4.33) into Eq. (4.26), for $l = K$, produces the following expression for the AHOT-N0 spatial weights of a thick cell as a function of the scaling parameter $\Delta$:

$$\alpha_{m,K} = \coth \left( \frac{\Delta}{\epsilon_{m,K}} \right) - \frac{\epsilon_{m,K}}{\Delta} \quad (4.35)$$

Similarly, substitution of Eqs. (4.32) and (4.34) into Eq. (4.26), for $l = N$, results in the following expression for the AHOT-N0 spatial weights of a thin cell as a function of the scaling parameter $\Delta$:
\[ \alpha_{m,N} = \coth \left( \frac{1}{\epsilon_{m,N} \Delta} \right) - \epsilon_{m,N} \Delta \]  

(4.36)

Finally, substitution of Eqs. (4.33) through (4.36) into Eqs. (4.27) through (4.31) produces the desired explicit expressions for the elements of matrix \( B^S \) as functions of the scaling parameter \( \Delta \).

**Diagonal elements:**

\[ B_{d,K}^S = (c_K \sigma_K \delta_K \Delta) - (c_K^2 \sigma_K \delta_K \Delta) \sum_{m=1}^{M} W_m \left( 1 + \coth \left( \frac{\Delta}{\epsilon_{m,K} \Delta} \right) - \frac{\epsilon_{m,K}}{\Delta} \right) \]  

(4.37)

\[ B_{d,N}^S = \left( c_N \sigma_N \delta_N \frac{1}{\Delta} \right) - \left( c_N^2 \sigma_N \delta_N \frac{1}{\Delta} \right) \sum_{m=1}^{M} W_m \left( 1 + \coth \left( \frac{1}{\epsilon_{m,N} \Delta} \right) - \frac{\epsilon_{m,N} \Delta}{\Delta} \right) \]  

(4.38)

**First off-diagonal elements:**

\[ B_{1,K \leftrightarrow N}^S = -c_K c_N \sum_{m=1}^{M/2} W_m \left| \mu_m \right|^{2} \left[ 1 + \coth \left( \frac{\Delta}{\epsilon_{m,K} \Delta} \right) \right] \]  

\[ = \left[ 1 + \coth \left( \frac{1}{\epsilon_{m,N} \Delta} \right) \right] \]  

(4.39)

**k\textsuperscript{th} off-diagonal elements with k ≥ 2 and k even:**

\[ B_{k,K \leftrightarrow N}^S = -4c_K^2 \sum_{m=1}^{M/2} W_m \left| \mu_m \right|^{2} \left[ \coth \left( \frac{\Delta}{\epsilon_{m,K} \Delta} \right) - 1 \right] \left[ 1 + \coth \left( \frac{1}{\epsilon_{m,N} \Delta} \right) \right] \]  

(4.40)
$B_{k,N \to N}^S = -4c_N^2 \sum_{m=1}^{M/2} w_m |\mu_m| \left[ \frac{1}{1 + \coth \left( \frac{1}{\epsilon_{m,N}} \Delta \right)} \right]^{k-1} \left\{ \begin{array}{c} \coth \left( \frac{1}{\epsilon_{m,N}} \Delta \right) - 1 \nonumber \\ \coth \left( \frac{\Delta}{\epsilon_{m,N}} \right) - 1 \end{array} \right\}^{k/2} \right] \tag{4.41}$

$k^{th}$ off-diagonal elements with $k > 2$ and $k$ odd:

$$B_{k,K \to N}^S = -4c_K c_N \sum_{m=1}^{M/2} w_m |\mu_m| \left[ \frac{1}{1 + \coth \left( \frac{1}{\epsilon_{m,K}} \Delta \right)} \right]^{k-1} \left\{ \begin{array}{c} \coth \left( \frac{\Delta}{\epsilon_{m,K}} \right) - 1 \nonumber \\ \coth \left( \frac{1}{\epsilon_{m,N}} \Delta \right) - 1 \end{array} \right\}^{k/2} \right] \tag{4.42}$$

Conducting an asymptotic analysis on the $B^S$ matrix elements for a periodic heterogeneous slab yields the following asymptotic behavior of the symmetric matrix $B^S$ elements in the limit in which the thick cells become thicker while the thin cells become thinner $(\Delta \to \infty)$.

$$B_{d,K}^S = (c_K \sigma_K \delta_K) \Delta + c_K^2 \left( \sum_{m=1}^{M/2} w_m |\mu_m| \right) + O \left( e^{- \sigma_K \delta_K \Delta/|\mu_{max}|} \right) \tag{4.43}$$

$$B_{d,N}^S = (c_N \sigma_N \delta_N) \frac{1}{\Delta} + O \left( \frac{1}{\Delta^2} \right) \tag{4.44}$$

$$B_{d,K \to N}^S = -\frac{c_K}{2} (c_N \sigma_N \delta_N) \frac{1}{\Delta} + O \left( \frac{1}{\Delta^2} \right) \tag{4.45}$$
\[
B_{2,k\leftrightarrow k}^S = -c_k^2 \left( \sum_{m=1}^{M/2} w_m \left| \mu_m \right| \right) + O\left( \frac{1}{\Delta} \right),
\]
(4.46)

\[
B_{k,k\leftrightarrow k}^S = -c_k^2 w_{\text{max}} \left| \mu_{\text{max}} \right| e^{-(k-2)\sigma_k \delta_k \Delta/2|\mu_{\text{max}}|} + O\left( \frac{e^{-(k-2)\sigma_k \delta_k \Delta/2|\mu_{\text{max}}|}}{\Delta} \right),
\]
(4.47)

\[k > 2 \text{ even}\]

\[
B_{k,N\leftrightarrow N}^S = -\left( c_N \sigma_N \delta_N \right)^2 \frac{w_{\text{max}} \left| \mu_{\text{max}} \right|}{\left( \frac{\mu_{\text{max}}}{\Delta} \right)^2} + O\left( \frac{e^{-k\sigma_k \delta_k \Delta/2|\mu_{\text{max}}|}}{\Delta^3} \right),
\]
(4.48)

\[k \geq 2 \text{ even}\]

\[
B_{k,K\leftrightarrow N}^S = -c_k \left( c_N \sigma_N \delta_N \right) w_{\text{max}} \frac{e^{-(k-1)\sigma_k \delta_k \Delta/2|\mu_{\text{max}}|}}{\Delta} + O\left( \frac{e^{-(k-1)\sigma_k \delta_k \Delta/2|\mu_{\text{max}}|}}{\Delta^2} \right),
\]
(4.49)

\[k > 2 \text{ odd}\]

where \(\mu_{\text{max}}\) and \(w_{\text{max}}\) were introduced in Eq. (3.102).

The result contained in Eq. (4.46) clearly points to the fact that, in the asymptotic limit considered, \(B^S\) acquires a pentadiagonal dominant structure. This behavior is due to the matrix elements on the second off-diagonal that couple the cell-averaged scalar fluxes in two thick cells separated by a single thin cell. These elements are finite to leading order. In contrast, other elements on the second off-diagonal that couple the cell-averaged scalar fluxes in two thin cells still vanish rapidly at an exponential rate, as indicated by Eq. (4.48) for \(k = 2\). This feature is not a consequence of the symmetrization procedure.
introduced in Eq. (4.1). In fact, it can be shown that the original \( B \) matrix approaches an analogous pentadiagonal structure in the same limit as \( \Delta \to \infty \).

As done in the previous chapter for the homogeneous case, the asymptotic results are first derived in Sec. 4.3.1. A verification that the results from the numerical implementation of the symmetrized \( B^s \) matrix are in line with the ones obtained analytically from the asymptotic analysis has also been successfully completed. The results of the numerical verification are presented in Sec. 4.3.2.

### 4.3.1 Derivation of the Asymptotic Results for the Elements of Matrix \( B^s \)

The derivation of the asymptotic results contained in Eqs. (4.43) through (4.49) is conducted using as a starting point the expressions for the elements of matrix \( B^s \) reported in Eqs. (4.37) through (4.42). The derivation is carried out for each type of matrix element separately and makes use of the techniques introduced in Ch. 3 to treat the thick cell limit and the thin cell limit for the \( B \) matrix elements, in Sec. 3.4.2 and in Sec. 3.4.3, respectively.

**Asymptotic analysis of the diagonal elements pertaining to a thick cell**

First the hyperbolic cotangents that appear in the numerator and denominator of Eq. (4.37) are written explicitly in terms of only negative exponentials. Performing the due simplifications and recalling that the quadrature weights satisfy the normalization condition in Eq. (3.2), the following expression is obtained:
\[ B_{iK}^S = (c_K \sigma_K \delta_K)(1 - c_K) \Delta + \left( c_K^2 \sigma_K \delta_K \right) \sum_{m=1}^{M} w_m \frac{\epsilon_{m,K}}{2} \left( 1 - e^{-2\Delta/\epsilon_{m,K}} \right) \]  \hspace{1cm} (4.50) \]

It is then convenient to write \( \epsilon_{m,K} \) explicitly in Eq. (4.50), using Eq. (4.32) for \( l = K \). Simplifying and rearranging terms:

\[ B_{iK}^S = (c_K \sigma_K \delta_K)(1 - c_K) \Delta + c_K^2 \left( \sum_{m=1}^{M} w_m |\mu_m| \right) - c_K^2 \left( \sum_{m=1}^{M} w_m |\mu_m| e^{- \sigma_K \delta_K \Delta/|\mu_{max}|} \right) \]  \hspace{1cm} (4.51) \]

Similar to what was done for the diagonal elements of matrix \( B \) in the thick cell limit, see Eq. (3.128), the asymptotic behavior of the diagonal elements \( B_{iK}^S \) as \( \Delta \rightarrow \infty \) is investigated by considering the following limit:

\[ \lim_{\Delta \rightarrow \infty} \left\{ B_{iK}^S - (c_K \sigma_K \delta_K)(1 - c_K) \Delta - c_K^2 \left( \sum_{m=1}^{M} w_m |\mu_m| \right) e^{\sigma_K \delta_K \Delta/|\mu_{max}|} \right\} \]  \hspace{1cm} (4.52) \]

Substitution of Eq. (4.51) into Eq. (4.52) leads to the following equation:

\[ \lim_{\Delta \rightarrow \infty} \left\{ B_{iK}^S - (c_K \sigma_K \delta_K)(1 - c_K) \Delta - c_K^2 \left( \sum_{m=1}^{M} w_m |\mu_m| \right) e^{\sigma_K \delta_K \Delta/|\mu_{max}|} \right\} = \]  \hspace{1cm} (4.53) \]

\[ = \lim_{\Delta \rightarrow \infty} \left\{ -c_K^2 \left( \sum_{m=1}^{M} w_m |\mu_m| e^{- \sigma_K \delta_K \Delta/(|\mu_{max}|-1)} \right) \right\} \]

Solving Eq. (4.53) for \( B_{iK}^S \) in the limit and using the result contained in Eq. (3.114), that derives from the ordering relations existing between the angles in the quadrature, confirms the expression for the diagonal elements asymptotic behavior reported in Eq. (4.43).
Asymptotic analysis of the diagonal elements pertaining to a thin cell

First the hyperbolic cotangents that appear in the numerator and denominator of Eq. (4.38) are written explicitly in terms of only negative exponentials. Performing the due simplifications and recalling that the quadrature weights satisfy the normalization condition in Eq. (3.2), the following expression is obtained:

\[ B_{iN}^s = (c_N \sigma_N \delta_N)(1-c_N) \frac{1}{\Delta} + (c_N^2 \sigma_N \delta_N) \sum_{m=1}^{M} \frac{w_{m,n}}{2} \left( 1 - e^{-2/\epsilon_{m,n} \Delta} \right) \]  (4.54)

In the limit as \( \Delta \to \infty \), which is a thin cell limit for an \( N \) cell, the exponential term appearing on the right hand side of Eq. (4.54) may be conveniently approximated by its Taylor series expansion truncated at the second order term:

\[ e^{-2/\epsilon_{m,n} \Delta} = 1 - \frac{2}{\epsilon_{m,n} \Delta} + \frac{1}{2} \left( \frac{2}{\epsilon_{m,n} \Delta} \right)^2 + O \left( \frac{1}{\Delta^3} \right) \]  (4.55)

Substituting this expansion truncated to second order into Eq. (4.54) and performing some elementary simplifications produces the following result:

\[ B_{iN}^s = (c_N \sigma_N \delta_N) \frac{1}{\Delta} - (c_N^2 \sigma_N \delta_N) \frac{1}{\Delta} - \sum_{m=1}^{M} \frac{w_{m,n}}{\epsilon_{m,n} \Delta} \frac{1}{\Delta^2} + O \left( \frac{1}{\Delta^3} \right) \]  (4.56)

Further simplification of the leading order terms proves that, to leading order, the expression for the diagonal elements \( B_{iN}^s \) asymptotic behavior is indeed given by Eq. (4.44).

Asymptotic analysis of the first off-diagonal elements

First the hyperbolic cotangents that appear in Eq. (4.39) are written explicitly in terms of only negative exponentials. Performing the usual simplifications:
\[ B_{1,K \leftrightarrow N}^{S} = -c_K c_N \sum_{m=1}^{M/2} w_m \mu_m \left( 1 - e^{-2\Delta/\epsilon_{m,K}} \right) \left( 1 - e^{-2/\epsilon_{m,N}\Delta} \right) \]  \hspace{1cm} (4.57)

In the limit as \( \Delta \to \infty \) the exponentials in the first parenthesis in Eq. (4.57) contribute infinitesimal terms that are higher order than the other contributions in the expression for \( B_{1,K \leftrightarrow N}^{S} \). In the same limit, the exponentials in the second parenthesis can be Taylor expanded in \( 1/\Delta \), truncating the expansion at the first order term. Substitution of the Taylor expansion truncated to first order into Eq. (4.57) produces the following expression:

\[ B_{1,K \leftrightarrow N}^{S} = -c_K c_N \sum_{m=1}^{M/2} w_m \mu_m \left[ 1 - 1 + \frac{2}{\epsilon_{m,N}\Delta} + O\left( \frac{1}{\Delta^2} \right) \right] \]  \hspace{1cm} (4.58)

Use of Eq. (4.32), for \( l = N \), into Eq. (4.58) leads to the equivalent result:

\[ B_{1,K \leftrightarrow N}^{S} = -c_K c_N \sigma_N \delta_N \left( \sum_{m=1}^{M/2} w_m \right) \frac{1}{\Delta} + O\left( \frac{1}{\Delta^2} \right) \]  \hspace{1cm} (4.59)

Finally, the equivalence of Eq. (4.59) with the asymptotic expression in Eq. (4.45) is a consequence of the normalization condition for the quadrature weights in Eq. (3.2).

**Asymptotic analysis of the \( k^{th} \) off-diagonal elements coupling two thick cells**

First the hyperbolic cotangents that appear in Eq. (4.40) are written explicitly in terms of only negative exponentials. Performing the usual simplifications and collecting terms, the following expression is obtained for \( k \geq 2 \) even:

\[ B_{k,K \leftrightarrow K}^{S} = -c_K c_K \sum_{m=1}^{M/2} w_m \mu_m \left( 1 - e^{-2\Delta/\epsilon_{m,K}} \right)^2 e^{-k/\epsilon_{m,N}\Delta} e^{-(k-2)/\epsilon_{m,K}} \]  \hspace{1cm} (4.60)
As evident from the latter expression, the asymptotic behavior of $B^S_{k,K \to K}$ is different for the cases $k = 2$ and $k > 2$. Therefore, the two cases will be treated separately in the following.

For the case $k = 2$, the expression in Eq. (4.60) reduces to:

$$B^S_{2,K \to K} = -c_2^2 \sum_{m=1}^{M/2} w_m \mu_m \left(1 - e^{-2\Delta/\epsilon_{m,K}}\right)^2 e^{-2/\epsilon_{m,N\Delta}}$$  \hspace{1cm} (4.61)

In the limit as $\Delta \to \infty$ the exponentials in the parenthesis in Eq. (4.61) contribute infinitesimal terms that are higher order than the other contributions in the expression for $B^S_{2,K \to K}$. In the same limit, the exponentials outside the parenthesis can be Taylor expanded, truncating the expansion at the first order term. Substitution of the Taylor expansion truncated to first order into Eq. (4.61) produces:

$$B^S_{2,K \to K} = -c_2^2 \sum_{m=1}^{M/2} w_m \mu_m \left[1 - \frac{2}{\epsilon_{m,N\Delta}} + O\left(\frac{1}{\Delta^2}\right)\right]$$  \hspace{1cm} (4.62)

The latter result confirms that, to leading order, the expression for $B^S_{2,K \to K}$ is that given in Eq. (4.46).

For the case $k > 2$, the asymptotic behavior of the elements $B^S_{k,K \to K}$ as $\Delta \to \infty$ is investigated by considering the following limit:

$$\lim_{\Delta \to \infty} \left\{B^S_{k,K \to K} e^{(k-2)\Delta/\epsilon_{max,K}}\right\} =$$

$$= \lim_{\Delta \to \infty} \left\{-c_2^2 \sum_{m=1}^{M/2} w_m \mu_m \left(1 - e^{-2\Delta/\epsilon_{m,K}}\right)^2 e^{-k/\epsilon_{m,N\Delta}} e^{-\left(k-2\right)\Delta(1/\epsilon_{m,K} - 1/\epsilon_{max,K})}\right\}$$  \hspace{1cm} (4.63)
where $\epsilon_{m,K}$ represents $\epsilon_{m,K}^{\max}$ evaluated for the discrete ordinate with cosine $\mu_{m,K}$, previously introduced in Eq. (3.102). By virtue of the result contained in Eq. (3.114), the limit equation in Eq. (4.63) reduces to:

$$\lim_{\Delta \to \infty} \left\{ B_{k,K+K}^{S} e^{(k-2)\Delta/\epsilon_{m,K}^{\max}} \right\} = \lim_{\Delta \to \infty} \left\{ -c_{k}^{2} w_{m} |\mu_{m}^{\max}| e^{-k/\epsilon_{m,N}^{\max}} \right\}$$  \hspace{1cm} (4.64)

The asymptotic behavior of $B_{k,K+K}^{S}$ is then determined by Taylor expanding the exponentials on the right hand side of Eq. (4.64), truncating the expansion at the first order term, and by solving the equation for $B_{k,K+K}^{S}$ in the limit as $\Delta \to \infty$. The following result is obtained:

$$B_{k,K+K}^{S} = -c_{k}^{2} w_{m} |\mu_{m}^{\max}| \left( 1 - \frac{k}{\epsilon_{m,N}^{\max}} \frac{1}{\Delta} + O \left( \frac{1}{\Delta^{2}} \right) \right) e^{-(k-2)\Delta/\epsilon_{m,K}^{\max}}$$  \hspace{1cm} (4.65)

When the explicit expressions for $\epsilon_{m,N}^{\max}$ and $\epsilon_{m,K}^{\max}$ are substituted in Eq. (4.65), it is confirmed that, to leading order, the expression for $B_{k,K+K}^{S}$ is that given in Eq. (4.47).

**Asymptotic analysis of the $k^{\text{th}}$ off-diagonal elements coupling two thin cells**

First the hyperbolic cotangents that appear in Eq. (4.41) are written explicitly in terms of only negative exponentials. Performing the usual simplifications and collecting terms, the following expression is obtained for $k \geq 2$ even:

$$B_{k,N+K}^{S} = -c_{N}^{2} \sum_{m=1}^{M/2} w_{m} |\mu_{m}| \left( 1 - e^{-2/\epsilon_{m,N}^{\max}} \right)^{2} e^{(k-2)/\epsilon_{m,N}^{\max}} e^{-k/\epsilon_{m,K}^{\max}}$$  \hspace{1cm} (4.66)

It is convenient to study the asymptotic behavior of the elements $B_{k,N+K}^{S}$, as $\Delta \to \infty$, by forming the following limit:
\[
\lim_{\Delta \to \infty} \left\{ B_{k,N}^{s} e^{\frac{k \Delta}{\epsilon_{\text{max},K}}} \right\} = \\
= \lim_{\Delta \to \infty} \left\{ -c_{N}^{2} \left( \sum_{m=1}^{M/2} w_{m} \mu_{m} \right) \left( 1 - e^{-\frac{2}{\epsilon_{m,N} \Delta}} \right)^{2} e^{-\frac{(k-2) \epsilon_{m,N} \Delta}{\epsilon_{\text{max},N} \Delta}} e^{-k \Delta (1/\epsilon_{m,K} - 1/\epsilon_{\text{max},K})} \right\}
\] (4.67)

By virtue of the result contained in Eq. (3.114), the limit equation in Eq. (4.67) reduces to:

\[
\lim_{\Delta \to \infty} \left\{ B_{k,N}^{s} e^{\frac{k \Delta}{\epsilon_{\text{max},K}}} \right\} = \\
= \lim_{\Delta \to \infty} \left\{ -c_{N}^{2} w_{\text{max}} \mu_{\text{max}} \left( 1 - e^{-\frac{2}{\epsilon_{\text{max},N} \Delta}} \right)^{2} e^{-\frac{(k-2) \epsilon_{\text{max},N} \Delta}{\epsilon_{\text{max},N} \Delta}} \right\}
\] (4.68)

The asymptotic behavior of \( B_{k,N}^{s} \) is then determined by Taylor expanding the exponentials on the right hand side of Eq. (4.68), truncating the expansion at the first order term, and by solving the equation for \( B_{k,N}^{s} \) in the limit as \( \Delta \to \infty \). The following result is obtained:

\[
B_{k,N}^{s} = -c_{N}^{2} w_{\text{max}} \mu_{\text{max}} \left( \frac{2}{\epsilon_{\text{max},N} \Delta} + O\left( \frac{1}{\Delta^{2}} \right) \right)^{2} \left( 1 - \frac{(k-2)}{\epsilon_{\text{max},N} \Delta} + O\left( \frac{1}{\Delta^{2}} \right) \right) e^{-\frac{k \Delta}{\epsilon_{\text{max},K}}} \] (4.69)

When the explicit expressions for \( \epsilon_{\text{max},N} \) and \( \epsilon_{\text{max},K} \) are substituted in Eq. (4.69), it is confirmed that, to leading order, the expression for \( B_{k,N}^{s} \) is that given in Eq. (4.48).

It is noted, as evident from Eq. (4.69), that for these matrix elements the case \( k = 2 \) does not represent, to leading order, a special case to be dealt with separately. Therefore, the expression for \( k = 2 \) is also contained in Eq. (4.48) and has an exponential behavior.
Asymptotic analysis of the \( k \)th off-diagonal elements coupling thick and thin cells

First the hyperbolic cotangents that appear in Eq. (4.42) are written explicitly in terms of only negative exponentials. Performing the usual simplifications and collecting terms, the following expression is obtained for \( k > 2 \) odd:

\[
B^S_{k, K+N} = -c_K c_N \sum_{m=1}^{M/2} W_m |\mu_m| \cdot \\
\left(1 - e^{-2\Delta/\epsilon_{m,K}}\right)\left(1 - e^{-2/\epsilon_{m,N}\Delta}\right) e^{-(k-1)/\epsilon_{m,N}\Delta - (k-1)/\epsilon_{m,K}}
\]

(4.70)

It is convenient to study the asymptotic behavior of the elements \( B^S_{k, K+N} \), as \( \Delta \to \infty \), by forming the following limit:

\[
\lim_{\Delta \to \infty} \left\{ B^S_{k, K+N} e^{(k-1)/\epsilon_{max,K}} \right\} = \lim_{\Delta \to \infty} \left\{ -c_K c_N \sum_{m=1}^{M/2} W_m |\mu_m| \cdot \\
\left(1 - e^{-2\Delta/\epsilon_{m,K}}\right)\left(1 - e^{-2/\epsilon_{m,N}\Delta}\right) e^{-(k-1)/\epsilon_{m,N}\Delta - (k-1)/\epsilon_{max,K}} \right\}
\]

(4.71)

By virtue of the result contained in Eq. (3.114), the limit equation in Eq. (4.71) reduces to:

\[
\lim_{\Delta \to \infty} \left\{ B^S_{k, K+N} e^{(k-1)/\epsilon_{max,K}} \right\} = \\
\lim_{\Delta \to \infty} \left\{ -c_K c_N W_{max} |\mu_{max}| \left(1 - e^{-2/\epsilon_{max,N}\Delta}\right) e^{-(k-1)/\epsilon_{max,N}\Delta} \right\}
\]

(4.72)

The asymptotic behavior of \( B^S_{k, K+N} \) is then determined by Taylor expanding the exponentials on the right hand side of Eq. (4.72), truncating the expansion at the first order term, and by solving the equation for \( B^S_{k, N+N} \) in the limit as \( \Delta \to \infty \). The following result is obtained:
\[ B^{S}_{k,K\rightarrow N} = -c_{K}c_{N}w_{\max}\mid\mu_{\max}\mid \]

\[
\left(\frac{2}{\varepsilon_{\max,N}} - \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right)\right) \left(1 - \frac{(k-1)}{\varepsilon_{\max,N}}\frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right)\right) e^{-\frac{(k-1)\Delta}{\varepsilon_{\max,K}}} \quad (4.73)
\]

When the explicit expressions for \( \varepsilon_{\max,N} \) and \( \varepsilon_{\max,K} \) are substituted in Eq. (4.73), it is confirmed that, to leading order, the expression for \( B^{S}_{k,K\rightarrow N} \) is that given in Eq. (4.49).

### 4.3.2 Numerical Verification

With reference to a slab subdivided into six computational cells in the usual order presented in Fig. 4.1, the results of the comparison between the analytic and the numeric results are reported in Figs. 4.3 and 4.4. The comparison has been performed by plotting, as a function of the parameter \( \Delta \), the ratio of the computed value for a certain matrix element and the numerical evaluation of the leading order of the expression obtained analytically for the same element in the asymptotic limit.

As expected, the ratio tends to a unit value as the parameter \( \Delta \) is progressively increased. An additional comment is worthwhile for the curves in Fig. 4.4. The non-fully-developed convergence to the unit horizontal asymptote is due to a numerical precision issue that arises in the evaluation of the elements on the second off-diagonal coupling two thin cells and beyond. As evident from the expressions of the off-diagonal elements of matrix \( \mathbf{B}^{S} \) in Eq. (4.20), these matrix elements happen to result from the multiplication by at least a factor \( q_{m,i} \), see Eq. (3.28), that is evaluated for a cell \( i \) which is an optically
thick computational cell. These same factors are in fact also present in the original expressions for matrix $\mathbf{B}$.

The term in the numerator of $q_{m,i}$ happens to become zero in finite arithmetic precision as soon as a certain threshold is reached for the value of the parameter $\Delta$. This threshold is in turn dependent on the choice for the arithmetic precision as was confirmed obtaining the same plots in the usual double precision employed in the calculations and in quadruple precision. The plots hereby reported result from calculations performed in quadruple precision. The fully developed asymptotic behavior would be obtained if higher arithmetic precision were employed.

![Graph](image)

*Fig. 4.3: Asymptotic behavior of matrix $\mathbf{B}^S$ elements.*
The results of the asymptotic analysis for periodically heterogeneous slabs confirm the physical intuition that the coupling of the cell-averaged scalar fluxes in two optically thick computational cells, separated by an interposed optically thin cell, should indeed be strong. In fact, a pentadiagonally dominated matrix structure is obtained in the limit in which the cell optical properties are pushed apart.

![Graph showing asymptotic behavior of matrix B elements](image)

*Fig. 4.4: Asymptotic behavior of matrix B^S elements (continued).*

As it will be shown in Sec. 4.4, this matrix structure can be used to understand some peculiar asymptotic properties possessed by the cell-averaged scalar fluxes of a periodically heterogeneous slab in the limit as $\Delta \to \infty$. At the same time, as pointed out in Ch. 1, this matrix structure appears puzzling in view of the efficient behavior of iterative methods based on low-order diffusive-like operators characterized by a
tridiagonal matrix structure, even in the presence of sharp material discontinuities. This apparent contradiction will be reconciled observing that, as already pointed out for Eq. (4.15), any algebraic manipulation of the system of equations in Eq. (1.27) that preserves the original exact cell-averaged scalar fluxes, would lead to a perfectly legitimate and equivalent matrix representation of the discrete integral transport operator. If an algebraic transformation exists that leads to a matrix representation characterized asymptotically by a tridiagonally dominant structure, then the original thesis would still be true.

The periodic nature of the structure and the fact that the elements on the second off-diagonal coupling two thin cells’ fluxes vanish exponentially as $\Delta \to \infty$, suggest the possibility of eliminating the elements on the second off-diagonal stripe coupling two thick cells’ fluxes by means of an exact algebraic manipulation. The investigation of this idea has led to the results presented in Secs. 4.5 and 4.6. These results confirm that an equivalent form indeed exists of the integral transport matrix characterized in the asymptotic limit as $\Delta \to \infty$ by a tridiagonally dominant structure.

4.4 Asymptotic Properties of the Cell-Averaged Scalar Fluxes

The expressions for the elements of matrices $\bar{A}$ and $B^s$ have been implemented in a computer code that builds and stores the matrices and directly solves Eq. (4.15). This code represents an evolution of the original code for the construction of matrices $A$ and $B$ and the direct solution of Eq. (1.27). As it was pointed out in Sec. 4.2, the systems of equations in Eq. (4.15) and in Eq. (1.27) are equivalent from an algebraic point of view.
Therefore, it is expected that the cell-averaged fluxes obtained from the numerical solution of the two systems of equations be equivalent to within the precision employed in the numeric computations. As it will be shown in the numerical results presented in Sec. 4.7, this expectation is indeed verified by the double precision computations implemented in the code.

In this section the emphasis is instead placed on the asymptotic properties possessed by the cell-averaged fluxes computed for periodically heterogeneous slabs with a uniform fixed source distribution, notably for the cases \( c_k = 1 \) and \( c_k < 1 \). These properties are at first illustrated referring to the numerical solutions obtained by solving two instances of the structure presented in Fig. 4.1, for the cases \( c_k = 1 \) and \( c_k = 0.5 \), respectively.

The first periodic slab is comprised of ten computational cells. It is assumed that \( \delta_k = \delta_N = 1 \), therefore \( \Delta x_k = \Delta \) while \( \Delta x_N = 1/\Delta \), and that \( \sigma_k = \sigma_N = 1 \). The scattering ratios are also assumed to be equal to each other and to have a unit value, \( c_k = c_N = 1 \), so that there is no absorption throughout the slab. To avoid the evaluation of cell-averaged scalar fluxes of the order of the scaling parameter \( \Delta \), the uniform fixed source in the computational cells is therefore scaled as \( 1/\Delta \). The cell-averaged fluxes obtained using the symmetric \( S_6 \) quadrature for increasing values of the scaling parameter \( \Delta \) are reported in Table 4.1.

A comparison of the cell-averaged scalar fluxes in Table 4.1 reveals the existence of two interesting features displayed by the solution in the asymptotic limit. First of all, the cell-averaged scalar fluxes pertaining to an internal thin cell are equal to the
arithmetic average of the cell-averaged fluxes in the two adjacent thick cells. Compare, for example, \( \tilde{\phi}_2 \) with the average of \( \tilde{\phi}_1 \) and \( \tilde{\phi}_3 \) for \( \Delta = 10^6 \). Finally, the cell-averaged flux pertaining to the last thin cell, at the right edge of the slab, becomes asymptotically equal to half the flux in the penultimate thick cell.

Table 4.1: Cell-averaged fluxes for a periodically heterogeneous slab with \( c_K = 1 \).

<table>
<thead>
<tr>
<th>( \Delta )</th>
<th>( \hat{\phi}_1 )</th>
<th>( \hat{\phi}_2 )</th>
<th>( \hat{\phi}_3 )</th>
<th>( \hat{\phi}_4 )</th>
<th>( \hat{\phi}_5 )</th>
<th>( \hat{\phi}_6 )</th>
<th>( \hat{\phi}_7 )</th>
<th>( \hat{\phi}_8 )</th>
<th>( \hat{\phi}_{10} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 10^0 )</td>
<td>15.90</td>
<td>26.07</td>
<td>33.49</td>
<td>38.41</td>
<td>40.87</td>
<td>40.87</td>
<td>38.41</td>
<td>33.49</td>
<td>26.07</td>
</tr>
<tr>
<td>( 10^1 )</td>
<td>9.93</td>
<td>13.38</td>
<td>16.59</td>
<td>17.87</td>
<td>18.92</td>
<td>18.03</td>
<td>16.92</td>
<td>13.86</td>
<td>10.58</td>
</tr>
<tr>
<td>( 10^2 )</td>
<td>9.81</td>
<td>12.80</td>
<td>15.77</td>
<td>16.78</td>
<td>17.77</td>
<td>16.79</td>
<td>15.80</td>
<td>12.85</td>
<td>9.88</td>
</tr>
<tr>
<td>( 10^4 )</td>
<td>9.81</td>
<td>12.75</td>
<td>15.69</td>
<td>16.67</td>
<td>17.65</td>
<td>16.67</td>
<td>15.69</td>
<td>12.75</td>
<td>9.81</td>
</tr>
<tr>
<td>( 10^6 )</td>
<td>9.80</td>
<td>12.75</td>
<td>15.69</td>
<td>16.67</td>
<td>17.65</td>
<td>16.67</td>
<td>15.69</td>
<td>12.75</td>
<td>9.80</td>
</tr>
</tbody>
</table>

The second periodic slab is also comprised of ten computational cells. The parameters are the same as for the previous case, except for the scattering ratio of the thick cells. In fact, in this case \( c_K = 0.5 \). Also, since the thick cells provide a significant absorption contribution, a unit uniform fixed source, independent of \( \Delta \) is assumed in the computational cells. The cell-averaged scalar fluxes obtained using the symmetric \( S_6 \) quadrature for increasing values of the scaling parameter \( \Delta \) are reported in Table 4.2.

Table 4.2: Cell-averaged fluxes for a periodically heterogeneous slab with \( c_K = 0.5 \).

<table>
<thead>
<tr>
<th>( \Delta )</th>
<th>( \hat{\phi}_1 )</th>
<th>( \hat{\phi}_2 )</th>
<th>( \hat{\phi}_3 )</th>
<th>( \hat{\phi}_4 )</th>
<th>( \hat{\phi}_5 )</th>
<th>( \hat{\phi}_6 )</th>
<th>( \hat{\phi}_7 )</th>
<th>( \hat{\phi}_8 )</th>
<th>( \hat{\phi}_{10} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 10^0 )</td>
<td>2.19</td>
<td>3.96</td>
<td>3.59</td>
<td>4.69</td>
<td>3.86</td>
<td>4.79</td>
<td>3.80</td>
<td>4.51</td>
<td>3.25</td>
</tr>
<tr>
<td>( 10^1 )</td>
<td>1.91</td>
<td>2.12</td>
<td>2.02</td>
<td>2.15</td>
<td>2.02</td>
<td>2.15</td>
<td>2.02</td>
<td>2.15</td>
<td>1.93</td>
</tr>
<tr>
<td>( 10^2 )</td>
<td>1.99</td>
<td>2.01</td>
<td>2.00</td>
<td>2.01</td>
<td>2.00</td>
<td>2.01</td>
<td>2.00</td>
<td>2.01</td>
<td>1.99</td>
</tr>
<tr>
<td>( 10^4 )</td>
<td>1.99</td>
<td>2.00</td>
<td>2.00</td>
<td>2.00</td>
<td>2.00</td>
<td>2.00</td>
<td>2.00</td>
<td>2.00</td>
<td>1.99</td>
</tr>
<tr>
<td>( 10^6 )</td>
<td>2.00</td>
<td>2.00</td>
<td>2.00</td>
<td>2.00</td>
<td>2.00</td>
<td>2.00</td>
<td>2.00</td>
<td>2.00</td>
<td>2.00</td>
</tr>
</tbody>
</table>
A comparison of the cell-averaged fluxes in Table 4.2 in the asymptotic limit indicates that, even for this case, the cell-averaged scalar fluxes pertaining to an internal thin cell are equal to the arithmetic average of the cell-averaged fluxes in the two adjacent thick cells. As a matter of fact, the equal values of the cell-averaged scalar fluxes pertaining to the thick computational cells can, as expected for a very thick cell, be interpreted as the ratio of the unit source in the cell divided by the absorption cross-section $\sigma_{a,k} = (1 - c_k)\sigma_k = 0.5$. In this case too, the cell-averaged flux pertaining to the last thin cell, at the right edge of the slab, appears asymptotically equal to half the flux in the penultimate thick cell.

The above results point to the fact that, as it may intuitively be expected, the solution for the slab is essentially driven by the optically thick cells that become more and more strongly coupled as the interposed thin cells are made thinner and thinner, by scaling the $\Delta$ parameter. In the remainder of this section it will be shown how the average property is intimately related to the asymptotic structures acquired by the $B^S$ and $\bar{A}$ matrices in the limit as $\Delta \to \infty$. More specifically, the asymptotic expressions for the elements of matrix $\bar{A}$ are presented in Sec. 4.4.1. The derivation of these results is similar to the derivation presented in Sec. 4.3.1 for the elements of matrix $B^S$ and will therefore be omitted, for brevity. Finally, Secs. 4.4.2 and 4.4.3 will contain a general derivation of the asymptotic properties of the cell-averaged scalar fluxes for the cases $c_k = 1$ and $c_k < 1$, respectively.
4.4.1 Asymptotic Results for the Elements of Matrix $\overline{A}$

The expressions for the matrix elements of matrix $\overline{A}$, pertaining to the periodically heterogeneous structure depicted in Fig. 4.1, are hereby reported in terms of the quantities introduced in Eqs. (4.25) and (4.26). The first off-diagonal elements are treated as a separate case in view of the results of the ensuing asymptotic analysis.

Diagonal elements:

$$\overline{A}_{l,l} = (c_l \Delta x_l) \sum_{m=1}^{M} w_m \frac{1 + \alpha_{m,l}}{1 + 2\kappa_{m,l} + \alpha_{m,l}}$$

First off-diagonal elements:

$$\overline{A}_{l,N \rightarrow K} = \frac{c_K}{\sigma_N} \sum_{m=1}^{M/2} w_m |\mu_m| \frac{2}{1 + 2\kappa_{m,K} + \alpha_{m,K} + 2\kappa_{m,N} + \alpha_{m,N}}$$

$$\overline{A}_{l,K \rightarrow N} = \frac{c_N}{\sigma_K} \sum_{m=1}^{M/2} w_m |\mu_m| \frac{2}{1 + 2\kappa_{m,K} + \alpha_{m,K} + 2\kappa_{m,N} + \alpha_{m,N}}$$

$k^{th}$ off-diagonal elements with $k > 1$ and $k$ even:

$$\overline{A}_{k,K \rightarrow K} = 4 \frac{c_K}{\sigma_K} \sum_{m=1}^{M/2} w_m |\mu_m| \left[ \frac{2\kappa_{m,K} + \alpha_{m,K} - 1}{1 + 2\kappa_{m,K} + \alpha_{m,K}} \right]^{k-1} \left[ \frac{2\kappa_{m,N} + \alpha_{m,N} - 1}{1 + 2\kappa_{m,N} + \alpha_{m,N}} \right]^{k}$$

$$\overline{A}_{k,N \rightarrow N} = 4 \frac{c_N}{\sigma_N} \sum_{m=1}^{M/2} w_m |\mu_m| \left[ \frac{2\kappa_{m,N} + \alpha_{m,N} - 1}{1 + 2\kappa_{m,N} + \alpha_{m,N}} \right]^{k-1} \left[ \frac{2\kappa_{m,K} + \alpha_{m,K} - 1}{1 + 2\kappa_{m,K} + \alpha_{m,K}} \right]^{k}$$
$k^{th}$ off-diagonal elements with $k > 1$ and $k$ odd:

$$
\overline{A}_{k,N\rightarrow K} = 4 \frac{c_K}{\sigma_N} \sum_{m=1}^{M/2} w_m |\mu_m| \left[ \frac{2\kappa_{m,K} + \alpha_{m,K} - 1}{2} \right]^{\frac{k-1}{2}} \left[ \frac{2\kappa_{m,N} + \alpha_{m,N} - 1}{2} \right]^{\frac{k-1}{2}} \left[ 1 + 2\kappa_{m,K} + \alpha_{m,K} \right]^{\frac{k+1}{2}} \left[ 1 + 2\kappa_{m,N} + \alpha_{m,N} \right]^{\frac{k+1}{2}} \tag{4.79}
$$

$$
\overline{A}_{k,K\rightarrow N} = 4 \frac{c_N}{\sigma_K} \sum_{m=1}^{M/2} w_m |\mu_m| \left[ \frac{2\kappa_{m,K} + \alpha_{m,K} - 1}{2} \right]^{\frac{k-1}{2}} \left[ \frac{2\kappa_{m,N} + \alpha_{m,N} - 1}{2} \right]^{\frac{k-1}{2}} \left[ 1 + 2\kappa_{m,K} + \alpha_{m,K} \right]^{\frac{k+1}{2}} \left[ 1 + 2\kappa_{m,N} + \alpha_{m,N} \right]^{\frac{k+1}{2}} \tag{4.80}
$$

Substitution of Eqs. (4.33) through (4.36) into Eqs. (4.74) through (4.80) produces the explicit expressions for the elements of matrix $\overline{A}$ as functions of the scaling parameter $\Delta$.

**Diagonal elements:**

$$
\overline{A}_{d,K} = (c_K \delta_K \Delta) \sum_{m=1}^{M} w_m \frac{1 + \coth \left( \frac{\Delta}{\epsilon_{m,K}} \right)}{1 + \coth \left( \frac{\Delta}{\epsilon_{m,K}} \right)} \tag{4.81}
$$

$$
\overline{A}_{d,N} = (c_N \delta_N \frac{1}{\Delta}) \sum_{m=1}^{M} w_m \frac{1 + \coth \left( \frac{1}{\epsilon_{m,N}} \frac{1}{\Delta} \right)}{1 + \coth \left( \frac{1}{\epsilon_{m,N}} \frac{1}{\Delta} \right)} \tag{4.82}
$$

**First off-diagonal elements:**

$$
\overline{A}_{l,N\rightarrow K} = \frac{c_K}{\sigma_N} \sum_{m=1}^{M/2} w_m |\mu_m| \left[ 1 + \coth \left( \frac{\Delta}{\epsilon_{m,K}} \right) \right]^{2} \left[ 1 + \coth \left( \frac{1}{\epsilon_{m,N}} \frac{1}{\Delta} \right) \right]^{2} \tag{4.83}
$$
\[ \overline{A}_{i,K \rightarrow N} = \frac{c_N}{\sigma_K} \sum_{m=1}^{M/2} W_m |\mu_m| \left[ \frac{2}{1 + \coth \left( \frac{\Delta}{\epsilon_{m,K}} \right)} \right] \left[ \frac{2}{1 + \coth \left( \frac{1}{\epsilon_{m,N}} \frac{1}{\Delta} \right)} \right] \] (4.84)

\[ \overline{A}_{k,K \leftrightarrow K} = \frac{4 c_K}{\sigma_K} \sum_{m=1}^{M/2} W_m |\mu_m| \left[ \frac{\coth \left( \frac{\Delta}{\epsilon_{m,K}} \right) - 1}{1 + \coth \left( \frac{\Delta}{\epsilon_{m,K}} \right)} \right] \left[ \frac{\coth \left( \frac{1}{\epsilon_{m,N}} \frac{1}{\Delta} \right) - 1}{1 + \coth \left( \frac{1}{\epsilon_{m,N}} \frac{1}{\Delta} \right)} \right] \] (4.85)

\[ \overline{A}_{k,N \rightarrow N} = \frac{4 c_N}{\sigma_N} \sum_{m=1}^{M/2} W_m |\mu_m| \left[ \frac{\coth \left( \frac{1}{\epsilon_{m,N}} \frac{1}{\Delta} \right) - 1}{1 + \coth \left( \frac{1}{\epsilon_{m,N}} \frac{1}{\Delta} \right)} \right] \left[ \frac{\coth \left( \frac{\Delta}{\epsilon_{m,K}} \right) - 1}{1 + \coth \left( \frac{\Delta}{\epsilon_{m,K}} \right)} \right] \] (4.86)

\[ \overline{A}_{k,N \rightarrow K} = \frac{4 c_K}{\sigma_N} \sum_{m=1}^{M/2} W_m |\mu_m| \left[ \frac{\coth \left( \frac{\Delta}{\epsilon_{m,K}} \right) - 1}{1 + \coth \left( \frac{\Delta}{\epsilon_{m,K}} \right)} \right] \left[ \frac{\coth \left( \frac{1}{\epsilon_{m,N}} \frac{1}{\Delta} \right) - 1}{1 + \coth \left( \frac{1}{\epsilon_{m,N}} \frac{1}{\Delta} \right)} \right] \] (4.87)
Conducting an asymptotic analysis for the $\mathbf{A}$ matrix elements for a periodic heterogeneous slab, yields the following asymptotic behavior of the matrix $\mathbf{A}$ elements in the limit in which the thick cells become thicker while the thin cells become thinner ($\Delta \to \infty$).

\[
\bar{A}_{d,K} = c_K \delta_K \Delta \frac{c_K}{\sigma_K} \left( \sum_{m=1}^{M/2} \left| \mu_m \right| \right) + O \left( e^{-\sigma_k \delta_k \Delta |\mu_{max}|} \right),
\]

(4.89)

\[
\bar{A}_{d,N} = c_N \sigma_N \left( \sum_{m=1}^{M/2} \left| \mu_m \right| \right) \frac{1}{\Delta^2} + O \left( \frac{1}{\Delta^3} \right),
\]

(4.90)

\[
\bar{A}_{1,N \to K} = \frac{1}{2} c_K \delta_N \frac{1}{\Delta} + O \left( \frac{1}{\Delta^2} \right),
\]

(4.91)

\[
\bar{A}_{1,K \to N} = \frac{1}{2} c_N \sigma_k \delta_N \frac{1}{\Delta} + O \left( \frac{1}{\Delta^2} \right),
\]

(4.92)

\[
\bar{A}_{2,K \to K} = \frac{c_K}{\sigma_N} \left( \sum_{m=1}^{M/2} \left| \mu_m \right| \right) + O \left( \frac{1}{\Delta} \right),
\]

(4.93)
The result contained in Eq. (4.93) indicates that, in the asymptotic limit considered, $\tilde{A}$ also acquires a pentadiagonal dominant structure. This behavior is due to the matrix elements on the second off-diagonal that couple the cell-averaged scalar fluxes in two thick cells separated by a single thin cell. These elements are finite to leading order. In contrast, other elements on the second off-diagonal that couple the cell-averaged scalar fluxes in two thin cells still vanish rapidly at an exponential rate, as indicated by Eq. (4.95) for $k = 2$.

The structure acquired to leading order by the $\tilde{A}$ matrix, in the asymptotic limit as $\Delta \to \infty$, is sketched in Fig. 4.5. All the elements that vanish exponentially, to leading
order, have been indicated as zeroes. The non-zero entries represent the leading order contributions to the $\tilde{A}$ matrix elements that occupy the corresponding positions in the matrix. Therefore, from Eqs. (4.89) through (4.93), it follows that:

\begin{equation}
\bar{k} = c_k \delta_k \Delta, \tag{4.98}
\end{equation}

\begin{equation}
\bar{n} = c_n \sigma_n \delta_n \alpha_i \frac{1}{\Delta^2}, \tag{4.99}
\end{equation}

\begin{equation}
\bar{f} = \frac{1}{2} c_k \delta_k \frac{1}{\Delta}, \tag{4.100}
\end{equation}

\begin{equation}
\bar{g} = \frac{1}{2} c_n \sigma_n \delta_n \frac{1}{\Delta}, \tag{4.101}
\end{equation}

\begin{equation}
\bar{s} = \frac{c_k}{\sigma_k} \beta_i, \tag{4.102}
\end{equation}

The quadrature-dependent constants $\alpha_i$ and $\beta_i$, introduced in Eqs. (4.99) and (4.102), respectively, have the following definitions:

\begin{equation}
\alpha_i = \left( \sum_{m=1}^{M/2} w_m |\mu_m| \right), \tag{4.103}
\end{equation}

\begin{equation}
\beta_i = \left( \sum_{m=1}^{M/2} w_m |\mu_m| \right) \tag{4.104}
\end{equation}
It is noted that $\bar{f}$ and $\bar{g}$ are not equal, therefore the pentadiagonal block of matrix $\tilde{A}$ is, in general, non-symmetric even in the asymptotic limit considered.

$$
\begin{bmatrix}
  k & \bar{f} & s & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 \\
  g & \bar{g} & \bar{g} & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 \\
  s & \bar{f} & k & \bar{f} & s & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & \bar{g} & \bar{p} & \bar{g} & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & \bar{s} & \bar{f} & k & \bar{f} & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 \\
  \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
  0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{bmatrix}
$$

*Fig. 4.5: Asymptotic structure of the $\tilde{A}$ matrix.*

### 4.4.2 Shuffling of the Cell-Averaged Scalar Fluxes for the Case $c_K = 1$

In order to study the asymptotic properties of the cell-averaged scalar fluxes in the asymptotic limit as $\Delta \to \infty$, it is convenient to consider an algebraic transformation of the system of equations in Eq. (4.15). The ordering of the $J$ equations in this system is
based on the natural ordering of the cell-averaged scalar fluxes in the periodic structure of Fig. 4.1. In this ordering, the odd computational cells are assumed to be thick while the even computational cells are assumed to be thin. The numerical evidence presented in Tables 4.1 and 4.2 suggests that, in the asymptotic limit, the cell-averaged scalar fluxes in the thin cells may be computed once the fluxes in the thick cells have been determined. In other words, the cell-averaged scalar fluxes in the thick cells appear to be the only independent variables. To investigate this conjecture, a transformation is introduced that changes the ordering of the equations so that the equations for the thick cells are indexed from 1 to \( J/2 \), while the equations for the thin cells are indexed from \((J/2+1)\) to \( J \). In other words, the cell-averaged scalar fluxes are reordered or “shuffled” according to the following transformation:

\[
\begin{pmatrix}
\phi_1 \\
\phi_2 \\
\phi_3 \\
\phi_4 \\
.. \\
.. \\
\phi_{J-1} \\
\phi_J
\end{pmatrix}
\rightarrow
\begin{pmatrix}
\phi_1 \\
\phi_2 \\
\phi_3 \\
\phi_4 \\
.. \\
.. \\
\phi_{J-1} \\
\phi_J
\end{pmatrix}
\]  

\[(4.105)\]

In the following, for brevity, the right hand side of Eq. (4.15) will be indicated as:

\[Q = \bar{A}q\]  

\[(4.106)\]

The components of the \( Q \) vector are shuffled consistently according to the transformation introduced for the cell-averaged scalar fluxes:
If the transformation is consistently applied to the elements of matrix $B^s$, leading to a transformed matrix $B'$, then the solution of the linear system:

$$B' \tilde{\phi}' = Q'$$

(4.108)

is perfectly equivalent to the original solution $\tilde{\phi}^\infty$ for the linear system in Eq. (4.15).

In view of the separation of the cell-averaged scalar fluxes pertaining to the thick cells from those pertaining to the thin cells obtained through the shuffling, it is convenient to define the following block vectors, each having $J/2$ components:

$$\tilde{\phi}_K = [\tilde{\phi}_1 \; \tilde{\phi}_3 \; \cdots \; \tilde{\phi}_{J-1}]^T$$

(4.109)

$$\tilde{\phi}_N = [\tilde{\phi}_2 \; \tilde{\phi}_4 \; \cdots \; \tilde{\phi}_J]^T$$

(4.110)

$$Q_K = [Q_1 \; Q_3 \; \cdots \; Q_{J-1}]^T$$

(4.111)

$$Q_N = [Q_2 \; Q_4 \; \cdots \; Q_J]^T$$

(4.112)
From Eqs. (4.105), (4.109) and (4.110), it follows that:

$$\tilde{\phi}' = \begin{pmatrix} \tilde{\phi}_K \\ \tilde{\phi}_N \end{pmatrix}$$  \hspace{1cm} (4.113)

Similarly, from Eqs. (4.107), (4.111) and (4.112), it follows that:

$$Q' = \begin{pmatrix} Q_K \\ Q_N \end{pmatrix}$$  \hspace{1cm} (4.114)

Matrix $B'$ can accordingly be written in block-matrix form:

$$B' = \begin{bmatrix} B_{KK} & B_{KN} \\ B_{NK} & B_{NN} \end{bmatrix},$$  \hspace{1cm} (4.115)

where each of the four blocks is a $(J/2 \times J/2)$ matrix.

Using Eqs. (4.113) through (4.115), the linear system in Eq. (4.108) is written as an equivalent system of two matrix equations in the unknown vectors $\tilde{\phi}_K$ and $\tilde{\phi}_N$:

$$\begin{cases} B_{KK}\tilde{\phi}_K + B_{KN}\tilde{\phi}_N = Q_K \\ B_{NK}\tilde{\phi}_K + B_{NN}\tilde{\phi}_N = Q_N \end{cases}$$  \hspace{1cm} (4.116)

The second equation in Eq. (4.116) can be used to relate $\tilde{\phi}_N$ to $\tilde{\phi}_K$:

$$\tilde{\phi}_N = (B_{NN})^{-1}Q_N - (B_{NN})^{-1}B_{NK}\tilde{\phi}_K$$  \hspace{1cm} (4.117)

Substituting Eq. (4.117) into the first equation in Eq. (4.116), the following equation in the unknown vector $\tilde{\phi}_K$ is obtained:

$$\begin{bmatrix} B_{KK} - B_{KN}(B_{NN})^{-1}B_{NK} \end{bmatrix}\tilde{\phi}_K = Q_K - B_{KN}(B_{NN})^{-1}Q_N$$  \hspace{1cm} (4.118)
For finite values of the $\Delta$ parameter, the block matrices in Eqs. (4.117) and (4.118) are dense matrices and Eq. (4.116) is a coupled system of equations in the unknown vectors $\tilde{\phi}_k$ and $\tilde{\phi}_N$. In the remainder of this section it will be shown, under the assumption of a uniform fixed source distribution $\mathbf{q}$ in Eq. (4.106), that in the asymptotic limit as $\Delta \to \infty$, it is possible to compute $\tilde{\phi}_k$ independently from $\tilde{\phi}_N$ (and $\mathbf{Q}_N$) using Eq. (4.118). Vector $\tilde{\phi}_N$ is then uniquely determined using Eq. (4.117). In order to derive these results, an asymptotic analysis is performed, to leading order, for the various terms appearing in Eqs. (4.117) and (4.118).

First, the source vectors $\mathbf{Q}_k$ and $\mathbf{Q}_N$ are considered. For the case $c_k = 1$, considered in this section, the uniform fixed source distribution vector $\mathbf{q}$ is scaled as $1/\Delta$:

$$q_i = 1/\Delta, \quad i = 1, \ldots, J$$  \hspace{1cm} (4.119)

Substituting Eq. (4.119) into Eq. (4.106) it follows that:

$$Q_i = \left(1/\Delta\right) \sum_{j=1}^{J} A_{i,j}, \quad i = 1, \ldots, J$$  \hspace{1cm} (4.120)

An inspection of the rows of matrix $\tilde{\mathbf{A}}$ pertaining to the thick cells, see Fig. 4.5, and the leading orders for $\overline{K}$, $\overline{F}$ and $\overline{S}$ in Eqs. (4.98), (4.100) and (4.102), respectively, produce the following asymptotic expressions for the components of vector $\mathbf{Q}_k$ for the case $c_k = 1$:

$$Q_{k,i} = \delta_k, \quad i = 1, \ldots, J/2$$  \hspace{1cm} (4.121)
The components of vector $\mathbf{Q}_N$ are therefore all equal, to leading order, and are $O(\Delta^0)$. An inspection of the rows of matrix $\mathbf{\bar{A}}$ pertaining to the thin cells, see Fig. 4.5, and the leading orders for $\bar{n}$ and $\bar{g}$ in Eqs. (4.99) and (4.101), respectively, produce the following asymptotic expressions for the components of vector $\mathbf{Q}_N$:

$$
\begin{align*}
Q_{N,i} & = c_N \frac{\sigma_N}{\sigma_k} \delta_N \frac{1}{\Delta^2}, \quad i = 1, \ldots, \left\lfloor \frac{J}{2} \right\rfloor - 1 \\
Q_{N,J/2} & = \frac{1}{2} c_N \frac{\sigma_N}{\sigma_k} \delta_N \frac{1}{\Delta^2}
\end{align*}
$$

(4.122)

The components of vector $\mathbf{Q}_N$ are all $O(\Delta^{-2})$. The coefficient multiplying $\Delta^{-2}$ in the $J/2$ component is half the coefficient multiplying $\Delta^{-2}$ in all the other components because only one $\bar{g}$ element appears in the equation for the last thin cell, as evident from Fig. 4.5.

In order to determine asymptotic expressions for the blocks of matrix $\mathbf{B}'$, first it is useful to sketch the structure acquired to leading order by matrix $\mathbf{B}'$, in the asymptotic limit as $\Delta \rightarrow \infty$, similar to what was done for $\mathbf{\bar{A}}$ in Fig. 4.5. The sketch is presented in Fig. 4.6 where as before the elements that vanish exponentially have been indicated as zeroes. The non-zero entries represent the leading order contributions to the $\mathbf{B}'$ matrix elements that occupy the corresponding positions in the matrix.
Therefore, from Eqs. (4.43) through (4.46), and using the short-hand notation $\beta_i$ for the quadrature-dependent quantity introduced in Eq. (4.104), it follows that for the case $c_k = 1$:

$$k = 2\beta_i$$

(4.123)

$$n = \left( c_N \sigma_N \delta_N \right)^{\frac{1}{2}}$$

(4.124)
\[
f = -\frac{1}{2} \left( c_N \sigma_N \delta_N \right) \frac{1}{\Delta}
\]  
\[s = -\beta_i \]  

The \( B' \) matrix, that corresponds to the \( B^s \) matrix in the transformation for the cell-averaged scalar fluxes defined by Eq. (4.105), can be obtained following a two-step process in which the rows of the \( B^s \) matrix are shuffled in the same order as the cell-averaged scalar fluxes in going from \( \phi^\infty \) to \( \phi' \). The asymptotic structure of the \( B^s \) matrix resulting from the application of this first transformation step to the \( B^s \) matrix, sketched in Fig. 4.6, is reported in Fig. 4.7. In the second transformation step the \( B' \) matrix is obtained by shuffling the columns of the \( B^s \) matrix in the same order as the cell-averaged scalar fluxes in going from \( \phi^\infty \) to \( \phi' \). The asymptotic structure of the resulting \( B' \) matrix is sketched in Fig. 4.8.

The asymptotic structures of the four blocks in which the \( B' \) matrix was subdivided in Eq. (4.115) are evident from Fig. 4.8. In order to write the expressions for the various blocks in a concise form, that is also useful for later algebraic manipulations, it is convenient to introduce the following three \((J/2 \times J/2)\) matrices, whose entries are independent of \( \Delta \).

The first matrix, indicated in the following as \( L \), is a lower triangular two-stripe matrix with ones on the diagonal and the first sub-diagonal stripes. The elements of the \( L \) matrix can be expressed using the Kronecker delta function:
\[ L_{i,j} = (\delta_{i-1,j} + \delta_{i,j}), \quad i, j = 1, \ldots, J / 2 \]  

\[
\begin{bmatrix}
 k & f & s & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 s & f & k & f & s & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & s & f & k & f & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & s & f & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & f & n & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & f & n & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{bmatrix}
\]

Fig. 4.7: Asymptotic structure of the $\overline{B}^s$ matrix.

The second matrix, indicated in the following as $U$, is an upper triangular two-stripe matrix with ones on the diagonal and the first super-diagonal stripes. The elements of the $U$ matrix are given by:

\[ U_{i,j} = (\delta_{i,j} + \delta_{i,j-1}), \quad i, j = 1, \ldots, J / 2 \]
The third and last matrix, indicated in the following as $T$, is a tridiagonal matrix, characterized by a diffusion-like coupling stencil, with entries of the integer 2 on the diagonal stripe and $(-1)$ entries on the sub- and super-diagonal stripes:

$$T_{i,j} = (-\delta_{i-1,j} + 2\delta_{i,j} - \delta_{i,j-1}), \quad i, j = 1, ..., J / 2$$

With reference to Fig. 4.8 and using Eqs. (4.123), (4.126) and (4.129), the $B_{kk}$ matrix has, to leading order, the following expression:
\[ B_{KK} = \beta_i T \]  

(4.130)

With reference to Fig. 4.8 and using Eqs. (4.125) and Eq. (4.127), the matrix has, to leading order, the following expression:

\[ B_{KN} = -\frac{1}{2} \left( c_n \sigma_N \delta_N \right) \frac{1}{\Delta} L \]  

(4.131)

With reference to Fig. 4.8 and using Eqs. (4.125) and (4.128), the matrix has, to leading order, the following expression:

\[ B_{NK} = -\frac{1}{2} \left( c_n \sigma_N \delta_N \right) \frac{1}{\Delta} U \]  

(4.132)

With reference to Fig. 4.8 and using Eq. (4.124), the matrix has, to leading order, the following expression:

\[ B_{NN} = \left( c_n \sigma_N \delta_N \right) \frac{1}{\Delta} I \]  

(4.133)

It is now possible to compare the orders of the various terms that appear in Eq. (4.118). As evident from Eq. (4.130), matrix \( B_{KK} \) is \( O(\Delta^0) \). The order of the second matrix contribution in the parenthesis on the left hand side of Eq. (4.118) can be determined using Eqs. (4.131) through (4.133). The following result is obtained:

\[ B_{KN} \left( B_{NN} \right)^{-1} B_{NK} = \frac{1}{4} \left( c_n \sigma_N \delta_N \right) \frac{1}{\Delta} LU \]  

(4.134)

It can easily be shown that the matrix resulting from the product of matrices \( L \) and \( U \) is a tridiagonal matrix whose elements on the diagonal stripe are all equal to 2 except for \( [LU]_{1,1} = 1 \), and whose entries on the super- and sub-diagonal stripes are all equal to 1. This result follows immediately from the definition of matrix multiplication.
(rows by columns) and from the definitions of \( L_{i,j} \) and \( U_{i,j} \) contained in Eqs. (4.127) and (4.128):

\[
\begin{bmatrix} L U \end{bmatrix}_{i,j} = \frac{1}{2} \sum_{k=1}^{J/2} L_{i,k} U_{k,j} = \frac{1}{2} \left[ \delta_{i,k} \delta_{k,j} + \delta_{i,k} \delta_{k,j-1} + \delta_{j-1,k} \delta_{k,j} + \delta_{j-1,k} \delta_{k,j-1} \right]
\]

(4.135)

Since \( B_{KK} \) is \( O(\Delta^0) \) while \( B_{KN} (B_{NN})^{-1} B_{NK} \) is only \( O(\Delta^{-1}) \), it is concluded that in the asymptotic limit as \( \Delta \to \infty \):

\[
B_{KK} - B_{KN} (B_{NN})^{-1} B_{NK} \sim B_{KK}
\]

(4.136)

As far as the right hand side of Eq. (4.118) is concerned, the result in Eq. (4.121) shows that \( Q_k \) is \( O(\Delta^0) \). Using Eqs. (4.122), (4.131) and (4.133), the following result is obtained for the components of the vector resulting from the second contribution on the right hand side of Eq. (4.118):

\[
\begin{align*}
\left[ B_{KN} (B_{NN})^{-1} Q_N \right]_1 &= \left( -\frac{1}{2} c_n \frac{\sigma_N}{\sigma_k} \delta_N \right) \frac{1}{\Delta_1^2} \\
\left[ B_{KN} (B_{NN})^{-1} Q_N \right]_i &= 2 \left( -\frac{1}{2} c_n \frac{\sigma_N}{\sigma_k} \delta_N \right) \frac{1}{\Delta_i^2}, \quad i = 2, \ldots, \left( \frac{J}{2} - 1 \right) \\
\left[ B_{KN} (B_{NN})^{-1} Q_N \right]_{J/2} &= \frac{3}{2} \left( -\frac{1}{2} c_n \frac{\sigma_N}{\sigma_k} \delta_N \right) \frac{1}{\Delta_{J/2}^2}
\end{align*}
\]

(4.137)

Since \( Q_k \) is \( O(\Delta^0) \) while \( B_{KN} (B_{NN})^{-1} Q_N \) is only \( O(\Delta^{-2}) \), it is concluded that in the asymptotic limit as \( \Delta \to \infty \):

\[
Q_k - B_{KN} (B_{NN})^{-1} Q_N \sim Q_k
\]

(4.138)

Substitution of Eqs. (4.136) and (4.138) into Eq. (4.118) produces the following interesting result:
\[ \mathbf{B}_{KK} \hat{\phi}_K \sim \mathbf{Q}_K \] (4.139)

It is therefore verified that in the asymptotic limit as \( \Delta \to \infty \) the cell-averaged scalar fluxes in the thick computational cells are decoupled from the fluxes in the thin cells. As a matter of fact, they can be determined, to within terms that are \( O(\Delta^{-1}) \), by inverting the diffusive tridiagonal matrix \( \mathbf{B}_{KK} \) on the vector containing the scaled fixed sources in the thick cells. Indicating with \( \mathbf{1} \) a vector of ones of dimension \( J/2 \), and substituting Eqs. (4.121) and (4.130) into Eq. (4.139), the following expression is obtained, to leading order, for vector \( \hat{\phi}_K \):

\[
\hat{\phi}_K = \frac{\delta_k}{\beta_i} \mathbf{T}^{-1} \mathbf{1}
\] (4.140)

Assuming a symmetric \( S_6 \) quadrature, for which \( \beta_i = 0.255 \), and \( \delta_k = 1 \), for the ten cell problem whose results have been presented in Table 4.1 for the case \( c_k = 1 \), the values obtained to two decimal places for the cell-averaged fluxes in the five thick cells using Eq. (4.140) are \( \hat{\phi}_1 = \hat{\phi}_6 = 9.80 \), \( \hat{\phi}_2 = \hat{\phi}_5 = 15.69 \) and \( \hat{\phi}_3 = 17.65 \). These results are in perfect agreement with those obtained for \( \Delta = 10^6 \) in Table 4.1.

Finally, a comparison is carried out for the orders of the various terms that appear on the right hand side of Eq. (4.117). From Eqs. (4.122) and (4.133) it follows that the first vector on the right hand side of Eq. (4.117) has the following components:

\[
\left[ \begin{array}{c}
\left( \mathbf{B}_{NN} \right)^{-1} \mathbf{Q}_N \\
\left( \mathbf{B}_{NN} \right)^{-1} \mathbf{Q}_N
\end{array} \right]_i = \frac{1}{\sigma_k} \frac{1}{\Delta}, \quad i = 1, \ldots, \left( \frac{J}{2} - 1 \right)
\] (4.141)
Therefore, \((B_{NN})^{-1}Q_N\) is a vector of \(O(\Delta^{-1})\). Using Eqs. (4.132) and (4.133), the second contribution on the right hand side of Eq. (4.117) can be expressed in the following way:

\[
(B_{NN})^{-1}B_{NK}\tilde{\phi}_K = -\frac{1}{2}U\tilde{\phi}_K
\]

(4.142)

The result in Eq. (4.140) implies that \(\tilde{\phi}_K\) is \(O(\Delta^0)\). From Eq. (4.142) it may therefore be concluded that \((B_{NN})^{-1}B_{NK}\tilde{\phi}_K\) is \(O(\Delta^0)\) and dominates over \((B_{NN})^{-1}Q_N\). It follows that, in the asymptotic limit as \(\Delta \to \infty\), Eq. (4.117) is properly approximated by:

\[
\tilde{\phi}_N \sim \frac{1}{2}U\tilde{\phi}_K
\]

(4.143)

The latter result verifies that the cell-averaged scalar fluxes pertaining to the thin cells are linearly dependent on the fluxes in the thick cells. Once \(\tilde{\phi}_K\) has been computed in the limit using Eq. (4.140), \(\tilde{\phi}_N\) is determined through Eq. (4.143). Interestingly enough, the matrix operator \((1/2)U\) is an “arithmetic average” operator. In fact, it is at first noted that matrix \(U\) may be defined using the following expression perfectly equivalent to Eq. (4.128):

\[
U_{i,j} = (\delta_{i,j} + \delta_{i+1,j}), \quad i, j = 1, \ldots, J/2
\]

(4.144)

Using Eq. (4.144), the matrix expression in Eq. (4.143) is then written for a single component:

\[
\phi_{N,i} = \frac{1}{2} \sum_{j=1}^{J/2} (\delta_{i,j} + \delta_{i+1,j}) \phi_{K,j}, \quad i = 1, \ldots, J/2
\]

(4.145)
The expressions for the components of vector $\phi_N$ resulting from Eq. (4.145) are

\[
\begin{align*}
\phi_{N,i,j} &= \frac{1}{2} (\phi_{K,i,j} + \phi_{K,i,j+1}), \quad i = 1, \ldots, \left(\frac{J}{2} - 1\right) \\
\phi_{N,J/2} &= \frac{1}{2} \phi_{K,J/2}
\end{align*}
\] (4.146)

It is therefore verified, under the assumption of a uniform fixed source distribution, that the cell-averaged flux for a thin internal cell is the arithmetic average of the fluxes in the two adjacent thick cells, while the cell-averaged flux in the last thin cell in the slab is half the flux in the preceding thick cell. This explains the results in Table 4.1. It is noted that the result in Eq. (4.146) is independent of the scattering ratio $c_N$ in the thin cells.

### 4.4.3 Shuffling of the Cell-Averaged Scalar Fluxes for the Case $c_K < 1$

The derivation follows the same conceptual steps outlined in the previous section, based on the idea of shuffling the cell-averaged scalar fluxes as in Eq. (4.105). For the case $c_K < 1$, considered in this section, the uniform unit fixed source distribution vector $\mathbf{q}$ is not scaled:

\[ q_i = 1, \quad i = 1, \ldots, J \] (4.147)

Substituting Eq. (4.147) into Eq. (4.106) it follows that:

\[ Q_i = \sum_{j=1}^{J} A_{i,j}, \quad i = 1, \ldots, J \] (4.148)
An inspection of the rows of matrix $\mathbf{A}$ pertaining to the thick cells, see Fig. 4.5, and the leading orders of $\bar{k}$, $\bar{f}$ and $\bar{s}$ in Eqs. (4.98), (4.100) and (4.102), produce the following asymptotic expressions for the components of vector $\mathbf{Q}_K$, for the case $c_K < 1$:

$$Q_{k,i} = c_K \delta_K \Delta, \quad i = 1, \ldots, J/2$$

(4.149)

The components of vector $\mathbf{Q}_K$ are therefore all equal, to leading order, and $O(\Delta)$. The components of vector $\mathbf{Q}_N$ have the same constant coefficients, as in Eq. (4.122), but a different scaling in $\Delta$ as a consequence of Eq. (4.147):

$$\begin{cases} Q_{N,i} = c_N \frac{\sigma_N}{\sigma_K} \delta_N \frac{1}{\Delta}, \quad i = 1, \ldots, \left(\frac{J}{2} - 1\right) \\ Q_{N,J/2} = \frac{1}{2} c_N \frac{\sigma_N}{\sigma_K} \delta_N \frac{1}{\Delta} \end{cases}$$

(4.150)

The $k$, $f$ and $s$ non-zero entries in the asymptotic matrix structure acquired by the $\mathbf{B}^\delta$ matrix in the asymptotic limit as $\Delta \to \infty$, sketched in Fig. 4.6, have a different expression for the case $c_K < 1$. In particular, the leading order contribution to $B^\delta_{d,K}$ in Eq. (4.43) is the $O(\Delta)$ term, therefore the expression for $k$ is modified as follows:

$$k = (c_K \sigma_K \delta_K)(1-c_K) \Delta$$

(4.151)

The expressions for $f$ and $s$ become:

$$f = \frac{-c_K}{2} (c_N \sigma_N \delta_N) \frac{1}{\Delta}$$

(4.152)

$$s = -c_K^2 \beta_f$$

(4.153)
The expression for \( n \) is instead the same as given in Eq. (4.124).

Since \( k \) is \( O(\Delta) \) while \( s \) is \( O(\Delta^0) \), only the elements on the diagonal stripe of the \( B_{kk} \) matrix are retained in the leading order asymptotic analysis that is performed in the following. Using Eq. (4.151), the expression for the \( B_{kk} \) matrix is therefore modified as follows:

\[
B_{kk} = (c_k \sigma_k \delta_k)(1-c_k)\Delta I \tag{4.154}
\]

The expressions for matrices \( B_{kn} \) and \( B_{nk} \) must also be modified to include the dependence on \( c_k \):

\[
B_{kn} = -\frac{c_k}{2} (c_N \sigma_N \delta_N) \frac{1}{\Delta} L \tag{4.155}
\]

\[
B_{nk} = -\frac{c_k}{2} (c_N \sigma_N \delta_N) \frac{1}{\Delta} U \tag{4.156}
\]

Matrix \( B_{nn} \) remains the same as in Eq. (4.133).

It is now possible to compare the orders of the various terms that appear in Eq. (4.118). As evident from Eq. (4.154), matrix \( B_{kk} \) is \( O(\Delta) \). The order of the second matrix contribution in the parenthesis on the left hand side of Eq. (4.118) can be determined using Eqs. (4.155), (4.156) and (4.133). The following result is obtained:

\[
B_{kn} (B_{nn})^{-1} B_{nk} = \left(\frac{c_k}{2}\right)^2 (c_N \sigma_N \delta_N) \frac{1}{\Delta} LU \tag{4.157}
\]
Since \( B_{kk} \) is \( O(\Delta) \) while \( B_{kn} (B_{nn})^{-1} B_{nk} \) is only \( O(\Delta^{-1}) \), it is concluded that the result in Eq. (4.136) holds true also for the case \( c_k < 1 \). As far as the right hand side of Eq. (4.118) is concerned, the result in Eq. (4.149) shows that \( Q_k \) is \( O(\Delta) \). Using Eqs. (4.133), (4.150) and (4.155), the following result is obtained for the components of the vector resulting from the second contribution on the right hand side of Eq. (4.118):

\[
\left[ B_{kn} (B_{nn})^{-1} Q_n \right]_i = \left( -\frac{c_k}{2} c_n \frac{\sigma_n}{\sigma_k} \frac{\delta_n}{\Delta} \right) \frac{1}{\Delta} \quad i = 1, \ldots, \left( J/2 \right)
\]

(4.158)

Since \( Q_k \) is \( O(\Delta) \) while \( B_{kn} (B_{nn})^{-1} Q_n \) is only \( O(\Delta^{-1}) \), it is concluded that the results in Eqs. (4.138) and (4.139) are also valid for the case in which the thick cells contain a neutron absorbing material. In particular, the cell-averaged scalar fluxes in the thick computational cells are decoupled from the fluxes in the thin cells. They can be determined, to within terms that are \( O(\Delta^{-1}) \), by inverting the diagonal matrix \( B_{kk} \) on the \( Q_k \) vector, containing the scaled fixed sources in the thick cells:

\[
\varphi_{k,j} = \frac{1}{(1-c_k) \sigma_k} \quad i = 1, \ldots, J/2
\]

(4.159)

Assuming \( c_k = 0.5 \) and \( \sigma_k = 1 \), the value of 2 obtained for the cell-averaged scalar fluxes in the thick cells is in agreement with those obtained for \( \Delta = 10^6 \) in Table 4.2.
Finally, a comparison is carried out for the asymptotic orders of the various terms that appear on the right hand side of Eq. (4.117). From Eqs. (4.133) and (4.150) it follows that the first vector on the right hand side of Eq. (4.117) has the following components:

\[
\begin{align*}
\left[ (B_{nn})^{-1} Q_n \right]_i &= \frac{1}{\sigma_k}, & i &= 1, \ldots, \left( \frac{J}{2} - 1 \right) \\
\left[ (B_{nn})^{-1} Q_n \right]_{T/2} &= \frac{1}{2} \frac{1}{\sigma_k}
\end{align*}
\] (4.160)

Therefore, \((B_{nn})^{-1} Q_n\) is a vector of \(O(\Delta^0)\). Using Eqs. (4.133) and (4.156), the second contribution on the right hand side of Eq. (4.117) can be expressed as:

\[
(B_{nn})^{-1} B_{nk} \tilde{\phi}_k = -\frac{c_k}{2} U \tilde{\phi}_k
\] (4.161)

As implied by Eq. (4.159), the \(\tilde{\phi}_k\) vector is \(O(\Delta^0)\). Therefore, for the case \(c_k < 1\) both contributions on the right hand side of Eq. (4.117) must be retained in the asymptotic analysis. Recalling that the matrix operator \((1/2)U\) is an “arithmetic average” operator, see Eq. (4.144), and substituting Eqs. (4.160) and (4.161) into Eq. (4.117), the following expressions for the components of vector \(\tilde{\phi}_n\) are obtained:

\[
\begin{align*}
\varphi_{n,i} &= \frac{1}{\sigma_k} + \frac{c_k}{2} (\varphi_{k,i} + \varphi_{k,i+1}), & i &= 1, \ldots, \left( \frac{J}{2} - 1 \right) \\
\varphi_{n,J/2} &= \frac{1}{2} \frac{1}{\sigma_k} + \frac{c_k}{2} \varphi_{k,J/2}
\end{align*}
\] (4.162)

Substitution of Eq. (4.159) in Eq. (4.162) produces the final result:
Comparing Eqs. (4.159) and (4.163) it is concluded, under the assumption of a uniform fixed source distribution, that the cell-averaged flux for a thin cell in the interior of the slab is the arithmetic average of the fluxes in the two adjacent thick cells. Also, the cell-averaged flux in the last thin cell on the right edge of the slab is half the flux in the preceding thick cell. This explains the results in Table 4.2. It is noted that the result in Eqs. (4.163) is independent of the scattering ratio $c_N$ in the thin cells.

4.5 Transformation of $B^S$ into an Asymptotically Tridiagonal Matrix

The transformation has been originally introduced considering the scalar form acquired by the linear system in Eq. (4.15) for a periodically heterogeneous slab comprised of six computational cells and then generalizing the transformation obtained. This same approach is presented here to illustrate the rationale of the transformation in a simple setting. A general result proving that the transformation eliminates the elements on the second off-diagonal coupling two thick computational cells while retaining the exponential nature of the asymptotic behavior of the other elements beyond the first off-diagonal, therefore leading to a matrix asymptotically characterized by a tridiagonal structure, will be given in Sec. 4.6.
As usual, the odd computational cells are assumed to be thick while the even computational cells are assumed to be thin. By virtue of the definition in Eq. (4.106), the scalar form of the system in Eq. (4.15), for a slab comprised of six computational cells, is the following:

\[
\begin{align*}
B_{15}^S \tilde{\phi}_1 + B_{14}^S \tilde{\phi}_2 + B_{13}^S \tilde{\phi}_3 + B_{12}^S \tilde{\phi}_4 + B_{11}^S \tilde{\phi}_5 + B_{10}^S \tilde{\phi}_6 &= Q_1 \\
B_{25}^S \tilde{\phi}_1 + B_{24}^S \tilde{\phi}_2 + B_{23}^S \tilde{\phi}_3 + B_{22}^S \tilde{\phi}_4 + B_{21}^S \tilde{\phi}_5 + B_{20}^S \tilde{\phi}_6 &= Q_2 \\
B_{35}^S \tilde{\phi}_1 + B_{34}^S \tilde{\phi}_2 + B_{33}^S \tilde{\phi}_3 + B_{32}^S \tilde{\phi}_4 + B_{31}^S \tilde{\phi}_5 + B_{30}^S \tilde{\phi}_6 &= Q_3 \\
B_{45}^S \tilde{\phi}_1 + B_{44}^S \tilde{\phi}_2 + B_{43}^S \tilde{\phi}_3 + B_{42}^S \tilde{\phi}_4 + B_{41}^S \tilde{\phi}_5 + B_{40}^S \tilde{\phi}_6 &= Q_4 \\
B_{55}^S \tilde{\phi}_1 + B_{54}^S \tilde{\phi}_2 + B_{53}^S \tilde{\phi}_3 + B_{52}^S \tilde{\phi}_4 + B_{51}^S \tilde{\phi}_5 + B_{50}^S \tilde{\phi}_6 &= Q_5 \\
B_{65}^S \tilde{\phi}_1 + B_{64}^S \tilde{\phi}_2 + B_{63}^S \tilde{\phi}_3 + B_{62}^S \tilde{\phi}_4 + B_{61}^S \tilde{\phi}_5 + B_{60}^S \tilde{\phi}_6 &= Q_6
\end{align*}
\]  

The elements on the second off-diagonal of the \( B^S \) matrix coupling two thick computational cells have been highlighted in the previous equations. It is desired to simultaneously eliminate the terms \( B_{31}^S \tilde{\phi}_1 \) and \( B_{53}^S \tilde{\phi}_5 \) from the third equation in the system. This will turn out to be possible in view of the periodical repetition of the computational cells in the slab.

The simultaneous elimination can be accomplished by replacing the third equation in Eq. (4.164) with the following combination of the third equation with the second and fourth equations in Eq. (4.164):

\[
-\left[ B_{21}^S + B_{41}^S \right] \cdot (3) + B_{31}^S \cdot \left[ (2) + (4) \right],
\]  

(4.165)
where \((n)\) refers to the \(n^{th}\) equation in Eq. (4.165).

The first contribution to Eq. (4.165) is constituted by the following equation:

\[-(B_{21}^S + B_{41}^S)B_{31}^S\tilde{\phi}_3 - (B_{21}^S + B_{41}^S)B_{32}^S\tilde{\phi}_2 - (B_{21}^S + B_{41}^S)B_{33}^S\tilde{\phi}_3 +
\]

\[= -(B_{21}^S + B_{41}^S)\bar{Q}_3 \]

The second contribution to Eq. (4.165) is constituted by the following equation:

\[B_{31}^S(B_{21}^S + B_{41}^S)\tilde{\phi}_1 + B_{31}^S(B_{22}^S + B_{42}^S)\tilde{\phi}_2 + B_{31}^S(B_{23}^S + B_{43}^S)\tilde{\phi}_3 +
\]

\[= B_{21}^S(Q_2 + Q_4) \]

Focusing on the first highlighted terms in Eq. (4.166) and in Eq. (4.167) respectively, the following result appears evident when these two contributions are summed together as required by Eq. (4.165):

\[-(B_{21}^S + B_{41}^S)B_{31}^S\tilde{\phi}_1 + B_{31}^S(B_{21}^S + B_{41}^S)\tilde{\phi}_1 = 0 \]

Focusing on the second highlighted terms in Eq. (4.166) and in Eq. (4.167) respectively, the following result is also true when these two contributions are summed together as required by Eq. (4.165):

\[-(B_{21}^S + B_{41}^S)B_{35}^S\tilde{\phi}_5 + B_{31}^S(B_{25}^S + B_{45}^S)\tilde{\phi}_5 = 0, \]

provided that \(B_{31}^S = B_{35}^S\), \(B_{21}^S = B_{45}^S\) and \(B_{41}^S = B_{25}^S\).
It is noted that the previous conditions are generally met for the periodically heterogeneous structure in Fig. 4.1. In fact, in view of the periodicity, the following relations hold:

\[ B_{i,i+2}^S = B_{i,i+2}^S = B_{2nd,K\rightarrow K}^S, \quad 2 < i \text{ odd} < (J-1) \quad (4.170) \]

\[ B_{j,j-1}^S = B_{k+1,k}^S = B_{1st,K+1N}^S, \quad 1 < j,k < J \quad (4.171) \]

\[ B_{j,j-3}^S = B_{k+3,k}^S = B_{3rd,K+3N}^S, \quad 3 < j,k < (J-2) \quad (4.172) \]

The previous transformation is appropriate for every equation pertaining to an internal thick cell. It is in fact evident from Fig. 4.1, that an internal K cell always has a preceding and a following cell. The first equation in Eq. (4.164) represents instead a special case since this cell is not preceded by any other cell, so a preceding equation is missing. One way of eliminating the term \( B_{13}^S \Phi_3 \) is that of exploiting the second equation for a thin cell. Specifically, the following combination of the two equations is considered:

\[ -B_{23}^S \cdot (1) + B_{13}^S \cdot (2) \quad (4.173) \]

That this transformation eliminates the term of interest from the first equation is evident in view of the following result:

\[ -B_{23}^S \cdot B_{13}^S + B_{13}^S \cdot B_{23}^S = 0 \quad (4.174) \]

The algebraic transformation that brings the original system of equations in Eq. (4.164), for the six cell case, into an equivalent system is summed up in Fig. 4.9.
Fig. 4.9: Algebraic transformation for a system of six equations in the $B^S$ matrix.

The recipe outlined in Fig. 4.9 can be translated in a straightforward way into a recipe for the construction of a transformed $B^S$ matrix, indicated in the following as $\tilde{B}$, and generalized to the case of a slab comprised of $J$ computational cells. The elements of matrix $\tilde{B}$ are obtained from the elements of $B^S$ using the relations in Eqs. (4.175) through (4.177).

\[
\begin{align*}
(1) & \rightarrow -B^S_{23} \cdot (1) + B^S_{13} \cdot (2) \\
(2) & \rightarrow (2) \\
(3) & \rightarrow -(B^S_{21} + B^S_{41}) \cdot (3) + B^S_{31} \cdot [(2) + (4)] \\
(4) & \rightarrow (4) \\
(5) & \rightarrow -(B^S_{43} + B^S_{63}) \cdot (5) + B^S_{53} \cdot [(4) + (6)] \\
(6) & \rightarrow (6)
\end{align*}
\]

\[
\begin{align*}
\tilde{B}_{i,j} & = B^S_{1,i} \cdot B^S_{2,j} - B^S_{2,i} \cdot B^S_{1,j}, \quad i = 1; \ 1 \leq j \leq J & \quad (4.175) \\
\tilde{B}_{i,j} & = B^S_{i,j}, \quad i \text{ even, } 2 \leq i \leq J; \ 1 \leq j \leq J & \quad (4.176) \\
\tilde{B}_{i,j} & = B^S_{i-1,j-2} \cdot \left( B^S_{i-1,i,j} + B^S_{i+1,j} \right) - \left( B^S_{i-1,j-2} + B^S_{i+1,j-2} \right) \cdot B^S_{i,j}, \quad i \text{ odd, } 3 \leq i \leq (J-1); \ 1 \leq j \leq J & \quad (4.177)
\end{align*}
\]
Recalling that the equations for the optically thin cells are the ones for \( i \) even, it can be seen that the original elements of matrix \( \mathbf{B}^s \) pertaining to these equations are retained in the transformation. The elements on the pentadiagonal of the thick cells equations pertaining to internal, i.e. non-boundary, thick cells are simultaneously eliminated by exploiting the equations for the two adjacent thin cells. The elimination of the single pentadiagonal element of the first equation, pertaining to the first thick cell at the boundary, is accomplished using only the right-adjacent thin cell equation. The same transformation is of course applied to the right hand side of the original system of equations and produces a transformed source vector \( \mathbf{Q} \) that will be indicated in the following as \( \tilde{\mathbf{Q}} \). The elements of vector \( \tilde{\mathbf{Q}} \) are obtained from the elements of \( \mathbf{Q} \) using the relations:

\[
\tilde{Q}_1 = B_{1,3}^s \cdot Q_2 - B_{2,3}^s \cdot Q_1, \quad i = 1; \ 1 \leq j \leq J
\]

\[
\tilde{Q}_i = Q_i, \quad i \text{ even}, \ 2 \leq i \leq J; \ 1 \leq j \leq J
\]

\[
\tilde{Q}_i = B_{i,2}^s \cdot (Q_{i-1} + Q_{i+1}) - (B_{i-1,j-2}^s + B_{i+1,j-2}^s) \cdot Q_i,
\]

\[
i \text{ odd}, \ 3 \leq i \leq (J - 1); \ 1 \leq j \leq J
\]

Finally, the transformed system of discretized transport equations in the \( \tilde{\mathbf{B}} \) matrix representation is:

\[
\tilde{\mathbf{B}} \tilde{\phi}^∞ = \tilde{\mathbf{Q}}
\]
Since this system has been obtained through legitimate exact algebraic transformations, it is equivalent to both the system in the $B^S$ representation, Eq. (4.15), and to the original system in the $B$ matrix representation, Eq. (1.27).

4.6 Asymptotic Analysis of the Elements of Matrix $\tilde{B}$

The objective of the algebraic transformation in Eqs. (4.175) through (4.177) is two-fold: ensuring the selective elimination of the asymptotically non-vanishing elements on the pentadiagonal stripe while guaranteeing that the desirable feature of rapid, exponentially vanishing elements in the limit is retained. In order to verify that both objectives are met by the transformation, an asymptotic analysis of the elements of $\tilde{B}$ is performed in the limit as $\Delta \to \infty$.

The results of the asymptotic analysis are hereby reported.

\begin{equation}
\tilde{B}_{1,3} = \frac{1}{2} c_k^2 (1 - c_k) \sigma_k \delta_k \sigma_N \delta_N + \frac{3}{2} \sum_{m=1}^{M/2} w_m |\mu_m| \left( c_k^2 \sigma_k \sigma_N \delta_N \frac{1}{\Delta} + O\left( \frac{1}{\Delta^2} \right) \right) \tag{4.182}
\end{equation}

\begin{equation}
\tilde{B}_{1,2} = - \sum_{m=1}^{M/2} w_m |\mu_m| \left( c_k^2 \sigma_k \sigma_N \delta_N \frac{1}{\Delta} + O\left( \frac{1}{\Delta^2} \right) \right) \tag{4.183}
\end{equation}

\begin{equation}
\tilde{B}_{1,3} = B_{1,3}^S \cdot B_{2,3}^S - B_{3,3}^S \cdot B_{1,3}^S = 0 \tag{4.184}
\end{equation}
\[
\tilde{B}_{1,1+k} = (c_K c_N \sigma_N \delta_N)^2 w_{max} \left( \sum_{m=1}^{M/2} w_m |\mu_m| - \frac{1}{2} \right) \frac{e^{-(k-1)\sigma_k \delta_k \Delta \sqrt{\mu_{max}}}}{\Delta^2} + \\
+ O \left( \frac{e^{-(k-1)\sigma_k \delta_k \Delta \sqrt{\mu_{max}}}}{\Delta^3} \right), \quad k \geq 3 \text{ odd, } 1+k \leq J
\]

\[
\tilde{B}_{1,1+k} = c_K^3 c_N \sigma_N \delta_N w_{max} \left( \sum_{m=1}^{M/2} w_m |\mu_m| - \frac{1}{2} \right) \frac{e^{-(k-2)\sigma_k \delta_k \Delta \sqrt{\mu_{max}}}}{\Delta} + \\
+ O \left( \frac{e^{-(k-2)\sigma_k \delta_k \Delta \sqrt{\mu_{max}}}}{\Delta^2} \right), \quad k > 2 \text{ even, } 1+k \leq (J-1)
\]

\[
i \text{ even, } 2 \leq i \leq J
\]

\[
\tilde{B}_{ij} = (c_N \sigma_N \delta_N) \frac{1}{\Delta} + O \left( \frac{1}{\Delta^2} \right)
\]

\[
\tilde{B}_{ij+1} = -\frac{c_K}{2} (c_N \sigma_N \delta_N) \frac{1}{\Delta} + O \left( \frac{1}{\Delta^2} \right)
\]

\[
\tilde{B}_{ij+k} = -(c_N \sigma_N \delta_N)^2 \frac{w_{max}}{\mu_{max}} \frac{e^{-k\sigma_k \delta_k \Delta \sqrt{\mu_{max}}}}{\Delta^2} + \\
+ O \left( \frac{e^{-k\sigma_k \delta_k \Delta \sqrt{\mu_{max}}}}{\Delta^3} \right), \quad k \geq 2 \text{ even, } i+k \leq J, \ 2 \leq i-k
\]
\[\tilde{B}_{i,j;k} = -c_K (c_N \sigma_N \delta_N) w_{\max} \frac{e^{-(k-1)\sigma_k \delta_k \Delta/2|\mu_{\max}|}}{\Delta} + \]

\[+ O\left( \frac{e^{-(k-1)\sigma_k \delta_k \Delta/2|\mu_{\max}|}}{\Delta^2} \right), \quad k > 1 \text{ odd, } i + k \leq (J - 1), \ 1 \leq i - k \] (4.190)

\[i \text{ odd, } \ 3 \leq i \leq (J - 1)\]

\[\tilde{B}_{i,i} = \frac{1}{2} c_K^2 (1-c_K) \sigma_K \delta_K c_N \sigma_N \delta_N + 2 \left( \sum_{m=1}^{M/2} w_m |\mu_m| \right) c_K^3 c_N \sigma_N \delta_N \frac{1}{\Delta} + O\left( \frac{1}{\Delta^2} \right) \] (4.191)

\[\tilde{B}_{i,i;2} = -\left( \sum_{m=1}^{M/2} w_m |\mu_m| \right) c_K^2 c_N \sigma_N \delta_N \frac{1}{\Delta} + O\left( \frac{1}{\Delta^2} \right) \] (4.192)

\[B_{i,i;2} = \left( B_{i-1,i;2}^S + B_{i+1,i;2}^S \right) - \left( B_{i-1,i-2}^S + B_{i+1,i-2}^S \right) \cdot B_{i,i;2}^S = 0 \] (4.193)

\[\tilde{B}_{i,j;2} = (c_K c_N \sigma_N \delta_N)^2 w_{\max} \left( \sum_{m=1}^{M/2} w_m |\mu_m| \right) \frac{1}{|\mu_{\max}|} - \frac{1}{2} \frac{e^{-(k-1)\sigma_k \delta_k \Delta/2|\mu_{\max}|}}{\Delta^2} + \]

\[+ O\left( \frac{e^{-(k-1)\sigma_k \delta_k \Delta/2|\mu_{\max}|}}{\Delta^3} \right), \quad k \geq 3 \text{ odd, } i + k \leq J, \ 2 \leq i - k \] (4.194)
\[
\tilde{B}_{i,j;k} = c_k^3 c_N \sigma_N \delta_N w_{\text{max}} \left( \sum_{m=1}^{M/2} w_m |\mu_m| - \frac{|\mu_{\text{max}}|}{2} \right) \frac{e^{- (k-2)\sigma_k \delta_k \Delta/2|\mu_{\text{max}}|}}{\Delta} + \\
+ O \left( \frac{e^{- (k-2)\sigma_k \delta_k \Delta/2|\mu_{\text{max}}|}}{\Delta^2} \right), \quad k > 2 \text{ even, } i+k \leq (J-1), \; 1 \leq i-k
\] (4.195)

These results verify that the transformed matrix is asymptotically characterized by a tridiagonally dominant structure as \( \Delta \to \infty \).

Note that the elements pertaining to the first thick cell are, in the limit and to leading order, the same as those for the internal thick cells for the case \( c_k < 1 \). However, the elements on the diagonal are different for the first cell from the elements on the diagonal for the internal thick cells for the case \( c_k = 1 \). Also, for \( c_k = 1 \), the matrix acquires, in the limit, a tridiagonal structure characterized by a diffusion-like coupling stencil. It may also be noted that the transformation leads to a \( \tilde{B} \) matrix that is no longer symmetric. As far as the tridiagonal block of the matrix is concerned, the symmetrization can easily be regained by multiplying either the thin-cell equations by the ratio of the first off-diagonal element pertaining to a thick-cell equation to the first off-diagonal element pertaining to a thin-cell equation or the thick-cell equations by the reciprocal of this ratio. This ratio appears to be constant to leading order and, therefore, does not modify the exponential order of the elements beyond the first off-diagonal. Hence the full matrix remains non-symmetric only to within rapidly vanishing exponential terms outside the tridiagonal block.

The techniques involved in the derivation of the above asymptotic results are the same employed in Sec. 4.3. Therefore, the intricacies of the derivation are omitted since
they do not provide any additional content from a conceptual point of view. A verification that the results from the numerical implementation of the transformed $\tilde{B}$ matrix are in line with the ones predicted analytically from the asymptotic analysis is presented in Sec. 4.7. The verification is based on results obtained from the solution of the transformed system in Eq. (4.181).

4.7 Numerical Results for Periodically Heterogeneous Slabs

The results of the asymptotic analysis performed for the case of periodically heterogeneous slabs point to the fact that the transformed $\tilde{B}$ matrix is characterized by a tridiagonally dominant structure in the limit in which the optically thick cells are made thicker while the optically thin cells are made thinner. Also the tridiagonal structure is approached at a fast exponential rate.

The availability of the full form of matrix $B$ and of the right hand side of the linear system of equations in Eq. (1.27) permits the evaluation of the impact of the various transformation steps performed on the matrix, from $B$ to $B^s$ and from $B^s$ to $\tilde{B}$, when calculations are performed numerically in finite (double precision) arithmetic. Also, as done in the case of a homogeneous slab in Sec. 3.5.2, the error introduced by the abrupt truncation of the transformed $\tilde{B}$ matrix into a tridiagonal structure for finite $\Delta$ is determined. The error is evaluated by computing the difference between the solution resulting from inversion of the truncated matrix and the solution from inverting the exact full matrix. The quantitative evaluation of this difference has been carried out following the same two measures used for the homogeneous case, see Sec. 3.5. The maximum
relative error in the cell-averaged scalar fluxes and the relative error in the neutron balance are reported, as a function of the parameter $\Delta$, in Figs. 4.10 and 4.11 respectively.

The geometric configuration employed to obtain the results in Figs. 4.10 and 4.11 is comprised of ten computational cells in a heterogeneous structure of the kind reported in Fig. 4.1 with a uniform unit source distribution in all cells, as for the source distribution $1^{10}$ that was defined in Sec. 3.5.2. All computations have been performed assuming $\delta_k = \delta_N = 1$, $\sigma_k = \sigma_N = 1$ and a level symmetric $S_6$ quadrature. Different combinations have been explored for the values of the scattering ratios in the thick and thin cells in both Figs. 4.10 and 4.11: $c_k = c_N = 1$ in A, $c_k = c_N = 0.8$ in B, $c_k = 0.8$, $c_N = 0.5$ in C and $c_k = 1$, $c_N = 0.5$ in D.

Case A is of particular interest since it is the most challenging for the iterative solution of the transport problem, in fact it is the case in which both layers K and N host a purely scattering material. Since in this case the scattering ratios in the thick and thin cells are assumed of unit value, the source has been scaled as the inverse of the parameter $\Delta$ to prevent round-off errors resulting from the unbounded growth of the flux as $\Delta \rightarrow \infty$. The same scaling has been used for the fixed source in the thick cells in case D, in view of the fact that, as shown in Sec. 4.4 the solution is driven by the cell-averaged fluxes in the thick cells.
Fig. 4.10: Flux difference for a periodically heterogeneous slab.
Fig. 4.10: (Continued).
Fig. 4.11: Neutron balance difference for a periodically heterogeneous slab.
As far as the impact of the various algebraic transformations on the accuracy of the solution is concerned, it is observed that this is numerically insignificant. The results
in both Figs. 4.10 and 4.11 show that the differences with respect to the solutions obtained from inversion of the original full $\mathbf{B}$ matrix, due to the various transformation steps, do have a noisy behavior that falls in a band around the machine epsilon. In contrast, the abrupt truncation of $\tilde{\mathbf{B}}$ introduces a significant error that for $\Delta < 30$ MFPs, as seen in both Figs. 4.10 and 4.11, is far larger than the insignificant noise background.

Note the sharp drop in the error that occurs around $\Delta \sim 30$ MFPs, as in the homogeneous case (see Sec. 3.5.2). This drop has an exponential behavior, as evident from the log-log plots. Above this threshold the error introduced by the abrupt truncation is no longer significant since the full $\tilde{\mathbf{B}}$ matrix is itself acquiring a tridiagonal structure.

### 4.8 Conclusion

Various algebraic transformations of the integral transport matrix $\mathbf{B}$ that preserve the solution $\tilde{\varphi}^\infty$ of Eq. (1.27) have been considered in this chapter. These transformations have been devised in order to effectively expose the asymptotic properties possessed by the discrete integral transport operator for an important class of heterogeneous slabs, namely periodically heterogeneous slabs. In particular, the asymptotic limit considered for these periodic structures is one in which the heterogeneity in the optical properties of adjacent computational cells is progressively pushed apart, i.e. the thick cells are made thicker while the thin cells are made thinner at a prescribed rate.

First the issue of symmetrizing the $\mathbf{B}$ matrix has been successfully addressed, identifying a general transformation that brings the $\mathbf{B}$ matrix into a symmetrized matrix, $\mathbf{B}^s$. The asymptotic properties of the elements of the $\mathbf{B}^s$ matrix have then been
investigated, as $\Delta \to \infty$, in the asymptotic limit for periodically heterogeneous slabs defined in Sec. 4.1. In this limit, it has been shown that the $\mathbf{B}^S$ matrix acquires a sparse pentadiagonal structure due to the matrix elements on the second off-diagonal that couple the cell-averaged scalar fluxes in two thick cells separated by a single thin cell. This result has confirmed the physical intuition that the coupling between two optically thick cells, separated by an interposed thin cell, should be strong and determines some notable asymptotic properties displayed by the numerically computed cell-averaged scalar fluxes for periodically heterogeneous slabs. In particular, numerical results obtained under the assumption of a uniform fixed source distribution, have shown that the cell-averaged flux for a thin internal cell is the arithmetic average of the fluxes in the two adjacent thick cells, while the cell-averaged flux in the last thin cell on the right edge of the slab is half the flux in the preceding thick cell. The latter results point to the fact that, as it may intuitively be expected, the solution for the slab is essentially driven by the optically thick cells that become more and more strongly inter-coupled as the interposed thin cells are made thinner and thinner, by scaling the $\Delta$ parameter.

In order to relate these asymptotic properties of the cell-averaged scalar fluxes to the asymptotic properties of the $\mathbf{B}^S$ matrix, an algebraic transformation, based on re-ordering the cell-averaged scalar fluxes from the natural ordering shown in Fig. 4.1 to a new ordering, has been considered. Specifically, the cell-averaged scalar fluxes in vector $\tilde{\varphi}^\infty$ have been shuffled so that the cell-averaged fluxes pertaining to the thick cells are grouped together and separated from those pertaining to the thin cells in a transformed vector $\varphi'$, as indicated in Eq. (4.107). Applying the same algebraic transformation to
both sides of the system of equations in Eq. (1.27), the equivalent system of equations in
Eq. (4.108) has been obtained. The latter algebraic system has then been cast in matrix
form as a system of two matrix equations in the unknown vectors \( \phi_k \) and \( \phi_N \), containing
the cell-averaged scalar fluxes in the thick cells and in the thin cells, respectively. The
study of the properties of this system, in the asymptotic limit as \( \Delta \to \infty \), has led to the
conclusion that the cell-averaged scalar fluxes in the thick computational cells can indeed
be computed independently from the fluxes in the thin cells. The cell-averaged scalar
fluxes pertaining to the thin cells are instead linearly dependent on the fluxes in the thick
cells. More specifically, the results of the asymptotic analysis have confirmed that, under
the assumption of a uniform fixed source distribution, the cell-averaged flux for a thin
cell in the interior of the slab is the arithmetic average of the fluxes in the two adjacent
thick cells. Also, the cell-averaged flux in the last thin cell on the right edge of the slab is
half the flux in the preceding thick cell.

The result that the \( B^8 \) matrix acquires a sparse pentadiagonal structure in the
asymptotic limit considered for periodically heterogeneous slabs appears in line with
physical intuition. However, this result needs to be reconciled with the successful results
of acceleration schemes that are based on low-order operators characterized by a
tridiagonal diffusion-like coupling stencil, even in the case of periodically heterogeneous
slabs. In this respect, the fundamental result obtained in this chapter is that the tridiagonal
structure of these low-order operators represents a good approximation of the full
transport operator not only for optically thick homogeneous slabs, as shown in the
previous chapter, but also in the case of periodically heterogeneous slabs, comprised of
optically thick and thin computational cells. Specifically, it has been shown that the $B^5$ matrix representing the integral transport operator is also amenable to algebraic transformations that lead to an equivalent matrix representation $\hat{B}$ that asymptotically approaches a tridiagonal structure in the limit of interest. Also, the algebraic transformations considered ensure that, like for the case of a homogeneous slab, the tridiagonal structure is approached at a fast exponential rate even for the periodically heterogeneous configuration considered.

The results obtained contribute to the basic understanding of the excellent convergence properties of acceleration methods for the neutron transport equation based on cell-centered preconditioners characterized by a diffusion-like coupling stencil even for the case of heterogeneous slabs. In fact, deterioration of the convergence properties of these acceleration schemes has been widely observed in the presence of sharp material discontinuities in multi-dimensional problems but not in one-dimensional problems. In this connection, the results presented in this chapter point to the existence of a low-order approximation to the full discrete integral transport operator characterized by a tridiagonal structure even in the case of a periodically heterogeneous slab.
Chapter 5

Integral Transport Matrix and AP Acceleration for Slabs

5.1 Introduction

The results of the asymptotic analysis for the elements of the integral transport matrix, presented in Chs. 3 and 4 for homogeneous and periodically heterogeneous slabs, respectively, indicate that in both cases the discrete integral operator acquires a sparse tridiagonal matrix structure in the asymptotic thick-cell limit. In other words, a strong local coupling exists between a cell’s average scalar flux and its nearest neighbors’, even in the presence of sharp material discontinuities across the separating edge. For homogeneous slabs, the tridiagonal matrix structure approached in the asymptotic limit is also characterized by a diffusion-like coupling stencil. The latter statement is also true for periodically heterogeneous slabs, but only in the case of purely scattering media.

The results of the structural analysis of the integral transport matrix are used in this chapter to provide insight into the excellent convergence properties of diffusion-based acceleration schemes in one-dimensional transport problems. More specifically, the acceleration scheme analyzed in this chapter is that based on the Adjacent-cell Preconditioner (AP) [19]. The AP formalism provides a recipe for the construction of a diffusive cell-centered tridiagonal preconditioner that has proved to work extremely well for acceleration purposes, especially for purely scattering media, both in homogeneous and heterogeneous cases.
The recipe for the construction of the AP matrix starts with the introduction of a suitably defined quantity, dependent on the geometric and material properties of a cell, that represents a sort of generalized “diffusion coefficient” for the cell. The expression for this quantity is derived from a Fourier analysis of the AP acceleration scheme, conducted for an infinite homogeneous medium, requiring that the acceleration step warrants the selective suppression of the “flat” error modes for the iterative algorithm. The latter are constant modes, i.e. modes independent from the wave-length introduced in the Fourier expansion of the iteration residuals, and are known to be the slowest converging modes in the basic Source Iteration algorithm. To address the more general case of a heterogeneous slab, the elements of the tridiagonal AP matrix are then constructed from the “diffusion coefficients” of the adjacent cells, using the traditional mixing formula known from Diffusion Theory.

Using this recipe, the expressions for the elements of the AP matrix, indicated in the following as $\mathbf{D}$, are first derived for the case of a homogeneous slab with uniform spatial mesh and compared, in the thick cell limit, with the corresponding asymptotic expressions for the elements in the tridiagonal block of the integral transport matrix $\mathbf{B}$, obtained in Ch. 3. A similar comparison is then conducted, in the asymptotic limit introduced in Ch. 4 for periodically heterogeneous slabs, between the expressions acquired by the elements of matrix $\mathbf{D}$ and the corresponding elements in the tridiagonal block of matrix $\mathbf{B}$. In both the homogeneous and periodically heterogeneous asymptotic regimes, it will be shown that the AP matrix limits exactly to the same tridiagonal structure acquired by the integral transport matrix for the case of purely scattering media. This is the case in which a diffusive behavior is expected for the integral transport matrix.
and the previous findings help therefore to clarify the immediate convergence behavior, namely convergence in two iterations, displayed by the AP acceleration scheme in the asymptotic limit.

The AP acceleration scheme displays excellent convergence properties even in the presence of absorbing media, both in homogeneous and heterogeneous problems. In the heterogeneous case, though, immediate convergence is lost even in the asymptotic limit. For this case, it will be shown that the discrepancy between the \( D \) matrix and the structure acquired in the limit by the integral transport matrix is responsible for the loss of immediate convergence. In particular, it will be shown that convergence in two-iterations is restored, in the limit, once the recipe for the construction of the AP matrix is modified so that the \( D \) matrix elements limit to the correct expressions acquired asymptotically by the elements of the integral transport matrix.

An outline of the chapter follows. A brief review of the AP formalism and an outline of the recipe for the construction of the AP matrix are given in Sec. 5.2. Asymptotic expressions are derived for the elements of the AP matrix in the thick cell limit for a homogeneous slab and contrasted with those obtained in the same limit by the elements in the tridiagonal block of the \( B \) matrix in Sec. 5.3. The asymptotic analysis is then extended to periodically heterogeneous slabs and a structural comparison is carried out with elements in the tridiagonal block of the \( \hat{B} \) matrix in Sec. 5.4. Section 5.5 concludes the chapter with a summary and discussion of the main results.
5.2 Recipe for the Construction of the AP Matrix

As usual in synthetic acceleration schemes, a single source iteration constitutes the high-order step in the acceleration scheme. The equations representing the fully discretized version of Eq. (1.12) may be expressed using the following compact matrix notation:

\[
\Phi^{(r+1/2)} = A \left( \sigma_s \Phi^{(r)} + q \right)
\]  

(5.1)

It is noted that the solution of the system of equations in Eq. (5.1) does not require building and storing the \( A \) matrix. In fact, as explained in Ch. 1, the scalar fluxes \( \Phi^{(r+1/2)} \) are obtained through the “mesh-sweep” algorithm discussed in Sec. 3.2. In other words, performing a mesh-sweep is equivalent to computing the matrix-vector multiplication on the right hand side of Eq. (5.1).

The low-order equations representing the fully discretized version of Eq. (1.21) in the AP formalism can also be expressed in compact matrix notation:

\[
\tilde{f} = D^{-1} C \left( \Phi^{(r+1/2)} - \Phi^{(r)} \right)
\]  

(5.2)

In Eq. (5.2), \( \tilde{f} \) is a vector containing the additive corrections to the cell-averaged scalar fluxes computed in the present iteration for the \( J \) computational cells. Matrix \( D \) is the AP preconditioner and represents a certain diffusive (hence tridiagonal) low-order approximation to the integral transport matrix \( B \). Matrix \( C \) is a diagonal matrix and represents an approximation to matrix \( A \sigma_s \) that is reminiscent of the diagonally dominated structure acquired by matrix \( A \) in the thick cell limit, as shown in Sec. 3.4.2.
The details of the derivation of the one-dimensional AP formalism are found in [19]. A brief outline of the recipe for the construction of the elements of matrices $D$ and $C$ is given in the following along with the expressions needed in the remainder of the chapter.

The expression for the “diffusion coefficient” of a generic computational cell $j$ in the spatial mesh is:

$$D_j = \frac{C_j}{4} \sum_{m=1}^{M} w_m (2\kappa_{m,j})(2\kappa_{m,j} + \alpha_{m,j})$$

The symbols used in Eq. (5.3) have the usual meaning. In particular, substituting Eqs. (1.23) and (1.25) into Eq. (5.3) and performing the usual algebraic manipulations for the hyperbolic cotangent in the spatial weights, it is possible to express $D_j$ in terms of the geometric and material properties of a cell:

$$D_j = c_j \sum_{m=1}^{M/2} w_m \left[ \frac{\beta_m}{\sigma_j \Delta x_j} \frac{1 + e^{-\sigma_j \Delta x_j / |\mu_m|}}{1 - e^{-\sigma_j \Delta x_j / |\mu_m|}} \right]$$

The diffusion coefficients pertaining to cell $j$ and to the adjacent cell $j+1$, or $j-1$, are mixed by way of the following non-dimensional mixing formula adapted from standard Diffusion Theory (it is noted that this formula is misprinted in Eq. (32.b) of [19]):

$$D_{o^j} = \frac{2\sigma_{j\pm1} \Delta x_{j\pm1}}{\sigma_{j\pm1} \Delta x_{j\pm1} D_j + \sigma_j \Delta x_j D_{j\pm1}}$$

The elements of the tridiagonal matrix $D$ pertaining to an internal computational cell are then assembled using the following expression:
\[
\begin{cases}
D_{j,j} = (1 - c_j) + D_{o}^{+j} + D_{o}^{-j} \\
D_{j,j+1} = -D_{o}^{+j} \\
D_{j,j-1} = -D_{o}^{-j}
\end{cases}, \quad j = 2, \ldots, (J - 1) \tag{5.6}
\]

The expressions for the elements pertaining to the left-most and right-most cells represent a particular case:

\[
\begin{cases}
D_{i,1} = (1 - c_i) + D_{o}^{+i} + D_i (1 - \Gamma_i) \\
D_{i,2} = -D_{o}^{+i}
\end{cases} \tag{5.7}
\]

\[
\begin{cases}
D_{j,j} = (1 - c_j) + D_{o}^{-j} + D_j (1 - \Gamma_j) \\
D_{j,j-1} = -D_{o}^{-j}
\end{cases} \tag{5.8}
\]

The \( \Gamma \) coefficients introduced in Eqs. (5.7) and (5.8) are computed according to the following formula:

\[
\Gamma_j = \frac{D_j \sigma_j \Delta x_j}{\frac{\beta_j \gamma_j}{D_j \sigma_j \Delta x_j} + 1} - 1, \quad j = 1, J \tag{5.9}
\]

The coefficient \( \beta_j \) is the quadrature-dependent constant that was introduced in Eq. (4.104). The \( \gamma \) coefficients appearing in Eq. (5.9) are defined for a generic cell in the following fashion:

\[
\gamma_j = \begin{cases}
c_j, & \sigma_j \Delta x_j \leq \bar{\delta} \\
1, & \sigma_j \Delta x_j > \bar{\delta}
\end{cases}, \quad j = 1, \ldots, J \tag{5.10}
\]

The dimensionless parameter \( \bar{\delta} \) has a value of 1.82 MFPs and was introduced in [19] as a cut-off parameter to adjust the right hand side of Eq. (5.2) according to the
optical thickness of the cell in question. Furthermore, the $\gamma$ coefficients are also the non-zero entries of the diagonal matrix $C$:

$$C_{j,j} = \gamma_j, \quad j = 1, \ldots, J$$ (5.11)

The updating formula that constitutes the closure of the AP acceleration scheme is also dependent on the cut-off parameter $\bar{\delta}$:

$$\phi_j^{(t+1)} = \begin{cases} \phi_j^{(t+1/2)} + \tilde{f}_j, & \sigma_j \Delta x_j \leq \bar{\delta} \\ \phi_j^{(t)} + \tilde{f}_j, & \sigma_j \Delta x_j > \bar{\delta} \end{cases}, \quad j = 1, \ldots, J$$ (5.12)

In Eq. (5.12) $\tilde{f}_j$ represents the $j$th element of vector $\tilde{f}$.

### 5.3 Asymptotic Analysis in the Thick Cell Limit for Homogeneous Slabs

Asymptotic expressions are derived for the elements of the $D$ matrix in the thick cell limit for a homogeneous slab with a uniform mesh and contrasted to the corresponding limit expressions for the elements in the tridiagonal block of the $B$ matrix derived in Sec. 3.4.2.

In the asymptotic limit as $\Delta \to \infty$ the “diffusion coefficient” for a cell acquires the following expression:

$$D = c\beta_l \frac{1}{\sigma \Delta} + O\left(\frac{e^{-\sigma \Delta \mu_{\text{max}}}}{\sigma \Delta}\right),$$ (5.13)

where $\mu_{\text{max}}$ was introduced in Eq. (3.102).

Applying the mixing formula in Eq. (5.5) the following result, as expected for a homogeneous slab, is obtained:
\[
D_o^{z,i} = \frac{2\sigma\Delta}{\frac{\sigma\Delta}{D} + \frac{\sigma\Delta}{D}} = D
\]  \hspace{1cm} (5.14)

Substituting Eqs. (5.13) and (5.14) into Eq. (5.6), the following asymptotic expressions are obtained for the elements of matrix \( \mathbf{D} \) pertaining to an internal cell:

\[
D_{j,j} = \left(1 - c\right) + 2c\beta_j \frac{1}{\sigma\Delta} + O\left(\frac{e^{-\sigma\Delta|\mu_{\text{max}}|}}{\sigma\Delta}\right)
\]

\[
D_{j,j-1} = D_{j,j+1} = -c\beta_j \frac{1}{\sigma\Delta} + O\left(\frac{e^{-\sigma\Delta|\mu_{\text{max}}|}}{\sigma\Delta}\right)
\]

\hspace{1cm} (5.15)

In order to obtain the asymptotic expressions for the elements pertaining to the boundary cells, first it is necessary to derive an asymptotic expression for the \( \Gamma \) coefficient of a cell. Substituting Eq. (5.13) into Eq. (5.9) and performing the standard asymptotic manipulations yields:

\[
\Gamma = \frac{c - 1}{c + 1} + O\left(\frac{e^{-\sigma\Delta|\mu_{\text{max}}|}}{c + 1}\right)
\]

\hspace{1cm} (5.16)

Using Eqs. (5.13), (5.14) and Eq. (5.16) into either Eq. (5.7) or Eq. (5.8) and performing some additional simplifications, the following expressions are obtained for the elements of matrix \( \mathbf{D} \) pertaining to a boundary cell in the asymptotic limit:

\[
D_{1,1} = D_{j,j} = \left(1 - c\right) + \left(\frac{c + 3}{c + 1}\right)c\beta_j \frac{1}{\sigma\Delta} + O\left(\frac{e^{-\sigma\Delta|\mu_{\text{max}}|}}{\sigma\Delta}\right)
\]

\[
D_{1,2} = D_{j,j-1} = -c\beta_j \frac{1}{\sigma\Delta} + O\left(\frac{e^{-\sigma\Delta|\mu_{\text{max}}|}}{\sigma\Delta}\right)
\]

\hspace{1cm} (5.17)
As it was shown in Sec. 3.4.2, in the same asymptotic limit matrix $B$ reduces to a tridiagonal matrix to within rapidly exponentially vanishing terms beyond the first off-diagonal band, see Eq. (3.101). The asymptotic expressions for the elements in the tridiagonal block of matrix $B$ are hereby summarized for ease of comparison with the expressions for the corresponding elements of matrix $D$. In particular, the expressions for the elements of matrix $B$ pertaining to an internal cell are:

$$B_{j,j} = (1-c) + 2c \beta_j \frac{1}{\sigma\Delta} + O\left(\frac{e^{-\sigma\Delta/|\mu_{max}|}}{\sigma\Delta}\right)$$

$$B_{j,j-1} = B_{j,j+1} = -c \beta_j \frac{1}{\sigma\Delta} + O\left(\frac{e^{-\sigma\Delta/|\mu_{max}|}}{\sigma\Delta}\right)
\quad, \quad j = 2, \ldots, (J-1) \quad (5.18)$$

The expressions for the elements of matrix $B$ pertaining to a boundary cell are:

$$B_{1,1} = B_{J,J} = (1-c) + 2c \beta_j \frac{1}{\sigma\Delta} + O\left(\frac{e^{-\sigma\Delta/|\mu_{max}|}}{\sigma\Delta}\right)$$

$$B_{1,2} = B_{J,J-1} = -c \beta_j \frac{1}{\sigma\Delta} + O\left(\frac{e^{-\sigma\Delta/|\mu_{max}|}}{\sigma\Delta}\right)
\quad (5.19)$$

Comparing Eqs. (5.15) and (5.18), it can be concluded that the elements of $D$ and $B$ pertaining to an internal cell have the same asymptotic behavior, to within rapidly vanishing exponential terms, for any value of the scattering ratio $c \leq 1$. The same conclusion can be drawn for the elements of $D$ and $B$ pertaining to a boundary cell but only for the case $c = 1$. A comparison of Eqs. (5.17) and (5.19), in fact, shows that the
diagonal elements of $D$ and $B$ converge to the same limit, $(1-c)$, to within terms that are only $O((\sigma \Delta)^{-1})$ for $c < 1$.

The previous findings for problems with homogeneous material composition may be summed up using the following compact matrix notation:

\[
D = B + O\left(\frac{e^{-\sigma \Delta/|\mu_{\text{max}}|}}{\sigma \Delta}\right), \quad c = 1
\]  \hspace{1cm} (5.20)

\[
D = B + O\left(\frac{1}{\sigma \Delta}\right), \quad c < 1
\]  \hspace{1cm} (5.21)

The results presented in Eqs. (5.20) and (5.21) help explain the superb convergence properties of the AP acceleration scheme in the homogeneous thick cell limit, as evidenced by the results presented in Tables 5.1 and 5.2 in terms of the number of iterations necessary to achieve convergence to within a specified convergence criterion.

The results in Table 5.1 refer to the case of a unit scattering ratio. They have been obtained with the AP1 iterative code [19] for the case of a slab subdivided in six computational cells with a unit value of the macroscopic total cross-section, using an $S_6$ symmetric quadrature and a value of $10^{-4}$ for the convergence parameter $\varepsilon$. A uniform unit source drives the problem and is scaled as $\Delta^{-1}$ for the case of a purely scattering material. Again vacuum boundary conditions are applied on both sides of the slab.
Table 5.1: Number of AP accelerated iterations for a homogeneous slab with $c = 1$.

<table>
<thead>
<tr>
<th>$\Delta$</th>
<th># of iterations</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>4</td>
<td>3</td>
</tr>
<tr>
<td>5</td>
<td>3</td>
</tr>
<tr>
<td>6</td>
<td>3</td>
</tr>
<tr>
<td>7</td>
<td>2</td>
</tr>
<tr>
<td>8</td>
<td>2</td>
</tr>
<tr>
<td>9</td>
<td>2</td>
</tr>
<tr>
<td>10</td>
<td>2</td>
</tr>
<tr>
<td>15</td>
<td>2</td>
</tr>
<tr>
<td>20</td>
<td>2</td>
</tr>
<tr>
<td>25</td>
<td>2</td>
</tr>
<tr>
<td>30</td>
<td>2</td>
</tr>
<tr>
<td>40</td>
<td>2</td>
</tr>
<tr>
<td>50</td>
<td>2</td>
</tr>
<tr>
<td>60</td>
<td>2</td>
</tr>
<tr>
<td>70</td>
<td>2</td>
</tr>
<tr>
<td>80</td>
<td>2</td>
</tr>
<tr>
<td>90</td>
<td>2</td>
</tr>
<tr>
<td>100</td>
<td>2</td>
</tr>
</tbody>
</table>

The results presented in Table 5.2 refer to the case of a uniform slab with scattering ratio $c = 0.8$. All other parameters are unchanged with respect to Table 5.1. It is noted that in both Tables 5.1 and 5.2 convergence in two iterations is obtained in the asymptotic limit as $\Delta \rightarrow \infty$. Since, as shown in Eqs. (5.20) and (5.21), $D$ becomes equal to $B$ in the limit as $\Delta \rightarrow \infty$, it is expected that the solution to Eq. (1.27) is obtained at the end of a single AP iteration, namely point-wise convergence is achieved, in the asymptotic limit. The results in Tables 5.1 and 5.2 do not contradict this expectation. In fact, it is noted that the AP1 iterative code starts with an initial guess $\phi^{(0)} = 0$ and obtains convergence when the difference between two successive scalar flux estimates is less
than the pre-assigned convergence criterion. Therefore, the first of the two AP iterations in Tables 5.1 and 5.2 obtains the solution to Eq. (1.27) while the second iteration is necessary to verify convergence to the solution to within the convergence parameter $\varepsilon$.

Convergence of the AP1 code in a single iteration could be obtained only if the scalar flux estimates at the end of the first iteration were compared directly to the solution to Eq. (1.27).

Table 5.2: Number of AP accelerated iterations for a homogeneous slab with $c = 0.8$.

<table>
<thead>
<tr>
<th>$\Delta$</th>
<th># of iterations</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^0$</td>
<td>5</td>
</tr>
<tr>
<td>$10^1$</td>
<td>3</td>
</tr>
<tr>
<td>$10^2$</td>
<td>3</td>
</tr>
<tr>
<td>$10^3$</td>
<td>3</td>
</tr>
<tr>
<td>$10^4$</td>
<td>2</td>
</tr>
<tr>
<td>$10^5$</td>
<td>2</td>
</tr>
<tr>
<td>$10^6$</td>
<td>2</td>
</tr>
</tbody>
</table>

While convergence in two iterations is obtained in the asymptotic limit both in Tables 5.1 and 5.2, it is evident that the asymptotic regime is approached at a much faster rate for the case of a purely scattering material than for the case in which absorption is present in the slab. Since in both cases convergence is eventually obtained in two iterations as $\Delta$ is increased, a quantity that is expected to give a quantitative indication on the rate at which the asymptotic regime is entered is the scalar flux residual at the end of the second iteration. The latter quantity is reported in Tables 5.3 and 5.4 for the cases $c = 1$ and $c = 0.8$, respectively.
Table 5.3: Scalar flux residual at the second AP accelerated iteration for a homogeneous slab with $c = 1$.

<table>
<thead>
<tr>
<th>$\Delta$</th>
<th>Residual @ 2\textsuperscript{nd} iteration</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$1.387 \times 10^{-2}$</td>
</tr>
<tr>
<td>2</td>
<td>$1.941 \times 10^{-2}$</td>
</tr>
<tr>
<td>3</td>
<td>$5.669 \times 10^{-3}$</td>
</tr>
<tr>
<td>4</td>
<td>$1.741 \times 10^{-3}$</td>
</tr>
<tr>
<td>5</td>
<td>$5.537 \times 10^{-4}$</td>
</tr>
<tr>
<td>6</td>
<td>$1.805 \times 10^{-4}$</td>
</tr>
<tr>
<td>7</td>
<td>$5.983 \times 10^{-5}$</td>
</tr>
<tr>
<td>8</td>
<td>$2.006 \times 10^{-5}$</td>
</tr>
<tr>
<td>9</td>
<td>$6.776 \times 10^{-6}$</td>
</tr>
<tr>
<td>10</td>
<td>$2.300 \times 10^{-6}$</td>
</tr>
<tr>
<td>15</td>
<td>$1.068 \times 10^{-8}$</td>
</tr>
<tr>
<td>20</td>
<td>$5.019 \times 10^{-11}$</td>
</tr>
<tr>
<td>25</td>
<td>$1.783 \times 10^{-13}$</td>
</tr>
<tr>
<td>30</td>
<td>$3.194 \times 10^{-14}$</td>
</tr>
<tr>
<td>40</td>
<td>$9.501 \times 10^{-14}$</td>
</tr>
<tr>
<td>50</td>
<td>$6.352 \times 10^{-14}$</td>
</tr>
<tr>
<td>60</td>
<td>$1.600 \times 10^{-13}$</td>
</tr>
<tr>
<td>70</td>
<td>$3.551 \times 10^{-14}$</td>
</tr>
<tr>
<td>80</td>
<td>$4.743 \times 10^{-14}$</td>
</tr>
<tr>
<td>90</td>
<td>$6.096 \times 10^{-14}$</td>
</tr>
<tr>
<td>100</td>
<td>$4.740 \times 10^{-13}$</td>
</tr>
</tbody>
</table>

Table 5.4: Scalar flux residual at the second AP accelerated iteration for a homogeneous slab with $c = 0.8$.

<table>
<thead>
<tr>
<th>$\Delta$</th>
<th>Residual @ 2\textsuperscript{nd} iteration</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^0$</td>
<td>$5.835 \times 10^{-2}$</td>
</tr>
<tr>
<td>$10^1$</td>
<td>$9.306 \times 10^{-3}$</td>
</tr>
<tr>
<td>$10^2$</td>
<td>$1.108 \times 10^{-3}$</td>
</tr>
<tr>
<td>$10^3$</td>
<td>$1.131 \times 10^{-4}$</td>
</tr>
<tr>
<td>$10^4$</td>
<td>$1.133 \times 10^{-5}$</td>
</tr>
<tr>
<td>$10^5$</td>
<td>$1.133 \times 10^{-6}$</td>
</tr>
<tr>
<td>$10^6$</td>
<td>$1.133 \times 10^{-7}$</td>
</tr>
</tbody>
</table>
The results in Tables 5.3 and 5.4 indicate that the asymptotic regime is approached at a fast exponential rate for the case of a purely scattering material, while it is approached at a linear rate for the case in which absorption is present in the slab. This is particularly evident comparing Fig. 5.1 with Fig. 5.2 in which the residual at the second iteration is plotted as a function of parameter $\Delta$ for $c=1$ and $c=0.8$, respectively.

![Graph showing residual vs $\Delta$ for AP accelerated iteration](image)

*Fig. 5.1: Scalar flux residual at the second AP accelerated iteration for a homogeneous slab with $c=1$.*

The curve plotted in Fig. 5.1 is very similar to the exponential curves obtained in the previous chapters. Notice in particular that once again the thick cell asymptotic regime is entered for a value of the $\Delta$ parameter corresponding to 30 MFPs. The residuals above $\Delta \sim 30$ MFPs exhibit once again finite arithmetic random noise. The fact
that the level of the noise is shifted higher than the machine epsilon is attributed to potential numerical precision issues in the code implementation for very large cells.

![Graph](image)

**Fig. 5.2:** Scalar flux residual at the second AP accelerated iteration for a homogeneous slab with $c = 0.8$.

The exponential behavior and the polynomial behavior displayed by the residual in Figs. 5.1 and 5.2, respectively, appear in turn to be a consequence of the different truncation orders predicted theoretically in Eqs. (5.20) and (5.21), for the cases $c = 1$ and $c < 1$, respectively. In particular, no exponential convergence is expected for the $c < 1$ case since matrices $D$ and $B$ differ to within $O\left(\left(\sigma\Delta\right)^{-1}\right)$ terms in the limit as $\Delta \to \infty$.

It is noted that the convergence of $D$ to $B$ within terms that are $O\left(\left(\sigma\Delta\right)^{-1}\right)$ is caused by the difference in the coefficients multiplying the $O\left(\left(\sigma\Delta\right)^{-1}\right)$ term in the
diagonal elements pertaining to the boundary cells of matrices \( D \) and \( B \). This difference is evident from comparing Eqs. (5.17) and (5.19).

The convergence of \( D \) to \( B \) within exponentially decaying terms can be restored, for the case \( c < 1 \), provided the recipe for the construction of the AP matrix presented in Sec. 5.2 is suitably modified. The modification must yield the correct coefficient in front of the \( O\left( (\sigma \Delta)^{-1} \right) \) term that would make the diagonal elements pertaining to the boundary cells of matrix \( D \) identical to those in the \( B \) matrix up to \( O\left( (\sigma \Delta)^{-1} \right) \). A possible way to obtain this result is by modifying the expression given in Eq. (5.9) for the \( \Gamma \) coefficients used to formulate the boundary equations.

The following modified definition is proposed:

\[
\tilde{\Gamma}_j = \frac{D_j \sigma_j \Delta x_j - 1}{D_j \sigma_j \Delta x_j + 1}, \quad j = 1, J
\]  

(5.22)

The new \( \tilde{\Gamma} \) coefficients are formally identical to the old \( \Gamma \) coefficients, except that they are based on the following definition:

\[
\tilde{\gamma}_j = c_j, \quad j = 1, J
\]  

(5.23)

It is noted that the \( \tilde{\gamma} \) coefficients in Eq. (5.23) differ from the \( \gamma \) coefficients in Eq. (5.10) by the fact that their definition is independent from the cut-off parameter \( \delta \).

Finally Eqs. (5.7) and (5.8) for the boundary cells are replaced by the following expressions where the \( \tilde{\Gamma} \) coefficients are used instead of the old \( \Gamma \) coefficients:
\[
\begin{align*}
\hat{D}_{1,1} &= (1-c_1) + D_o^{\tau_1} + D_1 \left( 1 - \bar{\Gamma}_1 \right) \\
\hat{D}_{1,2} &= -D_o^{\tau_1}
\end{align*}
\] (5.24)

\[
\begin{align*}
\tilde{D}_{j,j} &= (1-c_j) + D_o^{-j} + D_j \left( 1 - \bar{\Gamma}_j \right) \\
\tilde{D}_{j,j-1} &= -D_o^{-j}
\end{align*}
\] (5.25)

No other modifications are introduced with respect to the recipe presented in Sec. 5.2. Therefore the new matrix \( \hat{D} \) differs from the original AP matrix \( D \) only in the elements on the diagonal pertaining to the boundary cells. It is noted that matrix \( C \) and the update equations are also not modified.

By virtue of the modified definition in Eq. (5.23), the following asymptotic behavior results for the \( (1 - \bar{\Gamma}) \) coefficients appearing in Eqs. (5.24) and (5.25) in the thick cell limit for a homogeneous slab:

\[
1 - \bar{\Gamma} = 1 - \frac{1 - 1}{1 + 1} + O \left( e^{-\sigma \Delta / \mu_{\text{max}}} \right) = 1 + O \left( e^{-\sigma \Delta / \mu_{\text{max}}} \right)
\] (5.26)

The asymptotic behavior for the elements on the diagonal of \( \hat{D} \) pertaining to the boundary cells is therefore the following:

\[
\begin{align*}
\hat{D}_{1,1} &= D_{j,j} = (1 - c) + 2c \beta \frac{1}{\sigma \Delta} + O \left( \frac{e^{-\sigma \Delta / \mu_{\text{max}}}}{\sigma \Delta} \right) \\
\hat{D}_{1,2} &= D_{j,j-1} = -c \beta \frac{1}{\sigma \Delta} + O \left( \frac{e^{-\sigma \Delta / \mu_{\text{max}}}}{\sigma \Delta} \right)
\end{align*}
\] (5.27)

Comparison of Eq. (5.27) with Eq. (5.19) leads to the conclusion:
\[
\tilde{D} = B + \mathcal{O} \left( \frac{e^{-\sigma\Delta/|\mu_{\text{max}}|}}{\sigma\Delta} \right), \quad c \leq 1
\] (5.28)

In particular, it is noted that matrix \( \tilde{D} \) is coincident with matrix \( D \) for \( c = 1 \).

The modifications contained in Eqs. (5.22) through (5.25) are easily implemented in a modified version of the AP1 code. Since \( \tilde{D} \) and \( D \) are coincident for \( c = 1 \) the results obtained from the modified version for the case of a purely scattering medium are the same previously reported in Table 5.1 and in Fig. 5.1. The results obtained with the modified code for \( c = 0.8 \) are presented in Table 5.5 and in Fig. 5.3.

Table 5.5: Number of modified AP accelerated iterations for a homogeneous slab with \( c = 0.8 \).

<table>
<thead>
<tr>
<th>( \Delta )</th>
<th># of iterations</th>
<th>Residual @ 2\textsuperscript{nd} iteration</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5</td>
<td>5.835 \times 10^{-2}</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>1.421 \times 10^{-2}</td>
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<tr>
<td>3</td>
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</tr>
<tr>
<td>4</td>
<td>3</td>
<td>1.192 \times 10^{-3}</td>
</tr>
<tr>
<td>5</td>
<td>3</td>
<td>3.473 \times 10^{-4}</td>
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<tr>
<td>6</td>
<td>3</td>
<td>1.037 \times 10^{-4}</td>
</tr>
<tr>
<td>7</td>
<td>2</td>
<td>3.159 \times 10^{-5}</td>
</tr>
<tr>
<td>8</td>
<td>2</td>
<td>9.782 \times 10^{-6}</td>
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<tr>
<td>9</td>
<td>2</td>
<td>3.068 \times 10^{-6}</td>
</tr>
<tr>
<td>10</td>
<td>2</td>
<td>9.712 \times 10^{-7}</td>
</tr>
<tr>
<td>15</td>
<td>2</td>
<td>3.364 \times 10^{-9}</td>
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<tr>
<td>20</td>
<td>2</td>
<td>1.258 \times 10^{-11}</td>
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<tr>
<td>25</td>
<td>2</td>
<td>4.922 \times 10^{-14}</td>
</tr>
<tr>
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<td>2</td>
<td>9.250 \times 10^{-16}</td>
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<tr>
<td>40</td>
<td>2</td>
<td>9.160 \times 10^{-16}</td>
</tr>
<tr>
<td>50</td>
<td>2</td>
<td>9.105 \times 10^{-16}</td>
</tr>
<tr>
<td>60</td>
<td>2</td>
<td>9.068 \times 10^{-16}</td>
</tr>
<tr>
<td>70</td>
<td>2</td>
<td>9.042 \times 10^{-16}</td>
</tr>
<tr>
<td>80</td>
<td>2</td>
<td>2.220 \times 10^{-16}</td>
</tr>
<tr>
<td>90</td>
<td>2</td>
<td>8.883 \times 10^{-16}</td>
</tr>
<tr>
<td>100</td>
<td>2</td>
<td>8.994 \times 10^{-16}</td>
</tr>
</tbody>
</table>
The curve plotted in Fig. 5.3 shows that exponential convergence has been restored also for the case $c < 1$ as a result of the modifications to the recipe for the construction of the AP matrix introduced in Eqs. (5.22) through (5.25).

![Graph showing scalar flux residual at the second accelerated iteration for modified AP in a homogeneous slab with $c = 0.8$.](image)

**Fig. 5.3:** Scalar flux residual at the second accelerated iteration for modified AP in a homogeneous slab with $c = 0.8$.

### 5.4 Asymptotic Analysis for Periodically Heterogeneous Slabs

Asymptotic expressions are derived for the elements of the $\mathbf{D}$ matrix for periodically heterogeneous slabs in the limit introduced in Sec. 4.1. The resulting expressions are contrasted to the corresponding limit expressions for the elements in the tridiagonal block of matrix $\tilde{\mathbf{B}}$ obtained in Sec. 4.6.
In the asymptotic limit as $\Delta \to \infty$ the “diffusion coefficient” for a thick or K cell acquires the following expression:

$$D_K = c_K \beta_I \frac{1}{\sigma_K \delta_K} \frac{1}{\Delta} + O\left(\frac{e^{-\sigma_K \delta_K \Delta \mu_{max}}}{\Delta}\right) \quad (5.29)$$

In the same limit the “diffusion coefficient” for a thin or N cell is:

$$D_N = c_N \beta_I \frac{1}{(\sigma_N \delta_N)^2} \Delta^2 + O(\Delta) \quad (5.30)$$

The coefficient $\beta_I$ introduced in Eq. (5.30) is short-hand notation for the following quadrature-dependent constant:

$$\beta_I = \left(\sum_{m=1}^{M} w_m |\mu_m|^2\right) \quad (5.31)$$

In the case of a periodically heterogeneous slab the mixing formula produces two different results when applied to a K or an N cell respectively. Referring to the same structure introduced in Fig. 4.1, a K (N) cell is characterized by odd (even) values of index $j$, respectively. The mixing formula in Eq. (5.5) produces the following expression when applied to a K cell:

$$D_{\pm j} = \frac{2\sigma_N \Delta x_N}{\sigma_N \Delta x_N + \sigma_K \Delta x_K} \cdot D_K + \frac{\sigma_K \Delta x_K}{D_N}, \quad j \text{ odd} \quad (5.32)$$

Substituting Eqs. (5.29) and (5.30) in Eq. (5.32) along with the scaling with respect to $\Delta$ for $\Delta x_K$ and $\Delta x_N$, the following result is obtained after performing the due simplifications in the asymptotic limit:

$$D_{\pm j} = 2c_K \beta_I \frac{1}{\sigma_K \delta_K} \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right), \quad j \text{ odd} \quad (5.33)$$
The expression obtained by applying the mixing formula to an N cell is:

\[
D_o^{i,j} = \frac{2\sigma_k \Delta x_k}{\sigma_N \Delta x_N + \sigma_k \Delta x_k}, \quad j \ even \quad (5.34)
\]

The following result is obtained from the asymptotic analysis to Eq. (5.34):

\[
D_o^{i,j} = 2c_k \beta_i \frac{1}{\sigma_N \delta_N} \Delta + O\left(\Delta^0\right), \quad j \ even \quad (5.35)
\]

Substituting Eq. (5.33) into Eq. (5.6), the following asymptotic expressions are obtained for the elements of matrix \( D \) pertaining to an inner K cell:

\[
\begin{align*}
D_{j,j} &= (1 - c_k) + 4c_k \beta_i \frac{1}{\sigma_k \delta_k} \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right) \\
D_{j,j+1} &= D_{j,j-1} = -2c_k \beta_i \frac{1}{\sigma_k \delta_k} \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right) \\
\end{align*}
\]

Substituting Eq. (5.35) into Eq. (5.6), the following asymptotic expressions are obtained for the elements of matrix \( D \) pertaining to an inner N cell:

\[
\begin{align*}
D_{j,j} &= 4c_k \beta_i \frac{1}{\sigma_N \delta_N} \Delta + O\left(\Delta^0\right) \\
D_{j,j+1} &= D_{j,j-1} = -2c_k \beta_i \frac{1}{\sigma_N \delta_N} \Delta + O\left(\Delta^0\right) \\
\end{align*}
\]

The left-most cell found in the periodic arrangement in Fig. 4.1 is a K cell. The asymptotic expression for its \( \Gamma_k \) coefficient is therefore similar to that obtained in the thick cell limit in Eq. (5.16). The asymptotic behavior of \( (1 - \Gamma_k) \) is therefore:

\[
(1 - \Gamma_k) = \frac{2}{c_k + 1} + O\left(e^{-\sigma_k \Delta_k \mu_{\max}}\right) \quad (5.38)
\]
Using Eqs. (5.29), (5.34) and (5.38) in Eq. (5.7) and performing the due simplifications, the following expressions are obtained for the elements of matrix $D$ pertaining to the left-most boundary cell in the asymptotic limit:

\[
\begin{align*}
D_{1,1} &= (1-c_k) + 2\left(\frac{c_k + 2}{c_k + 1}\right)c_k \beta_i \frac{1}{\sigma_k \delta_k} \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right) \\
D_{1,2} &= -2c_k \beta_i \frac{1}{\sigma_k \delta_k} \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right)
\end{align*}
\] (5.39)

The right-most cell in the periodic arrangement in Fig. 4.1 is an $N$ cell. The asymptotic behavior determined for the $(1 - \Gamma_N)$ coefficient pertaining to this cell is:

\[
(1 - \Gamma_N) = 2 \frac{\beta_L}{\beta_{ii}} \sigma_N \delta_N \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right)
\] (5.40)

Using Eqs. (5.30), (5.35) and (5.40) in Eq. (5.8) and performing the due simplifications, the following expressions are obtained for the elements of matrix $D$ pertaining to the right-most boundary cell in the asymptotic limit:

\[
\begin{align*}
D_{j,j} &= 2(c_k + c_N) \beta_i \frac{1}{\sigma_N \delta_N} \Delta + O\left(\Delta^0\right) \\
D_{j,j-1} &= -2c_k \beta_i \frac{1}{\sigma_N \delta_N} \Delta + O\left(\Delta^0\right)
\end{align*}
\] (5.41)

As evident from a comparison of Eqs. (5.36) and (5.37), matrix $D$ is not in general a symmetric matrix, but it may be symmetrized in a straightforward fashion. In particular, to simplify the ensuing comparison with the integral transport matrix it is convenient to consider a symmetrized version of the AP matrix that retains the off-diagonal elements pertaining to a thick cell. This is accomplished by multiplying the equations for an $N$ cell
by the ratio of the off-diagonal element for a K cell to the off-diagonal element of an N cell. In the asymptotic limit as $\Delta \to \infty$ this ratio reduces to:

$$
-2c_k \beta_j \frac{1}{\sigma_k \delta_k} \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right) = \frac{\sigma_n \delta_n}{\sigma_k \delta_k} \frac{1}{\Delta^2} + O\left(\frac{1}{\Delta^3}\right)
$$

(5.42)

Indicating with $D^s$ the symmetrized AP matrix obtained through the aforementioned transformation, the asymptotic expressions obtained for the elements of this matrix are the following:

$$
\begin{align*}
D^s_{1,1} &= (1-c_k) + 2 \left(\frac{c_k + 2}{c_k + 1}\right) c_k \beta_j \frac{1}{\sigma_k \delta_k} \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right) \\
D^s_{1,2} &= -2c_k \beta_j \frac{1}{\sigma_k \delta_k} \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right) \\
D^s_{j,j} &= 4c_k \beta_j \frac{1}{\sigma_k \delta_k} \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right) \\
D^s_{j,j+1} &= D^s_{j,j-1} = -2c_k \beta_j \frac{1}{\sigma_k \delta_k} \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right)
\end{align*}
$$

(5.43)

$$
\begin{align*}
D^s_{j,j} &= (1-c_k) + 4c_k \beta_j \frac{1}{\sigma_k \delta_k} \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right) \\
D^s_{j,j+1} &= D^s_{j,j-1} = -2c_k \beta_j \frac{1}{\sigma_k \delta_k} \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right)
\end{align*}
$$

(5.44)

$$
\begin{align*}
D^s_{j,j} &= (1-c_k) + 4c_k \beta_j \frac{1}{\sigma_k \delta_k} \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right) \\
D^s_{j,j+1} &= D^s_{j,j-1} = -2c_k \beta_j \frac{1}{\sigma_k \delta_k} \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right)
\end{align*}
$$

(5.45)
\[
\begin{align*}
D_{j,j}^i &= 2(c_K + c_N)\beta_i \frac{1}{\sigma_k \delta_k} \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right) \\
D_{j,j+1}^i &= -2c_K\beta_i \frac{1}{\sigma_k \delta_k} \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right)
\end{align*}
\]

These equations confirm that \( D^s \) is indeed a symmetric matrix.

As it was shown in Sec. 4.6, in the same asymptotic limit matrix \( \tilde{\mathbf{B}} \) reduces to a tridiagonal matrix to within rapidly exponentially vanishing terms beyond the first off-diagonal. The asymptotic expressions for the elements in the tridiagonal block of matrix \( \tilde{\mathbf{B}} \) are hereby summarized using the definition of the \( \beta_i \) parameter to simplify the ensuing comparison with the expressions for the corresponding elements of matrix \( D^s \).

\[
\begin{align*}
\tilde{B}_{1,1} &= \frac{1}{2} c_k^2 (1 - c_k) \sigma_k \delta_k c_N \sigma_N \delta_N + \frac{3}{2} \beta c_k^3 c_N \sigma_N \delta_N \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right) \\
\tilde{B}_{1,2} &= -\beta c_k^2 c_N \sigma_N \delta_N \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right) \\
\tilde{B}_{j,j} &= c_N \sigma_N \delta_N \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right), \quad 2 \leq j \leq (J - 2) \quad j \text{ even} \\
\tilde{B}_{j,j+1} &= \tilde{B}_{j,j-1} = -\frac{c_k}{2} c_N \sigma_N \delta_N \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right)
\end{align*}
\]
\[
\begin{aligned}
\tilde{B}_{j,j} &= \frac{1}{2} c_k^2 (1-c_k) \sigma_k \delta_k c_n \sigma_n \delta_n + 2 \beta \delta c_k c_n \sigma_n \delta_n \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right) \\
\tilde{B}_{j,j+1} &= \tilde{B}_{j,j-1} = -\beta \delta c_k c_n \sigma_n \delta_n \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right)
\end{aligned}
\]

(5.49)

\[3 \leq j \leq (J-1) \text{ \ j odd}\]

\[
\begin{aligned}
\tilde{B}_{j,j} &= c_n \sigma_n \delta_n \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right) \\
\tilde{B}_{j,j-1} &= -\frac{c_k}{2} c_n \sigma_n \delta_n \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right)
\end{aligned}
\]

(5.50)

As stressed in Sec. 4.6 the \(\tilde{B}\) matrix is also in general non-symmetric. In view of the comparison with \(D^s\) it is convenient to symmetrize \(\tilde{B}\) following the same procedure used to obtain \(D^s\) from \(D\). This is accomplished by multiplying the equations for an N cell by the ratio of the off-diagonal element for a K cell to the off-diagonal element of an N cell in the \(\tilde{B}\) matrix. In the asymptotic limit as \(\Delta \to \infty\) this ratio reduces to:

\[
\frac{-\beta \delta c_k c_n \sigma_n \delta_n \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right)}{-\frac{c_k}{2} c_n \sigma_n \delta_n \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right)} = 2c_k \beta + O\left(\frac{1}{\Delta}\right)
\]

(5.51)

Indicating with \(\tilde{B}^s\) the symmetrized \(\tilde{B}\) matrix obtained through the aforementioned transformation, the asymptotic expressions obtained for the elements in the tridiagonal block of \(\tilde{B}^s\) are the following:
\[
\begin{align*}
\tilde{B}^s_{i,j} &= \frac{1}{2} c_K^2 \left( 1 - c_K \right) \sigma_K \delta_K \left( c_N \sigma_N \delta_N \right) + \frac{3}{2} \beta_j c_K^2 c_n \sigma_N \delta_N \frac{1}{\Delta} + O \left( \frac{1}{\Delta^2} \right) \\
\tilde{B}^s_{i,i+1} &= -\beta_j c_K^2 \left( c_N \sigma_N \delta_N \right) \frac{1}{\Delta} + O \left( \frac{1}{\Delta^2} \right) 
\end{align*}
\]
(5.52)

\[
\begin{align*}
\tilde{B}^s_{j,j} &= 2\beta_j c_K \left( c_N \sigma_N \delta_N \right) \frac{1}{\Delta} + O \left( \frac{1}{\Delta^2} \right) \\
\tilde{B}^s_{j,j+1} &= -\beta_j c_K^2 \left( c_N \sigma_N \delta_N \right) \frac{1}{\Delta} + O \left( \frac{1}{\Delta^2} \right) 
\end{align*}
\]
(5.53)

\[
\begin{align*}
\tilde{B}^s_{j,j} &= \frac{1}{2} c_K^2 \left( 1 - c_K \right) \sigma_K \delta_K \left( c_N \sigma_N \delta_N \right) + 2\beta_j c_K^3 \left( c_N \sigma_N \delta_N \right) \frac{1}{\Delta} + O \left( \frac{1}{\Delta^2} \right) \\
\tilde{B}^s_{j,j+1} &= -\beta_j c_K^2 \left( c_N \sigma_N \delta_N \right) \frac{1}{\Delta} + O \left( \frac{1}{\Delta^2} \right) 
\end{align*}
\]
(5.54)

\[
\begin{align*}
3 \leq j \leq (J - 1) & \quad j \text{ odd} \n\end{align*}
\]

Finally, before making a comparison with \( D^s \) it is convenient to rescale matrix \( \tilde{B}^s \) by multiplying its elements by the factor:
Indicating the rescaled matrix with the symbol $\tilde{B}^{s*}$, the following asymptotic expressions hold for the elements in the tridiagonal block of this matrix:

$$
\tilde{B}_{ij}^{s*} = c_K (1 - c_K) + 3 \beta_i c_k^2 \frac{1}{\sigma_k} \frac{1}{\delta_k \Delta} + O\left(\frac{1}{\Delta^2}\right)
$$

(5.57)

$$
\tilde{B}_{i,2}^{s*} = -2 \beta_i c_k \frac{1}{\sigma_k} \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right)
$$

(5.58)

$$
\tilde{B}_{j,j}^{s*} = 4 \beta_i \frac{1}{\sigma_k} \frac{1}{\delta_k \Delta} + O\left(\frac{1}{\Delta^2}\right)
$$

(5.59)

(5.60)
It is noted that both the transformations from $\tilde{B}$ to $\tilde{B}^s$ and from $\tilde{B}^s$ to $\tilde{B}^{s*}$ do not modify the exponential decay as $\Delta \to \infty$ of the elements beyond the first off-diagonal originally present in $\tilde{B}$. Therefore matrix $\tilde{B}^{s*}$ still approaches a tridiagonally dominated structure at a fast exponential rate in the asymptotic limit as $\Delta \to \infty$. It is also evident that if the same transformations are applied to both sides of Eq. (4.181) the original fluxes $\bar{\phi}^{s*}$ remain invariant. Therefore, matrix $\tilde{B}^{s*}$ is a legitimate representation of the integral transport matrix.

A comparison of the asymptotic expressions for the elements of $D^s$, Eqs. (5.43) through (5.46), with the corresponding ones for the elements of $\tilde{B}^{s*}$, Eqs. (5.57) through (5.60), leads to the following conclusions, depending on various possible combinations of the scattering ratios $c_k$ and $c_N$.

\[
D^s = \tilde{B}^{s*} + O\left(\frac{1}{\Delta^2}\right), \quad c_k = c_N = 1
\]  

(5.61)

\[
D^s = \tilde{B}^{s*} + O\left(\frac{1}{\Delta}\right), \quad c_k < 1, \quad c_N \leq 1
\]  

(5.62)

\[
D^s \neq \tilde{B}^{s*}, \quad c_k = 1, \quad c_N < 1
\]  

(5.63)

In the cases in which $c_k = 1$, matrix $\tilde{B}^{s*}$ acquires a tridiagonal structure still characterized by a diffusion-like coupling stencil, in the asymptotic limit. If also $c_N = 1$, the elements of $\tilde{B}^{s*}$ and $D^s$ are coincident, in the limit, up to the $O(\Delta^{-1})$ terms and may
differ for terms that are $O(\Delta^{-2})$, as indicated in Eq. (5.61). If instead $c_k = 1$ but $c_N < 1$, the terms that are $O(\Delta^0)$ in the two matrices are exact zeroes and equality of their tridiagonal blocks to within $O(\Delta^{-1})$ terms is lost. In fact, as evident from a comparison of Eq. (5.46) with Eq. (5.60), the diagonal elements pertaining to the last cell are different because of the presence of $c_N$ in Eq. (5.46). Hence the result reported in Eq. (5.63).

Finally, the result in Eq. (5.62) requires some explanation. When $c_k$ is less than unity both $D^s$ and $\tilde{B}^s*$ are to leading order dominated by the $O(\Delta^0)$ terms in the diagonal elements pertaining to the thick cells. If the elements of $\tilde{B}^s*$ pertaining to the thick cells are rescaled by dividing them by $c_k$, then equality of $D^s$ and $\tilde{B}^s*$ is regained within the leading $O(\Delta^0)$ terms, in the limit.

The analytic results in Eqs. (5.61) through (5.63) may help in reading the results reported in Table 5.6. These results have been obtained for a unit value of the $\delta_k$, $\delta_N$, $\sigma_k$ and $\sigma_N$ parameters. The slab is subdivided in six computational cells with a unit value of the macroscopic total cross-section, using the $S_6$ symmetric quadrature and a value of $10^{-4}$ for the convergence parameter $\epsilon$. A uniform unit source drives the problem and is scaled as $\Delta^{-1}$ in the thick cells containing a purely scattering material.

The results in Table 5.6 are obtained in the asymptotic regime considering two very large values of the $\Delta$ parameter. It is noted that convergence in two iterations is obtained for the case in which both $c_k$ and $c_N$ have a unit value. In the other cases convergence is achieved within more than two iterations, the worst case being the one in
which \( c_k = 1 \) while \( c_n < 1 \). The latter case corresponds to Eq. (5.63) and interestingly enough the greatest error in the convergence test performed at the end of the iterations is always in the right-most cell from the second iteration to the eleventh (and last) one. It was noted previously that the result in Eq. (5.63) is due to the fact that the diagonal elements pertaining to the right-most cell are actually different for \( \tilde{B}^{S*} \) and \( D^S \), because of the presence of \( c_n \) in Eq. (5.46).

### Table 5.6: Number of AP accelerated iterations for a periodically heterogeneous slab for very large \( \Delta \)

<table>
<thead>
<tr>
<th>( c_k )</th>
<th>( c_n )</th>
<th>( \Delta )</th>
<th># of iterations</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>1.0</td>
<td>( 10^5 )</td>
<td>2</td>
</tr>
<tr>
<td>1.0</td>
<td>1.0</td>
<td>( 10^6 )</td>
<td>2</td>
</tr>
<tr>
<td>0.8</td>
<td>0.8</td>
<td>( 10^5 )</td>
<td>3</td>
</tr>
<tr>
<td>0.8</td>
<td>0.8</td>
<td>( 10^6 )</td>
<td>3</td>
</tr>
<tr>
<td>0.8</td>
<td>0.5</td>
<td>( 10^5 )</td>
<td>3</td>
</tr>
<tr>
<td>0.8</td>
<td>0.5</td>
<td>( 10^6 )</td>
<td>3</td>
</tr>
<tr>
<td>1.0</td>
<td>0.5</td>
<td>( 10^5 )</td>
<td>11</td>
</tr>
<tr>
<td>1.0</td>
<td>0.5</td>
<td>( 10^6 )</td>
<td>11</td>
</tr>
</tbody>
</table>

A possible modification to the AP formalism that restores convergence in two iterations for all possible scattering ratio combinations in the asymptotic limit is presented in the following. Once again, the idea is that of restoring the equality of \( D^S \) to \( \tilde{B}^{S*} \) in the asymptotic limit up to terms that are \( O(\Delta^{-1}) \).

A procedure that allows obtaining the desired result starts by modifying Eqs. (5.6) through Eq. (5.8) for the construction of the elements of the \( D \) matrix in the case of a periodically heterogeneous slab. The modified equations for the internal cells are:
The modification consists of the division by \( c_k \) of the diagonal elements pertaining to an \( N \) cell in Eq. (5.64) and in the multiplication by \( c_k \) of the diagonal elements pertaining to a \( K \) cell in Eq. (5.65).

Similarly, the modified equations for the boundary cells become:

\[
\begin{align*}
\overline{D}_{j,1} & = c_k \left[ (1-c_k) + D_o^{+j} + D_o^{-j} \right] \\
\overline{D}_{j,2} & = -D_o^{+j} \\
\overline{D}_{j,j+1} & = -D_o^{+j} \quad , \quad 2 \leq j \leq (J-2) \quad j \text{ even} \\
\overline{D}_{j,j-1} & = -D_o^{+j}
\end{align*}
\]  

(5.65)

\[
\begin{align*}
\overline{D}_{j,j} & = \frac{1}{c_k} \left[ (1-c_N) + D_o^{+j} + D_o^{-j} \right] \\
\overline{D}_{j,(J-1)} & = -D_o^{-j}
\end{align*}
\]  

(5.67)

The following modified definition is proposed for the \( \Gamma \) coefficients used to formulate the boundary equations.

\[
\Gamma_i = \frac{D_i \sigma_i \Delta x_i}{\beta_i \overline{\gamma}_l} - 1, \quad l = K, N
\]  

(5.68)
The new $\Gamma$ coefficients are formally identical to the original $\Gamma$ coefficients, except that they are based on the following definition:

$$\overline{\gamma}_l = c_K, \quad l = K, N \quad (5.69)$$

The modifications introduced in Eqs. (5.64) through (5.69) yield a modified matrix $\overline{D}^8$ with the desired properties. First of all, due to the modified definition in Eq. (5.69), the following asymptotic behavior results for the $(1-\Gamma)$ coefficients for a $K$ and an $N$ cell:

$$(1-\Gamma_K) = 1 + O\left( e^{-\frac{\sigma_K \delta_N \Delta}{\mu_{\text{max}}}} \right) \quad (5.70)$$

$$(1-\Gamma_N) = 2 \frac{\beta_I}{\beta_{II}} \frac{c_K}{c_N} \sigma_N \delta_N \frac{1}{\Delta} + O\left( \frac{1}{\Delta^2} \right) \quad (5.71)$$

By virtue of the latter results, when the modified recipe is applied and the resulting matrix is symmetrized in the usual fashion, the elements of the new matrix $\overline{D}^8$ acquire the following expressions in the asymptotic limit:

$$\begin{align*}
\bar{D}_{1,1}^8 & = c_K (1-c_K) + 3c_K^2 \beta_I \frac{1}{\sigma_K \delta_K} \frac{1}{\Delta} + O\left( \frac{1}{\Delta^2} \right) \\
\bar{D}_{1,2}^8 & = -2c_K \beta_I \frac{1}{\sigma_K \delta_K} \frac{1}{\Delta} + O\left( \frac{1}{\Delta^2} \right)
\end{align*}$$

(5.72)
The expression in Eq. (5.72) is a consequence of Eqs. (5.66) and (5.70). The expressions in Eqs. (5.73) and (5.74) are a consequence of Eqs. (5.64) and (5.65) respectively. Finally the result in Eq. (5.75) derives from Eqs. (5.67) and (5.71).

Comparison of the asymptotic expressions in Eqs. (5.72) through Eq. (5.75), for the elements of $\bar{D}^s$, with the expressions in Eqs. (5.57) through (5.60), for the corresponding elements of $\hat{B}^{s*}$, leads to the following conclusion:

$$\bar{D}^s = \hat{B}^{s*} + O\left(\frac{1}{\Delta^2}\right), \quad c_k, c_N \leq 1$$ (5.76)
Preliminary numerical testing of the AP formalism based on the modified recipe indicates that, in order to restore convergence in two iterations for all possible combinations of $c_k$ and $c_N$, it is also necessary to introduce a modified matrix $\overline{C}$. A possible choice based on numerical testing is the following:

$$\overline{C}_{j,j} = c_k, \quad j = 1, \ldots, J$$  \hspace{1cm} (5.77)

It is noted that the expression in Eq. (5.77) may be obtained from Eq. (5.11) by using the new $\overline{\gamma}$ coefficients in place of the original $\gamma$ coefficients. It is therefore an easy modification of the original AP formalism to implement and still leads to a suitable diagonal matrix while improving the results shown in Table 5.6.

That Eq. (5.76) alone is not necessarily sufficient to restore immediate convergence in the asymptotic limit appears clear considering Eq. (1.21) in its fully discretized form. The exact solution is to be expected if the exact $A$ and $B$ matrices are utilized. Therefore not only should $D$ limit to $B$ in the asymptotic limit of interest, but $C$ should also approach the exact $A$ in the same limit. The vast majority of synthetic acceleration schemes utilize a diagonal approximation for $A$ that somehow corresponds to the physical intuition that the “scattering residual” should be a cell-based quantity. For this reason, more effort has been invested in the previous chapters, as well as in this chapter, in the study of the asymptotic properties of the $B$ matrix and of its equivalent representations for periodically heterogeneous structures than in the study of $A$. A similar study could be performed for the $A$ matrix and its equivalent representations, obtained applying the same transformations that have been introduced at various stages for $B$, and
would eventually indicate or justify analytically a certain choice for a low-order
approximation $\mathbf{C}$ to the $\mathbf{A}$ matrix.

When the further modification to the AP formalism presented in Eq. (5.77) is
implemented numerically, the results reported in Tables 5.7 through 5.10 are obtained,
using the same parameter settings used for Table 5.6.

**Table 5.7: Number of modified AP accelerated iterations and scalar flux residual at the
second iteration for the case $c_k = 1.0$ and $c_N = 1.0$.**

<table>
<thead>
<tr>
<th>$\Delta$</th>
<th># of iterations</th>
<th>Residual @ 2nd iteration</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^0$</td>
<td>4</td>
<td>$1.387 \times 10^{-2}$</td>
</tr>
<tr>
<td>$10^1$</td>
<td>4</td>
<td>$1.261 \times 10^{-2}$</td>
</tr>
<tr>
<td>$10^2$</td>
<td>3</td>
<td>$1.577 \times 10^{-3}$</td>
</tr>
<tr>
<td>$10^3$</td>
<td>3</td>
<td>$1.613 \times 10^{-4}$</td>
</tr>
<tr>
<td>$10^4$</td>
<td>2</td>
<td>$1.616 \times 10^{-5}$</td>
</tr>
<tr>
<td>$10^5$</td>
<td>2</td>
<td>$1.617 \times 10^{-6}$</td>
</tr>
<tr>
<td>$10^6$</td>
<td>2</td>
<td>$1.606 \times 10^{-7}$</td>
</tr>
</tbody>
</table>

**Table 5.8: Number of modified AP accelerated iterations and scalar flux residual at the
second iteration for the case $c_k = 0.8$ and $c_N = 0.8$.**

<table>
<thead>
<tr>
<th>$\Delta$</th>
<th># of iterations</th>
<th>Residual @ 2nd iteration</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^0$</td>
<td>9</td>
<td>$2.557 \times 10^{-1}$</td>
</tr>
<tr>
<td>$10^1$</td>
<td>4</td>
<td>$6.846 \times 10^{-2}$</td>
</tr>
<tr>
<td>$10^2$</td>
<td>3</td>
<td>$4.340 \times 10^{-3}$</td>
</tr>
<tr>
<td>$10^3$</td>
<td>2</td>
<td>$3.965 \times 10^{-4}$</td>
</tr>
<tr>
<td>$10^4$</td>
<td>2</td>
<td>$3.926 \times 10^{-5}$</td>
</tr>
<tr>
<td>$10^5$</td>
<td>2</td>
<td>$3.922 \times 10^{-6}$</td>
</tr>
<tr>
<td>$10^6$</td>
<td>2</td>
<td>$3.923 \times 10^{-7}$</td>
</tr>
</tbody>
</table>
Table 5.9: Number of modified AP accelerated iterations and scalar flux residual at the second iteration for the case \( c_K = 0.8 \) and \( c_N = 0.5 \).

<table>
<thead>
<tr>
<th>( \Delta )</th>
<th># of iterations</th>
<th>Residual @ 2(^{nd}) iteration</th>
</tr>
</thead>
<tbody>
<tr>
<td>10(^0)</td>
<td>9</td>
<td>5.308\times10^{-1}</td>
</tr>
<tr>
<td>10(^1)</td>
<td>4</td>
<td>4.957\times10^{-3}</td>
</tr>
<tr>
<td>10(^2)</td>
<td>3</td>
<td>6.763\times10^{-4}</td>
</tr>
<tr>
<td>10(^3)</td>
<td>2</td>
<td>6.991\times10^{-5}</td>
</tr>
<tr>
<td>10(^4)</td>
<td>2</td>
<td>7.015\times10^{-6}</td>
</tr>
<tr>
<td>10(^5)</td>
<td>2</td>
<td>7.017\times10^{-7}</td>
</tr>
<tr>
<td>10(^6)</td>
<td>2</td>
<td>7.018\times10^{-8}</td>
</tr>
</tbody>
</table>

Table 5.10: Number of modified AP accelerated iterations and scalar flux residual at the second iteration for the case \( c_K = 1.0 \) and \( c_N = 0.5 \).

<table>
<thead>
<tr>
<th>( \Delta )</th>
<th># of iterations</th>
<th>Residual @ 2(^{nd}) iteration</th>
</tr>
</thead>
<tbody>
<tr>
<td>10(^0)</td>
<td>11</td>
<td>6.226\times10^{-1}</td>
</tr>
<tr>
<td>10(^1)</td>
<td>5</td>
<td>5.502\times10^{-2}</td>
</tr>
<tr>
<td>10(^2)</td>
<td>3</td>
<td>5.894\times10^{-3}</td>
</tr>
<tr>
<td>10(^3)</td>
<td>3</td>
<td>5.938\times10^{-4}</td>
</tr>
<tr>
<td>10(^4)</td>
<td>2</td>
<td>5.943\times10^{-5}</td>
</tr>
<tr>
<td>10(^5)</td>
<td>2</td>
<td>5.944\times10^{-6}</td>
</tr>
</tbody>
</table>

The results contained in all four tables, in terms of number of iterations, confirm that the proposed modification of the AP formalism restores convergence in two iterations in the asymptotic limit for all four combinations of \( c_K \) and \( c_N \) originally considered in Table 5.6.

As done previously in Sec. 5.3, the residual in the second iteration has also been reported in Tables 5.7 through 5.10. It is noted that in all four cases the residual appears to decrease as \( \Delta^{-1} \). Further analysis would be required to eventually relate this result to
the analytical conclusion obtained in Eq. (5.76), and more generally to determine what relation exists between order of convergence of the preconditioner structure to the structure of the integral transport matrix and order of decrease of the residual, in the asymptotic limit. The presence of potential numerical precision issues in the numerical implementation should also be investigated since they may easily lead to a degradation of the order from $O\left(\Delta^{-2}\right)$ to $O\left(\Delta^{-1}\right)$ in the evaluation of the residual. In any case, it is explicitly pointed out that the result in Eq. (5.76) implies that exponential convergence, characteristic of the homogeneous case, is not attainable in the periodically heterogeneous case.

5.5 Conclusion

An asymptotic analysis has been conducted for the elements of the diffusive Adjacent-cell Preconditioner (AP) matrix $D$ both in the thick cell limit for a homogeneous slab with uniform spatial mesh and in the asymptotic limit introduced in Ch. 4 for periodically heterogeneous slabs. In both cases the resulting expressions for the elements of the $D$ matrix have been contrasted with the expressions obtained in the same asymptotic limits for the elements of the integral transport matrix.

The results of this comparison have indicated that the $D$ matrix is asymptotically capable to exactly capture the structure acquired by the integral transport matrix in all the limits in which the latter acquires a diffusive structure, namely homogeneous slabs and periodically heterogeneous slabs in which both the thick and the thin layer host a purely scattering material ($c_N = c_K = 1$). This comes as no surprise considering that the $D$ matrix
is inherently constructed to be a diffusive matrix, while the integral transport matrix acquires in general a non-diffusive stencil for periodically heterogeneous slabs containing absorbing materials.

These results provide an understanding of the immediate convergence behavior, namely convergence in two iterations, displayed by the AP acceleration scheme in the asymptotic limit for slabs hosting purely scattering materials, both in the homogeneous and periodically heterogeneous case. For periodically heterogeneous slabs containing absorbing materials, immediate convergence has been restored by amending the recipe for the construction of the $D$ matrix so that the correct asymptotic structure of the integral transport matrix is matched by the AP preconditioner in the asymptotic limit.

It is noted that the proposed modification has been more intended to explore the effect of replicating the correct structure of the integral transport operator in an acceleration scheme in limits of interest, by introducing simple modifications to the existing AP acceleration scheme, than for the interest of systematically modifying the AP formalism. In particular it was desired to test, as successfully done in this chapter, the expectation expressed in Ch. 1 that immediate convergence can be obtained in an asymptotic limit in which the low-order operator $M$, in this case the AP preconditioner, exactly limits to the integral transport operator.

The results presented in this chapter provide insight into the excellent convergence properties of diffusion-based acceleration schemes in one-dimensional transport problems and at the same time illustrate the potential benefit from using the integral transport matrix in devising novel synthetic acceleration schemes. Since existing acceleration schemes like AP and DSA have proven to be successful in treating highly
heterogeneous problems in slab geometry, the introduction of a novel acceleration scheme does not appear necessary in slab geometry. Therefore, the discussion of a novel acceleration scheme based on the integral transport matrix is deferred to the next chapters, in which the asymptotic properties of the integral transport matrix are studied in two-dimensional geometry.
Chapter 6

Integral Transport Matrix in Homogeneous Configurations in Two-Dimensional Geometry

6.1 Introduction

In this chapter, the study of the asymptotic properties of the integral transport matrix is extended to homogeneous configurations in two-dimensional geometry. First, exact analytic expressions are derived for the elements of the $B$ matrix that couple the cell-averaged scalar flux in cell $(i, j)$ with itself (self-coupling) and with the cell-averaged scalar fluxes in the first and second neighboring cells, with reference to the three-by-three two-dimensional Cartesian sub-mesh shown in Fig. 6.1. The derivation of these matrix elements is instrumental in devising a quantitative investigation of the strength of coupling of a cell’s average scalar flux to the scalar fluxes in its neighboring cells. Specifically, it is desired to study the strength of coupling as a function of computational-cell size and material properties in various asymptotic limits for homogeneous and periodically heterogeneous configurations in two-dimensional geometry. The results of the asymptotic analysis for homogeneous configurations are presented in this chapter while those referring to periodically heterogeneous configurations are discussed in the next chapter.

The same approach followed in Ch. 3 for slab geometry is extended here to two dimensions for obtaining the elements of the discrete transport operator. The three-by-
three spatial sub-mesh considered in Fig. 6.1 represents a simple setting for the construction effort, yet it also contains all the elements of interest in the analysis. In fact, as pointed out in Sec. 1.3, it is desired to investigate the strength of coupling of the cell-averaged scalar flux in cell \((i, j)\) to the scalar flux in its first diagonal neighbor, cell \((i+1, j+1)\). In the following we shall also refer to this coupling as cross-derivative coupling. Specifically, it is desired to contrast the strength of cross-derivative coupling to the strength of coupling of the cell-averaged scalar flux in cell \((i, j)\) with the scalar fluxes in its first Cartesian neighbors, cells \((i+1, j)\) and \((i, j+1)\). It has been shown earlier [20] that the latter elements are of the same order as the self-coupling elements on the diagonal of the transport matrix in the thick cell limit.

<table>
<thead>
<tr>
<th></th>
<th>((i, j + 2))</th>
<th>((i + 1, j + 2))</th>
<th>((i + 2, j + 2))</th>
</tr>
</thead>
<tbody>
<tr>
<td>((i, j + 1))</td>
<td>((i + 1, j + 1))</td>
<td>((i + 2, j + 1))</td>
<td></td>
</tr>
<tr>
<td>((i, j))</td>
<td>((i + 1, j))</td>
<td>((i + 2, j))</td>
<td></td>
</tr>
</tbody>
</table>

Fig. 6.1: A three-by-three two-dimensional Cartesian sub-mesh.
The asymptotic limits of interest for homogeneous two-dimensional configurations are a thick cell diffusive limit and a thin cell limit. The thick cell limit is obtained by scaling the size of a computational cell in the \( x \) and \( y \) directions, \( \Delta x \) and \( \Delta y \) respectively, as a dimensionless parameter \( \Delta \) times the appropriate length units and forming the limit of the matrix elements as \( \Delta \to \infty \). Similarly the thin cell limit is obtained by scaling \( \Delta x \) and \( \Delta y \) through a dimensionless parameter \( \delta \) and forming the limit of the matrix elements as \( \delta \to 0 \). Even for the two-dimensional case, the elements of matrix \( B \) are, in general, dependent on the product of a computational cell’s size in the \( x \) (\( y \)) direction and macroscopic total cross-section. In other words the elements of the \( B \) matrix depend on the optical thickness of the cell in the \( x \) (\( y \)) direction expressed in mean free paths. Therefore scaling the geometric cell widths is in the end equivalent to scaling the total cross-section alone or both parameters simultaneously.

For both limits, exact asymptotic expressions are obtained for the elements of the integral transport matrix coupling a cell-averaged scalar flux with the fluxes in neighboring cells up to the second neighbors. For cells beyond second neighbors estimates are obtained for the leading asymptotic order of the matrix elements relative to the cells’ optical thickness. The asymptotic estimates are verified by numerical tests.

The results obtained in the thick cell limit for homogeneous configurations show that elements pertaining to self-coupling and coupling with the first Cartesian neighbors are of the same order, satisfy a diffusion-like coupling stencil and dominate all other matrix elements in the optically thick cell limit. In particular, cross-derivative coupling with the first diagonal neighbors is of higher-order in the cell optical thickness. The
existence of this low-order five-banded approximation of the integral transport matrix points to a strong local coupling of a cell with its first Cartesian neighbors. It also provides further insight into the excellent convergence properties of diffusion based acceleration schemes in two-dimensional homogeneous configurations characterized by low absorption, in the optically thick cell limit.

Finally, the results obtained in the thin cell limit for homogeneous configurations indicate that the matrix acquires a diagonally dominated structure. In fact, similarly to what was pointed out for the one-dimensional case, the integral transport matrix tends to the identity matrix in this asymptotic limit. Also, the matrix elements outside the diagonal stripe have, in general, the same asymptotic behavior, since they are all \( O(\delta) \).

Differently from the one-dimensional case, though, the coefficient multiplying \( \delta \) in the leading order contribution is not the same for all the elements outside the diagonal stripe.

An outline of the chapter follows. The direct solution of the transport equation in its integral form for two-dimensional geometry is illustrated in Sec. 6.2. General analytic expressions for the elements of the matrix coupling a cell’s average flux with the fluxes in neighboring cells up to the second neighbors are derived in Sec. 6.3. A recursive algorithm for the numeric computation of the integral transport matrix is illustrated in Sec. 6.4. This algorithm has been coded and used in the numerical verification of the theoretically predicted asymptotic behavior of the matrix elements. The expressions acquired by the elements of the matrix in the homogeneous, uniform-mesh case are obtained in Sec. 6.5. The results of the asymptotic analysis in the thick cell limit and in
the thin cell limit are derived in Secs. 6.6 and 6.7, respectively. Finally, Sec. 6.8 contains some concluding remarks.

6.2 Direct Solution of the Transport Equation in Two-Dimensional Geometry

The construction of the matrix elements of the integral transport operator has been carried out using as a starting point the Source Iteration (SI) formulation. The governing equations comprise the three sets of equations constituting the Weighted Diamond Difference (WDD) spatially-discretized form of the one-group, steady-state, discrete ordinates approximation of the neutron transport equation in two-dimensional Cartesian geometry. As in the direct solution of the transport equation in slab geometry outlined in Sec. 3.2, a non-multiplying system with isotropic scattering and isotropic fixed source is also assumed in two-dimensional geometry.

The first set of equations represents a per cell statement of the balance of sources and sinks of neutrons that, in the most basic iterative approach to the solution of the transport equation, namely SI, may be expressed in the following form:

$$\kappa_{m,i,j} \left( \tilde{\psi}_{m,i,j}^{(f+1)} - \tilde{\psi}_{m,i,j}^{(f+1)} \right) + V_{m,i,j} \left( \psi_{m,i,j}^{(f+1)} - \psi_{m,i,j}^{(f+1)} \right) + \psi_{m,i,j}^{(f+1)} = c_{i,j} \tilde{\theta}_{i,j}^{(f)} + s_{i,j} \quad (6.1)$$

In these equations, \( \tilde{\theta}_{i,j}^{(f)} \) and \( \psi_{m,i,j}^{(f+1)} \) are the previous and present iterate of the scalar flux and \( m^{\text{th}} \) discrete ordinate angular flux averaged over cell \((i,j)\), respectively; \( \psi_{m,i,j}^{(f+1)} \) and \( \psi_{m,i,j}^{(f+1)} \) are the present iterate of the edge-averaged \( m^{\text{th}} \) angular flux, evaluated on the \( y \) \((x)\) equal to constant outgoing and incoming edge of
the cell, respectively; \( s_{i,j} = q_{i,j} / \sigma_{i,j} \) is the ratio of the fixed neutron source density averaged over cell \((i,j)\) to the macroscopic total cross-section in cell \((i,j)\); the macroscopic scattering cross-section for cell \((i,j)\) will be indicated by the symbol \( \sigma_{S_{i,j}} \) and \( c_{i,j} \) represents the scattering ratio, \( \sigma_{S_{i,j}} / \sigma_{i,j} \), for cell \((i,j)\); \( \kappa_{m,i,j} \) has been introduced to denote the reciprocal of the optical thickness of cell \((i,j)\) along the \( x \) coordinate:

\[
\kappa_{m,i,j} \equiv \left( \frac{\sigma_{i,j} \Delta x_i}{|\mu_m|} \right)^{-1}
\]  

(6.2)

In the previous relation \( \mu_m \) is the direction cosine of the \( m \)th discrete ordinate with respect to the \( x \) coordinate; \( \Delta x_i \) is the size of computational cell \((i,j)\) along the \( x \) coordinate. Analogously, \( \nu_{m,i,j} \) has been introduced to denote the reciprocal of the optical thickness of cell \((i,j)\) along the \( y \) coordinate:

\[
\nu_{m,i,j} \equiv \left( \frac{\sigma_{i,j} \Delta y_j}{|\eta_m|} \right)^{-1},
\]  

(6.3)

where \( \eta_m \) is the direction cosine of the \( m \)th discrete ordinate with respect to the \( y \) coordinate; \( \Delta y_j \) is the size of computational cell \((i,j)\) along the \( y \) coordinate.

Equation (6.1) is exact in the sense that it is obtained by direct integration of the continuous transport equation and using standard definitions of the edge- and cell-averaged fluxes and source. The terms on the left hand side of Eq. (6.1) represent the loss of neutrons from cell \((i,j)\) by streaming and collisions, while the terms on the right hand
side represent the sources from isotropic scattering, and external fixed sources, respectively.

The second set of equations in a generic WDD form of the discrete-variable transport equation provides an additional weighted-difference relation between the cell- and edge-averaged flux variables along the \( x \) coordinate:

\[
\psi^{(+)}_{m,i,j} = \left( \frac{1 + \alpha_{m,i,j}}{2} \right) \psi_{m,i,j} + \left( \frac{1 - \alpha_{m,i,j}}{2} \right) \psi_{m,i,j}
\]  

(6.4)

The dependence of the spatial weights \( \alpha_{m,i,j} \in [0,1] \) on the problem parameters is determined by the formalism of the underlying numerical spatial discretization method or simplifying assumptions applied directly to Eq. (6.4). Consistent with the treatment that has been carried out for slab geometry in the previous chapters, the results that will be presented in the following have been obtained using the Arbitrarily High Order Transport method of the Nodal type and 0-order spatial approximation (AHOT-N0). It is recalled that this is the lowest spatial-expansion order member of a class of spatial discretization methods whose order denotes the truncation order of the Legendre spatial-expansion of the flux within each cell, and in multi-dimensional cases on cell edges also [3]. In analogy to Eq. (1.25), the spatial weights for the AHOT-N0 method along the \( x \) coordinate are given by:

\[
\alpha_{m,i,j} = \coth \left( \frac{1}{2 \kappa_{m,i,j}} \right) - 2 \kappa_{m,i,j}
\]  

(6.5)

Finally, the third set of equations in the WDD form of the discrete-variable transport equation provides the additional weighted-difference relation between the cell- and edge-averaged flux variables along the \( y \) coordinate. This equation is needed in order
to obtain a closed system of equations in the variables introduced in the two-dimensional
discrete transport calculation and is expressed as follows:

\[
\psi^{(i+1)}_{m,i,j} = \left(1 + \frac{\beta_{m,i,j}}{2}\right)\psi^{\alpha^{(i+1)}}_{m,i,j} + \left(1 - \frac{\beta_{m,i,j}}{2}\right)\psi^{\beta^{(i+1)}}_{m,i,j}, \tag{6.6}
\]

where the spatial weights \(\beta_{m,i,j} \in [0,1]\) for the AHOT-N0 along the \(y\) coordinate are:

\[
\beta_{m,i,j} = \coth\left(\frac{1}{2v_{m,i,j}}\right) - 2v_{m,i,j} \tag{6.7}
\]

In Eqs. (6.1) through (6.7) the cell index \(i (j)\) varies from 1 to \(I (J)\), where \(I (J)\) is the number of computational cells along the \(x (y)\) coordinate. The discrete ordinate index \(m\) varies from 1 to \(M\), the number of discrete ordinates in the level symmetric \(S_N\) quadrature \(\{\mu_m, \eta_m, w_m\}\), where \(w_m\) are the quadrature weights [11].

It is noted that, in two-dimensional Cartesian geometries, the mirror symmetry of the angular flux about the plane formed by the \(x\) and \(y\) coordinates reduces to four the number of octants over which the angular dependence of the angular flux must be determined in the general three-dimensional case. Since a level symmetric quadrature satisfies reflective conditions across the \(x-z\) and \(y-z\) planes, only one octant needs actually be considered. Considering the octant characterized by \(x > 0\) and \(y > 0\) to fix ideas, if \((\mu_m, \eta_m)\) with \(\mu_m, \eta_m > 0\) specifies a direction in this octant then the ordinates for the other three octants are obtained by changing the signs of one or both direction cosines. The ordinate directions in a level symmetric \(S_N\) quadrature are also invariant to 90° rotations about any axis since they utilize the same set of \(N/2\) positive values of the
direction cosines with respect to each of the axes, namely $\mu_m = \eta_m$ for $m=1,\ldots,N/2$.

Quadratures in the $N/2$ positive $\mu_m$ are referred to as $S_N$ quadratures, for if the flux becomes dependent only on the direction cosine with respect to one coordinate axis, they reduce to the quadrature with $N$ ordinates introduced in Sec. 3.2 for slab geometry. There are $N(N+2)/8$ discrete ordinates per octant, therefore $M = N(N+2)/2$ is the total number of directions in the four octants in an $x$-$y$ geometry $S_N$ approximation with a symmetric quadrature set. The quadrature weights are also determined considering the octant with $\mu_m > 0$ and $\eta_m > 0$, and are usually normalized to one over the directions within this octant [11]. In the following, largely as a matter of convenience, the weights will be assumed to be renormalized to 1/4 per quadrant, so that the following normalization condition holds over the $M$ total directions considered in the two-dimensional problem:

$$\sum_{m=1}^{M} w_m = 1 \quad (6.8)$$

The level symmetric conditions require that all of the weights must be equal for directions in an octant obtained by permuting the direction cosines. In the numerical results presented in this and the next chapters, this condition is in particular met by employing level symmetric quadratures with equal weights, namely $w_m = w = 1/M$ for all $m$.

The solution of Eqs. (6.1), (6.4) and (6.6) for a single discrete ordinate over a given problem domain is conducted via the classical “mesh-sweep” algorithm. Closure of the iterative process is accomplished, in the SI scheme, by setting the values for the cell-
averaged scalar fluxes in the next iteration equal to the values obtained at the end of the present one.

The mesh-sweep algorithm amounts to the following procedure in two-dimensional geometry. The starting cell for each direction \((\mu_m, \eta_m)\) is one with two external boundary conditions where the incoming fluxes are explicitly (e.g., vacuum boundary conditions) or implicitly specified in terms of the outgoing fluxes at these boundaries (reflective, albedo) or outgoing at a related boundary (periodic boundary conditions). The incoming fluxes in Eqs. (6.1), (6.4) and (6.6) are set equal to the prescribed values in case explicit boundary conditions are specified, as it will be assumed in the following referring to vacuum boundary conditions on all four edges of the two-dimensional domain. In case of implicit boundary conditions, the incoming fluxes are set to previously computed outgoing fluxes, i.e. resulting from the mesh-sweep along directions \((-\mu_m, \eta_m)\) and/or \((\mu_m, -\eta_m)\) or the previous flux iterates when both boundary conditions are implicit, thus requiring iterations on the boundary conditions. The mesh-sweep algorithm then proceeds by recursively solving Eqs. (6.1), (6.4) and (6.6) simultaneously, for the cell-averaged fluxes and the outgoing edge-averaged fluxes, assigning the latter to the incoming cell-edge fluxes of the adjacent down-stream cells (angular flux continuity across cell edges) and repeating the process for all cells of the mesh. The equations expressing angular fluxes continuity are:

\[
\psi_{m,i+1,j}^{(f+1)} = \psi_{m,i,j}^{ov(f+1)}, \quad \mu_m > 0; i = 1, \ldots, (I - 1); j = 1, \ldots, J, \tag{6.9}
\]
A sketch illustrating the mesh-sweep algorithm for a discrete ordinate with \( \mu_m, \eta_m > 0 \) is depicted in Fig. 6.2. It is noted that the latter figure represents an extension to two dimensions of the sketch that was depicted in Fig. 3.1 for slab geometry. The numbering sequence indicated in Fig. 6.2 reflects the convention, commonly followed in transport calculations, of sweeping the mesh in the \( x \) direction first, namely along rows, one row at a time.

Upon completion of the mesh-sweep for all discrete ordinates the scalar flux is updated, as described shortly, and convergence of the iterations is tested, thus completing a single inner iteration. As indicated previously, closure of the iterative process is accomplished, in the SI scheme, by setting the values of the cell-averaged scalar fluxes in the next iteration equal to the values obtained at the end of the present one.

To illustrate mathematically how the mesh-sweep algorithm is used to solve the three sets of equations constituting the most general WDD form of the discrete ordinates approximation to the transport equation, it is convenient to express Eqs. (6.1), (6.4) and (6.6) in the following compact matrix form:

\[
\psi_{m,i,j}^{(\mu+1)} = \psi_{m,i,j}^{(\mu+1)}, \quad \mu_m < 0; i = 2, \ldots, I; j = 1, \ldots, J, \tag{6.10}
\]

\[
\psi_{m,i,j+1}^{(\mu+1)} = \psi_{m,i,j}^{(\mu+1)}, \quad \eta_m > 0; i = 1, \ldots, I; j = 1, \ldots, (J-1), \tag{6.11}
\]

\[
\psi_{m,i,j-1}^{(\mu+1)} = \psi_{m,i,j}^{(\mu+1)}, \quad \eta_m < 0; i = 1, \ldots, I; j = 2, \ldots, J \tag{6.12}
\]
\[ \mathbf{L}^0_{m,i,j} \begin{bmatrix} \tilde{\psi}^{(\ell)}_{m,i,j} & \tilde{\psi}^{\alpha \ell}_{m,i,j} & \tilde{\psi}^{\gamma \ell}_{m,i,j} \end{bmatrix}^T = \mathbf{S}^0_{m,i,j} \begin{bmatrix} \phi^{(\ell)}_{i,j} + s_{i,j} & \tilde{\psi}^{\alpha \ell}_{m,i,j} & \tilde{\psi}^{\gamma \ell}_{m,i,j} \end{bmatrix}^T, \]  

(6.13)

where \( s_{i,j} = s_{i,j} / c_{i,j} \).

Fig. 6.2: Order of sweeping a spatial mesh for \( \mu_m, \eta_m > 0 \).

Matrices \( \mathbf{L}^0_{m,i,j} \) and \( \mathbf{S}^0_{m,i,j} \) in Eq. (6.13) represent the discretized form of the “streaming plus collision” operator and of the “self-scattering” operator in the original continuous transport equation, respectively. The superscript on the matrices in Eq. (6.13) denotes the AHOT-N0 method that is utilized in all of the following discussion. The expressions for the two matrices are readily obtained from Eqs. (6.1), (6.4) and (6.6):
Inversion of matrix \( \mathbf{L}_{m,j}^0 \) is readily accomplished and allows to explicitly express \( \tilde{\psi}_{m,j}^{(\ell+1)} \), \( \tilde{\psi}_{m,i}^{ax,(\ell+1)} \) and \( \tilde{\psi}_{m,i}^{oy,(\ell+1)} \) in terms of \( \tilde{\phi}_{i,j} \), \( \tilde{\psi}_{m,i}^{\alpha} \), \( \tilde{\psi}_{m,i}^{y} \) and \( s_{i,j} \):

\[
\begin{bmatrix}
\tilde{\psi}_{m,i}^{(\ell+1)} \\
\tilde{\psi}_{m,i}^{ax,(\ell+1)} \\
\tilde{\psi}_{m,i}^{oy,(\ell+1)}
\end{bmatrix}
= \begin{bmatrix}
\gamma_{m,i}^{\alpha} & \gamma_{m,i}^{ax} & \gamma_{m,i}^{oy} \\
\gamma_{m,i}^{ax} & \gamma_{m,i}^{x} & \gamma_{m,i}^{y} \\
\gamma_{m,i}^{oy} & \gamma_{m,i}^{y} & \gamma_{m,i}^{y}
\end{bmatrix}
\begin{bmatrix}
\tilde{\phi}_{i,j}^{(\ell)} + s_{i,j} \\
\tilde{\psi}_{m,i}^{\alpha} \\
\tilde{\psi}_{m,i}^{y}
\end{bmatrix}
\]

The \( \gamma \) coefficients, representing the elements of matrix \( \Gamma_{m,i,j} = (\mathbf{L}_{m,j}^0)^{-1} \mathbf{S}_{m,j}^0 \),

are given by the following expressions:

\[
\gamma_{m,i,j}^{\alpha} = c_{i,j} \frac{(1+\alpha_{m,i,j})(1+\beta_{m,i,j})}{2\kappa_{m,i,j}(1+\beta_{m,i,j}) + 2v_{m,i,j}(1+\alpha_{m,i,j}) + (1+\alpha_{m,i,j})(1+\beta_{m,i,j})}
\]

\[
\gamma_{m,i,j}^{ax} = \frac{2v_{m,i,j}(1+\alpha_{m,i,j})}{2\kappa_{m,i,j}(1+\beta_{m,i,j}) + 2v_{m,i,j}(1+\alpha_{m,i,j}) + (1+\alpha_{m,i,j})(1+\beta_{m,i,j})}
\]

\[
\gamma_{m,i,j}^{oy} = \frac{2\kappa_{m,i,j}(1+\beta_{m,i,j})}{2\kappa_{m,i,j}(1+\beta_{m,i,j}) + 2v_{m,i,j}(1+\alpha_{m,i,j}) + (1+\alpha_{m,i,j})(1+\beta_{m,i,j})}
\]
\[ \gamma_{m,i,j}^{\alpha} = c_{i,j} \frac{2(1 + \alpha_{m,i,j})}{2 \kappa_{m,i,j} (1 + \beta_{m,i,j}) + 2 \nu_{m,i,j} (1 + \alpha_{m,i,j}) + (1 + \alpha_{m,i,j})(1 + \beta_{m,i,j})} \]  

(6.20)

\[ \gamma_{m,i,j}^{\beta} = \frac{2 \nu_{m,i,j} (1 + \alpha_{m,i,j}) + (2 \kappa_{m,i,j} + \alpha_{m,i,j} + 1)(\beta_{m,i,j} - 1)}{2 \kappa_{m,i,j} (1 + \beta_{m,i,j}) + 2 \nu_{m,i,j} (1 + \alpha_{m,i,j}) + (1 + \alpha_{m,i,j})(1 + \beta_{m,i,j})} \]  

(6.21)

\[ \gamma_{m,i,j}^{\gamma} = \frac{4 \kappa_{m,i,j}}{2 \kappa_{m,i,j} (1 + \beta_{m,i,j}) + 2 \nu_{m,i,j} (1 + \alpha_{m,i,j}) + (1 + \alpha_{m,i,j})(1 + \beta_{m,i,j})} \]  

(6.22)

\[ \gamma_{m,i,j}^{\delta} = c_{i,j} \frac{2(1 + \beta_{m,i,j})}{2 \kappa_{m,i,j} (1 + \beta_{m,i,j}) + 2 \nu_{m,i,j} (1 + \alpha_{m,i,j}) + (1 + \alpha_{m,i,j})(1 + \beta_{m,i,j})} \]  

(6.23)

\[ \gamma_{m,i,j}^{\varepsilon} = \frac{4 \nu_{m,i,j}}{2 \kappa_{m,i,j} (1 + \beta_{m,i,j}) + 2 \nu_{m,i,j} (1 + \alpha_{m,i,j}) + (1 + \alpha_{m,i,j})(1 + \beta_{m,i,j})} \]  

(6.24)

\[ \gamma_{m,i,j}^{\zeta} = \frac{2 \kappa_{m,j} (1 + \beta_{m,i,j}) + (2 \nu_{m,i,j} + \beta_{m,i,j} + 1)(\alpha_{m,i,j} - 1)}{2 \kappa_{m,i,j} (1 + \beta_{m,i,j}) + 2 \nu_{m,i,j} (1 + \alpha_{m,i,j}) + (1 + \alpha_{m,i,j})(1 + \beta_{m,i,j})} \]  

(6.25)

Closure of the iterative process is accomplished in the SI scheme by setting:

\[ \hat{\phi}_{i,j}^{(n+1)} = \sum_{m=1}^{M} w_{m} \psi_{m,i,j}^{(n+1)}, \quad i = 1, \ldots, I; j = 1, \ldots, J \]  

(6.26)
Equation (6.16) along with the appropriate continuity conditions, expressed by Eqs. (6.9) through (6.12), represent the standard mesh-sweep algorithm commonly used to solve the discretized integro-differential form of the discrete ordinates approximation of the neutron transport equation in two-dimensional geometry. Notice therefore that this algorithm is focused on the discrete-variable angular flux. In view of the linearity of these equations the operator performing the mesh-sweep is a linear operator. The weighted sum over angles of the discrete ordinate cell-averaged angular fluxes, performed in Eq. (6.26) to obtain the update of the cell-averaged scalar flux in the present iteration, is also a linear operator.

Similarly to what was illustrated in Ch. 1 for slab geometry, the composition of the mesh-sweep operator with the summation over angles operator that yields the cell-averaged scalar fluxes in two-dimensional geometry can also be viewed as a linear mapping of the scalar fluxes from the previous to the present iteration. Organizing the cell-averaged scalar fluxes in the two-dimensional mesh into a single vector, this mapping can be expressed using the same compact matrix notation introduced in Eq. (1.26). In the case of a two-dimensional mesh comprised of \((I \times J)\) spatial cells, Eq. (1.26) defines an \(A\) matrix that has dimensions \((I \times J) \times (I \times J)\). The two-dimensional integral transport discrete operator matrix \(B\) also has dimensions of \((I \times J) \times (I \times J)\) and is still defined by Eq. (1.28). Under the assumption that the iterative scheme converges, the \((I \times J)\) vector \(\bar{\phi}^\infty\), containing the limit of the iterates of the scalar fluxes, may therefore be computed as the solution of the linear system in Eq. (1.27), representing in this case the two-dimensional discrete approximation to the original
continuous integral transport equation. The latter may still be expressed using the compact operator formulation in Eq. (1.19) by extending to two dimensions the operators’ definitions.

6.3 Expressions for Certain Elements of Matrix $B$ in Two-Dimensional Geometry

In view of Eq. (1.28) the expressions for the elements of matrix $B$ may be readily obtained once the corresponding elements of matrix $A$ have been constructed. To this end it is convenient to rewrite the three sets of equations for the general WDD form of the discrete ordinates approximation to the transport equation, Eqs. (6.1), (6.4) and (6.6), in homogeneous form. This is accomplished by subtracting the sets of equations in two consecutive iterations, thus eliminating the fixed source $s_{n,j}$ and replacing the dependent discrete variables by their iterative residual counterparts. Accordingly the equations for the residual quantities may be derived from Eq. (6.13) in the following compact matrix form:

$$ L^0_{m,i,j} \begin{bmatrix} \psi_{m,i,j}^{(t+1)} & \phi_{m,i,j}^{(t+1)} & \phi_{m,i,j}^{(t+1)} \end{bmatrix}^T = S^0_{m,i,j} \begin{bmatrix} \phi_{i,j}^{(t)} & \psi_{m,i,j}^{(t+1)} & \psi_{m,i,j}^{(t+1)} \end{bmatrix}^T, \quad (6.27) $$

where, for example, $\psi_{m,i,j}^{(t+1)} = \psi_{m,i,j}^{(t+1)} - \psi_{m,i,j}^{(t)}$ is the mesh-sweep residual in the $m$th discrete ordinate angular flux averaged over cell $(i,j)$, and so on. Inversion of matrix $L^0_{m,i,j}$ produces the homogeneous form of Eq. (6.16) expressing the residuals $\psi_{m,i,j}^{(t+1)}$, $\phi_{m,i,j}^{(t+1)}$ and $\phi_{m,i,j}^{(t+1)}$ in terms of $\phi_{i,j}^{(t)}$, $\psi_{m,i,j}^{(t+1)}$ and $\psi_{m,i,j}^{(t+1)}$.
For the residual quantities too, the mesh-sweep algorithm proceeds by recursively solving Eq. (6.28) simultaneously for the residual cell-averaged flux and the residual outgoing edge-averaged fluxes. The latter are equated to the residual incoming edge-averaged fluxes of the adjacent down-stream cells; residual angular flux continuity across cell edges is a direct consequence of angular flux continuity across cell edges expressed by Eqs. (6.9) through (6.12).

As stated previously, explicit vacuum boundary conditions will be assumed on all four sides of the two-dimensional domain. Under this assumption, the starting point in the mesh-sweep algorithm for the discrete ordinates with positive director cosines is represented by the conditions:

\[
\psi^{(r+1)}_{m,i,j} = 0, \quad \eta_m > 0; i = 1, \ldots, I; \quad (6.29)
\]

\[
\psi^{(r+1)}_{m,i,j} = 0, \quad \mu_m > 0; j = 1, \ldots, J; \quad (6.30)
\]

applied to the residual of the incoming fluxes in the present iteration step, \((\ell + 1)\). Similar conditions apply for the discrete ordinates in the other three quadrants.

Closure of the iterative process is once again accomplished in the SI scheme for the residual quantities by setting:

\[
\phi^{(r+1)}_{i,j} = \sum_{m=1}^{M} W_m \psi^{(r+1)}_{m,i,j}, \quad i = 1, \ldots, I; j = 1, \ldots, J \quad (6.31)
\]
The composition of the mesh-sweep operator with the summation over angles operator can be viewed as a mapping of the residuals of the scalar fluxes from the previous iteration to the present iteration that represents the homogeneous form of Eq. (1.26). It is convenient to write this equation in terms of its components:

\[
\phi_{i,j}^{(f+1)} = \sum_{r=1}^{I} \sum_{s=1}^{J} A_{i,j,r,s} \sigma_{s,r} \phi_{r,s}^{(f)}, \quad i = 1, \ldots, I; j = 1, \ldots, J
\] (6.32)

Equation (6.32) provides a recipe for constructing the elements of the iteration matrix \( A \) by differentiating both sides of the equation with respect to the cell-averaged scalar flux residual in the previous iteration:

\[
A_{i,j,r,s} = \frac{1}{\sigma_{s,r}} \frac{\partial \phi_{i,j}^{(f+1)}}{\partial \phi_{r,s}^{(f)}}, \quad i, r = 1, \ldots, I; j, s = 1, \ldots, J
\] (6.33)

Note that, to within a factor \( 1/\sigma_{s,r} \), the elements of the SI iteration matrix \( A \) may be identified with the elements of the Jacobian matrix \( J \) for the linear transformation defined by Eq. (6.32):

\[
J_{i,j,r,s} = \frac{\partial \phi_{i,j}^{(f+1)}}{\partial \phi_{r,s}^{(f)}}, \quad i, r = 1, \ldots, I; j, s = 1, \ldots, J
\] (6.34)

Using Eq. (6.33) recursively in the mesh-sweep algorithm and applying angular flux continuity across cell-boundaries yields expressions for the elements of matrix \( A \). The elements of matrix \( B \) can then be obtained through the relationship:

\[
B_{i,j,r,s} = \delta_{i,r} \delta_{j,s} - A_{i,j,r,s} \sigma_{s,r}, \quad i, r = 1, \ldots, I; j, s = 1, \ldots, J
\] (6.35)

where \( \delta_{k,k'} \) is the Kronecker delta function; Eq. (6.35) is of course a direct consequence of Eq. (1.28).
In this and the next chapters on two-dimensional geometry, the focus will be on the \( \mathbf{B} \) matrix. Therefore, results will be presented only for this matrix. The general expressions for the elements of the \( \mathbf{B} \) matrix coupling the cell-averaged scalar flux in cell \((i,j)\) with the cell-averaged scalar fluxes in the neighboring cells, up to the second neighbors depicted in Fig. 6.1, are hereby reported.

**Self-coupling**

\[
B_{i,j,i,j} = 1 - \sum_{m=1}^{M} W_m \gamma_{m,i,j}^\alpha \gamma_{m,i,j}^\alpha (6.36)
\]

**Coupling with first neighbors**

\[
B_{i,j,i+1,j} = -\frac{1}{2} \sum_{m=1}^{M} W_m \gamma_{m,i,j}^\alpha \gamma_{m,i+1,j}^\alpha (6.37)
\]

\[
B_{i,j,i+1,j+1} = -\frac{1}{4} \sum_{m=1}^{M} W_m \left( \gamma_{m,i,j}^\alpha \gamma_{m,i+1,j+1}^\alpha + \gamma_{m,i,j}^\alpha \gamma_{m,i+1,j+1}^\alpha \gamma_{m,i+1,j+1}^\alpha \right) (6.38)
\]

**Coupling with second neighbors**

\[
B_{i,j,i+2,j} = -\frac{1}{2} \sum_{m=1}^{M} W_m \gamma_{m,i,j}^\alpha \gamma_{m,i+1,j}^\alpha \gamma_{m,i+2,j}^\alpha (6.39)
\]

\[
B_{i,j,i+2,j+1} = -\frac{1}{4} \sum_{m=1}^{M} W_m \left( \gamma_{m,i,j}^\alpha \gamma_{m,i+1,j}^\alpha \gamma_{m,i+1,j+1}^\alpha + \gamma_{m,i,j}^\alpha \gamma_{m,i+1,j+1}^\alpha \gamma_{m,i+2,j+1}^\alpha + \gamma_{m,i,j}^\alpha \gamma_{m,i+1,j}^\alpha \gamma_{m,i+2,j}^\alpha + \gamma_{m,i,j}^\alpha \gamma_{m,i+1,j}^\alpha \gamma_{m,i+2,j+1}^\alpha \right) (6.40)
\]
\[ B_{i,j,i+2,j+2} = -\frac{1}{4} \sum_{m=1}^{M} w_m \left( \gamma_{m,i,j}^{xx} \gamma_{m,i+1,j+1}^{xy} \gamma_{m,i+1,j+2}^{yy} \gamma_{m,i+1,j+2}^{xx} \gamma_{m,i+1,j+2}^{yy} \right) \]

\[ + \gamma_{m,i,j}^{yx} \gamma_{m,i+1,j+1}^{yx} \gamma_{m,i+1,j+2}^{yy} \gamma_{m,i+1,j+2}^{yx} \gamma_{m,i+1,j+2}^{yy} \]

\[ + \gamma_{m,i,j}^{xy} \gamma_{m,i+1,j+1}^{yx} \gamma_{m,i+1,j+2}^{yx} \gamma_{m,i+1,j+2}^{ yy} \gamma_{m,i+1,j+2}^{yx} \]

\[ + \gamma_{m,i,j}^{xy} \gamma_{m,i+1,j+1}^{xy} \gamma_{m,i+1,j+2}^{xx} \gamma_{m,i+1,j+2}^{yx} \gamma_{m,i+1,j+2}^{yx} \]

\[ + \gamma_{m,i,j}^{xy} \gamma_{m,i+1,j+1}^{xy} \gamma_{m,i+1,j+2}^{yx} \gamma_{m,i+1,j+2}^{yy} \gamma_{m,i+1,j+2}^{yx} \]

\[ + \gamma_{m,i,j}^{xy} \gamma_{m,i+1,j+1}^{xy} \gamma_{m,i+1,j+2}^{yx} \gamma_{m,i+1,j+2}^{yx} \gamma_{m,i+1,j+2}^{yy} \]

\[ + \gamma_{m,i,j}^{xy} \gamma_{m,i+1,j+1}^{xy} \gamma_{m,i+1,j+2}^{yx} \gamma_{m,i+1,j+2}^{yx} \gamma_{m,i+1,j+2}^{yy} \]  \hspace{1cm} (6.41)

It is noted that the expressions in Eqs. (6.36) through (6.41) are given for the neighbors in the lower half of the quadrant depicted in Fig. 6.1. Analogous expressions are obtained for the elements pertaining to the neighbors in the upper half of the quadrant.

Extensions to two-dimensional geometry of the “derivative” approach and of the constructive approach introduced in one-dimensional geometry in Secs. 3.3.1 and 3.3.2 respectively, have been utilized to evaluate the expressions in Eqs. (6.36) through (6.41). For brevity, the derivative approach, namely the approach based on explicitly computing the partial derivative in Eq. (6.33), is illustrated in the following only for the elements pertaining to self-coupling and coupling with the first neighbors. For the latter, the expressions obtained for the corresponding elements are also interpreted from a constructive point of view. The constructive approach is then used to justify the expressions obtained for the \( B \) matrix elements pertaining to the coupling with the second neighbors.

**Self-coupling**

The calculation of the elements \( A_{i,j,i,j} \) may be performed by applying Eq. (6.33) to the case \( r = i \) and \( s = j \):
\[ A_{i,j,i,j} = \frac{1}{\sigma_{s,i,j}} \frac{\partial \phi_{i,j}^{(r+1)}}{\partial \phi_{i,j}^{(r)}}, \quad i = 1,\ldots, I; \quad j = 1,\ldots, J \]  

(6.42)

The partial derivative in Eq. (6.42) may be evaluated using the following result obtained simply by differentiating both sides of Eq. (6.31) with respect to \( \phi_{i,j}^{(r)} \):

\[
\frac{\partial \phi_{i,j}^{(r+1)}}{\partial \phi_{i,j}^{(r)}} = \sum_{m=1}^{M} w_m \frac{\partial \psi_{m,i,j}^{(r+1)}}{\partial \phi_{i,j}^{(r)}}, \quad i = 1,\ldots, I; \quad j = 1,\ldots, J,
\]  

(6.43)

along with the following result deriving from the definition of \( \gamma_{m,i,j}^{ij} \) in Eq. (6.28):

\[
\frac{\partial \psi_{m,i,j}^{(r+1)}}{\partial \phi_{i,j}^{(r)}} = \gamma_{m,i,j}^{ij}, \quad m = 1,\ldots, M; \quad i = 1,\ldots, I; \quad j = 1,\ldots, J
\]  

(6.44)

Substitution of Eq. (6.43) and Eq. (6.44) into Eq. (6.42) produces the expression sought for \( A_{i,j,i,j} \). Use of the latter result in Eq. (6.35) proves that the expression for 

\( B_{i,j,i,j} \) is indeed given by Eq. (6.36).

**Coupling with first Cartesian neighbor**

The calculation of the elements \( A_{i,j,i+j} \) may be performed by applying Eq. (6.33) to the case \( r = i+1 \) and \( s = j \):

\[ A_{i,j,i+j} = \frac{1}{\sigma_{s,i+j}} \frac{\partial \phi_{i+j}^{(r+1)}}{\partial \phi_{i+j}^{(r)}}, \quad i = 1,\ldots, (I - 1); \quad j = 1,\ldots, J
\]  

(6.45)

In evaluating the partial derivative on the right hand side of Eq. (6.45) it must be noticed that the previous iterate of the scalar flux in cell \((i+1,j)\) contributes, or is coupled to the to-be-determined (in the present iterate) scalar flux in cell \((i,j)\) only
through the discrete ordinates in the two quadrants characterized by $\mu_m < 0$. Cell $(i, j)$ influences cell $(i+1, j)$ when the two-dimensional structure is swept from left to right along $\mu_m > 0$, while cell $(i+1, j)$ influences cell $(i, j)$ when the structure is swept from right to left along $\mu_m < 0$. Keeping in mind this observation, the partial derivative on the right hand side of Eq. (6.45) is evaluated by differentiating with respect to $\phi_{r+1,j}^{(i)}$ both sides of Eq. (6.31), taking the sum only over the discrete ordinates in the quadrants $(\mu_m < 0, \eta_m > 0)$ and $(\mu_m < 0, \eta_m < 0)$, since the remaining partial derivatives are all equal to zero. This partial sum is expressed using the following notation:

$$\frac{\partial \phi_{r+1,j}^{(i+1)}}{\partial \phi_{r+1,j}^{(i)}} = \sum_{\mu_m < 0} w_m \frac{\partial \psi_{m,i,j}^{(i+1)}}{\partial \phi_{r+1,j}^{(i)}}$$

(6.46)

The system of equations in Eq. (6.28), along with the continuity condition for residual quantities deriving from Eq. (6.10) may be used to express $\psi_{m,i,j}^{(i+1)}$ as a function of $\phi_{r+1,j}^{(i)}$. The first equation in the system is first written for cell $(i, j)$ and $\mu_m < 0$:

$$\psi_{m,i,j}^{(i+1)} = \gamma_{m,i,j}^{\mu} \phi_{r+1,j}^{(i)} + \gamma_{m,i,j}^{\psi} \psi_{m,i,j}^{(i+1)} + \gamma_{m,i,j}^{\gamma} \psi_{m,i,j}^{\gamma} + \gamma_{m,i,j}^{\psi} \psi_{m,i,j}^{\psi} , \quad \mu_m < 0$$

(6.47)

The partial derivatives on the right hand side of Eq. (6.46) can be directly calculated using Eq. (6.47) along with the continuity condition and noting that, for $\mu_m < 0$, both $\phi_{r+1,j}^{(i)}$ and $\psi_{m,i,j}^{(i+1)}$ are independent from $\phi_{r+1,j}^{(i)}$:  

$$\frac{\partial \phi_{r+1,j}^{(i+1)}}{\partial \phi_{r+1,j}^{(i)}} = \sum_{\mu_m < 0} w_m \gamma_{m,i,j}^{\gamma} \frac{\partial \psi_{m,i,j}^{(i+1)}}{\partial \phi_{r+1,j}^{(i)}}$$

(6.48)
The partial derivatives on the right hand side of Eq. (6.48) are then calculated using the third equation in the system of equations in Eq. (6.28) written for cell \((i+1, j)\) and \(\mu_m < 0\):

\[
\psi_{m,i+1,j}^{\mu} = \gamma_{m,i+1,j}^{\当下} \phi_{i+1,j}^{(t)} + \gamma_{m,i+1,j}^{\当下} \psi_{m,i+1,j}^{\当下} + \gamma_{m,i+1,j}^{\当下} \psi_{m,i+1,j}^{\当下}, \quad \mu_m < 0
\] (6.49)

Notice that \(\psi_{m,i+1,j}^{\当下} \) and \(\psi_{m,i+1,j}^{\当下} \) contain the information on how previously swept cells influence cell \((i+1, j)\) and depend (linearly) only on the previous iterate of the scalar flux residual (assuming vacuum boundary conditions) up to cells \((i+1, j+1)\) and \((i+2, j)\), respectively, but not on \(\phi_{i+1,j}^{(t)}\). Therefore, using Eq. (6.49) in Eq. (6.48) it follows that:

\[
\frac{\partial \phi_{i+1,j}^{(t)}}{\partial \phi_{i+1,j}^{(t)}} = \sum_{\mu_m < 0} \omega_{m} \gamma_{m,i+1,j}^{\当下} \gamma_{m,i+1,j}^{\当下}
\] (6.50)

Under the assumption of a level symmetric quadrature introduced in Sec. 6.2, Eq. (6.50) can be written in yet another equivalent form. The latter is based on the observation that the discrete ordinates in the two quadrants characterized by \(\mu_m < 0\) are half the total number \(M\) of discrete ordinates in the quadrature:

\[
\frac{\partial \phi_{i+1,j}^{(t)}}{\partial \phi_{i+1,j}^{(t)}} = \frac{1}{2} \sum_{m=1}^{M} \omega_{m} \gamma_{m,i+1,j}^{\当下} \gamma_{m,i+1,j}^{\当下}
\] (6.51)

Substitution of Eq. (6.51) into Eq. (6.45) produces the expression sought for \(A_{i,j,i+1,j}\). Use of the latter result in Eq. (6.35) proves that the expression for \(B_{i,j,i+1,j}\) is indeed given by Eq. (6.37).
Similar to the constructive approach introduced in Sec. 3.3.2 for slab geometry, a constructive interpretation can be given for the expression of $B_{i,j,i+1,j}$ contained in Eq. (6.37). This interpretation is based on the “transport path” depicted in Fig. 6.3.

As evident in Fig. 6.3, the past iterate of the cell-averaged scalar flux residual in cell $(i+1, j)$, $\phi_{i+1,j}^{(i)}$, contributes to the present iterate of the cell-averaged scalar flux residual in cell $(i, j)$, $\phi_{i,j}^{(i+1)}$, only through the discrete ordinates in the two quadrants characterized by $\mu_m < 0$. Coefficient $\gamma_{m,i+1,j}^{aw}$ represents the partial contribution of $\phi_{i+1,j}^{(i)}$ to the outgoing edge-averaged angular flux residual leaving cell $(i+1, j)$, $\psi_{m,i+1,j}^{aw\,(i+1)}$. Due to angular flux continuity, the latter is also the incoming edge-averaged residual, $\psi_{m,i,j}^{aw\,(i+1)}$, entering cell $(i, j)$ and contributing to $\phi_{i,j}^{(i)}$ via coefficient $\gamma_{m,i,j}^{aw}$. The corresponding $B_{i,j,i+1,j}$ matrix element is obtained as the sum over the discrete ordinates with $\mu_m < 0$ of the product of the two $\gamma$ coefficients multiplied by the corresponding weight in the quadrature. Notice, in fact, that the expression in Eq. (6.50) may be interpreted as the result of a derivative chain rule applied along the transport path depicted in Fig. 6.3:
\[
\frac{\partial \phi^{(i+1)}_{i,j}}{\partial \phi^{(i)}_{i+1,j}} = \sum_{m \mu < 0} w_m \left( \frac{\partial \phi^{(i+1)}_{i,j}}{\partial \psi^{(i+1)}_{m,j+1,i}} \right) \left( \frac{\partial \psi^{(i+1)}_{m,j+1,i}}{\partial \phi^{(i)}_{i+1,j}} \right) = \sum_{m \mu < 0} w_m \gamma^{\mu}_{m,j} \gamma^{\nu}_{m,i+1,j+1} \quad (6.52)
\]

**Coupling with first diagonal neighbor**

The calculation of the elements \( A_{i,j+1,i+1} \) may be performed by applying Eq. (6.33) to the case \( r = i+1 \) and \( s = j+1 \):

\[
A_{i,j+1,i+1} = \frac{1}{\sigma_{S,i+1,j+1}} \frac{\partial \phi^{(i+1)}_{i,j}}{\partial \phi^{(i)}_{i+1,j+1}}, \quad i = 1,\ldots,(I-1); \quad j = 1,\ldots,(J-1) \quad (6.53)
\]

In evaluating the partial derivative on the right hand side of Eq. (6.53) it must be noticed that the previous iterate of the scalar flux residual in cell \((i+1, j+1)\) contributes, or is coupled to the to-be-determined (in the present iterate) scalar flux residual in cell \((i, j)\) only through the discrete ordinates in the quadrant characterized by \(\mu_m, \eta_m < 0\). Cell \((i+1, j+1)\) influences cell \((i, j)\) when the structure is swept from right to left along \(\mu_m < 0\) and from top to bottom along \(\eta_m < 0\). Keeping in mind this observation, the partial derivative on the right hand side of Eq. (6.53) may be evaluated by taking the partial derivative with respect to \(\phi^{(i)}_{i+1,j+1}\) of both sides of Eq. (6.31). The sum in the latter equation is taken only over the discrete ordinates in the \((\mu_m < 0, \eta_m < 0)\) quadrant, since the remaining partial derivatives are all equal to zero. This partial sum is expressed using the following notation:

\[
\frac{\partial \phi^{(i+1)}_{i,j}}{\partial \phi^{(i)}_{i+1,j+1}} = \sum_{m \mu \eta < 0} w_m \frac{\partial \psi^{(i+1)}_{m,i,j}}{\partial \phi^{(i)}_{i+1,j+1}} \quad (6.54)
\]
The system of equations in Eq. (6.28), along with the continuity conditions for residual quantities deriving from Eqs. (6.10) and (6.12), are used to express $\psi_{m,i,j}^{(r+1)}$ as a function of $\phi_{r+1,i,j}^{(r)}$. The first equation in the system is first written for cell $(i,j)$ and $\mu_m, \eta_m < 0$:

$$\psi_{m,i,j}^{(r+1)} = \gamma_{m,i,j}^{\alpha \alpha} \phi_{r+1,i,j}^{(r)} + \gamma_{m,i,j}^{\alpha \alpha} \psi_{m,i,j}^{(r+1)} + \gamma_{m,i,j}^{\gamma \gamma} \psi_{m,i,j}^{(r+1)}, \quad \mu_m, \eta_m < 0 \quad (6.55)$$

The partial derivatives on the right hand side of Eq. (6.54) can be directly calculated using Eq. (6.55) along with the continuity conditions and noting that, for $\mu_m, \eta_m < 0$, both $\psi_{m,i,j}^{(r+1)}$ and $\psi_{m,i,j}^{(r+1)}$ depend on $\phi_{r+1,i,j}^{(r)}$ while $\phi_{r+1,i,j}^{(r)}$ is independent from $\phi_{r+1,i,j}^{(r)}$:

$$\frac{\partial \phi_{r+1,i,j}^{(r)}}{\partial \phi_{r+1,i,j}^{(r)}} = \sum_{\mu_m, \eta_m < 0} \mathcal{W}_m \left( \gamma_{m,i,j}^{\alpha \alpha} \frac{\partial \psi_{m,i+1,j}^{(r+1)}}{\partial \phi_{r+1,i,j}^{(r)}} + \gamma_{m,i,j}^{\gamma \gamma} \frac{\partial \psi_{m,i,j}^{(r+1)}}{\partial \phi_{r+1,i,j}^{(r)}} \right) \quad (6.56)$$

The partial derivatives in the first term on the right hand side of Eq. (6.56) are then calculated using the third equation in the system of equations in Eq. (6.28) written for cell $(i+1,j)$ and $\mu_m, \eta_m < 0$:

$$\psi_{m,i+1,j}^{(r+1)} = \gamma_{m,i+1,j}^{\alpha \alpha} \phi_{r+1,i+1,j}^{(r)} + \gamma_{m,i+1,j}^{\alpha \alpha} \psi_{m,i+1,j}^{(r+1)} + \gamma_{m,i+1,j}^{\gamma \gamma} \psi_{m,i+1,j}^{(r+1)}, \quad \mu_m, \eta_m < 0 \quad (6.57)$$

For the discrete ordinates in the $(\mu_m < 0, \eta_m < 0)$ quadrant, $\psi_{m,i+1,j}^{(r+1)}$ depends on $\phi_{r+1,i+1,j}^{(r)}$ only through $\psi_{m,i+1,j}^{(r+1)}$. Using the continuity condition for residual quantities deriving from Eq. (6.12), the following expression is obtained:

$$\frac{\partial \psi_{m,i+1,j}^{(r+1)}}{\partial \phi_{r+1,i+1,j}^{(r)}} = \gamma_{m,i+1,j}^{\alpha \alpha} \frac{\partial \psi_{m,i+1,j}^{(r+1)}}{\partial \phi_{r+1,i+1,j}^{(r)}}, \quad \mu_m, \eta_m < 0 \quad (6.58)$$
The partial derivatives on the right hand side of Eq. (6.58) can then be readily evaluated using the second equation in the system of equations in Eq. (6.28) written for cell \((i+1, j+1)\) and \(\mu_m, \eta_m < 0\):

\[
\psi^{\alpha (i+1)}_{m,i+1,j+1} = \gamma^{xa}_{m,i+1,j+1} \phi^{(i)}_{i+1,j+1} + \gamma^{xx}_{m,i+1,j+1} \psi^{ix (i+1)}_{m,i+1,j+1} + \gamma^{yy}_{m,i+1,j+1} \psi^{iy (i+1)}_{m,i+1,j+1}, \quad \mu_m, \eta_m < 0
\]

(6.59)

Once again, notice that neither \(\psi^{ix (i+1)}_{m,i+1,j+1}\) nor \(\psi^{iy (i+1)}_{m,i+1,j+1}\) depend on \(\phi^{(i)}_{i+1,j+1}\), therefore the following result is obtained:

\[
\frac{\partial \psi^{\alpha (i+1)}_{m,i+1,j+1}}{\partial \phi^{(i)}_{i+1,j+1}} = \gamma^{xa}_{m,i+1,j+1}, \quad \mu_m, \eta_m < 0
\]

(6.60)

Substitution of Eq. (6.60) into Eq. (6.58) produces an expression in terms of \(\gamma\) coefficients only:

\[
\frac{\partial \psi^{\alpha (i+1)}_{m,i+1,j}}{\partial \phi^{(i)}_{i+1,j+1}} = \gamma^{xa}_{m,i+1,j+1} \gamma^{xa}_{m,i+1,j+1}, \quad \mu_m, \eta_m < 0
\]

(6.61)

Following a similar procedure it can be shown that the partial derivatives in the second term on the right hand side of Eq. (6.56) evaluates to:

\[
\frac{\partial \psi^{\alpha (i+1)}_{m,i+1,j}}{\partial \phi^{(i)}_{i+1,j+1}} = \gamma^{ya}_{m,i+1,j+1} \gamma^{ya}_{m,i+1,j+1}, \quad \mu_m, \eta_m < 0
\]

(6.62)

Finally, substitution of Eqs. (6.61) and (6.62) into Eq. (6.56) leads to:

\[
\frac{\partial \phi^{(i+1)}_{i,j}}{\partial \phi^{(i)}_{i+1,j+1}} = \sum_{\mu_m, \eta_m < 0} w_m \left( \gamma^{ya}_{m,i,j+1} \gamma^{ya}_{m,i+1,j} \gamma^{ya}_{m,i+1,j+1} + \gamma^{ax}_{m,i,j} \gamma^{ax}_{m,i+1,j} \gamma^{ax}_{m,i+1,j+1} \right)
\]

(6.63)
Under the assumption of a level symmetric quadrature introduced in Sec. 6.2, Eq. (6.63) can be written in an equivalent form. The latter is based on the observation that the contribution to the sum from the discrete ordinates in the quadrant characterized by \(\mu_m, \eta_m < 0\), are a quarter of the total sum from all \(M\) discrete ordinates in the quadrature:

\[
\frac{\partial \phi^{(i+1)}_{i,j}}{\partial \phi^{(i)}_{i+1,j+1}} = \frac{1}{4} \sum_{m=1}^{M} w_{m} \left( \gamma_{m,i,j}^{\alpha x} \gamma_{m,i+1,j}^{\alpha x} + \gamma_{m,i,j}^{\alpha y} \gamma_{m,i+1,j+1}^{\alpha y} + \gamma_{m,i,j}^{\alpha x} \gamma_{m,i+1,j+1}^{\alpha x} + \gamma_{m,i,j+1}^{\alpha y} \gamma_{m,i+1,j}^{\alpha y} \right)
\]  \quad (6.64)

Substitution of Eq. (6.64) into Eq. (6.53) produces the sought expression for \(A_{i,j,i+1,j+1}\). Use of the latter result in Eq. (6.35) proves that the expression for \(B_{i,j,j+1,j+1}\) is indeed given by Eq. (6.38).

![Diagram](image)

**Fig. 6.4:** Transport paths for the calculation of \(B_{i,j,j+1,j+1}\).

The transport paths involved in the constructive derivation of Eq. (6.38) are depicted in Fig. 6.4. It is noted that the two different paths that have to be considered in
this case represent a topological counterpart to the branching in the evaluation of the partial derivatives on the right hand side of Eq. (6.56).

**Second neighbors**

The expressions in Eqs. (6.39) through (6.41), for the elements of matrix $B$ coupling the cell-averaged scalar flux in cell $(i, j)$ to the fluxes in its second neighboring cells, have been derived analytically by extending the procedure for the first neighbors that was outlined in detail above. The intricacies of the derivative approach are omitted in favor of a graphical representation of the transport paths involved in the constructive derivation of those same expressions. Specifically, the transport paths involved in the constructive derivation of Eqs. (6.39) and (6.40) are reported in Figs. 6.5 and 6.6, respectively. Finally, the six transport paths that have to be considered in the derivation of Eq. (6.41) are reported in Figs. 6.7 and 6.8.

Fig. 6.5: Transport paths for the calculation of $B_{i,j,i+2,j}$. 
Fig. 6.6: Transport paths for the calculation of $B_{i,j,i+2,j,1}$.

Fig. 6.7: Transport paths for the calculation of $B_{i,j,i+2,j,2}$. 
The recipe for constructing the $B$ matrix elements may be used to compute the elements pertaining to coupling with neighbors that are farther than the second. However, the analytic procedure quickly becomes very complicated the farther the two cells considered are from one another. Hence the task of determining a general closed analytic expression for the $B$ matrix elements is abandoned in favor of an algorithmic approach for the numeric evaluation of the integral transport matrix, as presented in the next section. Also, an estimate of the increasing infinitesimal order of the matrix elements as a function of the distance from the self-cell can in most cases be obtained by simply reasoning on the leading order of the $\gamma$ coefficients with respect to $\Delta$. In fact, as evident from the results obtained in this section, the expressions for the elements of the $B$ matrix

Fig. 6.8: Transport paths for the calculation of $B_{i,j,i+2,j+2}$ (continued).
result in general from the sum of products of the $\gamma$ coefficients corresponding to the various paths that can connect two cells in the transport computation, over the directions in the quadrature and over all the possible paths.

6.4 An Algorithm for Computing the SI Jacobian Matrix in One Mesh-Sweep

Equations (6.33) and (6.34) readily imply the following relationship between the Jacobian matrix $J$ and the $A$ matrix:

$$J = A \sigma_s$$

(6.65)

Consequently, Eq. (6.35) implies the following relationship between the Jacobian matrix and the $B$ matrix:

$$B = I - J$$

(6.66)

Therefore, the problem of numerically computing the elements of the $A$ and $B$ matrices is equivalent to the problem of evaluating the elements of the Jacobian matrix. In this respect, a first numerical approach that can be utilized for the numerical computation of the elements of the integral transport matrix is Automatic Differentiation (AD). This approach has been implemented in [40] using an AD system, such as GRESS [41], to compute the Jacobian matrix for given test problems and for the AHOT-N family of transport methods. Once the $J$ matrix has been computed, the $A$ and $B$ matrices are readily obtained through Eqs. (6.65) and (6.66) and the limit of the iterates of the scalar flux vector $\Phi^\infty$ can be computed solving Eq. (1.27) by directly inverting the integral transport matrix. Since the solution vector $\Phi^\infty$ is free from iteration convergence error,
and subject only to truncation and round-off errors, the purpose in [40] was that of generating accurate benchmark solutions to transport test problems.

Another algorithmic approach for the numeric evaluation of the Jacobian matrix was proposed in reference [40]. The latter is a recursive algorithm for the computation of the Jacobian matrix from the computational cells’ $\Gamma_{m,i,j}^N$ matrices of the AHOT-N in one mesh-sweep. As part of this research effort, the latter algorithm has been coded for the AHOT-N0 method in order to numerically evaluate the $A$ and $B$ matrices for this spatial discretization in two-dimensional geometry. This code serves the purpose of extending to two-dimensional geometry the numerical capability of obtaining the solution vector $\phi^\infty$ by directly solving Eq. (1.27), in analogy to what was done in Sec 3.3.3 for slab geometry. Since the code allows evaluating the elements of the integral transport matrix, it has also been used to verify the theoretical predictions of the asymptotic analysis performed in this chapter and in the following, as shown in Sec. 6.6.2. In the following this code will be referred to as the NS code, where NS stands for “No Sweep”. The latter notation derives from the fact that the code allows to compute the solution vector $\phi^\infty$ without iterations. It may actually appear as a misnomer when one considers that the algorithm implemented in the code computes $J$ in a mesh-sweep, and is actually similar to the “mesh-sweep” algorithm. Instead of accumulating angular fluxes in the scalar fluxes, though, in this case the $\gamma$ coefficients of the various cells in the spatial mesh are accumulated in the elements of the Jacobian matrix.
The main ideas of the algorithm originally proposed in [40] are detailed in Sec. 6.4.1 for the case of the AHOT-N0 spatial discretization, referring to the notation introduced in this chapter.

6.4.1 Computation of \( J \) from \( \Gamma^0 \) in One Mesh-Sweep

Consider the formal relation in Eq. (6.16) for a given discrete ordinate direction of index \( m \), with \( 1 \leq m \leq M \). For any WDD (Weighted Diamond Difference) transport method, including in particular AHOT-N0, the \( \Gamma_{m,i,j}^0 \) matrix appearing in Eq. (6.16) is a \((3 \times 3)\) matrix. To fix ideas, the expressions that will be written in the following refer to the case of a discrete ordinate characterized by \( \mu_m, \eta_m > 0 \). Therefore, cell \((1,1)\) in the lower left corner of the spatial mesh is the cell at the mesh corner at which all incoming angular fluxes are known. As usual in this work, vacuum boundary conditions are assumed on all four sides of the two-dimensional Cartesian mesh.

For arbitrary cell \((i, j)\), suppose the matrix operators:

\[
X_{m,i,j,i',j'} = \frac{\partial \psi_{m,i,j}^{(i+1)}}{\partial \phi_{i,j}^{(i)}}
\]

(6.67)

with \( 1 \leq i' \leq i \) and \( 1 \leq j' < j \), and:

\[
Y_{m,i,j,i',j'} = \frac{\partial \psi_{m,i,j}^{(i+1)}}{\partial \phi_{i,j}^{(i)}}
\]

(6.68)

with \( 1 \leq i' < i \) and \( 1 \leq j' \leq j \), are known.
It is possible to derive a recursive relation for these two matrices that is then updated throughout a mesh-sweep and used to compute the $J$ matrix by appending the correct $\gamma$ coefficients in the corresponding $J$ matrix element. As it will become apparent in the following, in this approach the possible branching paths that should be considered analytically, as pointed out in Sec. 6.3, are therefore automatically accounted for through the sweeping sequence. Due to their recursive nature, the $X$ and $Y$ matrices must at first be initialized, at $i=1$, $j=2$ for Eq. (6.67) and at $i=2$, $j=1$ for Eq. (6.68). For the case of vacuum boundary conditions considered here, and applying angular flux continuity, it follows from Eq. (6.16) written for cell $(1,1)$ that:

$$X_{m,1,2,1,1} = \frac{\partial \tilde{\psi}_{m,1,2}^{(i+1)}}{\partial \tilde{\phi}_{1,1}^{(i)}} = \frac{\partial \tilde{\psi}_{m,1,1}^{(i+1)}}{\partial \tilde{\phi}_{1,1}^{(i)}} = \gamma_{m,1,1}^{\alpha}$$

(6.69)

$$Y_{m,2,1,1,1} = \frac{\partial \tilde{\psi}_{m,2,1}^{(i+1)}}{\partial \tilde{\phi}_{1,1}^{(i)}} = \frac{\partial \tilde{\psi}_{m,1,1}^{(i+1)}}{\partial \tilde{\phi}_{1,1}^{(i)}} = \gamma_{m,1,1}^{\beta}$$

(6.70)

To compute the iteration Jacobian, the derivatives of the discrete ordinates angular fluxes are accumulated throughout a mesh-sweep. In fact, substitution of Eq. (6.31) into Eq. (6.34) yields:

$$J_{k,j,i,j'} = \sum_{m=1}^{M} w_m \frac{\partial \tilde{\psi}_{m,i,j}^{(i+1)}}{\partial \tilde{\phi}_{i,j'}^{(i)}}$$

(6.71)

As noted in Sec. 6.3, due to the hyperbolic nature of the transport operator the $m^{th}$ discrete ordinate angular flux in a given cell depends only on the old iterate of the scalar
flux in upstream cells for each discrete direction. Hence, for a discrete ordinate with 
\( \mu_m, \eta_m > 0 \), it is:

\[
\frac{\partial \psi_{m,i,j}^{(r+1)}}{\partial \phi_{i',j'}^{(r)}} = 0, \quad i' > i \text{ or } j' > j
\]

(6.72)

As the mesh-sweep proceeds to cell \((i, j)\), the contribution of the angular
direction \(m\) to the diagonal element of the Jacobian matrix, \(J_{i,j,i,j}\), is computed by
differentiating Eq. (6.16) to obtain:

\[
\frac{\partial \psi_{m,i,j}^{(r+1)}}{\partial \phi_{i,j}^{(r)}} = \gamma_{m,i,j}^{aa}
\]

(6.73)

This contribution is accumulated in \(J_{i,j,i,j}\) straightaway, since it only depends on
cell \((i, j)\). On the other hand, in order to compute the contribution of the angular
direction \(m\) to an off-diagonal element of the Jacobian matrix \(J_{i,j,i',j'}\), it is observed that
the dependence of \(\psi_{m,i,j}^{(r+1)}\) on \(\phi_{i,j}^{(r)}\), for \(i' < i\) and \(j' < j\), results from its dependence on the
incoming angular fluxes \(\psi_{m,i,j}^{ix(r+1)}\) and \(\psi_{m,i,j}^{iy(r+1)}\). The partial derivative of \(\psi_{m,i,j}^{(r+1)}\) with respect
to \(\phi_{i,j}^{(r)}\) can be evaluated using the derivative chain rule:

\[
\frac{\partial \psi_{m,i,j}^{(r+1)}}{\partial \phi_{i,j}^{(r)}} = \frac{\partial \psi_{m,i,j}^{(r+1)}}{\partial \psi_{m,i,j}^{ix(r+1)}} \frac{\partial \psi_{m,i,j}^{ix(r+1)}}{\partial \phi_{i,j}^{(r)}} + \frac{\partial \psi_{m,i,j}^{(r+1)}}{\partial \psi_{m,i,j}^{iy(r+1)}} \frac{\partial \psi_{m,i,j}^{iy(r+1)}}{\partial \phi_{i,j}^{(r)}}
\]

(6.74)

The partial derivatives of \(\psi_{m,i,j}^{(r+1)}\) with respect to \(\psi_{m,i,j}^{ix(r+1)}\) and \(\psi_{m,i,j}^{iy(r+1)}\) are
immediately obtained from Eq. (6.16). They are equal to \(\gamma_{m,i,j}^{ax}\) and \(\gamma_{m,i,j}^{ay}\), respectively.
Substitution of the latter result, along with the definitions in Eqs. (6.67) and (6.68), into Eq. (6.74) yields:

$$\frac{\partial \tilde{\psi}^{i+1}_{m,i,j}}{\partial \tilde{\phi}^{(l)}_{i,j'}} = \gamma_{m,i,j}^{ax} X_{m,i,j,i',j'} + \gamma_{m,i,j}^{ay} Y_{m,i,j,i',j'}$$ (6.75)

Provided matrices $X_{m,i,j,i',j'}$ and $Y_{m,i,j,i',j'}$ are known, as assumed earlier, the expression in Eq. (6.75) is readily computed and the corresponding contribution can be accumulated in $J_{i,j,i',j'}$. Therefore, all that is left to close the algorithm is to indicate the recursive relations used to update matrices $X_{m,i,j,i',j'}$ and $Y_{m,i,j,i',j'}$, before moving to the next computational cell in the mesh-sweep, starting from the initialization conditions in Eqs. (6.69) and (6.70).

The update of matrices $X$ and $Y$ is again based on the continuity of the angular flux across cell edges:

$$X_{m,i,j+1,i',j'} = \frac{\partial \tilde{\psi}^{ax(\{+1\}}_{m,i,j+1}}{\partial \tilde{\phi}^{(l)}_{i',j'}} = \frac{\partial \tilde{\psi}^{ax(\{+1\}}_{m,i,j}}{\partial \tilde{\phi}^{(l)}_{i',j'}}$$ (6.76)

$$Y_{m,i+1,j,i',j'} = \frac{\partial \tilde{\psi}^{ay(\{+1\}}_{m,i+1,j}}{\partial \tilde{\phi}^{(l)}_{i',j'}} = \frac{\partial \tilde{\psi}^{ay(\{+1\}}_{m,i,j}}{\partial \tilde{\phi}^{(l)}_{i',j'}}$$ (6.77)

The update is performed in two stages. First, in each step of the mesh-sweep a new element will be appended to each matrix in Eqs. (6.76) and (6.77), representing the present computational cell $(i,j)$. For $i'=i$ and $j'=j$, the value of the appended element follows directly from Eq. (6.16):
Second, for all other $i'$ and $j'$ the update is accomplished by compounding the present $X$ and $Y$ matrices with the derivative of the outgoing edge-averaged fluxes with respect to the incoming edge-averaged fluxes as computed from Eq. (6.16). Specifically, the partial derivative of $\tilde{\psi}_{m,i,j}^{\alpha(x+1)}$ with respect to $\tilde{\phi}_{i,j}^{(t)}$ in Eq. (6.76) can be evaluated using the derivative chain rule:

$$X_{m,i,j+1,i,j} = \frac{\partial \tilde{\psi}_{m,i,j}^{\alpha(x+1)}}{\partial \tilde{\phi}_{i,j}^{(t)}} = \gamma_{m,i,j}^{\alpha} \quad (6.78)$$

$$Y_{m,i+1,j,i,j} = \frac{\partial \tilde{\psi}_{m,i,j}^{\alpha(y+1)}}{\partial \tilde{\phi}_{i,j}^{(t)}} = \gamma_{m,i,j}^{\alpha} \quad (6.79)$$

The partial derivatives of $\tilde{\psi}_{m,i,j}^{\alpha(x+1)}$ with respect to $\tilde{\psi}_{m,i,j}^{\alpha}$ and $\tilde{\psi}_{m,i,j}^{\alpha(y+1)}$ are immediately obtained from Eq. (6.16). They are equal to $\gamma_{m,i,j}^{\alpha}$ and $\gamma_{m,i,j}^{\alpha(y+1)}$, respectively. Substitution of the latter result, along with the definitions in Eqs. (6.67) and (6.68), into Eq. (6.80) yields:

$$X_{m,i,j+1,i',j'} = \gamma_{m,i,j}^{x} X_{m,i,j,i',j'} + \gamma_{m,i,j}^{y} Y_{m,i,j,i',j'} \quad (6.81)$$

Following a similar procedure, the following analogous recursive relation is obtained for the $Y$ matrix:

$$Y_{m,i+1,j,i,j'} = \gamma_{m,i,j}^{x} X_{m,i,j,i',j} + \gamma_{m,i,j}^{y} Y_{m,i,j,i',j'} \quad (6.82)$$

The latter equation closes the recursive relation for the $X$ and $Y$ matrices.
It is noted that the previous derivation applies to a cell \((i, j)\) in the interior of the mesh, namely for \(1 < i < I\) and \(1 < j < J\). Since dealing with the boundary cells is in the end a matter of proper “book-keeping” in the coding of the algorithm, the details are omitted. It is also noted that the dot products in Eqs. (6.75), (6.81) and (6.82) are performed for each element in the arrays used to store the \(X\) and \(Y\) matrices. Also, since the elements of the Jacobian matrix are accumulated immediately, there is no reason to store the arrays \(X\) and \(Y\) between sweeps, i.e. they can be overwritten by subsequent angular directions. Similarly, the elements of the \(\Gamma_{m,i,j}^0\) matrix are not needed beyond the present cell \((i, j)\) and angular direction \(m\). Therefore, the array used to store the elements of the latter matrix can also be overwritten in the coding of the algorithm.

Finally, as it was indicated in Fig. 6.2, it is common in transport calculations to sweep the mesh in the \(x\) direction first, namely along rows, one row at a time. Therefore, only one copy of the \(Y\) array needs be kept and overwritten as the sweep progresses, since the outgoing \(x\) equal to constant surface at which \(Y\) is updated coincides with the incoming surface where it is used in precisely the next cell in the sweep. In contrast, the \(X\) array is computed on a surface but not used until the entire row is swept, i.e. \(I\) cells later in the sweep process. Hence it is necessary to store \(I\) different \(X\) arrays, one for each \(i = 1, \ldots, I\). Once each of these arrays is used, it can be overwritten and used for the vertically adjacent cell.

In concluding this section, it is noted that, as it was done in Sec. 3.3.3 for the code developed in slab geometry for the numerical solution of Eq. (1.27) via direct inversion of the \(B\) matrix, the cell-averaged fluxes computed via the NS code have been
successfully compared with those obtained using SI with a conveniently small value for the convergence criterion. Since the latter results served more as a debugging tool for the NS code and do not add further content to the discussion conducted in Sec. 3.3.3, they are not presented here. The NS code is instead used in Sec. 6.6.2 to numerically evaluate the elements of the $B$ matrix in order to verify the predictions of the asymptotic analysis.

6.5 Expressions for Certain Elements of Matrix $B$ in Homogeneous Configurations

In the homogeneous, uniform-mesh case all the computational cells in which the two-dimensional domain is subdivided are characterized by the same geometric and physical properties. Therefore the spatial indices $i$ and $j$ may be dropped in the expressions referring to parameters characterizing a generic computational cell. More specifically, the symbol $\Delta x$ ($\Delta y$) will be used to indicate the size of each computational cell in the $x$ ($y$) direction, $\sigma$ and $\sigma_s$ will represent the macroscopic total and scattering cross-sections, respectively, and $c$ is the scattering ratio. The reciprocal of the optical thickness for a generic cell along the $m^{th}$ discrete ordinate is denoted by $\kappa_m$, where $\kappa_m = |\mu_m|/(\sigma \Delta x)$, in the $x$ direction and by $\nu_m$, where $\nu_m = |\eta_m|/(\sigma \Delta y)$, in the $y$ direction.

In terms of the parameters introduced for the homogeneous, uniform-mesh case the expressions for the AHOT-N0 spatial weights along the $x$ and $y$ coordinates, contained in Eqs. (6.5) and (6.7), respectively, become:
In order to write compact expressions for the $B$ matrix elements, it is convenient to introduce the following definitions:

\[ \varepsilon_{m,i} = 2\kappa_m, \quad m = 1, \ldots, M \]  
(6.85)

\[ \varepsilon_{m,2} = 2\nu_m, \quad m = 1, \ldots, M \]  
(6.86)

\[ \chi_{m,1} = \varepsilon_{m,1} / (1 + \alpha_m), \quad m = 1, \ldots, M \]  
(6.87)

\[ \chi_{m,2} = \varepsilon_{m,2} / (1 + \beta_m), \quad m = 1, \ldots, M \]  
(6.88)

Substitution of Eqs. (6.85) through (6.88) into Eqs. (6.36) through (6.41) produces the expressions for the $B$ matrix elements in the homogeneous, uniform-mesh case.

**Self-coupling**

\[ B_{1,i,j,i} = 1 - c \sum_{m=1}^{M} w_m \frac{1}{1 + \sum_{k=1}^{2} \chi_{m,k}} \]  
(6.89)
Coupling with first neighbors

\[
B_{i,j,i+1,j} = -c \sum_{m=1}^{M} \frac{w_m \chi_{m,1}^2}{\varepsilon_{m,1}} \frac{1}{\left[1 + \sum_{k=1}^{2} \chi_{m,k}\right]^2}
\]  
(6.90)

\[
B_{i,j+1,i+1,j} = -2c \sum_{m=1}^{M} \frac{w_m \chi_{m,1} \chi_{m,2}}{\varepsilon_{m,1} \varepsilon_{m,2}} \frac{1}{\left[1 + \sum_{k=1}^{2} \chi_{m,k}\right]^3}
\]  
(6.91)

Coupling with second neighbors

\[
B_{i,j,i+2,j} = -c \sum_{m=1}^{M} w_m \chi_{m,1}^3 \left[ (1 + \alpha_m) \chi_{m,1} + (\alpha_m - 1)(1 + \chi_{m,2}) \right] \frac{1}{\left[1 + \sum_{k=1}^{2} \chi_{m,k}\right]^3}
\]  
(6.92)

\[
B_{i,j,j+2,j+1} = -2c \sum_{m=1}^{M} \frac{w_m \chi_{m,1}^2 \chi_{m,2}^2}{\varepsilon_{m,1}^2 \varepsilon_{m,2}^2} \left[ (2 + \alpha_m) \chi_{m,1} + (\alpha_m - 1)(1 + \chi_{m,2}) \right] \frac{1}{\left[1 + \sum_{k=1}^{2} \chi_{m,k}\right]^4}
\]  
(6.93)

\[
B_{i,j+1,j+2,j+1} = -2c \sum_{m=1}^{M} \frac{w_m \chi_{m,1} \chi_{m,2}^3 \xi_{m,1,2}}{\varepsilon_{m,1}^2 \varepsilon_{m,2}^2} \frac{\xi_{m,1,2}}{\left[1 + \sum_{k=1}^{2} \chi_{m,k}\right]^5}
\]  
(6.94)

The symbol \(\xi_{m,1,2}\) introduced in Eq. (6.94) is a short-hand notation for:

\[
\xi_{m,1,2} = \left\{ (2 + \alpha_m)(\beta_m - 1) \chi_{m,1}^2 + (\alpha_m - 1)[(\beta_m - 1) + (2 + \beta_m) \chi_{m,2}](1 + \chi_{m,2}) + \chi_{m,1}[(1 + 2\alpha_m)(\beta_m - 1) + (8 + \alpha_m + \beta_m + 2\alpha_m\beta_m) \chi_{m,2}] \right\}
\]  
(6.95)
The expressions in Eqs. (6.89) through (6.95) are given for the neighbors in the lower half of the quadrant depicted in Fig. 6.1. The expressions for the elements pertaining to the neighbors in the upper half of the quadrant are obtained by replacing the subscript 1 with 2 in the coefficients $\varepsilon$ and $\chi$, and by replacing $\alpha_m$ with $\beta_m$ in Eqs. (6.89) through (6.95).

### 6.6 Asymptotic Analysis in the Thick Cell Limit for Homogeneous Configurations

An asymptotic analysis is conducted on the $B$ matrix elements for a homogeneous configuration with a uniform mesh to study the asymptotic behavior of the $B$ matrix elements in the thick cell limit. The latter is obtained by scaling the cell widths in the $x$ and $y$ directions as $\Delta x = \delta_x \Delta$ and $\Delta y = \delta_y \Delta$, respectively, where $\delta_x$ and $\delta_y$ are fixed dimensional parameters, having dimensions of length, while $\Delta$ is a non-dimensional parameter. The asymptotic thick cell limit is obtained in the limit as $\Delta \to \infty$.

The techniques employed in this asymptotic analysis have already been discussed in Sec. 3.4.2 for the one-dimensional case. For brevity, the intricacies related to extending the analysis to two-dimensional geometry will be omitted in the following. It is noted that the analysis can be greatly simplified by observing that in the asymptotic limit as $\Delta \to \infty$, the spatial weights for the AHOT-N0 satisfy the following relations [20]:

$$\alpha_m = 1 - 2\kappa_m + O\left[\exp\left(-1/\kappa_m\right)\right] \quad (6.96)$$

$$\beta_m = 1 - 2\nu_m + O\left[\exp\left(-1/\nu_m\right)\right] \quad (6.97)$$
Substitution of Eqs. (6.96) and (6.97) into Eqs. (6.89) through (6.95) produces expressions for the elements of the $B$ matrix in terms of only $\kappa_m$ and $\nu_m$. The latter are then written explicitly in terms of the quadrature parameters, material and geometric properties and the scaling parameter $\Delta$. Finally, the following asymptotic expressions are obtained for the $B$ matrix elements in the limit as $\Delta \to \infty$.

**Self-coupling**

$$B_{i,j,i,j} = (1 - c) + c \sum_{m=1}^{M} w_m \left( \frac{\mu_m}{\sigma \delta_x} + \frac{\eta_m}{\sigma \delta_y} \right) \frac{1}{\Delta} + O \left( \frac{1}{\Delta^2} \right)$$  \hspace{1cm} (6.98)

**Coupling with first neighbors**

$$B_{i,j,i+1,j} = -\frac{c}{2} \sum_{m=1}^{M} w_m \frac{\mu_m}{\sigma \delta_x} \frac{1}{\Delta} + O \left( \frac{1}{\Delta^2} \right)$$  \hspace{1cm} (6.99)

$$B_{i,j,i+1,j+1} = -\frac{c}{2} \sum_{m=1}^{M} w_m \frac{\mu_m}{\sigma \delta_x} \frac{\eta_m}{\sigma \delta_y} \frac{1}{\Delta^2} + O \left( \frac{1}{\Delta^3} \right)$$  \hspace{1cm} (6.100)

**Coupling with second neighbors**

$$B_{i,j,i+2,j} = \frac{c}{2} \sum_{m=1}^{M} w_m \left( \frac{\mu_m}{\sigma \delta_x} \right)^2 \frac{\eta_m}{\sigma \delta_y} \frac{1}{\Delta^3} + O \left( \frac{1}{\Delta^4} \right)$$  \hspace{1cm} (6.101)

$$B_{i,j,i+2,j+1} = -\frac{c}{4} \sum_{m=1}^{M} w_m \left( \frac{\mu_m}{\sigma \delta_x} \right)^2 \frac{\eta_m}{\sigma \delta_y} \frac{1}{\Delta^3} + O \left( \frac{1}{\Delta^4} \right)$$  \hspace{1cm} (6.102)

$$B_{i,j,i+2,j+2} = -\frac{c}{2} \sum_{m=1}^{M} w_m \left( \frac{\mu_m}{\sigma \delta_x} \right)^2 \left( \frac{\eta_m}{\sigma \delta_y} \right)^2 \frac{1}{\Delta^4} + O \left( \frac{1}{\Delta^5} \right)$$  \hspace{1cm} (6.103)
As in the previous sections, the results in Eqs. (6.98) through (6.103) are given for the neighbors in the lower half of the quadrant depicted in Fig. 6.1. The expressions for the elements pertaining to the neighbors in the upper half of the quadrant are obtained by replacing $\delta_x$ with $\delta_y$ and $|\mu_m|$ with $|\eta_m|$, respectively.

A comparison of Eqs. (6.98) and (6.99) shows that the elements of the $B$ matrix pertaining to coupling of a generic cell $(i,j)$ with itself and with its first Cartesian neighbors, satisfy the following relation in the asymptotic thick cell limit:

$$B_{i,j,i,j} \sim (1-c) - B_{i,j,i+1,j} - B_{i,j,i-1,j} - B_{i,j,i,j+1} - B_{i,j,j-1}$$  \hspace{1cm} (6.104)$$

This relation is familiar from Diffusion Theory and represents the extension to two-dimensional geometry of the result obtained in Eq. (3.103) for homogeneous, uniform-mesh slabs.

Comparing Eq. (6.100) with Eqs. (6.98) and (6.99), it is evident that coupling of a cell’s averaged scalar flux with its first diagonal neighbors is of higher order, in the inverse of a cell optical thickness, with respect to self-coupling and coupling with the first Cartesian neighbors. The results reported in Eqs. (6.101) through (6.103) for the second neighbors confirm the intuitive expectation, for this type of scaling, that the farther the neighbor, the weaker the coupling. Additional quantitative insight into this intuitive behavior will be given in Sec. 6.6.1, in which asymptotic estimates are obtained for the strength of coupling with neighbors beyond the second.
6.6.1 Asymptotic Estimates for the Strength of Coupling with Far Neighbors

Even though expressions for the $B$ matrix elements pertaining to the coupling of a cell’s averaged scalar flux with neighbors beyond the second have not been obtained in closed analytical form, it is still possible to obtain an estimate of their increasing asymptotic order as a function of the distance from the self-cell. In fact, no matter how intricate they are, the expressions for the elements of the $B$ matrix result in general from the sum of products of the $\gamma$ coefficients, previously introduced in Eq. (6.28), that correspond to the various paths that can connect two cells in the transport computation, over the directions in the quadrature and over all the possible paths. Therefore, an estimate of the increasing infinitesimal order of the $B$ matrix elements can be obtained by simply reasoning on the leading order of the $\gamma$ coefficients with respect to $1/\Delta$.

In the homogeneous, uniform-mesh case all the computational cells in which the two-dimensional domain is subdivided are characterized by the same geometric and physical properties. Therefore the spatial indices $i$ and $j$ may be dropped in the expressions for the $\gamma$ coefficients, characterizing a generic computational cell, in Eqs. (6.17) through (6.25). Following the same steps outlined in the previous section for the asymptotic analysis of the $B$ matrix elements in the thick cell limit, asymptotic expressions are obtained for the $\gamma$ coefficients.

$$
\gamma_{m}^{ia} = c - c\left(\frac{\mu_{m}}{\sigma\delta_{x}} + \frac{\eta_{m}}{\sigma\delta_{y}}\right)\frac{1}{\Delta} + O\left(\frac{1}{\Delta^{2}}\right)
$$ (6.105)
\[
\gamma_{m}^{xx} = \frac{|\eta_m|}{\sigma \delta_y} \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right) \quad (6.106)
\]

\[
\gamma_{m}^{yy} = \frac{|\mu_m|}{\sigma \delta_x} \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right) \quad (6.107)
\]

\[
\gamma_{m}^{xy} = -c - c \frac{|\mu_m|}{\sigma \delta_x} \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right) \quad (6.108)
\]

\[
\gamma_{m}^{yx} = -\frac{|\mu_m|}{\sigma \delta_x} \frac{|\eta_m|}{\sigma \delta_y} \frac{1}{\Delta^2} + O\left(\frac{1}{\Delta^4}\right) \quad (6.109)
\]

\[
\gamma_{m}^{yy} = \frac{|\mu_m|}{\sigma \delta_x} \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right) \quad (6.110)
\]

\[
\gamma_{m}^{xx} = -c - c \frac{|\eta_m|}{\sigma \delta_y} \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right) \quad (6.111)
\]

\[
\gamma_{m}^{yx} = \frac{|\eta_m|}{\sigma \delta_y} \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right) \quad (6.112)
\]

\[
\gamma_{m}^{yy} = -\frac{|\mu_m|}{\sigma \delta_x} \frac{|\eta_m|}{\sigma \delta_y} \frac{1}{\Delta^2} + O\left(\frac{1}{\Delta^4}\right) \quad (6.113)
\]
From the previous results it is evident that $\gamma^u_m$ and $\gamma^u_m$ are $O(\Delta^0)$; $\gamma^{uu}_m$ and $\gamma^{uu}_m$ are $O(\Delta^{-1})$; finally $\gamma^{uu}_m$ are $O(\Delta^{-2})$, $u,v=x$ or $y$. Therefore, only those products of $\gamma$ coefficients that contain the minimum number of $\gamma^{uu}_m$ coefficients will contribute to the leading order of the corresponding $B$ matrix element. The related “dominant” transport paths can be easily identified and the corresponding leading order for the $B$ matrix element determined from the order of the $\gamma$ coefficients.

To fix ideas, the concept of dominant transport paths is outlined at first for the second neighbors. Three of the six transport paths that connect a cell to its second purely diagonal neighbor, originally sketched in Fig. 6.7, are depicted in Fig. 6.9. The additive contributions to the order that each single path contributes to the $B_{i,j,i+2,j+2}$ element are indicated for the $\gamma$ coefficient that correspond to each segment constituting the path. By adding the contributions for each path it is concluded that the purely diagonal path (solid line) dominates the other two transport paths (dashed lines). The same conclusion can be drawn for the purely diagonal path of the other three transport paths contributing to $B_{i,j,i+2,j+2}$, previously sketched in Fig. 6.8. These two purely diagonal paths determine the $O(\Delta^{-4})$ leading order previously obtained in Eq. (6.103) from the asymptotic analysis.

The dominant path contributing to the leading order of $B_{i,j,i+2,j+1}$ is sketched in Fig. 6.10, again using a solid line. This S-shaped path determines the $O(\Delta^{-3})$ leading order previously obtained in Eq. (6.102) from the asymptotic analysis.
Fig. 6.9: Dominant transport path contributing to the leading order of $B_{i,j;i+2,j+2}$ in the thick cell limit.

Fig. 6.10: Dominant transport path contributing to the leading order of $B_{i,j;i+2,j+1}$ in the thick cell limit.
Finally, for the case of the second Cartesian neighbor, the dominant path is of course coincident with the only possible transport path, sketched in Fig. 6.11. This straight path determines the $O\left(\Delta^{-3}\right)$ leading order previously obtained in Eq. (6.101) from the asymptotic analysis for $B_{i,j,i+2,j}$.

![Fig. 6.11: Dominant transport path contributing to the leading order of $B_{i,j,i+2,j}$ in the thick cell limit.](image)

It is noted that the leading order is the same for $B_{i,j,i+2,j+1}$ and $B_{i,j,i+2,j}$, $O\left(\Delta^{-3}\right)$, while $B_{i,j,i+2,j+2}$, namely the element pertaining to coupling with the second purely diagonal neighbor, is one order higher $O\left(\Delta^{-4}\right)$. This result is not restricted to the second neighbors. In the following it will in fact be shown that for all $r^{th}$ neighboring cells, i.e. cells that can be reached by traversing a minimum of $r$ intervening cells, a different estimate is obtained for the purely diagonal neighbor and for all the other neighbors with the same $r$, respectively. In fact, with reference to a quadrant, it can be proved that:

$$O\left(B_{i,j,i+r,j+r}\right) = O\left(\Delta^{-2r}\right)$$  \hspace{1cm} (6.114)

$$O\left(B_{i,j,i+r,j+r-k}\right) = O\left(\Delta^{-\left(2r-1\right)}\right)$$  \hspace{1cm} (6.115)
independent of \( k \), for \( 1 \leq k \leq r \).

The results in Eqs. (6.114) and (6.115) are given for the neighbors in the lower half of the quadrant depicted in Fig. 6.1. The same results hold true for the elements pertaining to the neighbors in the upper half of the quadrant. Therefore, a derivation of the latter results is given in the following considering only the neighbors in the lower half of the quadrant. In the derivation it is convenient to distinguish between the case of a purely diagonal neighbor of order \( r \), treated at first, and the other neighbors of the same order, considered at last.

**Purely diagonal neighbor of order \( r \)**

Any path that connects cell \((i, j)\) with cell \((i+r, j+r)\) traverses a total number of \((2r+1)\) cells and is made up of \((2r+1)\) segments corresponding to the product of \((2r+1)\) \(\gamma\) coefficients. In fact, starting from cell \((i+r, j+r)\), \(r\) interfaces between columns in the Cartesian mesh and \(r\) interfaces between rows in the Cartesian mesh have to be crossed by any path that ends in cell \((i, j)\). These \(2r\) crossings account for \(2r\) segments in any possible path while an additional segment lies in the destination cell \((i, j)\). This result is verified, for the case of the second purely diagonal neighbor \((r = 2)\), by the transport paths depicted in Figs. 6.7 and 6.8, each comprised of 5 segments.

As noted above, the contribution to the \(B\) matrix element \(B_{i,j,i+r,j+r}\) that couples the cell-averaged scalar flux in cell \((i, j)\) to the cell-averaged scalar flux in cell \((i+r, j+r)\), from a path connecting the two cells, results from the product of \((2r+1)\) \(\gamma\) coefficients. As evident from Figs. 6.7 and 6.8, the first and last coefficients in the
product can only be of the type $\gamma^u_m$ and $\gamma^v_m$, respectively, where $u = x$ or $y$. The remaining $(2r-1)$ coefficients in the product may be of the type $\gamma^v_m$ or $\gamma^u_m$, where $u, v = x$ or $y$. As obtained previously, the $\gamma^u_m$ coefficients are $O(\Delta^{-1})$ while the $\gamma^v_m$ coefficients are $O(\Delta^{-2})$. It follows that, of all the possible paths connecting cells $(i, j)$ and $(i + r, j + r)$ that one would have to consider, only two are going to contribute to the leading order of the corresponding $B$ matrix element. These are the purely diagonal paths corresponding to products that contain only $\gamma^v_m$ coefficients and no $\gamma^u_m$ coefficients. Any other path will contain at least a $\gamma^v_m$ coefficient and will be of higher order in the reciprocal of $\Delta$. To fix ideas, the two dominant paths for the purely diagonal third neighbor are depicted using a solid line in Fig. 6.12. The two paths in dashed lines are the ones contributing the highest order contributions to the corresponding $B$ matrix element, or, in other words, the weakest ones.

Since $\gamma^u_m$ and $\gamma^v_m$ are $O(\Delta^0)$ and $O(\Delta^{-1})$ respectively while the $\gamma^v_m$ coefficients are $O(\Delta^{-1})$, the contribution to the leading order of $B_{i,j,i+r,j+r}$ due to the purely diagonal paths can be immediately obtained:

$$O(B_{i,j,i+r,j+r}) = O(\Delta^0) \cdot \left[ O(\Delta^{-1}) \cdot \ldots \cdot O(\Delta^{-1}) \right] \cdot O(\Delta^{-1}) = O(\Delta^{-2r}) \quad (6.116)$$

This proves the result contained in Eq. (6.114).
**Fig. 6.12:** Dominant (solid lines) and weakest paths for a purely diagonal third neighbor in the thick cell limit.

**Other neighbors of order** $r$

Any path that connects cell $(i, j)$ with cell $(i+r, j+r-k)$, with $1 \leq k \leq r$, traverses a total number of $(2r-k+1)$ cells and is made up of $(2r-k+1)$ segments corresponding to the product of $(2r-k+1)$ $\gamma$ coefficients. In fact, starting from cell $(i+r, j+r-k)$, $r$ interfaces between columns in the Cartesian mesh and $(r-k)$ interfaces between rows in the Cartesian mesh have to be crossed by any path that ends in cell $(i, j)$. These $(2r-k)$ crossings account for $(2r-k)$ segments in any possible path while an additional segment lies in the destination cell $(i, j)$, giving a total of $(2r-k+1)$ segments. This result is verified, for the case of the second Cartesian neighbor $(r, k = 2)$,
by the single transport path depicted in Fig. 6.5, which is comprised of 3 segments. It is also verified, for the case of the intermediate second neighbor \((r = 2, k = 1)\), by the transport paths depicted in Fig. 6.6, each comprised of 4 segments.

As noted above, the contribution to the B matrix element \(B_{i,j,i+r,j+r-k}\), that couples the cell-averaged scalar flux in cell \((i,j)\) to the cell-averaged scalar flux in cell \((i+r, j+r-k)\), from a path connecting the two cells, results from the product of \((2r-k+1)\) \(\gamma\) coefficients. As evident from Figs. 6.5 and 6.6, the first and last coefficients in the product can only be of the type \(\gamma_{m}^{u}x\) and \(\gamma_{m}^{v}y\), respectively, where \(u = x\) or \(y\). The remaining \((2r-k-1)\) coefficients in the product may be of the type \(\gamma_{m}^{uv}\) or \(\gamma_{m}^{uv}\), where \(u,v = x\) or \(y\). It is recalled that the \(\gamma_{m}^{uv}\) coefficients are \(O(\Delta^{-1})\) while the \(\gamma_{m}^{uv}\) coefficients are \(O(\Delta^{-2})\). It follows that, of all the possible paths connecting cells \((i,j)\) and \((i+r, j+r-k)\) that one would have to consider, only one is going to contribute to the leading order of the corresponding B matrix element. This is the S-shaped path corresponding to products that contain the maximum possible number of \(\gamma_{m}^{uv}\) coefficients and the minimum possible number of \(\gamma_{m}^{uv}\) coefficients. Any other path will be of higher order in the reciprocal of \(\Delta\). To fix ideas, the dominant paths for the non-purely diagonal third neighbors are depicted in Fig. 6.13. Of course, for the case of the third Cartesian neighbor, the S-shaped path reduces to the only possible path, that is a straight path.
Fig. 6.13: Dominant paths for the non-purely diagonal third neighbors in the thick cell limit.

Of the \((2r-k-1)\) intermediate factors in the product of the \(\gamma\) coefficients corresponding to an S-shaped path, \((k-1)\) are \(\gamma_m^{uu}\) coefficients. In fact, as exemplified in Fig. 6.13 for the neighbors of order 3, the number of \(\gamma_m^{uu}\) coefficients decreases by one unit at a time going from \((r-1)\), for the Cartesian neighbor corresponding to \(k = r\), to a value of 0, for the neighbor of order \(r\) corresponding to \(k = 1\). The remaining \(2(r-k)\) intermediate factors can be interpreted as the product of \((r-k)\) binomials of the form \(\left(\gamma_m^{uv} \gamma_m^{vu}\right)\). Since \(\gamma_m^{uu}\) and \(\gamma_m^{uu}\) are \(O(\Delta^0)\) and \(O(\Delta^{-1})\), respectively, while \(\gamma_v^{uv}\) and \(\gamma_v^{uu}\) are
\(O(\Delta^{-1})\) and \(O(\Delta^{-2})\), respectively, the contribution to the leading order of \(B_{i,j,i+r,j+r-k}\) due to the S-shaped path can be immediately obtained:

\[
O(B_{i,j,i+r,j+r-k}) =
\]

\[
= O(\Delta^0) [O(\Delta^{-2}) \ldots O(\Delta^{-2})] [O(\Delta^{-2}) \ldots O(\Delta^{-2})] O(\Delta^{-1}) =
\]

\[
\text{ } | (r-k) \text{ times } | | (k-1) \text{ times } |
\]

\[
= O(\Delta^{-(2r-2k+2k-1)}) = O(\Delta^{-(2r-1)})
\]

This proves the result contained in Eq. (6.115) and explains why the order of \(B_{i,j,i+r,j+r-k}\) is independent from \(k\). A more intuitive explanation of this independence may be gained from Fig. 6.13. It is noted that the same number of columns in the Cartesian mesh is interposed between the starting cell and the ending cell. Each S-shaped path intersects a column with either a single straight \(\gamma_{\nu\mu}^m\) segment that is \(O(\Delta^{-2})\) or with two skewed \(\gamma_{\nu\nu}^m\), \(\gamma_{\mu\mu}^m\) segments, each of order \(O(\Delta^{-1})\). It follows that the \(B\) matrix elements coupling the cell-averaged scalar flux in cell \((i,j)\) with any of the non-purely diagonal neighbors of order \(r\) is the same and can only depend on \(r\).

The results of the asymptotic analysis are summarized in Fig. 6.14. The leading order is shown for the \(B\) matrix elements coupling cell \((1,1)\) in the bottom-left corner with up to the fourth neighbors. Due to the symmetry of the observed order about the diagonal cells \((i,i)\), only sub-diagonal entries are included in Fig. 6.14.
These results show that, in the limit $\Delta \rightarrow \infty$, the elements in the $B$ matrix pertaining to the coupling of a cell’s averaged scalar flux with itself and with its first Cartesian neighbors dominate over all the other elements in the matrix. By virtue of the result in Eq. (6.104), it is concluded that in the thick cell limit for the homogeneous case the full transport operator represented by matrix $B$ acquires a five-banded block matrix structure characterized by a diffusion-like coupling stencil. This result provides further insight into the superior convergence properties of diffusion-based acceleration schemes in two-dimensional geometry, in the homogeneous case. Specifically, the convergence properties of the Adjacent-cell Preconditioner (AP) in the asymptotic thick cell limit for the homogeneous, uniform-mesh case in two-dimensional geometry are discussed in Sec. 7.2.3.

Fig. 6.14: Summary of asymptotic results for the homogeneous thick cell limit.
In concluding this section it is also noted that, quite differently from the one-dimensional case, the results obtained in the asymptotic thick cell limit for the two-dimensional case indicate that no exponential decay is obtained for the elements of the $B$ matrix coupling a cell with neighboring cells beyond the first neighbors. These findings provide further insight into the peculiar asymptotic behavior possessed by the AHOT-N0 integral transport matrix in homogeneous slab geometry as opposed to multi-dimensional geometry, originally pointed out by Azmy in [20].

6.6.2 Numerical Verification

In order to verify the results from the asymptotic analysis, the NS code has been used to numerically evaluate the $B$ matrix elements for a homogeneous problem characterized by a $5 \times 5$ spatial mesh. A square mesh is considered in order to reduce the matrix elements of interest to those pertaining to the coupling of cells comprised in half a quadrant, as in Fig. 6.14.

In Fig. 6.15 we present the behavior of the $B$ matrix elements computed with the above algorithm for cells up to the second neighbors. The case depicted in Fig. 6.15 is based on an $S_6$ level symmetric quadrature with equal weights, $\sigma = 1$, $\delta_x = \delta_y = 1$, and $c = 0.5$. It is evident that the $B$ matrix elements approach the theoretically predicted asymptotes of Eqs. (6.98) through (6.103) summarized in Fig. 6.14, for values of $\Delta$ larger than $\sim 10$, thus verifying our asymptotic analysis.
The asymptotic behavior of the $\mathbf{B}$ matrix elements corresponding to the third and fourth neighboring cells was also successfully verified against the analytic orders of Eqs. (6.114) and (6.115), reported in Fig. 6.14. The $\mathbf{B}$ matrix elements pertaining to coupling with the third neighbors computed with the NS code are reported in Fig. 6.16. It is noted that all the elements pertaining to coupling with the non-purely diagonal third neighbors are clustered together and are characterized by the same order as a function of $\Delta$. Noting that there are two decades between each grid-line for the vertical axis, and counting decades between two successive values of the $\Delta$ parameter in the asymptotic regime, it is evident that the points corresponding to these elements are separated by five decades for each decade increase in $\Delta$. This is in line with the $O(\Delta^{-5})$ predicted in...
Fig. 6.14, for the non-purely diagonal neighbors of order \( r = 3 \). In contrast, the decades for the purely diagonal neighbor are six and confirm the \( O(\Delta^{-6}) \) predicted in Fig. 6.14, for the strength of coupling with the third purely diagonal neighbor.

Finally, the \( \mathbf{B} \) matrix elements pertaining to coupling with the fourth neighbors computed with the NS code are reported in Fig. 6.17. Even for this case, the points corresponding to the non-purely diagonal neighbors of order \( r = 4 \) are all clustered together. Counting decades it is verified that the \( \mathbf{B} \) matrix elements pertaining to coupling with the fourth non-purely diagonal neighbors are \( O(\Delta^{-7}) \), while the matrix element corresponding to the purely diagonal neighbor is \( O(\Delta^{-8}) \).
Fig. 6.17: Numerically computed values of $B$ matrix elements for the fourth neighbors in the thick cell limit.

The latter results are also in line with the theoretical predictions summarized in Fig. 6.14, for the case $r = 4$.

### 6.7 Asymptotic Analysis in the Thin Cell Limit for Homogeneous Configurations

An asymptotic analysis is conducted on the $B$ matrix elements for a homogeneous configuration with a uniform mesh to study their asymptotic behavior in the thin cell limit. The latter is obtained by scaling the cell widths in the $x$ and $y$ directions as $\Delta x = \delta_x \delta$ and $\Delta y = \delta_y \delta$, respectively, where $\delta_x$ and $\delta_y$ are fixed dimensional parameters, having dimensions of length, while $\delta$ is a non-dimensional parameter. The asymptotic thin cell limit is obtained as $\delta \to 0$. 
The techniques employed in this asymptotic analysis have already been discussed in Sec. 3.4.3 for the one-dimensional case. Specifically, as in slab geometry, the exponentials brought about by the hyperbolic cotangents of the AHOT-N0 spatial weights, see Eq. (6.5) and (6.7), must be expanded in a Taylor series in the thin cell limit. For brevity, the intricacies related to extending the analysis to two-dimensional geometry will be omitted in the following. First the elements of the $B$ matrix, whose expressions for the homogeneous case were obtained in Eqs. (6.89) through (6.95), are written explicitly in terms of the quadrature parameters, the material and geometric properties and the scaling parameter $\delta$. Finally, the following asymptotic expressions are obtained for the $B$ matrix elements in the limit as $\delta \to 0$.

**Self-coupling**

\[
B_{i,i,i,j} = 1 - \frac{c}{2} \sum_{m=1}^{M} w_m \frac{1}{\left| \mu_m \right| + \left| \eta_m \right|} \frac{1}{\sigma^2} \delta + O(\delta^2) \tag{6.118}
\]

**Coupling with first neighbors**

\[
B_{i,i,j+1,j} = -\frac{c}{2} \sum_{m=1}^{M} w_m \frac{\left| \mu_m \right|}{\sigma^2} \left( \frac{1}{\sigma^2} + \left| \eta_m \right| \right) \delta + O(\delta^2) \tag{6.119}
\]

\[
B_{i,i,j+1,j+1} = -\frac{c}{2} \sum_{m=1}^{M} w_m \frac{\left| \mu_m \right|}{\sigma^2} \left( \frac{1}{\sigma^2} + \left| \eta_m \right| \right) \delta + O(\delta^2) \tag{6.120}
\]
Coupling with second neighbors

\[ B_{i,j,i+2,j} = -\frac{c}{2} \sum_{m=1}^{M} w_m \left( \frac{\mu_m}{\sigma^2_{\delta_x}} \left( \frac{\mu_m}{\sigma_{\delta_x}} + \frac{\eta_m}{\sigma_{\delta_y}} \right) \right)^3 \delta + O(\delta^2) \quad (6.121) \]

\[ B_{i,j,i+2,j+1} = -c \sum_{m=1}^{M} w_m \left( \frac{\mu_m}{\sigma^2_{\delta_x}} \left( \frac{\mu_m}{\sigma_{\delta_x}} + \frac{\eta_m}{\sigma_{\delta_y}} \right) \right)^4 \delta + O(\delta^2) \quad (6.122) \]

\[ B_{i,j,i+2,j+2} = -2c \sum_{m=1}^{M} w_m \left( \frac{\mu_m}{\sigma^2_{\delta_x}} \left( \frac{\mu_m}{\sigma_{\delta_x}} + \frac{\eta_m}{\sigma_{\delta_y}} \right) \right)^5 \delta + O(\delta^2) \quad (6.123) \]

As in the previous sections, the results in Eqs. (6.118) through (6.123) are given for the neighbors in the lower half of the quadrant depicted in Fig. 6.1. The expressions for the elements pertaining to the neighbors in the upper half of the quadrant are obtained by replacing \( \delta_x \) with \( \delta_y \) and \( |\mu_m| \) with \( |\eta_m| \), respectively.

It is noted that the leading order of \( B_{i,j,i+2,j} \), whose asymptotic expression was obtained in Eq. (6.121), can be \( O(\delta^2) \) for the case of a square mesh, \( \delta_x = \delta_y \), and of the level symmetric \( S_2 \) quadrature, \( |\mu_m| = |\eta_m| \) for \( m = 1,4 \). Similarly, the leading order of
Eq. (6.122), becomes $O\left(\delta^2\right)$ for the case of a rectangular mesh with $\delta_x = 2\delta_y$ and of the level symmetric $S_2$ quadrature. It is expected that analogous exact algebraic cancellations can result for other elements of the $B$ matrix, for a particular choice of the widths $\delta_x$ and $\delta_y$ of a computational cell in a uniform spatial mesh, when the level symmetric $S_2$ is employed.

For a level symmetric quadrature of order higher than two, both for rectangular and square meshes, it is evident from the expressions contained in Eqs. (6.119) through (6.123), that all the $B$ matrix elements pertaining to coupling of a cell’s averaged scalar flux with neighboring cells up to the second neighbors are $O(\delta)$. The only exception to this asymptotic behavior is constituted by the elements pertaining to self-coupling. As evident from Eq. (6.118), the latter are $O(\delta^0)$.

As for the homogeneous thick cell limit, estimates for the infinitesimal order of the $B$ matrix elements pertaining to coupling with neighboring cells beyond the second neighbors can be obtained by reasoning on the leading order of the $\gamma$ coefficients with respect to $\delta$. As it will become apparent in the following, the treatment of the homogeneous thin cell limit is more complicated than the study of the homogeneous thick cell limit. Specifically, it is not possible to obtain a unified prediction that covers all the possible choices of parameters with regard to the quadrature order and the aspect ratio of the computational cells in the uniform spatial mesh.

The asymptotic expressions obtained for the $\gamma$ coefficients in the homogeneous, uniform-mesh thin cell limit are:
\[
\gamma_m^{xa} = c \frac{1}{\left(\frac{\mu_m}{\sigma \delta_x} + \frac{\eta_m}{\sigma \delta_y}\right)} \delta + O(\delta^2)
\]  
(6.124)

\[
\gamma_m^{ax} = \frac{|\eta_m|}{\sigma \delta_y} \frac{1}{\left(\frac{\mu_m}{\sigma \delta_x} + \frac{\eta_m}{\sigma \delta_y}\right)} + O(\delta)
\]  
(6.125)

\[
\gamma_m^{ay} = \frac{|\mu_m|}{\sigma \delta_x} \frac{1}{\left(\frac{\mu_m}{\sigma \delta_x} + \frac{\eta_m}{\sigma \delta_y}\right)} + O(\delta)
\]  
(6.126)

\[
\gamma_m^{ca} = c \frac{1}{\left(\frac{\mu_m}{\sigma \delta_x} + \frac{\eta_m}{\sigma \delta_y}\right)} \delta + O(\delta^2)
\]  
(6.127)

\[
\gamma_m^{cx} = -\frac{|\eta_m|}{\sigma \delta_y} \frac{|\mu_m|}{\sigma \delta_x} \frac{1}{\left(\frac{\mu_m}{\sigma \delta_x} + \frac{\eta_m}{\sigma \delta_y}\right)} + O(\delta)
\]  
(6.128)

\[
\gamma_m^{cy} = 2 \frac{|\mu_m|}{\sigma \delta_x} \frac{1}{\left(\frac{\mu_m}{\sigma \delta_x} + \frac{\eta_m}{\sigma \delta_y}\right)} + O(\delta)
\]  
(6.129)
\[ \gamma_{m}^{xx} = c \frac{1}{\left( \mu_{m} \pm \eta_{m} \right)} \delta + O(\delta^2) \]  

\[ \gamma_{m}^{yy} = 2 \frac{1}{\sigma \delta_{x}} \left( \frac{\mu_{m}}{\sigma \delta_{x}} + \frac{\eta_{m}}{\sigma \delta_{y}} \right) + O(\delta) \]  

\[ \gamma_{m}^{xy} = \frac{1}{\sigma \delta_{x} \sigma \delta_{y}} \left( \frac{|\mu_{m}|}{\sigma \delta_{x}} - \frac{|\eta_{m}|}{\sigma \delta_{y}} \right) + O(\delta) \]  

It is noted that, as evident from Eqs. (6.128) and (6.132), the leading order of the coefficients \( \gamma_{m}^{xx} \) and \( \gamma_{m}^{yy} \) is characterized by the presence of a negative sign between the two terms in its numerator. This negative sign complicates the analysis and limits the scope of the predictions that can be made on the leading order of the \( \mathbf{B} \) matrix elements, based on the asymptotic behavior of the \( \gamma \) coefficients. For one thing, the leading order of coefficients \( \gamma_{m}^{xx} \) and \( \gamma_{m}^{yy} \) can become \( O(\delta) \), instead of \( O(\delta^0) \), for a square mesh, \( \delta_x = \delta_y \), and a discrete ordinate characterized by \( |\mu_{m}| = |\eta_{m}| \). This result explains why the case of a square mesh and a level symmetric \( S_2 \) quadrature is peculiar, as pointed out earlier considering Eq. (6.121) for the Cartesian neighbor \( B_{i,j,i+2,j} \). The negative sign effecting the named difference also has a subtler consequence. Even if the \( O(\delta^0) \) term of the \( \gamma_{m}^{xx} \) and \( \gamma_{m}^{yy} \) coefficients is not an exact zero, the superposition of products of the \( \gamma \)
coefficients over the discrete ordinates in the quadrature and over the various transport
paths can yield an algebraic cancellation of the leading order of the corresponding \( B \)
matrix element that would otherwise be predicted considering only the leading order of
the \( \gamma \) coefficients. This fact was pointed out earlier analyzing the exact asymptotic
expression for \( B_{i,j,i+2,j+1} \) in Eq. (6.122), for the case of a rectangular mesh with \( \delta_x = 2\delta_y \)
and of the level symmetric \( S_2 \) quadrature. This complication is brought about by the fact
that the \( \gamma_m^{xy} \) and \( \gamma_m^{yx} \) coefficients are also \( O(\delta^0) \), as evident from Eqs. (6.129)
and (6.131). Therefore, differently from the homogeneous thick cell limit, none of the
three transport paths in Fig. 6.6 dominates over the others, and all have to be considered
in determining the leading order of \( B_{i,j,i+2,j+1} \). It is the negative sign in the numerator of
the leading \( O(\delta^0) \) contribution to the \( \gamma_m^{xy} \) coefficients, over two of the three paths in
Fig. 6.6, that is in the end responsible for the \( O(\delta^2) \) for \( B_{i,j,i+2,j+1} \), for the case \( \delta_x = 2\delta_y \).
But this result can only be predicted through a detailed algebraic calculation of the
contributions to \( B_{i,j,i+2,j+1} \) from the various paths. The leading order that would be
predicted for \( B_{i,j,i+2,j+1} \), for the case \( \delta_x = 2\delta_y \), based on the leading orders of the \( \gamma \)
coefficients, is instead \( O(\delta) \), as sketched in Fig. 6.18.

The potential for algebraic cancellations resulting from the cumulative effect of
various transport paths contributing to a certain \( B \) matrix element is present for the case
of the \( S_2 \) quadrature for rectangular meshes and potentially for quadratures of order
higher than two in the case of a square mesh. For these cases, an estimate of the leading
order of the $B$ matrix elements based on the leading order of the $\gamma$ coefficients could lead to overestimating the leading order of some of the matrix elements. Notwithstanding, there are two notable cases in which a correct estimate of the leading order of the $B$ matrix elements can still be obtained through simple arguments based on the leading order of the $\gamma$ coefficients. As it will be detailed in the following, the first case is the more general case of a level symmetric quadrature of order greater than two and of a rectangular mesh. The second case is the more specific case of a square mesh for the level symmetric $S_2$ quadrature.

![Diagram](image.png)

Fig. 6.18: Additive order of $\gamma$ coefficients for $B_{i,j,i+2,j+1}$ for rectangular cells in the thin cell limit.

For rectangular meshes and level symmetric quadratures of order greater than two, the $\gamma_{uu}^m$, $\gamma_{uv}^m$ and $\gamma_{uu}^m$ coefficients are all $O(\delta^3)$, while the $\gamma_{uv}^m$ coefficients are $O(\delta)$, with $u,v = x$ or $y$. The $\gamma_{uu}^m$ coefficient is also $O(\delta)$ but represents a particular case since it only contributes to the $B_{i,j,i,j}$ diagonal elements, pertaining to self-coupling,
whose order is $O(\delta^0)$, as obtained in Eq. (6.118). Therefore, no matter how far in the mesh a cell $(r,s)$ is from cell $(i,j)$, the predicted leading order for the corresponding $B_{r,i,j,r,s}$ matrix element, based on the leading order of the $\gamma$ coefficients, is in any case $O(\delta)$. Even for this case, as noted previously, the numerator of the leading $O(\delta^0)$ contribution to the order of the $\gamma_m^{\delta^0}$ coefficients is characterized by a negative sign. In this case, though, this negative sign cannot lead to an algebraic cancellation of the predicted leading order of the $B$ matrix elements, thanks to the contribution of the discrete ordinates in the quadrature characterized by $|\mu_m| \neq |\eta_m|$, under the assumption of a rectangular mesh, namely $\delta_x \neq \delta_y$. In fact, even though a level symmetric quadrature contains both $(\mu_m, \eta_m)$ and $(\eta_m, \mu_m)$, and the contributions from these discrete ordinates may potentially lead to an algebraic cancellation, the latter is prevented by the fact that the denominator of the $O(\delta^0)$ contribution to the order of $\gamma_m^{\delta^0}$ is different for $(\mu_m, \eta_m)$ and $(\eta_m, \mu_m)$, under the assumption $\delta_x \neq \delta_y$. It follows that the contributions to the predicted leading order, $O(\delta)$, for the off-diagonal $B$ matrix elements due to $(\mu_m, \eta_m)$ and $(\eta_m, \mu_m)$ cannot exactly cancel each other in general. This explains, for example, why the leading order for Eq. (6.122) is still $O(\delta)$, even for the case of a rectangular mesh with $\delta_x = 2\delta_y$, for a level symmetric quadrature of order greater than two.

The results of the thin-cell asymptotic analysis are summarized in Fig. 6.19. The leading order is shown for the $B$ matrix elements coupling cell $(1,1)$ in the bottom-left
corner with up to the fourth neighbors. Due to the symmetry of the observed order about the diagonal cells \((i,i)\), only sub-diagonal entries are included in Fig. 6.19.

![Diagram](image)

**Fig. 6.19:** Asymptotic results in the thin cell limit for a quadrature of order \(n > 2\).

Numerical evidence indicates that the results summarized in Fig. 6.19 are also valid in the case of a square mesh. Therefore, for the case of a level symmetric quadrature of order greater than two, the structure acquired by the \(B\) matrix in the thin cell limit for a two-dimensional homogeneous, uniform-mesh configuration is similar to the structure acquired by the integral transport matrix in the same limit in slab geometry, see Sec. 3.4.3. As for the one-dimensional case, matrix \(B\) is again approaching the identity matrix \(I\) in the thin cell limit. Yet, there is a fundamental difference between the two-dimensional case and the one-dimensional case. While in the one-dimensional case all the off-diagonal elements are equal to leading order, namely they are characterized by the
same coefficient multiplying $\delta$, in the two-dimensional case a different coefficient is found, as evident comparing Eqs. (6.119) through (6.123). Further research is necessary in order to ascertain if a generalized formulation of the transformation that was introduced in Sec. 3.6, allowing to bring matrix $B$ into a matrix asymptotically dominated by its diagonal to within $O(\delta^2)$ off-diagonal elements in the one-dimensional case, can be identified for the more general two-dimensional case.

Finally, the case of a square mesh and a level symmetric $S_2$ quadrature is considered. For this case the $\gamma_{m}^{uv}$ and $\gamma_{m}^{vu}$ coefficients are $O(\delta^0)$, while the $\gamma_{m}^{uu}$ and $\gamma_{m}^{uu}$ coefficients are $O(\delta)$, with $u,v = x$ or $y$. Interestingly enough, the $O(\delta)$ contribution to the $\gamma_{m}^{uu}$ coefficients does not contain a difference for the case $m = n$ and $\delta_x = \delta_y$:

$$\gamma_{m}^{xx} = \gamma_{m}^{yy} = -\frac{1}{6} \frac{1}{\sigma \delta_x + \sigma \delta_y} \delta + O(\delta^2)$$ (6.133)

Therefore, the concept of a dominant transport path can be applied to treat this particular case, similarly to what was done for the asymptotic thick cell limit. The dominant paths are once again those paths that correspond to products of the $\gamma$ coefficients that contain the minimum number of $\gamma_{m}^{uu}$ coefficients. The latter paths are the same as indicated in the previous section for a purely diagonal neighbor and for the other neighbors of a certain order $r$. The only difference lies in the additive order for the $\gamma$ coefficients to be attached to the segments forming a dominant path, as illustrated in Figs. 6.20 and 6.21 for the case of the purely diagonal neighbor and of the other neighbors of order three, respectively.
Fig. 6.20: Dominant paths for a purely diagonal third neighbor in the thin cell limit for the $S_2$ quadrature and a square mesh.

The results of the thin-cell asymptotic analysis for the $S_2$ quadrature and a square mesh are summarized in Fig. 6.22. The leading order is shown for the $B$ matrix elements coupling cell (1,1) in the bottom-left corner with up to the fourth neighbors. Due to the symmetry of the observed order about the diagonal cells $(i, i)$, only sub-diagonal entries are included in Fig. 6.22.

The increasing infinitesimal order predicted in Fig. 6.22, going from the purely diagonal neighbor of a given order $r$ to the Cartesian neighbor of the same order, has also been observed numerically. Specifically, the Mathematica [42] notebook described in Sec. 7.3.1 has been used to compute the elements of the $B$ matrix for very small $\delta$ and
the structure acquired by the matrix for different quadratures and cell’s aspect ratios confirmed the fundamental difference between the “leading order patterns” reported in Figs. 6.19 and 6.22, respectively. It is suggested that a more systematic numerical investigation of the theoretical predictions for the thin cell limit be conducted as part of the further research envisioned for this asymptotic limit in two-dimensional geometry.

Fig. 6.21: Dominant paths for the other third neighbors in the thin cell limit for the $S_2$ quadrature and a square mesh.
6.8 Conclusion

The coupling of a cell-averaged scalar flux with the fluxes in neighboring spatial cells characteristic of Weighted Diamond Difference (WDD) transport methods has been investigated in the optically thick and thin cell limits for homogeneous problems in two-dimensional geometry. In particular the Arbitrarily High Order Transport method of the Nodal Type with 0-order (AHOT-N0) spatial approximation has been considered. For this spatial discretization, exact and asymptotic expressions have been derived for the
matrix elements of the integral transport matrix coupling a cell-averaged scalar flux with the fluxes in neighboring cells up to the second neighbors. For cells beyond second neighbors estimates have been obtained for the leading asymptotic order of the matrix elements in terms of the cells’ optical thickness. A recursive algorithm has been illustrated and coded for the numeric computation of the integral transport matrix in one mesh-sweep. This permitted numerical verification of the theoretically predicted asymptotic behavior with increasing cell optical thickness.

The results obtained in the homogeneous optically thick cell limit confirm the common understanding that the asymptotic order of the coupling decreases (gets weaker) the farther apart the considered cells. Notably, it provides quantitative estimates of this canonical behavior [24] for the AHOT-N0 spatial discretization of the transport equation in the homogeneous, optically thick cell limit. Moreover, these estimates provide further insight into the excellent convergence properties of diffusion-based acceleration schemes in homogeneous optically thick multi-dimensional problems. In fact, it has been shown that in the thick cell limit for the homogeneous case the integral transport matrix \( \mathbf{B} \) acquires a five-banded block matrix structure characterized by a diffusion-like coupling stencil. The existence of this low-order five-banded approximation of the integral transport matrix points to a strong local coupling of a cell with its first Cartesian neighbors. In particular, it has been shown that cross-derivative coupling with the first diagonal neighbors is of higher-order in the cell optical thickness than self-coupling and coupling with the first Cartesian neighbors. While this result was intuitively expected for the homogeneous medium thick cell limit, it is important to stress that it is not necessarily true in general. Specifically, in the next chapter it will be shown that this behavior is no
longer true for the case of periodically heterogeneous configurations in two-dimensional geometry.

The results obtained in the homogeneous thin cell limit indicate that, similarly to the result obtained in Ch. 3 for the one-dimensional case, the $B$ matrix approaches the identity matrix $I$ in this asymptotic limit. Also, the matrix elements outside the diagonal stripe have, for level symmetric quadratures of order greater than two, the same asymptotic behavior, since they are all $O(\delta)$. Differently from the one-dimensional case, though, the coefficient multiplying $\delta$ in the leading order contribution is not the same for all the elements outside the diagonal stripe. Further research is necessary in order to ascertain if a generalized formulation of the transformation that was introduced in Sec. 3.6, allowing to reduce matrix $B$ into a matrix asymptotically dominated by its diagonal with $O(\delta^2)$ off-diagonal elements in the one-dimensional case, can be identified for the more general two-dimensional case.
Chapter 7

A Novel Synthetic Acceleration Scheme for the PHI Configuration in Two-Dimensional Geometry

7.1 Introduction

The study of the asymptotic properties of the integral transport matrix initiated in Ch. 6 for the case of homogeneous material, uniform-mesh two-dimensional configurations is extended in this chapter to the Periodic Horizontal Interface (PHI) configuration shown in Fig. 7.1.

\[ \begin{array}{cccccc}
  K & K & K & K & K & K \\
  N & N & N & N & N & N \\
  K & K & K & K & K & K \\
  N & N & N & N & N & N \\
  K & K & K & K & K & K \\
  N & N & N & N & N & N \\
\end{array} \]

\[ \delta_y \quad \delta_x \]

Fig. 7.1: Periodic Horizontal Interface (PHI) Configuration.
In this periodically heterogeneous two-dimensional configuration, layers of two different materials are stacked in the $y$ direction in an alternating fashion. The asymptotic limit considered for these periodic structures is one in which the heterogeneity in the optical properties of vertically adjacent computational cells is progressively pushed apart, i.e. the cells in the thick layers are made thicker while those in the thin layers are made thinner at a prescribed rate. As indicated in Fig. 7.1, in the following it will be assumed that the bottom-most layer is optically thin while the top-most one is optically thick, considering an even number of layers in the $y$ direction. This assumption in no way limits the generality of the results that will be presented.

The following choice has been made for the geometric and material properties of a thick cell and of a thin cell, denoted by $K$ and $N$, respectively:

- **K cell**: $\delta_x, \delta_y, \Sigma_K = \sigma_K \Delta, c_K$

- **N cell**: $\delta_x, \delta_y, \Sigma_N = \sigma_N / \Delta, c_N$

The scattering ratios and the geometric properties of the cells are assumed as fixed parameters, and a uniform mesh is assumed for simplicity. The total cross-sections are scaled according to the dimensionless parameter $\Delta$. The total cross-section vanishes like $\Delta^{-1}$ in the thin layer and diverges like $\Delta$ in the thick layer, in the limit as $\Delta \to \infty$.

It is noteworthy that it is the alternating pattern of optically thin and thick layers that gives the PHI configuration its name, and a different scaling of the parameters could be considered, provided it results in a sharp discontinuity in the neutron MFP in two adjacent layers. For example, a scaling where the cells’ width in the $y$ direction is also scaled as $\Delta^{-2}$ is studied in Appendix A. The latter was introduced in [10] to devise a
particle transport problem for which there exists no preconditioner with a cell-centered diffusion coupling stencil that is unconditionally stable and robust. The scaling proposed in this chapter was selected since it satisfies the following three criteria: 1) it represents a natural extension to two-dimensional configurations of the scaling that was introduced in Ch. 4 for periodically heterogeneous slabs. In fact, since the expressions for the $B$ matrix elements are only dependent on the number of neutron MFPs in a computational cell, the choice of scaling the cell’s geometrical width is equivalent to scaling the total cross-sections; 2) as it will be shown in the next section, this scaling also defines a transport problem for which the Adjacent-cell Preconditioner (AP) displays a lack of unconditional robustness; 3) differently form the scaling considered in [10], the scaling proposed in this chapter does not favor leakage for any finite manifestation of the PHI configuration in the asymptotic limit of interest. Therefore, it is more relevant from an application standpoint. As a matter of fact, the conclusion of the Fourier analysis for the scaling defined in [10] holds only for an infinite number of PHI layers where there is no leakage. For any finite configuration, in contrast, the height of the problem domain becomes thinner in the same asymptotic limit causing leakage to dominate the spectral properties, thus producing rapid convergence of the SI or AP iterations. As it will be apparent in the following, the scaling considered in this chapter does not have this drawback.

The terms *stable* and *robust* have the same meaning as in [10]. Specifically, the term stable has the standard meaning of iterative convergence for arbitrary initial guess; the term robust implies convergence in a number of iterations that does not increase with problem size. Hence stability requires the spectral radius to be smaller than 1, while robustness requires it to be significantly smaller than 1, independent of problem size. The
PHI configuration represents an important example of a multi-dimensional configuration in which diffusion-based acceleration schemes lose their robustness, while remaining unconditionally stable. The analysis conducted in this chapter refers in particular to the AP preconditioner in two-dimensional geometry [20]. After presenting the AP formalism, a Fourier analysis is conducted for the AP acceleration scheme for the PHI configuration. It is noted that the case of a homogeneous configuration is also contained in this Fourier analysis as the case in which the two layers acquire the same material properties. Results of the Fourier analysis are therefore obtained and contrasted for the homogeneous thick cell limit, considered in Ch. 6, and for the asymptotic limit defined for the PHI configuration to illustrate the crisis of the AP formalism in moving from the homogeneous to the periodically heterogeneous case. In both cases the predictions of the Fourier analysis are also verified with results from a two-dimensional transport code that implements the AP acceleration scheme. The spectral analysis conducted in [10] had shown that the error modes that are responsible for the crisis of the AP preconditioner in the PHI configuration are high/low frequency modes in the $x/y$ direction, which in the following will also be referred to as longitudinal modes. For the new scaling proposed in this chapter it is verified that the latter modes are the offending modes responsible for the AP failure to robustly accelerate convergence in the PHI configuration.

The study of the asymptotic properties of the integral transport matrix is conducted for the PHI configuration in order to shed light on the fundamental mechanisms that are involved in the loss of robustness of the AP formalism. The results of the asymptotic analysis conducted for the matrix elements of the $B$ matrix confirm that elements outside the five-banded block of the integral transport matrix are indeed no
longer negligible in the asymptotic limit considered for the PHI configuration. In particular cross-derivative coupling of a cell in a thin layer with its diagonal neighbors appears of the same order in $\Delta$ as self-coupling and coupling with the Cartesian neighbors. Another distinctive feature of the asymptotic limit for PHI is that the integral transport matrix acquires a sparse matrix structure that is non-local. In other words, a cell-averaged scalar flux in the PHI configuration can be coupled with the same strength to other fluxes in the spatial mesh independent from the distance between the respective cells in the mesh. It so happens, for example, that a cell in a thin layer can be coupled to all the cells in the adjacent thick layer independent from their position in the layer, a circumstance we refer to as long-range coupling.

These findings provide insight into one of the important issues that prompted this research effort, namely the crisis of diffusion-based preconditioners that has been observed in multi-dimensional problems but not in one-dimensional problems. The fundamental difference between one-dimensional periodically heterogeneous configurations, considered in Ch. 4, and the PHI configuration lies in the fact that, while the integral transport matrix acquires a local structure in the asymptotic limit in slab geometry, the locality is lost in the two-dimensional case. In other words, while a strong coupling between two layers in the one-dimensional case depicted in Fig. 4.1 translates in a strong coupling between two computational cells (a layer coincides with a single cell in the one-dimensional spatial mesh), it entails a strong coupling with many cells in the two-dimensional case depicted in Fig. 7.1.

The results of the asymptotic analysis for the PHI configuration help to understand why the offending modes for the AP preconditioner are longitudinal. While
doing so, they also expose the structural deficiency of the low-order approximation to the integral transport matrix represented by diffusion-based preconditioners. As it will be detailed in the following, longitudinal modes that involve two adjacent layers are sustained because the coupling of the two layers through the elements of the integral transport matrix involves cross-derivative coupling, as exposed by the results of the asymptotic analysis. From a spectral point of view, the matrix elements coupling two vertical Cartesian neighbors in the adjacent layers, can only contribute a dependence on frequency in the $y$ direction. Yet, a low-order diffusive approximation to the structure of the integral transport matrix assumes that only self-coupling and coupling of a cell to its first Cartesian neighbors are important. Therefore, the AP preconditioner couples two adjacent layers in the PHI configuration only through vertical neighbors and is structurally inadequate to cope with modes sustained by the two-layers that are high frequency in the $x$ direction.

The conjecture explored in the final part of this chapter is that robustness of the AP formalism can be restored provided the structure of the preconditioner is amended by abandoning the diffusion paradigm and extending its traditional five-point stencil (in two-dimensional geometry) to a nine-point stencil that accounts for coupling of a cell with its first diagonal neighbors. Preliminary results of the Fourier analysis conducted for the proposed novel acceleration scheme show that, for the model problem considered at the beginning of this chapter in which a crisis of the traditional AP formalism is observed, robustness is regained for the amended acceleration scheme. The new acceleration scheme has also been implemented in the two-dimensional transport code and numerical
results from the code are successfully contrasted with the predictions of the Fourier analysis, thus verifying the latter.

An outline of the chapter follows. A summary of the AP formalism in two-dimensional geometry and the results of the Fourier analysis for the AP acceleration scheme, both in the homogeneous thick cell limit and in the asymptotic limit for the PHI configuration, are presented in Sec. 7.2. A discussion of the offending error modes for the AP acceleration scheme in the PHI configuration is presented in Sec. 7.3. The results of the asymptotic analysis for the integral transport matrix in the PHI configuration are obtained in Sec. 7.4. The results of the spectral analysis and of the structural asymptotic analysis lead to the conjecture, on the importance of accounting for cross-derivative coupling in the PHI configuration, discussed in Sec. 7.5. An extension of the AP formalism to account for cross-derivative coupling is introduced in Sec. 7.6. A Fourier analysis is conducted for the novel acceleration scheme and verified with the results from the implementation of the scheme in a two-dimensional transport code in Sec. 7.7. Finally, some concluding remarks are presented in Sec. 7.8.

7.2 Loss of Unconditional Robustness of the AP Scheme for the PHI Configuration

The details of the derivation of the two-dimensional AP formalism are found in [20]. A brief outline of the recipe for the AP acceleration scheme is presented in Sec. 7.2.1. A Fourier analysis for the AP acceleration scheme for the PHI configuration was originally conducted in [10]. The analysis is outlined in Sec. 7.2.2 and has been implemented in a Mathematica [42] notebook, see Appendix B, for the computation of
the spectral radius as a function of the parameter $\Delta$, for the scaling of the PHI configuration introduced in Sec. 7.1. As it will become apparent in the following, the Fourier analysis for the PHI configuration contains also the homogeneous case, as a special case in which the two layers in the PHI configuration have the same material properties. The Mathematica notebook has been written to allow for different material and geometric properties and various scaling of the parameters. The results of the Fourier analysis for the homogeneous thick cell limit case are presented in Sec. 7.2.3 to illustrate the success of the AP formalism in treating homogeneous configurations with low absorption in this asymptotic limit. The predictions of the Fourier analysis are also verified with results from the two-dimensional AP2 transport code [20] that implements the AP acceleration scheme. Finally, the results of the Fourier analysis for the PHI configuration are presented in Sec. 7.2.4. These results confirm the loss of unconditional robustness suffered by the AP acceleration scheme for the scaling of the PHI configuration proposed in Sec. 7.1. Even for this case the predictions of the Fourier analysis are verified by the results obtained from the AP2 code.

7.2.1 The AP Formalism in Two-Dimensional Geometry

As usual in synthetic acceleration schemes, a single source iteration constitutes the high-order step in the acceleration scheme:

$$\phi^{(r+1/2)} = A \left( \sigma_s \phi^{(r)} + q \right)$$

(7.1)
The low-order equations for the additive correction computed in the AP formalism, expressed in compact matrix notation, are:

$$\tilde{f} = D^{-1}C\left(\phi^{(i+1/2)} - \phi^{(i)}\right)$$  \hspace{1cm} (7.2)

Closure of the two-dimensional AP acceleration scheme is given by the update equation:

$$\tilde{\phi}^{(i+1)} = \tilde{\phi}^{(i+1/2)} + \tilde{f}$$  \hspace{1cm} (7.3)

The details of the derivation of the two-dimensional AP formalism are found in [20]. It is also noted that the two-dimensional AP formalism represents an extension to two-dimensional geometry of the one-dimensional AP formalism outlined in Sec. 5.2. A brief outline of the recipe for the construction of the elements of matrices $D$ and $C$ is given in the following along with the expressions needed in the remainder of this chapter.

The expressions for the “diffusion coefficients” in the $x$ and $y$ directions for a generic computational cell $(i, j)$ in the spatial mesh are:

$$D_{x_{i,j}} = \sigma_{x_{i,j}} \left(\Delta x_i\right)^2 \frac{1}{4} \sum_{m=1}^{M} w_m \left(2\kappa_{m,i,j} + \alpha_{m,i,j}\right)$$

$$i = 1, \ldots, I; \ j = 1, \ldots, J$$  \hspace{1cm} (7.4)

$$D_{y_{i,j}} = \sigma_{y_{i,j}} \left(\Delta y_j\right)^2 \frac{1}{4} \sum_{m=1}^{M} w_m \left(2\nu_{m,i,j} + \beta_{m,i,j}\right)$$

$$i = 1, \ldots, I; \ j = 1, \ldots, J$$  \hspace{1cm} (7.5)
It is noted that while the one-dimensional AP formalism detailed in Sec. 5.2 was formulated in a non-dimensional form, the expressions for the “diffusion coefficients”, in Eqs. (7.4) and (7.5), and the expressions that will be given in the following for the mixing formulas and for the elements of matrices \( D \) and \( C \) are in dimensional form [20].

The elements of the \( D \) matrix pertaining to cell \((i, j)\) in the interior of the Cartesian mesh, for \( i = 2, \ldots, (I-1) \) and \( j = 2, \ldots, (J-1) \), are obtained by mixing the “diffusion coefficients” via dimensional mixing formulas adapted from standard Diffusion Theory:

\[
D_{o,x}^{\pm i,j} = \frac{2\Delta y_j}{\frac{\Delta x_{\pm i,j}}{D_{i,j}^{\pm i,j}} + \frac{\Delta x_i}{D_{i,j}^{\pm i,j}}} , \quad (7.6)
\]

\[
D_{o,y}^{i,j} = \frac{2\Delta x_i}{\frac{\Delta y_{i,j}}{D_{i,j}^{i,j}} + \frac{\Delta y_j}{D_{i,j}^{i,j}}} \quad (7.7)
\]

The elements of the five-diagonal banded matrix \( D \) pertaining to an internal computational cell are then assembled using the following expression:

\[
\begin{align*}
D_{i,j,i+j} &= \sigma_{i,j} \Delta x_j \Delta y_j (1 - c_{i,j}) + D_{o,x}^{i,j} + D_{o,x}^{-i,j} + D_{o,y}^{i,j} + D_{o,y}^{-i,j} \\
D_{i,j,i+1,j} &= -D_{o,x}^{i,j} \\
D_{i,j,i-1,j} &= -D_{o,x}^{-i,j} \\
D_{i,j,i,j+1} &= -D_{o,y}^{i,j} \\
D_{i,j,i,j-1} &= -D_{o,y}^{-i,j}
\end{align*} \quad (7.8)
\]
Vacuum boundary conditions are assumed on all four sides of the two-dimensional domain. For the cells at the domain boundary Larsen’s prescription [17] adapted to two-dimensional geometry is employed. The following quadrature dependent constant is computed:

$$\beta = \frac{1}{2} \sum_{m=1}^{M} w_m |\mu_m|$$ (7.9)

Fictitious cells are assumed on the periphery of the problem domain, with the preconditioning expression relating them to the boundary cells via the $\Gamma$ factors defined by:

$$\Gamma_{i,j}^x = \left( \frac{D_{i,j}^x / \beta \Delta x_j}{D_{i,j}^x / \beta \Delta x_j + 1} \right)^{-1}, \quad (7.10)$$

$$\Gamma_{i,j}^y = \left( \frac{D_{i,j}^y / \beta \Delta y_j}{D_{i,j}^y / \beta \Delta y_j + 1} \right)^{-1}, \quad (7.11)$$

in analogy with the one-dimensional case, see Eq. (5.9). The following quantities are then defined for the boundary cells in terms of the $\Gamma$ factors:

$$D_{\beta,i,j}^{x,j} = D_{i,j}^x \left( 1 - \Gamma_{i,j}^x \right) \frac{\Delta x_j}{\Delta y_j}$$ (7.12)

$$D_{\beta,i,j}^{x,i} = D_{i,j}^x \left( 1 - \Gamma_{i,j}^x \right) \frac{\Delta x_i}{\Delta y_j}$$ (7.13)
\[ D_{\beta,y}^{i+J} = D_{\beta,y}^y \left( 1 - \Gamma_{i,j}^y \right) \frac{\Delta y_j}{\Delta x_i} \]  
(7.14)

\[ D_{\beta,y}^{i,-1} = D_{\beta,y}^y \left( 1 - \Gamma_{i,j}^y \right) \frac{\Delta y_i}{\Delta x_i} \]  
(7.15)

The elements of the D matrix pertaining to a corner cell are then assembled using the following expressions:

\[
\begin{align*}
D_{1,1,1,1} &= \sigma_{i,j} \Delta x_i \Delta y_j \left( 1 - c_{i,j} \right) + D_{o,x}^{+1,1} + D_{o,y}^{-1,1} + D_{\beta,x}^{1,+1} + D_{\beta,y}^{1,-1} \\
D_{1,1,2,1} &= -D_{o,x}^{1,+1} \\
D_{1,1,1,2} &= -D_{o,y}^{1,-1}
\end{align*}
\]  
(7.16)

\[
\begin{align*}
D_{1,1,l,l} &= \sigma_{i,j} \Delta x_i \Delta y_j \left( 1 - c_{i,j} \right) + D_{\beta,x}^{+1,l} + D_{\beta,y}^{-1,l} + D_{o,x}^{l,+1} + D_{o,y}^{l,-1} \\
D_{1,1,l,-1} &= -D_{o,x}^{l,-1} \\
D_{1,1,l,2} &= -D_{o,y}^{l,+1}
\end{align*}
\]  
(7.17)

\[
\begin{align*}
D_{1,l,1,j} &= \sigma_{i,j} \Delta x_i \Delta y_j \left( 1 - c_{i,j} \right) + D_{o,x}^{+1,j} + D_{\beta,y}^{-1,j} + D_{o,x}^{1,+j} + D_{o,y}^{1,-j} \\
D_{1,l,2,j} &= -D_{o,x}^{1,+j} \\
D_{1,l,1,j-1} &= -D_{o,y}^{1,-j}
\end{align*}
\]  
(7.18)

\[
\begin{align*}
D_{1,l,l,j} &= \sigma_{i,j} \Delta x_i \Delta y_j \left( 1 - c_{i,j} \right) + D_{\beta,x}^{+1,j} + D_{\beta,y}^{-1,j} + D_{o,x}^{l,+j} + D_{o,y}^{l,-j} \\
D_{1,l,l,-1} &= -D_{o,x}^{l,-j} \\
D_{1,l,l,j-1} &= -D_{o,y}^{l,+j}
\end{align*}
\]  
(7.19)

Finally, the recipe for the other edge cells is:
\[ i = 2, \ldots, (I-1); j = 1 \]

\[
\begin{align*}
D_{i,i,i} &= \sigma_{i,i} \Delta x_i \Delta y_j (1-c_{i,i}) + D_{o,x}^{+i} + D_{o,x}^{-i} + D_{o,y}^{i+} + D_{o,y}^{i-} \\
D_{i,i,i+1} &= -D_{o,x}^{+i+1} \\
D_{i,i,i-1} &= -D_{o,x}^{-i} \\
D_{i,i,i+2} &= -D_{o,y}^{i+} \\
\end{align*}
\]

(7.20)

\[ i = 2, \ldots, (I-1); j = J \]

\[
\begin{align*}
D_{i,j,i} &= \sigma_{i,j} \Delta x_i \Delta y_j (1-c_{i,j}) + D_{o,x}^{+i} + D_{o,x}^{-i} + D_{o,y}^{i+} + D_{o,y}^{i-} \\
D_{i,j,i+1} &= -D_{o,x}^{+i+1} \\
D_{i,j,i-1} &= -D_{o,x}^{-i} \\
D_{i,j,i+J} &= -D_{o,y}^{i+} \\
\end{align*}
\]

(7.21)

\[ i = 1; j = 2, \ldots, J-1 \]

\[
\begin{align*}
D_{i,j,i} &= \sigma_{i,j} \Delta x_i \Delta y_j (1-c_{i,j}) + D_{o,x}^{+i+1} + D_{o,x}^{i+1} + D_{o,y}^{i+1} + D_{o,y}^{i+1} \\
D_{i,j,2} &= -D_{o,x}^{+i+1} \\
D_{i,j,i+1} &= -D_{o,y}^{i+1} \\
D_{i,j,i-1} &= -D_{o,y}^{i+1} \\
\end{align*}
\]

(7.22)

\[ i = I; j = 2, \ldots, J-1 \]

\[
\begin{align*}
D_{i,j,i} &= \sigma_{i,j} \Delta x_i \Delta y_j (1-c_{i,j}) + D_{o,x}^{+i+1} + D_{o,x}^{i+1} + D_{o,y}^{i+1} + D_{o,y}^{i+1} \\
D_{i,j,I-1} &= -D_{o,x}^{i+1} \\
D_{i,j,I+j} &= -D_{o,y}^{i+1} \\
D_{i,j,I-j-1} &= -D_{o,y}^{i+1} \\
\end{align*}
\]

(7.23)

Similar to the one-dimensional case, the C matrix is a diagonal scattering matrix.

In dimensional form the elements of this matrix are:
As usual in two-dimensional transport calculations, it is assumed that the cell-averaged scalar fluxes are ordered in the $\Phi$ vector according to their natural order, namely one row at a time. Therefore, the placement of the elements in the $D$ matrix corresponding to natural ordering of the cell-averaged scalar fluxes is accomplished through the simple mapping:

$$C_{i,j,i,j} = \sigma_{i,j} \Delta x_i \Delta y_j c_{i,j}, \quad i = 1,\ldots,I; j = 1,\ldots,J$$  \hspace{1cm} (7.24)

$$D_{u,v} = D_{i,j,r,s}$$  \hspace{1cm} (7.25)

$$u = i + I (j - 1)$$  \hspace{1cm} (7.26)

$$v = r + I (s - 1)$$  \hspace{1cm} (7.27)

In concluding it is noted that in the AP2 code the $D$ matrix is stored as a sparse matrix and inverted using MA28 routines from the Harwell Subroutine Library [43].

### 7.2.2 Fourier Analysis of the AP Scheme for the PHI Configuration

As observed in [10], the standard approach for determining the spectrum of iterative schemes typically applies to a model configuration composed of an infinite uniform mesh and a single, homogeneous material. The iteration residual in the discrete variables in such configurations possess spatial periodicity in multiples of the mesh size that permits decomposition into Fourier modes. Orthogonality of the Fourier modes
permits their separation so that each mode can be considered separately, providing an expression for the iteration eigenvalue in terms of the problem parameters.

The same principles are applicable for the PHI configuration depicted in Fig. 7.1, except that in the $y$ direction the periodicity is in multiples of $2\delta_y$, and the variables in each layer are decomposed separately as indicated in Fig. 7.2.

\[ \phi_{N}^{(\ell)} = \Phi_{N}^{(\ell)} \] (7.28)

**Fig. 7.2:** Two-cell system for the Fourier analysis of the PHI configuration.

Therefore, the following Fourier ansatz is formulated for the variables in Fig. 7.2 assuming, for simplicity and without any loss of generality, that the origin of the $(x,y)$ coordinate system is coincident with the center of the N cell:
\[ \phi_\lambda^{(f)} = \Phi_\lambda^{(f)} \exp \left[ \hat{i} \text{sgn} (\eta_m) \hat{\lambda}_y \delta_y \right] \] (7.29)

\[ \psi_m^{(f+1)} = \psi_m^{(f+1)} \] (7.30)

\[ \psi_{m,K}^{(f+1)} = \Psi_{m,K}^{(f+1)} \exp \left[ \hat{i} \text{sgn} (\eta_m) \lambda_x (\delta_x / 2) \right] \] (7.31)

\[ \psi_{m,N}^{(f+1)} = \Psi_{m,N}^{(f+1)} \exp \left[ -\hat{i} \text{sgn} (\mu_m) \lambda_x (\delta_x / 2) \right] \] (7.32)

\[ \psi_{m,N}^{(f+1)} = \Psi_{m,N}^{(f+1)} \exp \left[ \hat{i} \text{sgn} (\mu_m) \lambda_x (\delta_x / 2) \right] \] (7.33)

\[ \psi_{m,K}^{(f+1)} = \Psi_{m,K}^{(f+1)} \exp \left[ -\hat{i} \text{sgn} (\mu_m) \lambda_x (\delta_x / 2) + \hat{i} \text{sgn} (\eta_m) \lambda_y \delta_y \right] \] (7.34)

\[ \psi_{m,K}^{(f+1)} = \Psi_{m,K}^{(f+1)} \exp \left[ \hat{i} \text{sgn} (\mu_m) \lambda_x (\delta_x / 2) + \hat{i} \text{sgn} (\eta_m) \lambda_y \delta_y \right] \] (7.35)

\[ \psi_{m,N}^{(f+1)} = \Psi_{m,K}^{(f+1)} \exp \left[ -\hat{i} \text{sgn} (\eta_m) \lambda_y (\delta_y / 2) \right] \] (7.36)

\[ \psi_{m,K}^{(f+1)} = \Psi_{m,K}^{(f+1)} \exp \left[ -\hat{i} \text{sgn} (\eta_m) \lambda_y (\delta_y / 2) \right] \] (7.37)
\[ \psi_{m,N}^{\alpha(\pm)} = \Psi_{m,N}^{\alpha(\pm)} \exp\left[ i \text{sgn} (\eta_m) \lambda_x \left( \delta_x / 2 \right) \right] \] (7.38)

\[ \psi_{m,k}^{\pm x(\pm)} = \Psi_{m,N}^{\pm x(\pm)} \exp\left[ i \text{sgn} (\eta_m) \lambda_y \left( \delta_y / 2 \right) \right] \] (7.39)

It is noted that the Fourier ansatz incorporates both the continuity of the angular flux at the material interface between the two cells and the periodicity of the angular flux at the boundaries of the two-cell system in Fig. 7.2. In Eqs. (7.28) through (7.39) the uppercase symbols denote the Fourier coefficients of the corresponding variable, \( i = \sqrt{-1} \) is the imaginary unit, \( \text{sgn} (\cdot) \) is the signum function and \( \lambda_x, \lambda_y \) are the Fourier variables in the \( x \) and \( y \) direction, respectively.

It is noted that the continuity and periodicity conditions reduce the original twelve variables in physical space to eight variables in Fourier space. Therefore, when the Fourier ansatz is substituted in the system of equations comprised of the two balance equations and the four WDD relations written for the two-cell system:

\[ \kappa_{m,l} \left( \psi_{m,l}^{\alpha x(\pm)} - \psi_{m,l}^{\alpha y(\pm)} \right) + \nu_{m,l} \left( \psi_{m,l}^{\alpha y(\pm)} - \psi_{m,l}^{\alpha x(\pm)} \right) + \psi_{m,l}^{(\pm)} = c_l \phi_{\delta}^{(\pm)}, \quad l = N, K, \] (7.40)

\[ \psi_{m,l}^{(\pm)} = \left( \frac{1 + \alpha_{m,l}}{2} \right) \psi_{m,l}^{\alpha x(\pm)} + \left( \frac{1 - \alpha_{m,l}}{2} \right) \psi_{m,l}^{\alpha y(\pm)}, \quad l = N, K, \] (7.41)

\[ \psi_{m,l}^{(\pm)} = \left( \frac{1 + \beta_{m,l}}{2} \right) \psi_{m,l}^{\alpha y(\pm)} + \left( \frac{1 - \beta_{m,l}}{2} \right) \psi_{m,l}^{\alpha x(\pm)}, \quad l = N, K, \] (7.42)
it is possible to eliminate four of the Fourier coefficients, specifically \( \Psi_{m,N}^{x(r+1)} \), \( \Psi_{m,N}^{y(r+1)} \), \( \Psi_{m,K}^{x(r+1)} \), and \( \Psi_{m,K}^{y(r+1)} \), and relate the remaining four cell-centered variables through the remaining two equations. Therefore, it is convenient to introduce the vectors:

\[
\Phi^{(r)} = \begin{pmatrix} \Phi_N^{(r)} \\ \Phi_K^{(r)} \end{pmatrix}
\]  

(7.43)

\[
\Psi_m^{x(r+1)} = \begin{pmatrix} \psi_{m,N}^{x(r+1)} \\ \psi_{m,K}^{x(r+1)} \end{pmatrix}
\]  

(7.44)

It is noted that, both from an analytical and a computational point of view, it is easier at first to express the scalar variables as a function of the angular variables:

\[
\Phi^{(r)} = G F_m \Psi_m^{(r+1)}
\]  

(7.45)

Matrices \( G \) and \( F_m \) introduced in the previous equation are:

\[
G = \begin{bmatrix} 1/c_N & 0 \\ 0 & 1/c_K \end{bmatrix}
\]  

(7.46)

\[
F_m = I + F_m^x + F_m^y
\]  

(7.47)

Matrices \( F_m^x \) and \( F_m^y \) have the following expressions:
\[ F_m^x = i \text{sgn}(\mu_m) \sin \left( \frac{r}{2} \right). \]

\[
\begin{bmatrix}
2\kappa_{m,N} & 0 \\
\cos \left( \frac{r}{2} \right) + i \text{sgn}(\mu_m) \alpha_{m,N} \sin \left( \frac{r}{2} \right) & 0 \\
0 & 2\kappa_{m,K} \\
\cos \left( \frac{r}{2} \right) + i \text{sgn}(\mu_m) \alpha_{m,K} \sin \left( \frac{r}{2} \right)
\end{bmatrix}
\] (7.48)

\[ F_m^y = \left[ (\beta_{m,N} + \beta_{m,K}) \cos(s) + i \text{sgn}(\eta_m) (1 + \beta_{m,N} \beta_{m,K}) \sin(s) \right]^{-1}. \]

\[
\begin{bmatrix}
2\nu_{m,N} & -2\nu_{m,N} \\
\left[ \cos(s) + i \text{sgn}(\eta_m) \beta_{m,K} \sin(s) \right]^{-1} & 2\nu_{m,K} \\
-2\nu_{m,K} & \left[ \cos(s) + i \text{sgn}(\eta_m) \beta_{m,N} \sin(s) \right]^{-1}
\end{bmatrix}
\] (7.49)

Also, in Eqs. (7.48) and (7.49) the definitions \( r \equiv \lambda, \delta \) and \( s \equiv \lambda, \gamma, \delta \) are utilized.

Inverting the matrices product in Eq. (7.45) and using the definition of scalar flux:

\[ \Phi^{(t+1)} = \sum_{m=1}^{M} W_m \Psi_m^{(t+1)}, \] (7.50)

It is possible to relate the present and the old iterates of the scalar variables:

\[ \Phi^{(t+1)} = J \Phi^{(t)} \] (7.51)

The Jacobian matrix \( J \) is obtained from matrices \( G \) and \( F_m \):

\[ J = \sum_{m=1}^{M} W_m \left[ G F_m \right]^{-1} = \sum_{m=1}^{M} W_m F_m^{-1} G^{-1} \] (7.52)
Of course, the inverse of the $G$ matrix is a diagonal matrix whose non-zero elements are the scattering ratios in the two layers:

$$G^{-1} = \begin{bmatrix} c_N & 0 \\ 0 & c_K \end{bmatrix}$$  \hspace{1cm} (7.53)

As pointed out in Eq. (6.65) $J = A\sigma_s$, and the Jacobian matrix is once again recognized as the iteration matrix for the basic SI scheme in Eq. (7.1). For a given order of the level symmetric quadrature, and for given values of the $\delta_s$, $\delta_y$, $\sigma_K$, $\sigma_N$, $c_K$ and $c_N$ parameters, the spectral radius for SI is obtained as a function of the scaling parameter $\Delta$ introduced in Sec. 7.1 for the PHI configuration:

$$\rho_{SI} = \rho_{SI}(\Delta) = \max_{r,s} \left[ \text{Abs} \left[ \text{Eig} \left[ J(r,s,\Delta) \right] \right] \right]$$  \hspace{1cm} (7.54)

A spectral radius less than or equal to 1 implies stability of the iterative scheme. Also, the smaller the spectral radius, the faster the convergence rate of the iterative scheme. The expressions for the $G$ and $F_m$ matrices have been coded in the Mathematica notebook and employed to compute and plot the spectral radius $\rho_{SI}$ as a function of the $\Delta$ parameter. The result presented in Fig. 7.3 refers to the case of the $S_6$ level symmetric quadrature of equal weights, and for the following choice of problem parameters: $\delta_s = \delta_y = 1$, $\sigma_K = \sigma_N = 1$, $c_K = c_N = 0.99999999$. The problem defined by this choice of the parameters for the PHI configuration will be referred to in the following as the model problem. The choice of 0.99999999 for the value of the scattering ratios is justified in the following.
Fig. 7.3: Spectral radius of SI for a PHI configuration with $c_K = c_N = 0.99999999$.

The conclusion reached in [10] that the spectral radius $\rho_{SI} = c_K = c_N$ is therefore also true for the new scaling of the PHI configuration as a function of the $\Delta$ parameter introduced in Sec. 7.1. It is noted that the result in Fig. 7.3 represents the spectral counterpart of the practical interpretation of the inefficiency of the SI scheme, in configurations characterized by no leakage, as in the infinite medium Fourier analysis, and very low absorption, that was given in Sec. 1.1. The spectral radius is in fact equal to the scattering ratio.
The Fourier analysis for the two-dimensional AP formalism introduced in Sec. 7.2.1 is readily formulated by writing the high-order, low-order and update equations in Fourier space:

\[ \Phi^{(t+1/2)} = J \Phi^{(t)} \]  

(7.55)

\[ f = D^{-1}C\left( \Phi^{(t+1/2)} - \Phi^{(t)} \right) \]  

(7.56)

\[ \Phi^{(t+1)} = \Phi^{(t+1/2)} + f \]  

(7.57)

The AP matrix \( D \) in Eq. (7.56) written, for the two-cell system in Fig. 7.2, in Fourier space is:

\[
D = \begin{bmatrix}
D_{d,N} + 2D_{ax,N} \cos(r) & 2D_{oy} \cos(s) \\
2D_{oy} \cos(s) & D_{d,K} + 2D_{ax,K} \cos(r)
\end{bmatrix}
\]  

(7.58)

The elements of the \( D \) matrix are obtained by applying the recipe for the construction of the AP matrix outlined in Sec. 7.2.1 to the two-cell system. It is convenient to index the “diffusion coefficients” with respect to the material index:

\[
D_x^y = \Sigma_{\gamma} \delta^y_x \frac{1}{4} \sum_{m=1}^{M} w_m \left( 2\kappa_{m,i} \right) \left( 2\kappa_{m,i} + \alpha_{m,i} \right), \quad l = N, K
\]  

(7.59)

\[
D_y^y = \Sigma_{\gamma} \delta^y_x \frac{1}{4} \sum_{m=1}^{M} w_m \left( 2\nu_{m,i} \right) \left( 2\nu_{m,i} + \beta_{m,i} \right), \quad l = N, K
\]  

(7.60)

Applying the dimensional mixing formula:
Applying the stability condition \[10\] for the flat error eigenmodes, \( r,s = 0 \):

\[
D_{l,j} = \Sigma_l \delta_l \delta_j \left(1 - c_l \right) - 2D_{l,x_j} - 2D_{l,y_j}, \quad l = N,K
\] (7.63)

Finally, the diagonal \( C \) matrix acquires the expression:

\[
C = \begin{bmatrix}
\Sigma_N \delta_x \delta_y c_N & 0 \\
0 & \Sigma_K \delta_x \delta_y c_K
\end{bmatrix}
\] (7.64)

Eliminating \( \Phi^{(t+1/2)} \) from Eqs. (7.55) through Eq. (7.57) it is possible to find the expression that maps \( \Phi^{(t)} \) into \( \Phi^{(t+1)} \) for the AP acceleration scheme:

\[
\Phi^{(t+1)} = \left[ \mathbf{J} + \mathbf{D}^{-1} \mathbf{C} \right] \Phi^{(t)}
\] (7.65)

Therefore, the iteration matrix for the AP scheme is:

\[
\mathbf{T}_{AP} = \mathbf{J} + \mathbf{D}^{-1} \mathbf{C} \left( \mathbf{J} - \mathbf{I} \right)
\] (7.66)

It was shown in \[10\] that in case of perfect scattering, \( \mathbf{G}^{-1} = \mathbf{I} \), if matrix \( \mathbf{D} \) is not singular at the origin of Fourier space, \( r = s = 0 \), then the spectral radius of \( \mathbf{T}_{AP} \) is bounded from below by 1, implying lack of both stability and robustness. The stability condition for the flat error eigenmodes in Eq. (7.63) ensures the vanishing of the determinant of \( \mathbf{D} \) at the origin of Fourier space, for \( c_K = c_N = 1 \). In this connection, we
further point out that the integral transport matrix, $\mathbf{B} = \mathbf{I} - \mathbf{J}$, for the AHOT-N0 method is also singular at the origin of Fourier space for the degenerate case $c_K = c_N = 1$, corresponding to a purely non-dissipative system. Therefore, the stability condition appears to be required in order for the low-order approximation $\mathbf{D}$ to match the behavior of the high-order transport operator $\mathbf{B}$ at the origin of Fourier space. Since $\mathbf{D}$ becomes non-invertible, for $c_K = c_N = 1$, at $r = s = 0$, the behavior of the acceleration scheme can be studied around the origin of Fourier space only in the limit as $c_K, c_N \to 1$. That’s why a value of 0.99999999 has been selected for $c_K$ and $c_N$ in the model problem. The latter is sufficiently close to 1 to instigate the crisis of the AP acceleration scheme for the PHI configuration, as illustrated in Sec. 7.2.4, without resulting in a singular $\mathbf{D}$ matrix in the Fourier analysis.

For a given order of the level symmetric quadrature, and for given values of the $\delta_x$, $\delta_y$, $\sigma_N$, $c_K$ and $c_N$ parameters, the spectral radius for AP is obtained as a function of the scaling parameter $\Delta$ introduced in Sec. 7.1 for the PHI configuration:

$$\rho_{AP} = \rho_{AP} (\Delta) = \max_{r,s} \left[ \text{Abs} \left[ \text{Eig} \left[ \mathbf{T}_{AP} (r,s,\Delta) \right] \right] \right]$$

(7.67)

The equations for the AP scheme have also been implemented in the Mathematica notebook. The results of the Fourier analysis for PHI are presented in Sec. 7.2.4. Before considering the periodically heterogeneous case, it is worthwhile to discuss the results of the Fourier analysis for the homogeneous thick cell limit. These results are presented in the next section.
7.2.3 Results for Homogeneous Configurations in the Asymptotic Thick-Cell Limit

Let us assume that the material properties of the two cells in Fig. 7.2 are the same and such that \( \Sigma_N = \Sigma_K = \alpha \Delta \) and \( c_N = c_K = c \). Under this assumption the PHI configuration reduces to a homogeneous configuration whose cells are characterized by the properties of the thick layer. From the integral transport matrix point of view, the latter scaling is perfectly equivalent to the homogeneous asymptotic thick-cell limit that was studied in Sec. 6.6.

The result obtained for the AP spectral radius considering this scaling for the case of the \( S_6 \) level symmetric quadrature of equal weights, and for the choice of problem parameters \( \delta_x = \delta_y = 1, \sigma = 1, c = 0.99999999 \), is presented in Fig. 7.4.

The result in Fig. 7.4 illustrates the superb convergence properties of the AP formalism in the homogeneous thick cell limit, even in the case of very low absorption, \( c \approx 1 \). In fact, it is evident that the spectral radius tends to zero in the limit as \( \Delta \to \infty \). These spectral properties are in turn determined by the fact that, as it was shown in Sec. 6.6, in the thick cell limit the integral transport matrix \( B \) acquires a five-banded diffusive structure. Similar to the result that was obtained in Sec. 5.3 for the one-dimensional AP, it could be shown that the five-banded diffusive structure approached by the \( B \) matrix in the limit is coincident with the non-dimensional form of the two-dimensional AP preconditioner.

The predictions of the Fourier analysis for the parameter values considered in Fig. 7.4 have been verified with the two-dimensional AP2 transport iterative code [20]. The code has been slightly modified to add the capability of obtaining an accurate \( L_2 \)
norm estimate of the spectral radius with power iteration, introducing a convergence criterion on the spectral radius. The objective, in this case, is therefore to measure the spectral radius instead of converging the cell-averaged scalar fluxes to within a certain convergence criterion.

![Graph](image)

*Fig. 7.4: Spectral radius of AP for a homogeneous configuration with $c = 0.99999999$.*

For the case of vacuum boundary conditions considered in Table 7.1, the fixed source is set equal to zero everywhere and the possible error modes that can be sustained by the spatial mesh are excited by a delta-like initial guess at the center of the mesh for the cell-averaged scalar fluxes. Specifically, the cell-averaged scalar fluxes are assumed to be zero everywhere except for the four cells surrounding the central point of the entire
mesh, where a unit flux initial guess is assumed. It is noted that the transport solution for this homogeneous transport problem is trivial and is coincident with zero scalar fluxes in all cells. Therefore, the initial guess perturbs the flux iterates away from the zero uniform solution. As usual, the spectral radius is computed as the square root of the ratio of the $L_2$ norm of the iterative residual in a given iterate to that in the previous iterate [44]. The convergence criterion for the spectral radius is fixed at $\rho_\varepsilon = 1 \times 10^{-5}$ and the pre-set maximum number of iterations is 500. In order to approach the ideal situation of an infinite medium considered in the Fourier analysis, a sequence of square meshes of increasing size is considered, going from a $10 \times 10$ to a $160 \times 160$ mesh. The values reported in the last row of the table are the values of the spectral radius predicted by the Fourier analysis for a certain value of the $\Delta$ parameter.

*Table 7.1: Spectral radius of AP for a homogeneous configuration ($c = 0.99999999$).*

<table>
<thead>
<tr>
<th>$I \times J$</th>
<th>$10^0$</th>
<th>$10^1$</th>
<th>$10^2$</th>
<th>$10^3$</th>
<th>$10^4$</th>
<th>$10^5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10x10</td>
<td>0.103</td>
<td>9.99x10^{-2}</td>
<td>1.06x10^{-2}</td>
<td>1.06x10^{-3}</td>
<td>1.07x10^{-4}</td>
<td>1.05x10^{-5}</td>
</tr>
<tr>
<td>20x20</td>
<td>0.117</td>
<td>0.106</td>
<td>1.12x10^{-2}</td>
<td>1.12x10^{-3}</td>
<td>1.12x10^{-4}</td>
<td>1.09x10^{-5}</td>
</tr>
<tr>
<td>40x40</td>
<td>0.123</td>
<td>0.107</td>
<td>1.13x10^{-2}</td>
<td>1.12x10^{-3}</td>
<td>1.12x10^{-4}</td>
<td>1.10x10^{-5}</td>
</tr>
<tr>
<td>80x80</td>
<td>0.124</td>
<td>0.108</td>
<td>1.13x10^{-2}</td>
<td>1.12x10^{-3}</td>
<td>1.12x10^{-4}</td>
<td>1.10x10^{-5}</td>
</tr>
<tr>
<td>160x160</td>
<td>0.124</td>
<td>0.108</td>
<td>1.13x10^{-2}</td>
<td>1.12x10^{-3}</td>
<td>1.12x10^{-4}</td>
<td>1.10x10^{-5}</td>
</tr>
<tr>
<td>Fourier</td>
<td>0.125</td>
<td>0.109</td>
<td>1.15x10^{-2}</td>
<td>1.16x10^{-3}</td>
<td>1.16x10^{-4}</td>
<td>1.16x10^{-5}</td>
</tr>
</tbody>
</table>

As expected, the estimated values of the spectral radius for a certain $\Delta$ increase as the dimensions of the problem increase, effecting reduced neutron losses by leakage, and are bounded above by the value predicted by the Fourier analysis. For a given $\Delta$ the $10 \times 10$ structure is leakage dominated, especially at the smaller values of the $\Delta$
parameter, while the effect of the leakage becomes less and less important as the problem size is increased.

A transport problem has also been considered for the same meshes and for the same parameters selected in Fig. 7.4, by introducing a uniform unit fixed source in all computational cells. In this case, the scalar fluxes are converged with a convergence criterion $\varepsilon_\phi = 10^{-5}$ and a pre-set maximum number of iterations equal to 50. The number of iterations consumed to reach convergence is reported in Table 7.2, for the same sequence of meshes considered in Table 7.1.

Table 7.2: Number of AP iterations for a homogeneous configuration ($c = 0.99999999$).

<table>
<thead>
<tr>
<th>$I \times J$</th>
<th>$10^0$</th>
<th>$10^1$</th>
<th>$10^2$</th>
<th>$10^3$</th>
<th>$10^4$</th>
<th>$10^5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10 \times 10$</td>
<td>5</td>
<td>5</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>2</td>
</tr>
<tr>
<td>$20 \times 20$</td>
<td>5</td>
<td>5</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>2</td>
</tr>
<tr>
<td>$40 \times 40$</td>
<td>5</td>
<td>5</td>
<td>3</td>
<td>3</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>$80 \times 80$</td>
<td>5</td>
<td>5</td>
<td>3</td>
<td>3</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>$160 \times 160$</td>
<td>5</td>
<td>5</td>
<td>3</td>
<td>3</td>
<td>2</td>
<td>2</td>
</tr>
</tbody>
</table>

From the results in Table 7.2 it is evident that immediate convergence of the AP accelerated iterations, namely convergence in two iterations, is achieved in the asymptotic limit as $\Delta \to \infty$. 
7.2.4 Results for the PHI Configuration in the Asymptotic Limit

The result of the Fourier analysis of the AP accelerated iterations for the scaling of the PHI configuration introduced in Sec. 7.1 and the model problem defined by the quadrature and parameter values selected for SI in Fig. 7.3, is presented in Fig. 7.5.

![Graph of spectral radius vs. Δ for a PHI configuration with $c_K = c_N = 0.99999999$.](image)

*Fig. 7.5: Spectral radius of AP for a PHI configuration with $c_K = c_N = 0.99999999$.*

The result in Fig. 7.5 illustrates the loss of unconditional robustness of the AP scheme when applied to the PHI configuration. In the limit as $Δ → ∞$ the spectral properties of the acceleration scheme approach those of the unaccelerated SI scheme, for $c_K → 1$. More precisely, by loss of unconditional robustness it is meant that, for every small $ε > 0$, there exists a value of $Δ$ large enough to yield a spectral radius for the AP
accelerated iterations equal to $1 - \varepsilon$. This behavior is very different from what was observed in the previous section for the case of homogeneous configurations, where the spectral radius is far smaller than 1 for all meshes and material properties.

The $L_2$ estimates of the spectral radius obtained from the AP2 code for increasing mesh size with vacuum boundary conditions are contrasted with the values predicted from the Fourier analysis in Table 7.3. The convergence criterion for the spectral radius is $\varepsilon_p = 1 \times 10^{-5}$ and the pre-set maximum number of iterations is 500.

<table>
<thead>
<tr>
<th>$I \times J$</th>
<th>$10^0$</th>
<th>$10^1$</th>
<th>$10^2$</th>
<th>$10^3$</th>
<th>$10^4$</th>
<th>$10^5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10×10</td>
<td>0.103</td>
<td>0.530</td>
<td>0.703</td>
<td>0.724</td>
<td>0.726</td>
<td>0.725</td>
</tr>
<tr>
<td>20×20</td>
<td>0.117</td>
<td>0.655</td>
<td>0.871</td>
<td>0.898</td>
<td>0.901</td>
<td>0.900</td>
</tr>
<tr>
<td>40×40</td>
<td>0.123</td>
<td>0.725</td>
<td>0.938</td>
<td>0.969</td>
<td>0.972</td>
<td>0.970</td>
</tr>
<tr>
<td>80×80</td>
<td>0.124</td>
<td>0.755</td>
<td>0.960</td>
<td>0.989</td>
<td>0.992</td>
<td>0.991</td>
</tr>
<tr>
<td>160×160</td>
<td>0.124</td>
<td>0.768</td>
<td>0.969</td>
<td>0.994</td>
<td>0.996</td>
<td>0.995</td>
</tr>
<tr>
<td>Fourier</td>
<td>0.125</td>
<td>0.781</td>
<td>0.976</td>
<td>0.997</td>
<td>0.999</td>
<td>0.998</td>
</tr>
</tbody>
</table>

Table 7.3: Spectral radius of AP for a PHI configuration ($c_K = c_N = 0.99999999$).

The number of iterations consumed to reach convergence of the scalar fluxes for the same problem driven by a unit fixed source in all computational cells is reported in Table 7.4. The scalar fluxes are converged with a convergence criterion $\varepsilon_\phi = 10^{-5}$ and a pre-set maximum number of iterations equal to 50.

It is noted that convergence is not achieved for the larger meshes with $\Delta > 10^2$. The results in both Table 7.3 and Table 7.4 confirm also that the scaling proposed for the PHI configuration in Sec. 7.1 does not favor leakage in the asymptotic limit. In fact, differently from what was observed in similar tables built in [10] for the scaling of the
PHI configuration considered there, no significant decrease is observed, either in the spectral radius or in the number of iterations, along the rows of Tables 7.3 and 7.4.

Table 7.4: Number of AP iterations for a PHI configuration ($c_K = c_N = 0.99999999$).

<table>
<thead>
<tr>
<th>$I \times J$</th>
<th>$10^0$</th>
<th>$10^1$</th>
<th>$10^2$</th>
<th>$10^3$</th>
<th>$10^4$</th>
<th>$10^5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10\times10</td>
<td>5</td>
<td>18</td>
<td>29</td>
<td>31</td>
<td>32</td>
<td>32</td>
</tr>
<tr>
<td>20\times20</td>
<td>5</td>
<td>23</td>
<td>&gt;50</td>
<td>&gt;50</td>
<td>&gt;50</td>
<td>&gt;50</td>
</tr>
<tr>
<td>40\times40</td>
<td>5</td>
<td>25</td>
<td>&gt;50</td>
<td>&gt;50</td>
<td>&gt;50</td>
<td>&gt;50</td>
</tr>
<tr>
<td>80\times80</td>
<td>5</td>
<td>28</td>
<td>&gt;50</td>
<td>&gt;50</td>
<td>&gt;50</td>
<td>&gt;50</td>
</tr>
<tr>
<td>160\times160</td>
<td>5</td>
<td>31</td>
<td>&gt;50</td>
<td>&gt;50</td>
<td>&gt;50</td>
<td>&gt;50</td>
</tr>
</tbody>
</table>

7.3 Offending Error Modes for the AP Scheme in the PHI Configuration

It was proven in [10], for the scaling of the PHI configuration considered there, that the offending error modes that are responsible for the loss of robustness of the AP formalism are modes that are nearly flat in the $y$ direction, $s \sim 0$, and characterized by a high frequency in the $x$ direction, $r \sim \pi/2$. A similar conclusion holds for the new scaling of the PHI configuration considered in this chapter and could be proven following the same approach outlined in [10]. In the following an alternative numerical verification of this conclusion is delineated that is based on a physical space, as opposed to Fourier space, interpretation of the nature of the offending modes.
7.3.1 Error Modes for a 6×6 PHI Configuration with Periodic Boundary Conditions

The first step of the numerical verification is the computation of the maximum absolute eigenvalue for the 36 error modes that can be sustained by a PHI configuration with a 6×6 mesh, having periodic boundary conditions on all four sides of the problem domain, as depicted in Fig. 7.6.

Fig. 7.6: A 6×6 PHI configuration with all periodic boundary conditions.

The periodic boundary conditions eliminate the influence of particle leakage at the domain boundaries, as in an infinite medium. The transport problem for the PHI configuration sketched in Fig. 7.6 is solved in physical space with the objective of building the 36×36 iteration matrix for the AP formalism corresponding to this particular instance of the PHI configuration. To avoid iterating over the implicit periodic boundary conditions, the direct solution of the transport problem is carried out with the
aid of Mathematica. At first the 36×36 Jacobian is built by solving, for each quadrant in angular space, the system of equations constituted by the 36 balance equations plus the 72 WDD relations plus the 12 periodicity conditions and the 60 continuity conditions for the 36 computational cells. Similar to the procedure outlined in Sec. 7.2.2 for the Fourier analysis, the 36×36 matrices corresponding to the Fₘ matrices of the Fourier analysis are obtained at first and then accumulated in the J matrix. It is noted, in passing, that the latter is another possible approach for the construction of the Jacobian matrix, along with Automatic Differentiation (AD) and the “No Sweep” algorithm previously described in Sec. 6.4. Subsequently, the AP matrix D for the case of periodic boundary conditions and the diagonal C matrix are constructed and used to assemble the iteration matrix for the AP acceleration scheme via Eq. (7.66). Finally, the maximum value of the magnitude of the eigenvalues of the iteration matrix is obtained as a function of the scaling parameter Δ, using the same quadrature and parameter values of the model problem. The plot corresponds to the solid line in Fig. 7.7.

It is noted that the error modes that can be sustained by the 6×6 PHI configuration are only a subset of all the possible modes that can be sustained by an infinite mesh and that are accounted for by the Fourier ansatz introduced in the spectral analysis in Sec. 7.2.2. That is the reason why the curve in Fig. 7.7 saturates to a value that is lower than 0.99999999. The latter value would be ideally approached by considering a sequence of I×I meshes with increasing I, that would contain a larger number of cells and would be capable of sustaining higher frequency modes, as it will be illustrated in the following section.
Fig. 7.7: Maximum eigenvalue of AP for a 6×6 and a 6×2 PHI configurations ($c_K = c_N = 0.99999999$).

The 6×6 PHI configuration in Fig. 7.6 can be obtained by repeating three times in the y direction a smaller 6×2 PHI configuration comprised only of an N and K layer, as sketched in Fig. 7.8.

A subset of the 36 modes for the PHI configuration is thus constituted by those modes in which these three stripes of two layers oscillate in exactly the same way. It is noted that the resulting collective mode for the 6×6 PHI configuration is essentially flat in the y direction, since it repeats itself every two layers, while it involves up to 6 cells in the x direction. Modes that are sustained by the smaller 6×2 PHI configuration in Fig. 7.8 are therefore the longitudinal modes for the 6×6 PHI configuration. These
modes can be isolated and studied by assembling the 12×12 AP iteration matrix for the two-layer PHI configuration with periodic boundary conditions sketched in Fig. 7.8. The maximum value of the magnitude of the eigenvalues of the latter iteration matrix is obtained as a function of the scaling parameter Δ, and is also plotted, using asterisks, in Fig. 7.7.

![Diagram of PHI configuration with periodic boundary conditions](image)

**Fig. 7.8: A 2×6 PHI configuration with all periodic boundary conditions.**

It is noted that the two curves in Fig. 7.7 corresponding to the 6×6 case and to the 6×2 cases are coincident. This means that the maximum eigenvalue for the AP acceleration scheme for the 6×6 configuration is actually contributed by the longitudinal modes. Therefore, in the following section the analysis will focus only on the modes that can be sustained by an I×2 PHI configuration for increasing values of I. As noted above, this allows exploring longitudinal modes of increasing frequency in physical space.
7.3.2 High Frequency Longitudinal Error Modes and Crisis of the AP Formalism

The calculation of the maximum eigenvalue illustrated for the 6×2 case, is repeated for the 10×2, 15×2 and 20×2 cases, respectively. Since the curves obtained for the maximum eigenvalue are all essentially flat between $\Delta = 10^3$ and $\Delta = 10^5$, as evident for the 6×2 case in Fig. 7.7, the value of the maximum eigenvalue obtained for $\Delta = 10^5$ is reported in Table 7.5 for the various meshes. All the other parameters have the same values as in the model problem.

Table 7.5: Maximum eigenvalue of AP for longitudinal modes of increasing frequency.

<table>
<thead>
<tr>
<th>Max Eigenvalue</th>
<th>6×2</th>
<th>10×2</th>
<th>15×2</th>
<th>20×2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.622</td>
<td>0.804</td>
<td>0.894</td>
<td>0.935</td>
</tr>
</tbody>
</table>

As the number of cells in the $x$ direction is increased and higher frequency longitudinal modes can be sustained, the maximum eigenvalue increases and gets closer to the $\sim 1$ value of the spectral radius predicted by the Fourier analysis. This value would ideally be recovered in the limit as $I \rightarrow \infty$ for the $I \times 2$ mesh. It is noted that a value of 0.935 is already reached for $I = 20$.

These results confirm the fundamental role played by high frequency longitudinal modes in instigating the crisis, namely the loss of robustness, of the AP acceleration scheme in the PHI configuration for the scaling introduced in Sec. 7.1.
7.4 Asymptotic Analysis of the Integral Transport Matrix in the PHI Configuration

In order to gain a basic understanding of the fundamental causes that lead to the deterioration in the spectral properties of the AP preconditioner, an asymptotic analysis is conducted for the elements of the integral transport matrix for the PHI configuration.

In view of their importance in the asymptotic analysis, as pointed out in Ch. 6, asymptotic expressions are first derived for the $\gamma$ coefficients for a cell in the thick and in the thin layers, respectively. The asymptotic expressions for the $\gamma$ coefficients for a cell in the thick layer are the same as those obtained for the $\gamma$ coefficients in the homogeneous thick cell limit in Sec. 6.6, provided $c = c_k$ and $\sigma = \sigma_k$. As noted earlier for the elements of the $B$ matrix, the $\gamma$ coefficients for a generic cell $(i, j)$ also are functions of $\sigma_{i,j} \Delta x_i$ and $\sigma_{i,j} \Delta y_j$, namely of the number of MFPs in the $x$ and $y$ direction. Therefore, scaling either $\sigma_{i,j}$ or $\Delta x_i, \Delta y_j$ as proportional to $\Delta$ produce equivalent results in the limit as $\Delta \to \infty$. Analogously, the asymptotic expressions for the $\gamma$ coefficients for a cell in the thin layer are equivalent to those obtained for the $\gamma$ coefficients in the homogeneous thin cell limit in Sec. 6.7, provided $c = c_N$, $\sigma = \sigma_N$ and $\Delta = 1/\delta$.

Similar to what was pointed out in Ch. 4 for heterogeneous slabs, the integral transport matrix $B$ is in general non-symmetric for two-dimensional heterogeneous configurations. Reasoning on the general expressions for the $\gamma_{m,i,j}$ and $\gamma_{n,i,j}$ coefficients, where $u = x$ or $y$, it appears that symmetrization of the matrix elements can be accomplished via the relationship:
The latter can be interpreted as a straightforward generalization of Eq. (4.1) for the one-dimensional $B$ matrix. At least initially though, it is preferred to consider the structure acquired, in the asymptotic limit for the PHI configuration, by the elements of the non-symmetric $B$ matrix. In fact, it is desired to investigate the different strength of coupling of a cell-averaged scalar flux with its surrounding neighbors, depending on whether the cell lies in a thick layer or in a thin layer. Specifically, the strength of coupling of a cell-averaged scalar flux with its surrounding neighbors is studied in Sec. 7.4.1 for a cell in a thick layer and in Sec. 7.4.2 for a cell in a thin layer, respectively.

7.4.1 Coupling of a Thick Cell’s Average Scalar Flux with its Neighbors

Exact analytic expressions were derived in Sec. 6.3 for the elements of the $B$ matrix coupling a cell’s average flux in cell $(i, j)$ with the fluxes in its neighboring cells up to the second neighbors. With reference to the PHI configuration sketched in Fig. 7.1, for $j$ even the cell is in a thick layer as indicated in Fig. 7.9.

The general expressions for the $B$ matrix elements in Eqs. (6.36) through (6.41) are evaluated for the material properties of the K and N layers in the PHI configuration, expressing them in terms of the configuration’s parameters, and studied in the limit as $\Delta \to \infty$ for the scaling introduced in Sec. 7.1.

$$B_{i,j,l,m}^S = \left(c_{i,j} \sigma_{i,j} \Delta x_i \Delta y_j \right) B_{i,j,l,m}$$ (7.68)
The following asymptotic expressions are obtained for the $B$ matrix elements pertaining to a cell $(i, j)$ in a thick layer:

**Self-coupling**

$$B_{i,j,i,j} = (1 - c_k) + c_k \sum_{m=1}^{M} w_m \left( \frac{|\mu_m|}{\sigma_k \delta_x} + \frac{|\eta_m|}{\sigma_k \delta_y} \right) \frac{1}{\Delta} + O\left( \frac{1}{\Delta^2} \right)$$  \hspace{1cm} (7.69)

**Coupling with first neighbors**

$$B_{i,j,i+1,j} = -\frac{c_k}{2} \sum_{m=1}^{M} w_m \frac{|\mu_m|}{\sigma_k \delta_x} \frac{1}{\Delta} + O\left( \frac{1}{\Delta^2} \right)$$  \hspace{1cm} (7.70)

$$B_{i,j,i,j+1} = -\frac{c_N}{2} \sum_{m=1}^{M} w_m \left( \frac{|\eta_m|}{\sigma_N \delta_x} + \frac{|\eta_m|}{\sigma_N \delta_y} \right) \frac{1}{\Delta^2} + O\left( \frac{1}{\Delta^3} \right)$$  \hspace{1cm} (7.71)
\[ B_{i,j+1,j+1} = -\frac{c_N}{2} \sum_{m=1}^{M} W_m \left( \frac{\mu_m}{\sigma_N \delta_x} \right) \left( \frac{\eta_m}{\sigma_k \delta_y} \right) \frac{1}{\Delta^2} + O\left( \frac{1}{\Delta^3} \right) \]  

(7.72)

Coupling with second neighbors

\[ B_{i,j+2,j} = \frac{c_K}{2} \sum_{m=1}^{M} W_m \left( \frac{\mu_m}{\sigma_k \delta_x} \right)^2 \frac{\eta_m}{\sigma_k \delta_y} \frac{1}{\Delta^3} + O\left( \frac{1}{\Delta^4} \right) \]  

(7.73)

\[ B_{i,j+1,j+2} = -\frac{c_K}{2} \sum_{m=1}^{M} W_m \left[ \left( \frac{\eta_m}{\sigma_N \delta_x} \right) - \left( \frac{\mu_m}{\sigma_N \delta_x} \right) \left( \frac{\eta_m}{\sigma_k \delta_y} \right) \right] \frac{1}{\Delta} + O\left( \frac{1}{\Delta^2} \right) \]  

(7.74)

\[ B_{i,j+2,j+1} = -\frac{c_N}{2} \sum_{n=1}^{M} W_n \left( \frac{\mu_m}{\sigma_N \delta_x} \right) \left[ \left( \frac{\mu_m}{\sigma_N \delta_x} \right) - \left( \frac{\eta_m}{\sigma_N \delta_y} \right) \right] \frac{\eta_m}{\sigma_k \delta_y} \frac{1}{\Delta^2} \]  

+ \( O\left( \frac{1}{\Delta^3} \right) \)  

(7.75)

\[ B_{i,j+1,j+2} = -\frac{c_K}{2} \sum_{m=1}^{M} W_m \left( \frac{\mu_m}{\sigma_N \delta_x} \right) \left( \frac{\eta_m}{\sigma_N \delta_y} \right) \left( \frac{\eta_m}{\sigma_k \delta_y} \right) \frac{1}{\Delta^2} + O\left( \frac{1}{\Delta^3} \right) \]  

(7.76)
As noted in Sec. 6.7, due to the negative sign in the numerator of the $\gamma_{m,N}^{uu}$ coefficients, where $u = x$ or $y$, the case of a level symmetric $S_2$ quadrature is a peculiar case. Since the numerical results discussed in this chapter are for an $S_6$ quadrature, the results discussed in the following are for a quadrature of order higher than two. That same negative sign is responsible for the different behavior that is observed, even for higher order quadratures, for square cells as opposed to rectangular cells. For example, as evident from Eq. (7.75), the $B_{i,j,j+2,j+2}$ element is $O(\Delta^{-2})$ for a rectangular cell, but becomes $O(\Delta^{-3})$ for a square cell due to an exact algebraic cancellation of the leading order term for a level symmetric quadrature of any order.

To distinguish the square case from the rectangular case it is convenient to define the aspect ratio $R = \delta_y / \delta_x$ for a computational cell. Obviously, $R = 1$ for a square cell, while $R \neq 1$ for a rectangular cell. Using this definition, the results of the asymptotic analysis are summarized in Fig. 7.10.

As done in Ch. 6, the estimates of the strength of coupling of a thick cell’s scalar flux with the neighbors beyond second are based on the leading order of the $\gamma$ coefficients for the two layers and on numerical studies.
Since the $\gamma_{\mu,\nu}^{m,K}$ coefficients are $O(\Delta^{-1})$ and the $\gamma_{\mu,\nu}^{m,K}$ coefficients are $O(\Delta^{-2})$, where $\mu, \nu = x$ or $y$, a decrease in the infinitesimal order (weaker coupling) is expected moving in the $y$ direction beyond the second neighbors. That is the reason why only elements pertaining to coupling with neighbors in the first three layers are considered in Fig. 7.10. The persistence of the infinitesimal order in the $x$ direction, pointing to a long-range coupling in this direction, is brought about by the fact that the $\gamma_{\mu,\nu}^{m,N}$ and $\gamma_{\mu,\nu}^{m,N}$ coefficients are $O(\Delta^0)$. This circumstance is illustrated in Fig. 7.11, for the $O(\Delta^{-1})$ coupling with the cells belonging to the layer with $j=4$, by sketching the dominant paths that connect the various cells in this layer with cell $(1,2)$. Therefore, the coupling of a thick cell with the elements in the next thick layer can be of the same order as self-coupling and coupling with the first Cartesian neighbors.

**Fig. 7.10: Strength of coupling of a thick cell’s average flux with its neighbors for PHI.**

<table>
<thead>
<tr>
<th>$j=5$</th>
<th>$j=4$</th>
<th>$j=3$</th>
<th>$j=2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$r=3$</td>
<td>$r=2$</td>
<td>$r=1$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$O(\Delta^{-1})$</td>
<td>$O(\Delta^{-2}) &lt; O(\Delta^{0})$</td>
<td>$O(\Delta^{-2})$</td>
</tr>
<tr>
<td></td>
<td>$O(\Delta^{-1})$</td>
<td>$O(\Delta^{-2})$</td>
<td>$O(\Delta^{-3})$</td>
</tr>
<tr>
<td></td>
<td>$O(\Delta^{-1})$</td>
<td>$O(\Delta^{-3})$</td>
<td>$O(\Delta^{-5})$</td>
</tr>
<tr>
<td></td>
<td>$O(\Delta^{-1})$</td>
<td>$O(\Delta^{-3})$</td>
<td>$O(\Delta^{-7})$</td>
</tr>
<tr>
<td>$i=1$</td>
<td>$i=2$</td>
<td>$i=3$</td>
<td>$i=4$</td>
</tr>
<tr>
<td>$r=1$</td>
<td>$r=2$</td>
<td>$r=3$</td>
<td>$r=4$</td>
</tr>
</tbody>
</table>
Finally, an explanation is given for the “oscillation” of the order of coupling with
the cells in the adjacent thin-cell layer evident in Fig. 7.10, for the case \( R = 1 \). This result
is again a consequence of the negative sign in the numerator of the \( \gamma_{m,N} \) coefficients. A
dominant path connecting a cell in the thin layer to cell \((1, 2)\) is again a straight path
along the thin layer that bends in cell \((1, 3)\) and enters cell \((1, 2)\). For a cell characterized
by \( i > 2 \) even, an even number of \( \gamma_{m,N}^{\text{ev}} \) coefficients are multiplied along the path and no
exact algebraic cancellation can result for the \( O(\Delta^0) \) leading term resulting from the
superposition of all the possible discrete ordinates (even power of
\( (|\mu_m|/\sigma_n \delta_x - |\eta_m|/\sigma_n \delta_y) \)). For a cell characterized by \( i > 2 \) odd, an odd number of \( \gamma_{m,N}^{\text{ov}} \)
coefficients are instead multiplied along the path and this leads to algebraic cancellation
of the \( O(\Delta^0) \), for a level symmetric quadrature. Finally, this same behavior does not

Fig. 7.11: Dominant paths connecting a thick cell to the cells in the next thick layer.
occur, even for square cells, for the dominant paths depicted in Fig. 7.11 thanks to the extra coefficients that have to be multiplied along the longer paths needed to reach these farther neighbors. As evident, for example, from Eq. (7.77), these extra coefficients result in an expression that is not invariant under the exchange of $|\mu_m|$ with $|\eta_m|$, and vice versa.

### 7.4.2 Coupling of a Thin Cell’s Average Scalar Flux with its Neighbors

Exact analytic expressions were derived in Sec. 6.3 for the elements of the $B$ matrix coupling a cell’s average flux in cell $(i,j)$ with the fluxes in its neighboring cells up to the second neighbors. With reference to the PHI configuration sketched in Fig. 7.1, for $j$ odd the cell is in a thick layer as indicated in Fig. 7.12.

![Fig. 7.12: First and second neighboring cells for cell $(i,j)$ in a thin layer.](image)

The general expressions for the $B$ matrix elements in Eqs. (6.36) through (6.41) are evaluated for the material properties of the K and N layers in the PHI configuration, expressing them in terms of the configuration’s parameters, and studied in the limit as $\Delta \to \infty$ for the scaling introduced in Sec. 7.1.
The following asymptotic expressions are obtained for the $B$ matrix elements pertaining to a cell $(i, j)$ in a thin layer:

**Self-coupling**

$$B_{i,j,i,j} = 1 - \frac{c_N}{2} \sum_{m=1}^{M} W_m \frac{1}{\frac{|\mu_m|}{\sigma_N \delta_x} + \frac{|\eta_m|}{\sigma_N \delta_y}} \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right) \quad (7.78)$$

**Coupling with first neighbors**

$$B_{i,j,i+1,j} = -\frac{c_N}{2} \sum_{m=1}^{M} W_m \frac{\frac{|\mu_m|}{\sigma_N \delta_x}}{\frac{|\mu_m|}{\sigma_N \delta_x} + \frac{|\eta_m|}{\sigma_N \delta_y}} \frac{1}{\Delta} + O\left(\frac{1}{\Delta^2}\right) \quad (7.79)$$

$$B_{i,j,i,j+1} = -\frac{c_K}{2} \sum_{m=1}^{M} W_m \left[\frac{\mu_m}{\sigma_N \delta_x} \left(\frac{\eta_m}{\sigma_N \delta_y}\right)\right] + O\left(\frac{1}{\Delta}\right) \quad (7.80)$$

$$B_{i,j,i+1,j+1} = -\frac{c_K}{2} \sum_{m=1}^{M} W_m \left[\frac{\mu_m}{\sigma_N \delta_x} \left(\frac{\eta_m}{\sigma_N \delta_y}\right)\right] + O\left(\frac{1}{\Delta}\right) \quad (7.81)$$
Coupling with second neighbors

\begin{align*}
B_{i,j,i+2,j} &= -\frac{c_N}{2} \sum_{m=1}^{M} w_m \left( \frac{|\mu_m|}{\sigma_N \delta_x} \frac{|\mu_m|}{\sigma_N \delta_x} - \frac{|\eta_m|}{\sigma_N \delta_y} \right) \frac{1}{\Delta} + O \left( \frac{1}{\Delta^2} \right) \quad (7.82)
\end{align*}

\begin{align*}
B_{i,j,i,j+2} &= \frac{c_N}{2} \sum_{m=1}^{M} w_m \left( \frac{|\mu_m|}{\sigma_N \delta_y} \frac{|\mu_m|}{\sigma_K \delta_x} \frac{|\eta_m|}{\sigma_K \delta_x} + \frac{|\eta_m|}{\sigma_N \delta_y} \right)^2 \frac{1}{\Delta^3} + O \left( \frac{1}{\Delta^4} \right) \quad (7.83)
\end{align*}

\begin{align*}
B_{i,j,i+2,j+1} &= -\frac{c_K}{2} \sum_{m=1}^{M} w_m \left( \frac{|\mu_m|}{\sigma_N \delta_x} \frac{|\eta_m|}{\sigma_N \delta_y} \left[ \frac{|\mu_m|}{\sigma_K \delta_x} \frac{|\eta_m|}{\sigma_K \delta_y} \right] - \frac{|\eta_m|}{\sigma_N \delta_y} \right) \frac{1}{\Delta} + O \left( \frac{1}{\Delta^2} \right) \quad (7.84)
\end{align*}

\begin{align*}
B_{i,j,i+1,j+2} &= \frac{c_N}{4} \sum_{m=1}^{M} w_m \left( \frac{|\eta_m|}{\sigma_N \delta_y} \right)^3 \left[ \frac{3}{\sigma_N \delta_x} - \frac{|\eta_m|}{\sigma_K \delta_x} \frac{|\eta_m|}{\sigma_K \delta_y} \right] \frac{1}{\Delta^3} + O \left( \frac{1}{\Delta^4} \right) \quad (7.85)
\end{align*}
The results of the asymptotic analysis are summarized in Fig. 7.13. The explanations for the main features displayed by the results summarized in Fig. 7.13 are similar to the explanations given in the previous section.

\[
B_{i,j+2,i+2} = c_N \sum_{m=1}^{M} W_m \left( \frac{|\mu_m|}{\sigma_N \delta_x} \right) \left( \frac{|\eta_m|}{\sigma_N \delta_y} \right) \left[ \left( \frac{|\mu_m|}{\sigma_N \delta_x} \right)^2 \left( \frac{|\eta_m|}{\sigma_N \delta_y} \right) + \left( \frac{|\eta_m|}{\sigma_N \delta_y} \right)^2 \right] \frac{1}{\Delta^3} 
\]

\[
+ O \left( \frac{1}{\Delta^4} \right)
\]

The results in Fig. 7.13 indicate that the coupling of a thin cell’s scalar flux with the scalar fluxes in the next thick layer can be of the same order as self-coupling and coupling with the first Cartesian neighbors. In particular, the coupling with the first

\[
\begin{array}{cccccc}
  j = 4 & r = 3 & K & O(\Delta^{-3}) & O(\Delta^{-3}) & O(\Delta^{-3}) \\
  j = 3 & r = 2 & N & O(\Delta^{-1}) & O(\Delta^{-1}) & O(\Delta^{-1}) \\
  j = 2 & r = 1 & K & O(\Delta^0) & O(\Delta^0) & O(\Delta^0) \\
  j = 1 & i = 1 & c_N \leq 1 & O(\Delta^{-1}) & O(\Delta^{-1}) & O(\Delta^{-1}) \\
  & i = 2 & & & & \\
  & i = 3 & & & & \\
  & i = 4 & & & & \\
  & i = 5 & & & & \\
  & r = 1 & & & & \\
  & r = 2 & & & & \\
  & r = 3 & & & & \\
  & r = 4 & & & & \\
\end{array}
\]

Fig. 7.13: Strength of coupling of a thin cell’s average flux with its neighbors for PHI.
diagonal neighbor is always of the same order as self-coupling and coupling with the first Cartesian neighbor in the y direction.

7.5 Conjecture on the Importance of Cross-Derivative Coupling for PHI

In this section the main findings of the spectral analysis for the AP acceleration scheme and of the asymptotic analysis for the elements of the integral transport matrix are used to gain a basic understanding of the mechanisms that lead to deterioration of the spectral properties of the AP acceleration scheme for the PHI configuration.

In Sec. 7.2.2 a general expression has been obtained for the Jacobian matrix $J$. For a given quadrature order and for given values of the $\delta_x$, $\delta_y$, $\sigma_k$, $\sigma_n$, $c_k$ and $c_n$ parameters:

$$ J = J(r,s,\Delta) $$

(7.87)

As pointed out in Sec. 6.4, the simple relationship $B = I - J$ permits obtaining the expression for the integral transport matrix. In view of Eq. (7.87):

$$ B = B(r,s,\Delta) = \begin{bmatrix} B_{NN}(r,s,\Delta) & B_{NK}(r,s,\Delta) \\ B_{KN}(r,s,\Delta) & B_{KK}(r,s,\Delta) \end{bmatrix} $$

(7.88)

In Sec. 7.3 it has been shown that, in the asymptotic limit for the PHI configuration, the offending modes for the AP acceleration scheme are high frequency longitudinal modes. The latter modes are almost flat in the y direction, $s \sim 0$, and have a strong dependence on $r$. It is important to observe that these modes happen to be offending modes also for SI in the PHI configuration. It is traditionally recognized that
for homogeneous model configurations the flattest modes, characterized by \( r, s \sim 0 \), are the slowest converging modes and cause the spectral radius of SI to be coincident with the scattering ratio of the homogeneous medium. This result is true also for the case of the PHI configuration. In the asymptotic limit as \( \Delta \to \infty \), though, also the high frequency longitudinal modes contribute an eigenvalue that is equal to the scattering ratio, assuming \( c_K = c_N \). More generally, as it was observed in [10] for the Fourier analysis of SI for the PHI configuration, one peculiar feature of the PHI case is the diminishing range of the spectrum with increasing material discontinuity. Specifically, for each Fourier mode, identified by \( r \) and \( s \), the larger (in absolute value) of the two corresponding eigenvalues of the \( J \) matrix increases toward the value of the scattering ratio, assuming \( c_K = c_N \), for increasing values of the scaling parameter \( \Delta \). In other words, the infimum of the absolute value of the spectrum over the Fourier space approaches its supremum, i.e. the value of the scattering ratio, as the material discontinuity increases. The latter observations on the behavior of SI are important because they indicate that in the asymptotic limit for PHI, the high-order step in the AP acceleration scheme, namely a sweep of the mesh, is not capable of attenuating the high frequency longitudinal modes. This circumstance is quite different from what happens in the homogeneous model configuration where, loosely speaking, the high-order mesh-sweep attenuates the high frequency component of the spectrum, while the low-order step (for a diffusive preconditioner) takes care of the low frequency modes.

In Sec. 7.4 the strength of coupling between the cell-averaged scalar fluxes in neighboring cells has been investigated in the asymptotic limit for the PHI configuration
by studying the asymptotic properties of the $B$ matrix elements. In the following the focus will be in particular on the asymptotic results for the coupling of cells that lie in two adjacent layers, one hosting a thick material the other hosting a thin material. In fact, as shown in Sec. 7.3, the latter are the cells that support high frequency longitudinal modes. The results of the asymptotic analysis for the $B$ matrix elements for the PHI configuration in the limit as $\Delta \to \infty$ indicate that a cell in the thin layer is coupled to the adjacent thick layer not only through coupling with its vertical Cartesian neighbor but also through coupling with its first diagonal neighbor and possibly with farther neighbors in the thick layer. In contrast, the coupling of a cell in a thick layer with the cells in the adjacent thin layer appears to be of negligible order. It follows that the off-diagonal element $B_{NK}$ plays a significant role in determining the coupling between two adjacent layers in the asymptotic limit. The previous results of the asymptotic analysis are summarized by the mathematical expression:

$$\lim_{\Delta \to \infty} B_{NK} (r, s, \Delta) = 2B_{ov,NK} \cos(s) + 4B_{osy,NK} \cos(r) \cos(s) + ...$$  \hspace{1cm} (7.89)$$

In Eq. (7.89), $B_{ov,NK}$ and $B_{osy,NK}$ indicate the asymptotic expressions for the $B$ matrix elements pertaining to the coupling of a thin cell’s average flux to its vertical Cartesian neighbor and to its first diagonal neighbor in a thick layer, respectively. The latter expressions are contained in Eqs. (7.80) and (7.81), respectively. Notice that other elements of the $B$ matrix can in general contribute to the expansion on the right hand side of Eq. (7.89). In fact, as summarized in Fig. 7.13, the strength of coupling of a thin cell’s scalar flux with fluxes in the adjacent thick layer farther than the first diagonal neighbor
can be of the same order as the coupling with the vertical Cartesian neighbor and the first diagonal neighbor.

From Eq. (7.89) it follows that:

\[
\lim_{\Delta \to \infty} \frac{\partial B_{NK}(r,s,\Delta)}{\partial r} \neq 0 \tag{7.90}
\]

In contrast, for the AP matrix \(D\) it has been shown in Sec. 7.2.2 that:

\[
D(r,s,\Delta) = \begin{bmatrix}
D_{NN}(r,\Delta) & D_{NK}(s,\Delta) \\
D_{KN}(s,\Delta) & D_{KK}(r,\Delta)
\end{bmatrix} \tag{7.91}
\]

In particular, \(D_{NK}(s,\Delta) = 2D_{oy} \cos(s)\) does not depend on \(r\) implying:

\[
\lim_{\Delta \to \infty} \frac{\partial D_{NK}(s,\Delta)}{\partial r} = 0 \tag{7.92}
\]

The above findings lead to the formulation of the following conjecture on the crisis of the AP formalism, and potentially of other diffusion-based preconditioning schemes, in the asymptotic limit of the PHI configuration. We believe that this crisis is due to a structural deficiency of the preconditioner. Specifically, the low-order operator ignores the strong cross-derivative coupling between the cells in two adjacent layers, displayed by the full integral transport operator. Hence it appears inadequate in attenuating high frequency longitudinal modes because these modes are sustained by two adjacent layers exclusively through cross-derivative coupling. In fact, as evident from Eq. (7.89), the \(B_{oy,NK}\) elements, and potentially others, account for the dependence on \(r\) of \(B_{NK}\) in the asymptotic limit \(\Delta \to \infty\), but not the \(B_{oy,NK}\) elements. The latter elements only contribute to the dependence of \(B_{NK}\) on \(s\). Yet, they are the only elements of the integral transport matrix, coupling cells in two adjacent layers hosting different materials,
accounted for by the five-point stencil matrix of the diffusive two-dimensional AP preconditioner. Therefore, we also believe that extended low-order operators that account for cross-derivative coupling have the potential to recover acceleration robustness in the asymptotic limit of the PHI configuration.

Different directions may be taken to test the above conjecture by devising a novel acceleration scheme that accounts for cross-derivative coupling. A new acceleration scheme based on extending the AP formalism is illustrated in the next section. The preliminary results of the investigation of this acceleration scheme, presented in the remainder of the chapter, confirm the validity of the above conjecture. Another direction that may be pursued in future research, no longer based on the AP formalism, is suggested in Sec. 8.3.

### 7.6 Extension of the AP Formalism to Account for Cross-Derivative Coupling

Since the AP acceleration scheme works extremely well for homogeneous configurations in the thick cell limit, it is desired to preserve this nice feature of the AP formalism while at the same time extending the structure of the AP preconditioner to improve the spectral properties of the method for the PHI configuration. Specifically, it is desired to extend the structure of the AP preconditioner $D$ to a nine-point stencil matrix $P$ that incorporates the coupling of a cell’s average flux to its first diagonal neighbors:

$$
P = \begin{bmatrix}
P_{d,N} + 2D_{\text{ox},N} \cos(r) & 2D_{\text{oy}} + 4P_{\text{ox},\text{Nk}} \cos(r) \cos(s) \\
2D_{\text{oy}} + 4P_{\text{ox},\text{KN}} \cos(r) \cos(s) & P_{d,K} + 2D_{\text{ox},K} \cos(r)
\end{bmatrix}
$$

(7.93)
The recipe for the construction of the elements of the $P$ matrix that couple a cell’s average flux to its first Cartesian neighbors is the same as for the AP preconditioner. Therefore, the expressions for $D_{ox,l}$, where $l = N, K$, and $D_{oy}$ are the same as in Eqs. (7.61) and (7.62), respectively. The diagonal elements are constructed by extending the stability condition for the flat error eigenmodes, originally discussed in [10] for the $D$ matrix, to incorporate the coupling with the four diagonal neighbors:

$$
P_{d,N} = \sum_N \delta_x \delta_y (1-c_N) - 2D_{ox,N} - 2D_{oy} - 4P_{oxy,NK} \quad (7.94)
$$

$$
P_{d,K} = \sum_K \delta_x \delta_y (1-c_K) - 2D_{ox,K} - 2D_{oy} - 4P_{oxy,KN} \quad (7.95)
$$

For the moment, the elements pertaining to cross-derivative coupling, $P_{oxy,NK}$ and $P_{oxy,KN}$ are left unspecified. They are allowed to be possibly different. Also, it is ideally desired that they vanish for the case of a homogeneous configuration so that the $P$ matrix reduces to the $D$ matrix and the traditional AP formalism that is highly efficient in homogeneous media is recovered.

Two questions must then be addressed: 1) Does the inclusion of $P_{oxy,NK}$ and $P_{oxy,KN}$ improve the spectral properties of the extended AP formalism for the PHI configuration? 2) If yes, how are these elements built as a function of a configuration’s parameters? The preliminary results presented in the remainder of the chapter address these two questions for the model problem introduced in Sec. 7.2 to illustrate the crisis of the AP formalism in the PHI configuration.
Initially, in order to address question 1, the maximum eigenvalue for the acceleration scheme obtained by replacing the traditional AP preconditioner $D$ with the $P$ matrix is computed, as a function of $P_{o\gamma,NK}$ and $P_{o\gamma,KN}$, for the $10 \times 2$ PHI configuration with periodic boundary conditions on all four sides considered in Sec. 7.3.2, assuming $\Delta=10^4$ as in Table 7.5. The parametric study is conducted using a coarse scale for varying the unknown preconditioner elements, $-10^6 \leq P_{o\gamma,NK}, P_{o\gamma,KN} \leq +10^6$, with two-decade intervals for each parameter. The search is then refined around the local minimum for the maximum eigenvalue. The results of the parametric study indicate the existence of an optimal value for the maximum eigenvalue of 0.422, that corresponds to $P_{o\gamma,NK} \sim -10^4$ and $P_{o\gamma,KN} \sim 0$. This result represents a first encouraging, though still incomplete, answer to question 1. In fact, the value of the maximum eigenvalue has been reduced with respect to the value of 0.804 that was obtained for the traditional AP preconditioner in Table 7.5.

The above result is also used to guide the search for a possible answer to question 2. Since for $\Delta=10^4$ $P_{o\gamma,NK} \sim -10^4$ and $P_{o\gamma,KN} \sim 0$, it is conjectured that $P_{o\gamma,NK} \sim O(\Delta)$ while $P_{o\gamma,KN}$ is infinitesimal in $\Delta$, in the limit as $\Delta \to \infty$. It is also noted that this fairly asymmetric behavior of the $P_{o\gamma,NK}$ and $P_{o\gamma,KN}$ elements, in the asymptotic limit of PHI, is similar to the asymptotic behavior of the elements of the integral transport matrix $B$ pertaining to coupling with the first diagonal neighbors. Specifically, it follows from Eqs. (7.81) and Eq. (7.72) that $B_{o\gamma,NK} \sim O(\Delta^6)$ while $B_{o\gamma,KN} \sim O(\Delta^{-2})$, respectively. The general recipe for constructing these elements of the $B$ matrix for given values of the
problem’s parameters is known from Sec. 6.3. Applying Eq. (6.38) to the PHI configuration:

\[
B_{\text{oxy}, NK} = -\frac{1}{4} \sum_{m=1}^{M} W_m \left( \gamma_{m,N}^{\text{xy}} \gamma_{m,K}^{\text{xy}} \gamma_{m,N}^{\text{xy}} + \gamma_{m,N}^{\text{xy}} \gamma_{m,K}^{\text{xy}} \gamma_{m,N}^{\text{xy}} \gamma_{m,K}^{\text{xy}} \right) \tag{7.96}
\]

\[
B_{\text{oxy}, KN} = -\frac{1}{4} \sum_{m=1}^{M} W_m \left( \gamma_{m,K}^{\text{xy}} \gamma_{m,N}^{\text{xy}} \gamma_{m,N}^{\text{xy}} \gamma_{m,K}^{\text{xy}} \gamma_{m,K}^{\text{xy}} \gamma_{m,N}^{\text{xy}} \right) \tag{7.97}
\]

In view of the above discussion it appears that \( B_{\text{oxy}, NK} \) and \( B_{\text{oxy}, KN} \) can serve the purpose of constructing \( P_{\text{oxy}, NK} \) and \( P_{\text{oxy}, KN} \), respectively, when properly re-scaled to account for the different scaling with \( \Delta \), due to the dimensional form of the AP preconditioner. Specifically, the following expressions are proposed for \( P_{\text{oxy}, NK} \) and \( P_{\text{oxy}, KN} \):

\[
P_{\text{oxy}, NK} = \frac{\left| \Sigma_K - \Sigma_N \right|}{\Sigma_K} \Sigma_k \delta_k \delta_B B_{\text{oxy}, NK} \tag{7.98}
\]

\[
P_{\text{oxy}, KN} = \frac{\left| \Sigma_K - \Sigma_N \right|}{\Sigma_K} \Sigma_n \delta_n \delta_B B_{\text{oxy}, KN} \tag{7.99}
\]

The multiplication of the dimensionless \( B \) matrix elements by the product of a macroscopic cross-section times an area is necessary to obtain the correct dimensions for the elements of the dimensional \( P \) matrix. Since for the scaling of the PHI configuration introduced in Sec. 7.1 \( \Sigma_N \sim O(\Delta^{-1}) \) and \( \Sigma_K \sim O(\Delta) \), it follows that in general \( P_{\text{oxy}, NK} \sim O(\Delta) \) while \( P_{\text{oxy}, NK} \sim O(\Delta^{-3}) \), as desired. For the particular case of a
homogeneous configuration $\Sigma_k = \Sigma_N$, and from Eqs. (7.98) and (7.99) it is concluded that $P_{\text{oxy},Nk} = P_{\text{oxy},Kn} = 0$, therefore $P$ reduces to the traditional AP preconditioner $D$.

The proposed recipe for constructing the elements of the $P$ matrix as a function of the parameters of the PHI configuration is tested at first for the same longitudinal modes for which the traditional AP formalism was shown to lose robustness in Sec. 7.3.2. Since the novel acceleration scheme proposed is obtained by amending the traditional AP preconditioner by incorporating the elements of the $B$ matrix coupling a cell’s average flux to its first diagonal neighbors, in the following this scheme will be referred to as APB. The results obtained for the APB scheme, for the same problems considered for the traditional AP scheme in Table 7.5 for $\Delta = 10^4$, are presented in Table 7.6.

<table>
<thead>
<tr>
<th>Max Eigenvalue</th>
<th>6x2</th>
<th>10x2</th>
<th>15x2</th>
<th>20x2</th>
</tr>
</thead>
<tbody>
<tr>
<td>6x2</td>
<td>0.515</td>
<td>0.550</td>
<td>0.544</td>
<td>0.550</td>
</tr>
</tbody>
</table>

While for the AP scheme the value of the maximum eigenvalue appeared to increase toward an almost unit value for increasing frequency of the longitudinal modes, the maximum eigenvalue for the APB scheme appears to be bounded by a value of $\sim 0.55$, which is much less than 1. Therefore, it appears that amending the recipe for the construction of the AP preconditioner to account for cross-derivative coupling can restore robustness of the amended AP formalism by attenuating the offending modes for the traditional AP scheme. In the next section it is also verified that this result is true for all possible modes and frequencies by performing a Fourier analysis for the novel APB scheme for the model problem. The latter result completes the positive answer to question
1, namely it has been shown that the inclusion of $P_{\text{oxy}, NK}$ and $P_{\text{oxy}, KN}$ significantly improves the spectral properties of the extended AP formalism for an instance of the PHI configuration for which it was shown that the traditional AP acceleration scheme loses its robustness. Specifically, acceleration robustness has been regained for the APB preconditioner for the model problem considered in this chapter.

Before concluding this section, it is also noted that the APB formalism proposed in this section, and further generalized in the next section for a finite mesh with vacuum boundary conditions, represents a positive answer to question 2, namely a simple recipe is proposed to build the elements pertaining to cross-derivative coupling as a function of a configuration’s parameters, at least for homogeneous and PHI configurations. This recipe is easy to implement and works for the model problem considered in this chapter. Notwithstanding, this recipe is not necessarily optimal, since a value of 0.55 was obtained instead of the optimum 0.422 for the $10 \times 2$ mesh, and needs to be tested for more general choices vs problem’s parameters, as further discussed in Sec. 8.3. Finally, since the proposed recipe incorporates the elements from the integral transport matrix $B$ pertaining to coupling with the first diagonal neighbors while preserving the mixing formula approach of the “diffusion coefficients” of the traditional AP formalism adapted from Diffusion Theory, the resulting APB preconditioner may be regarded as a sort of discrete hybrid diffusion-transport operator. Further research is also needed to dwell on the potential philosophical implications of the proposed scheme, and its applicability to other diffusion-based acceleration schemes.
7.7 Fourier Analysis and Numerical Results for the Novel Acceleration Scheme

The Fourier analysis for the APB scheme introduced in the previous section is similar to the Fourier analysis for the AP scheme that was conducted in Sec. 7.2.2. Specifically, the high-order equations and the update equations are the same as Eqs. (7.55) and (7.57), respectively. The low-order equations for the novel acceleration scheme are:

\[
\Phi^{(i+1/2)} = P^{-1} C (\Phi^{(i+1/2)} - \Phi^{(i)}) ,
\]

(7.100)

where the \( P \) matrix is the matrix previously defined in Eq. (7.93), while \( C \) is the same matrix defined in Eq. (7.64) for the traditional AP formalism.

Eliminating \( \Phi^{(i+1/2)} \) from Eqs. (7.55), (7.100) and (7.57) it is possible to find the expression that maps \( \Phi^{(i)} \) into \( \Phi^{(i+1)} \) for the APB acceleration scheme:

\[
\Phi^{(i+1)} = \left[ J + P^{-1} C (J - I) \right] \Phi^{(i)}
\]

(7.101)

Therefore, the iteration matrix for APB is:

\[
T_{APB} = J + P^{-1} C (J - I)
\]

(7.102)

For a given order of the level symmetric quadrature, and for given values of the \( \delta_x, \delta_y, \sigma_k, c_k \) and \( c_N \) parameters, the spectral radius for APB is obtained as a function of the scaling parameter \( \Delta \) introduced in Sec. 7.1 for the PHI configuration:

\[
\rho_{APB} = \rho_{APB} (\Delta) = \max_{r,s} \left[ \text{Abs} \left[ \text{Eig} \left[ T_{APB} (r, s, \Delta) \right] \right] \right]
\]

(7.103)

The equations for the Fourier analysis of the APB scheme have also been implemented in the *Mathematica* notebook and solved for the homogeneous thick cell
limit and for the PHI configuration. In view of Eqs. (7.98) and (7.99), the result for the homogeneous case is the same as that obtained in Sec. 7.2.3 for the AP scheme, for the same choice of problem’s parameters. The result of the Fourier analysis of the APB accelerated iterations for the scaling of the PHI configuration introduced in Sec. 7.1 and the model problem defined in Sec. 7.2.2 is presented in Fig. 7.14.

![Figure 7.14: Spectral radius of APB for a PHI configuration with $c_K = c_N = 0.99999999$.](image)

The results of the Fourier analysis confirm that the value of the spectral radius has been reduced to ~0.55 for the APB acceleration scheme in the asymptotic limit of the PHI configuration analyzed in this chapter. For this model problem, robustness of the accelerated iterations is restored thanks to the inclusion of cross-derivative coupling in
the APB preconditioner. The latter result verifies the conjecture that was formulated in Sec. 7.5.

The APB acceleration scheme has also been implemented in the original AP2 code as a new option in order to test the predictions of the Fourier analysis both for homogeneous and PHI configurations. The elements of the $P$ matrix pertaining to a cell $(i,j)$ in the interior of the Cartesian mesh, for $i = 2, ..., (I-1)$ and $j = 2, ..., (J-1)$, are obtained using the same equations introduced in Sec. 7.2.1 to build the elements effecting coupling to Cartesian neighbors for the traditional AP preconditioner and generalizing the expressions proposed in Sec. 7.6 for the additional elements of the APB preconditioner that account for cross-derivative coupling. Specifically, the following cross-derivative terms are defined:

$$P_{\text{xy}}^{\pm i, \pm j} = -\frac{|\sigma_{i,j} - \sigma_{\pm i, \pm j}|}{\max(\sigma_{i,j}, \sigma_{\pm i, \pm j})} \sigma_{\pm i, \pm j} \Delta x_{\pm i} \Delta y_{\pm j} B_{i,j, \pm i, \pm j}, \quad (7.104)$$

in terms of the elements of the integral transport matrix that couple cell $(i,j)$ to its first diagonal neighbors defined in Sec. 6.3:

$$B_{i,j, \pm i, \pm j} = -\frac{1}{4} \sum_{m=1}^{M} w_m \left( \gamma_{m,i,j}^{\text{xy}} \gamma_{m,i,j}^{\text{xy}} + \gamma_{m,i,j}^{\text{xy}} \gamma_{m,i,j}^{\text{xy}} + \gamma_{m,j,i}^{\text{xy}} \gamma_{m,j,i}^{\text{xy}} + \gamma_{m,j,i}^{\text{xy}} \gamma_{m,j,i}^{\text{xy}} \right), \quad (7.105)$$

The elements of the nine-diagonal banded matrix $P$ pertaining to an internal computational cell are then assembled using the following expression:
\[
\begin{aligned}
\begin{pmatrix}
P_{i,j,j} &= \sigma_{i,j} \Delta x_i \Delta y_j \left(1 - c_{i,j}\right) + D_{o,x}^{i,j} + D_{o,y}^{i,j} + D_{o,x}^{i,-j} + \\
&+ D_{o,y}^{i,j} + P_{o,x}^{i,j} + P_{o,y}^{i,j} + P_{o,x}^{i,-j} + P_{o,y}^{i,-j} \\
P_{i,j,j+1} &= -D_{o,x}^{i,j} \\
P_{i,j,j-1} &= -D_{o,x}^{i,j} \\
P_{i,j,j,j+1} &= -D_{o,y}^{i,j} \\
P_{i,j,j,j-1} &= -D_{o,y}^{i,j} \\
P_{i,j,j+1,j+1} &= -P_{o,x}^{i,j,j} \\
P_{i,j,j,j+1,j+1} &= -P_{o,x}^{i,j,j} \\
P_{i,j,j-1,j+1} &= -P_{o,y}^{i,j,j} \\
P_{i,j,j-1,j-1} &= -P_{o,y}^{i,j,j} \\
P_{i,j,j+1,j-1} &= -P_{o,y}^{i,j,j} \\
P_{i,j,j+1,j-1} &= -P_{o,y}^{i,j,j}
\end{pmatrix},
\end{aligned}
\]

(7.106)

where \(D_{o,x}^{i,j}\) and \(D_{o,y}^{i,j}\) are obtained by mixing the “diffusion coefficients”, defined in Eqs. (7.4) and (7.5), via the usual dimensional mixing formulas, introduced in Eqs. (7.6) and (7.7), for the traditional AP formalism.

A prescription must then be introduced to construct the elements of the \(P\) matrix pertaining to the boundary cells, under the assumption of vacuum boundary conditions. The Fourier analysis does not give any prescription on the boundaries, since it refers to an infinite configuration. Preliminary numerical evidence suggests that, similar to the treatment of the Cartesian neighbors in the AP formalism, it is necessary to consider some sort of fictitious diagonal neighboring cells, for a cell at the domain boundary, also when computing the \(P_{i,j,i,j}\) elements for the boundary cells. In fact, failing to do so resulted in an unstable acceleration scheme. Currently the fictitious cells are considered to have the same properties of available internal diagonal neighboring cells for a cell at the domain boundary. This prescription is easy to implement and, as evident from the numerical results presented below, it appears to work well in numerical experiments. As
indicated in Sec. 8.3, further research is needed in the future to either obtain a rigorous justification of this result or derive a more accurate prescription to implement vacuum boundary conditions for the nine-point stencil preconditioner $P$. As heuristic justification for the fact that the elements pertaining to self-coupling for the $P$ preconditioner need not necessarily be different for a cell on the boundary and for an internal cell is based on the observation that such a circumstance appears to be true for the integral transport operator. In fact, the derivation of the expression for the $B$ matrix element $B_{i,j,i,j}$, pertaining to self-coupling, in Sec. 6.3 is the same whether cell $(i, j)$ is an internal cell or a boundary cell.

Therefore, the elements of the $P$ matrix pertaining to a corner cell are assembled using the following expressions:

\[
\begin{align*}
P_{1,1,1,1} &= \sigma_{i,1} \Delta x_i \Delta y_j \left( 1 - c_{i,1} \right) + D_{a,x}^{+1} + D_{a,y}^{-1} + D_{\beta,x}^{+1} + D_{\beta,y}^{-1} + 4P_{o,xy}^{+1} \\
P_{1,1,2,1} &= -D_{a,x}^{+1} \\
P_{1,1,1,2} &= -D_{a,y}^{-1} \\
P_{1,1,2,2} &= -P_{o,xy}^{-1}
\end{align*}
\] (7.107)

\[
\begin{align*}
P_{1,1,l,1} &= \sigma_{i,1} \Delta x_i \Delta y_j \left( 1 - c_{l,1} \right) + D_{\beta,x}^{+1} + D_{a,x}^{-1} + D_{a,y}^{+1} + D_{\beta,y}^{-1} + 4P_{o,xy}^{+1} \\
P_{1,1,l-1,1} &= -D_{a,x}^{-1} \\
P_{1,1,l,2} &= -D_{a,y}^{+1} \\
P_{1,1,l-1,2} &= -P_{o,xy}^{-1}
\end{align*}
\] (7.108)
\[
\begin{align*}
P_{1,j,1} &= \sigma_{x,j} \Delta x_i \Delta y_j \left(1 - c_{1,j}\right) + D_{o,x}^{+,J} + D_{o,y}^{-,J} + D_{o,y}^{+,J} + D_{o,y}^{-,J} + 4P_{o,xy}^{+,J} \\
P_{1,j,2} &= -D_{o,x}^{+,J} \\
P_{1,j,1,J-1} &= -D_{o,y}^{-,J} \\
P_{1,j,1,J-1} &= -P_{o,xy}^{+,J}
\end{align*}
\] (7.109)

\[
\begin{align*}
P_{j,j,1} &= \sigma_{x,j} \Delta x_i \Delta y_j \left(1 - c_{1,j}\right) + D_{o,x}^{+,J} + D_{o,x}^{-,J} + D_{o,y}^{+,J} + D_{o,y}^{-,J} + 4P_{o,xy}^{+,J} \\
P_{j,j,1,J} &= -D_{o,x}^{-,J} \\
P_{j,j,1,J} &= -D_{o,y}^{-,J} \\
P_{j,j,1,J} &= -P_{o,xy}^{-,J}
\end{align*}
\] (7.110)

Similarly, the recipe for the other edge cells is:

\[
i = 2, ..., (I-1); j = 1
\]

\[
\begin{align*}
P_{i,1,1} &= \sigma_{i,1} \Delta x_i \Delta y_{1} \left(1 - c_{i,1}\right) + D_{o,x}^{+,i,1} + D_{o,x}^{-,i,1} + D_{o,y}^{+,i,1} + D_{o,y}^{-,i,1} + 2P_{o,xy}^{+,i,1} + 2P_{o,xy}^{+,i,1} \\
P_{i,1,i+1,1} &= -D_{o,x}^{+,i,1} \\
P_{i,1,i-1,1} &= -D_{o,x}^{-,i,1} \\
P_{i,1,i,2} &= -D_{o,x}^{+,i,1} \\
P_{i,1,i-1,2} &= -D_{o,xy}^{+,i,1} \\
P_{i,1,i+1,2} &= -D_{o,xy}^{+,i,1}
\end{align*}
\] (7.111)

\[
i = 2, ..., (I-1); j = J
\]

\[
\begin{align*}
P_{i,j,1} &= \sigma_{i,j} \Delta x_i \Delta y_{J} \left(1 - c_{i,j}\right) + D_{o,x}^{+,J} + D_{o,x}^{-,J} + D_{o,y}^{+,J} + D_{o,y}^{-,J} + \\
&\quad + 2P_{o,xy}^{+,J} + 2P_{o,xy}^{+,J} \\
P_{i,j,i+1,J} &= -D_{o,x}^{+,J} \\
P_{i,j,i-1,J} &= -D_{o,x}^{-,J} \\
P_{i,j,i,J-1} &= -D_{o,x}^{+,J} \\
P_{i,j,i,J-1} &= -D_{o,xy}^{-,J} \\
P_{i,j,i+1,J} &= -D_{o,xy}^{+,J}
\end{align*}
\] (7.112)
\[ i = 1; j = 2, \ldots, J - 1 \]

\[
P_{1,j,1,j} = \sigma_{1,j} \Delta x_i \Delta y_j \left( 1 - c_{1,j} \right) + D_{\beta,x}^{1,j} + D_{\beta,x}^{-1,j} + D_{\beta,y}^{1,j} + D_{\beta,y}^{-1,j} + 2P_{o,x}^{1,j} + 2P_{o,x}^{-1,j}
\]

\[
P_{1,j,2,j} = -D_{o,x}^{1,j}
\]

\[
P_{1,j,1,j+1} = -D_{o,y}^{1,j+1}
\]

\[
P_{1,j,1,j-1} = -D_{o,y}^{-1,j}
\]

\[
P_{1,j,2,j-1} = -P_{o,y}^{1,j-1}
\]

\[
P_{1,j,2,j+1} = -P_{o,y}^{1,j+1}
\]

\[ i = I; j = 2, \ldots, J - 1 \]

\[
P_{I,j,I,j} = \sigma_{I,j} \Delta x_i \Delta y_j \left( 1 - c_{I,j} \right) + D_{\beta,x}^{I,j} + D_{\beta,x}^{-I,j} + D_{\beta,y}^{I,j} + D_{\beta,y}^{-I,j} + 2P_{o,x}^{I,j} + 2P_{o,x}^{-I,j}
\]

\[
P_{I,j,I-1,j} = -D_{o,x}^{I,j}
\]

\[
P_{I,j,I,j+1} = -D_{o,y}^{I,j+1}
\]

\[
P_{I,j,I,j-1} = -D_{o,y}^{-I,j}
\]

\[
P_{I,j,I-1,j-1} = -P_{o,y}^{I,j-1}
\]

\[
P_{I,j,I-1,j+1} = -P_{o,y}^{I,j+1}
\]

Finally, the recipe for constructing the diagonal \( C \) matrix is the same as in Eq. (7.24).

In view of Eq. (7.104), the results for the homogeneous case are the same as those obtained for the AP scheme for the sequence of meshes considered in Table 7.1, for the estimate of the spectral radius, and in Table 7.2 for the number of iterations, for the same choice of the homogeneous problem’s parameters. In fact, for a homogeneous configuration the APB scheme reduces to the traditional AP scheme.
The $L_2$ estimates of the spectral radius obtained from the AP2 code for increasing mesh size with vacuum boundary conditions are contrasted with the values predicted from the Fourier analysis for the model problem in Table 7.7. The convergence criterion for the spectral radius is $\epsilon_\rho = 1 \times 10^{-5}$ and the pre-set maximum number of iterations is 500.

Table 7.7: Spectral radius of APB for a PHI configuration ($c_K = c_N = 0.99999999$).

<table>
<thead>
<tr>
<th>$I \times J$</th>
<th>$10^0$</th>
<th>$10^1$</th>
<th>$10^2$</th>
<th>$10^3$</th>
<th>$10^4$</th>
<th>$10^5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10x10</td>
<td>0.103</td>
<td>0.413</td>
<td>0.481</td>
<td>0.488</td>
<td>0.489</td>
<td>0.488</td>
</tr>
<tr>
<td>20x20</td>
<td>0.117</td>
<td>0.452</td>
<td>0.519</td>
<td>0.527</td>
<td>0.528</td>
<td>0.527</td>
</tr>
<tr>
<td>40x40</td>
<td>0.123</td>
<td>0.470</td>
<td>0.534</td>
<td>0.542</td>
<td>0.543</td>
<td>0.542</td>
</tr>
<tr>
<td>80x80</td>
<td>0.124</td>
<td>0.470</td>
<td>0.539</td>
<td>0.547</td>
<td>0.548</td>
<td>0.547</td>
</tr>
<tr>
<td>160x160</td>
<td>0.124</td>
<td>0.470</td>
<td>0.540</td>
<td>0.548</td>
<td>0.549</td>
<td>0.548</td>
</tr>
<tr>
<td>Fourier</td>
<td>0.125</td>
<td>0.471</td>
<td>0.541</td>
<td>0.549</td>
<td>0.550</td>
<td>0.549</td>
</tr>
</tbody>
</table>

The number of iterations consumed to reach convergence of the scalar fluxes for the same problem driven by a unit fixed source in all computational cells is reported in Table 7.8. The scalar fluxes are converged with a convergence criterion $\epsilon_\phi = 10^{-5}$ and a pre-set maximum number of iterations equal to 50.

While the traditional AP scheme did not converge for $\Delta > 10^2$, as evident from Table 7.4, convergence has been restored for the same model problem with the APB scheme, as indicated by the results in Table 7.8. Thus, it is verified that amending the traditional AP formalism to account for cross-derivative coupling has resulted in a novel acceleration scheme that is more resilient to adverse material discontinuity for the model problem considered within the PHI configuration.
Table 7.8: Number of APB iterations for a PHI configuration ($c_K = c_N = 0.99999999$).

<table>
<thead>
<tr>
<th>$I \times J$</th>
<th>$10^0$</th>
<th>$10^1$</th>
<th>$10^2$</th>
<th>$10^3$</th>
<th>$10^4$</th>
<th>$10^5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10×10</td>
<td>5</td>
<td>13</td>
<td>14</td>
<td>14</td>
<td>14</td>
<td>14</td>
</tr>
<tr>
<td>20×20</td>
<td>5</td>
<td>14</td>
<td>15</td>
<td>16</td>
<td>16</td>
<td>16</td>
</tr>
<tr>
<td>40×40</td>
<td>5</td>
<td>15</td>
<td>16</td>
<td>16</td>
<td>16</td>
<td>16</td>
</tr>
<tr>
<td>80×80</td>
<td>5</td>
<td>15</td>
<td>17</td>
<td>17</td>
<td>17</td>
<td>17</td>
</tr>
<tr>
<td>160×160</td>
<td>5</td>
<td>15</td>
<td>17</td>
<td>17</td>
<td>17</td>
<td>17</td>
</tr>
</tbody>
</table>

7.8 Conclusion

A study of the asymptotic properties of the integral transport matrix $B$ has been conducted for a new scaling of the Periodic Horizontal Interface (PHI) configuration defined in Sec. 7.1, in order to gain a basic understanding of the mechanisms that lead to the degradation of the spectral properties of the two-dimensional AP acceleration scheme observed in the PHI configuration with increasing material discontinuity. As illustrated in Sec. 7.2, by performing a Fourier analysis of the AP acceleration scheme for the PHI configuration and by numerical testing, the degradation of the spectral properties of the AP accelerated iterations manifests itself as a loss of unconditional robustness. In Sec. 7.3 it has also been shown that the error eigenmodes for the iteration residuals of the scalar flux that are responsible for the loss of unconditional stability of the AP acceleration scheme are high frequency longitudinal modes, namely in the $x$ direction, sustained by two thick and thin adjacent layers in the PHI configuration.
The results of the asymptotic analysis conducted in Sec. 7.4 for the matrix elements of the B matrix have confirmed that elements outside the five-banded block of the integral transport matrix are not negligible in the asymptotic limit considered for the PHI configuration. In particular cross-derivative coupling of a cell in a thin layer with its diagonal neighbors is of the same order in the scaling parameter $\Delta$ as the self-coupling and coupling with the Cartesian neighbors. Only cross-derivative coupling between two adjacent layers can account for high frequency longitudinal modes but the diffusive AP preconditioner ignores cross-derivative coupling *tout court*. Therefore, the findings of the spectral analysis combined with those of the asymptotic analysis sustain the conjecture that prompted this research effort, namely that the crisis of the two-dimensional AP preconditioner is due to a structural deficiency of this low-order approximation of the discrete integral transport operator.

In Sec. 7.5, it was also conjectured that amending the AP formalism to account for cross-derivative coupling could result in an acceleration scheme more resilient to adverse material discontinuities. In order to verify this proposition, an extension of the AP formalism has been suggested in Sec. 7.6 amounting to a nine-point stencil preconditioner that accounts for coupling of a cell’s average flux to its first diagonal neighbors. In particular, the additional elements in the stencil pertaining to cross-derivative coupling have been constructed utilizing the elements of the integral transport matrix pertaining to coupling of a cell’s average flux with its first diagonal neighbors, appropriately scaled. For this reason, the novel acceleration scheme has been denominated APB.
Preliminary results of the Fourier analysis for the APB acceleration scheme, for the same model problem considered at the beginning of the chapter to illustrate the crisis of the AP acceleration scheme in the PHI configuration, have confirmed a significant improvement in the spectral properties of the novel acceleration scheme. Specifically, robustness of the accelerated iterations has been restored for the PHI configuration. The predictions of the Fourier analysis have also been verified by the numerical results obtained by the implementation of the APB formalism in a two-dimensional transport code to test the novel acceleration scheme.

While further testing is required to assess potential limitations of the novel acceleration scheme for a wider range of parameters, and further research is needed to generalize the APB formalism and optimize the additional preconditioner elements, the results presented in this chapter constitute a first encouraging step in the quest for extended low-order approximations of the integral transport operator, unconstrained by the diffusion paradigm, that are more resilient to adverse material discontinuities in multi-dimensional geometry.
Chapter 8

Concluding Discussion

8.1 Summary of Work

The objective of this work was to derive expressions for the elements of the matrix representing a certain angular ($S_N$) and spatial discretized form of the neutron integral transport operator. The asymptotic properties of these elements have then been investigated in homogeneous and periodically heterogeneous limits in one-dimensional and two-dimensional geometries. The objective of the asymptotic study conducted in one-dimensional (or slab) geometry was to obtain further insight into the excellent convergence properties displayed by a notable class of diffusion-based acceleration schemes for the iterative solution of neutral particle transport problems, namely the one-dimensional Adjacent-cell Preconditioner (AP) acceleration scheme. The latter has proven to be highly effective not only for homogeneous model problems but also for heterogeneous slabs with unbounded material discontinuities, of which periodically heterogeneous slabs represent a notable example. The objective of the asymptotic analysis for two-dimensional configurations was to gain a basic understanding of the mechanisms that lead to degradation of the excellent spectral properties displayed by the two-dimensional AP acceleration scheme for homogeneous model problems when the same scheme is employed in the solution of two-dimensional periodically heterogeneous
configurations with unbounded material discontinuities. Specifically, it was desired to test the conjecture that while the one-dimensional AP preconditioner represents a valid approximation of the discrete integral transport operator both for homogeneous and periodically heterogeneous slabs, the two-dimensional AP preconditioner maintains this property for homogeneous configurations but loses it for periodically heterogeneous structures. In particular, it was conjectured that the crisis of the AP formalism in two-dimensional periodically heterogeneous problems depends on the fact that the diffusion-based AP preconditioner ignores cross-derivative coupling, i.e. coupling of a cell’s average flux to that of its diagonal neighbors. It was also conjectured that amending the AP formalism to account for cross-derivative coupling had the potential to improve the spectral properties of the amended acceleration scheme, by producing a scheme that is more resilient in the presence of unbounded material discontinuities in two-dimensional periodically heterogeneous problems. The above conjectures have been investigated in the chapters of this thesis as follows.

The most basic scheme for the iterative solution of neutral particle transport problems, namely Source Iteration (SI), was detailed in Ch. 1 along with synthetic acceleration methods devised to speed-up the convergence of SI. This chapter served the purpose of stressing the fact that the preconditioners employed in synthetic acceleration schemes, for the determination of the scalar flux variable, can be identified as low-order approximations of the integral transport operator. Hence the main purpose of Ch. 1 was to elaborate the intimate connection between study of the properties of the $S_N$–equivalent integral transport discrete operator, the $B$ matrix, and the iterative acceleration of neutral particle transport methods. The other purpose of this introductory chapter was to review
the AHOT-N0 spatial approximation and to give an outline for the remainder of the thesis by reviewing the main results obtained in one- and two-dimensional geometry.

A review of the literature relevant to this work was given in Ch. 2 with the dual intent of illustrating the historical background that has led to this research effort and of indicating the potential connections of this work with other areas of current active research in computational methods for neutral particle transport.

Exact analytic expressions for the elements of the integral transport matrix were derived for one-dimensional geometry in Ch. 3. The asymptotic properties of these elements as a function of computational-cell size were then investigated for homogeneous, uniform-mesh slabs in the thick cell limit and in the thin cell limit. The results obtained in the thick cell limit prove that the $B$ matrix acquires a tridiagonally dominated structure characterized by a diffusion-like coupling stencil. Interestingly enough, in slab geometry the $B$ matrix displays this asymptotic behavior at a fast exponential rate, manifested by the exponential vanishing of the elements beyond the first off-diagonal with increasing cell thickness. The exponential nature of this convergence is strictly related to the AHOT-N0 spatial discretization utilized in the analysis and does not extend to other WDD discretization schemes. It is also characteristic of this spatial discretization in slab geometry, since it does not carry over to multi-dimensional geometry. In contrast, in the thin limit the $B$ matrix acquires a diagonally dominated structure that is approached at a much slower linear rate that is identical for all the off-diagonal elements. Notwithstanding, it was shown that it is possible to identify an exact algebraic manipulation that transforms $B$ into a matrix that acquires a diagonally dominated structure at a faster quadratic rate in the thin cell limit.
The study of the asymptotic properties of the integral transport matrix was extended to periodically heterogeneous slabs in Ch. 4. Specifically, the asymptotic limit considered is one in which the heterogeneity in the optical properties of adjacent computational cells is progressively pushed apart, i.e. the thick cells are made thicker while the thin are made thinner at a prescribed rate. In this asymptotic limit it was shown that the discrete integral transport operator is approximated by a sparse matrix characterized by a pentadiagonal structure. This result confirms physical intuition, suggesting that the coupling between two optically thick cells, separated by an interposed thin cell, should be strong. It was also used to obtain an analytical derivation of some notable asymptotic properties displayed by the numerically computed cell-averaged scalar fluxes for periodically heterogeneous slabs. However, as it was shown in the last part of Ch. 4, the matrix representing the integral transport operator is also amenable to algebraic transformations that lead to a matrix representation that asymptotically approaches a tridiagonal structure in the limit of interest. Also, the algebraic transformations considered ensure that, like for the case of a homogeneous slab, the tridiagonal structure is approached at a fast exponential rate even for the periodically heterogeneous configuration considered. The latter results contribute to the basic understanding of the excellent convergence properties of acceleration methods for the neutron transport equation based on cell-centered preconditioners characterized by a diffusion-like coupling stencil even for the case of heterogeneous slabs. In fact, deterioration of the convergence properties of these acceleration schemes has been widely observed in the presence of sharp material discontinuities in multi-dimensional problems but not in one-dimensional problems. In this connection, the results presented
in Ch. 4 point to the existence of a low-order approximation to the full discrete integral transport operator characterized by a tridiagonal structure even in the case of a periodically heterogeneous slab.

The results of the structural analysis of the integral transport matrix obtained in the previous two chapters were then used in Ch. 5 to provide insight into the excellent convergence properties of diffusion-based acceleration schemes in one-dimensional transport problems. More specifically, the acceleration scheme analyzed in Ch. 5 is that based on the Adjacent-cell Preconditioner (AP) formalism. The results of this comparison indicated that the AP preconditioner is asymptotically capable of exactly capturing the structure acquired by the integral transport matrix in all the limits in which the latter acquires a diffusive structure, namely homogeneous slabs and periodically heterogeneous slabs in which both the thick and the thin layers host a purely scattering material. This comes as no surprise considering that the AP preconditioner is inherently constructed to be a diffusive matrix, while the integral transport matrix acquires in general a non-diffusive stencil for periodically heterogeneous slabs containing absorbing materials. The previous results provide an understanding of the immediate convergence behavior, namely convergence in two iterations, displayed by the AP acceleration scheme in the asymptotic limit for slabs hosting purely scattering materials, both in the homogeneous and periodically heterogeneous cases. For periodically heterogeneous slabs containing absorbing materials, immediate convergence has been restored by amending the recipe for the construction of the AP matrix so that the correct asymptotic structure of the integral transport matrix is matched by the AP preconditioner in the asymptotic limit.
The study of the asymptotic properties of the integral transport matrix was extended to homogeneous configurations in two-dimensional geometry in Ch. 6. First, exact analytic expressions were derived for the elements of the $B$ matrix that couple the cell-averaged scalar flux in a cell with itself (self-coupling) and with the cell-averaged scalar fluxes in the first and second neighboring cells, with reference to a three-by-three two-dimensional Cartesian sub-mesh. This spatial mesh represents a simple setting for the construction effort, yet it also contains all the elements of interest in the analysis. As pointed out earlier, it was desired to investigate the strength of coupling of the cell-averaged scalar flux in a cell with the scalar fluxes in its first diagonal neighbors (cross-derivative coupling) and to contrast it with the strength of coupling with the scalar fluxes in its cell’s first Cartesian neighbors. The asymptotic limits of interest for homogeneous, uniform-mesh two-dimensional configurations are a thick cell diffusive limit and a thin cell limit. For both limits, exact asymptotic expressions were obtained for the elements of the integral transport matrix coupling a cell-averaged scalar flux with the fluxes in neighboring cells up to the second neighbors. For cells beyond second neighbors, estimates were obtained for the leading asymptotic order of the matrix elements relative to the cells’ optical thickness. The asymptotic estimates were also verified by numerical tests. The results obtained in the thick cell limit for homogeneous configurations show that elements pertaining to self-coupling and coupling with the first Cartesian neighbors are of the same order, satisfy a diffusion-like coupling stencil and dominate all other matrix elements in the optically thick cell limit. In particular, cross-derivative coupling with the first diagonal neighbors is of higher-order in the cell optical thickness. The existence of this low-order five-banded approximation of the integral transport matrix
points to a strong local coupling of a cell with its first Cartesian neighbors. It also provides further insight into the excellent convergence properties of diffusion-based acceleration schemes in two-dimensional homogeneous configurations characterized by low absorption, in the optically thick cell limit. Finally, the results obtained in the thin cell limit for homogeneous configurations indicate that the $B$ matrix acquires a diagonally dominated structure. In fact, similar to what was pointed out for the one-dimensional case, the integral transport matrix approaches the identity matrix $I$ in this asymptotic limit. Also, the matrix elements outside the diagonal stripe have, in general, the same asymptotic behavior. In contrast to the one-dimensional case, though, the coefficient of the leading order contribution is not the same for all the off-diagonal elements.

Finally, a study of the asymptotic properties of the integral transport matrix $B$ was conducted in Ch. 7 via a new asymptotic scaling of the uniform-mesh Periodic Horizontal Interface (PHI) configuration as proposed in Sec. 7.1. The objective of this study was to gain a basic understanding of the mechanisms that lead to the degradation of the spectral properties of the two-dimensional AP acceleration scheme observed in the PHI configuration for asymptotically increasing material discontinuity. For the proposed scaling, it was verified, by performing a Fourier analysis for the AP acceleration scheme for the PHI configuration and by numerical testing, that the degradation of the spectral properties of the AP accelerated iterations manifests itself as a loss of unconditional robustness. It was also verified that the error eigenmodes of the iteration residuals of the scalar flux that are responsible for the loss of unconditional stability of the AP acceleration scheme are high frequency longitudinal modes, namely in the $x$ direction, sustained by two thick and thin adjacent layers in the PHI configuration. The results of
the asymptotic analysis conducted for the elements of the $B$ matrix have confirmed that elements outside the five-banded block of the integral transport matrix are not negligible in the asymptotic limit considered for the PHI configuration. In particular, cross-derivative coupling of a cell in a thin layer with its diagonal neighbors appears to be of the same order as self-coupling and coupling with the Cartesian neighbors. Only cross-derivative coupling between two adjacent layers can account for high frequency longitudinal modes, yet the diffusive AP preconditioner ignores cross-derivative coupling 
*tout court*. Therefore, the findings of the spectral analysis combined with those of the asymptotic analysis sustain the conjecture that prompted this research effort, namely that the crisis of the two-dimensional AP preconditioner is due to a structural deficiency of this low-order approximation of the discrete integral transport operator. It was also conjectured that amending the AP formalism to account for cross-derivative coupling could result in an acceleration scheme more resilient to adverse material discontinuities.

In order to verify this intuition, an extension of the AP formalism has been proposed by constructing a nine-point stencil preconditioner that accounts for coupling of a cell’s average flux with its first diagonal neighbors. In particular, the additional elements in the stencil pertaining to cross-derivative coupling were constructed utilizing the elements of the integral transport matrix pertaining to coupling of a cell’s average flux with its first diagonal neighbors. For this reason, the novel acceleration scheme was denominated APB. Preliminary results of the Fourier analysis for the APB acceleration scheme confirmed a significant improvement in the spectral properties of the novel acceleration scheme. Specifically, robustness of the accelerated iterations has been restored for the PHI configuration. The predictions of the Fourier analysis were also verified by the
numerical results obtained by the implementation of the APB formalism in a two-dimensional transport code for the testing of the novel acceleration scheme.

A summary of some fundamental conclusions that descend from the previous findings is given in the next section. Finally, suggestions for possible avenues of research to be investigated in future work are delineated in Sec. 8.3.

8.2 Conclusions

The results of this research have shown that in one-dimensional problems, both homogeneous and periodically heterogeneous, and in homogeneous two-dimensional problems containing optically thick cells, the discrete integral transport operator acquires a sparse matrix structure, implying a strong local coupling of a cell-averaged scalar flux only with its nearest Cartesian neighbors. These results provide further insight into the excellent convergence properties of diffusion-based acceleration schemes for this broad class of transport problems. In particular, they explain why the deterioration of the convergence properties of diffusion-based acceleration schemes, widely observed in the presence of sharp material discontinuities in multi-dimensional problems, has never been encountered in one-dimensional problems. In contrast, the results of the asymptotic analysis for two-dimensional periodically heterogeneous problems point, in general, to a sparse but non-local matrix structure due to a strong long-range coupling of a cell’s average flux with its neighboring cells, independent of the distance between the named cells within the mesh. In particular, the latter results have confirmed the conjecture that cross-derivative coupling of a cell’s average flux with its diagonal neighbors, while
negligible in the homogeneous case, plays a fundamental role in the two-dimensional periodically heterogeneous case. In fact, cross-derivative coupling appears instrumental in determining the mechanisms involved in the loss of robustness of diffusion-based acceleration schemes in the presence of sharp material discontinuities in multi-dimensional problems. Finally, the results of the asymptotic analysis have been employed to amend the structure of the diffusive cell-centered Adjacent-cell Preconditioner (AP) to account for cross-derivative coupling by including elements, outside the diffusive stencil, that couple a cell’s average flux with its first diagonal neighbors. Preliminary results of the Fourier analysis conducted for the novel acceleration scheme show that robustness is regained for the amended preconditioner. The new acceleration scheme has also been implemented in a two-dimensional transport code and numerical results from the code have successfully verified the predictions of the Fourier analysis. The latter findings appear encouraging in the quest for extended low-order operators, unconstrained by the diffusive approximation, that are more resilient to adverse material-discontinuity effects in multi-dimensional problems.

8.3 Suggestions for Future Work

There are many avenues along which future research could proceed from this work. They are outlined in the following paragraphs.

**Integral transport matrix in one-dimensional geometry**: for the AHOT-N0 spatial discretization considered in this work it is desirable to extend the results of the
asymptotic analysis from uniform meshes to non-uniform meshes. In particular, for the homogeneous thin cell limit it is worthwhile investigating whether it is possible or not to extend the transformation of the integral transport matrix that led to a diagonally dominated equivalent matrix to within $O(\delta^2)$ off-diagonal elements for the uniform-mesh case, see Sec. 3.6, to the case of non-uniform meshes. It is stressed that the thin cell limit that was studied in Ch. 3 is also a thin slab limit that favors leakage for any finite mesh configuration. There exists another thin cell limit, corresponding for example to the problem of mesh refinement, which is not necessarily a thin slab limit. The computational cells become thinner and thinner, but the domain does not and leakage is not favored by the scaling. As illustrated in Appendix A, mesh refinement implies a sequence of meshes and matrices of increasing size that corresponds to an asymptotic limit in which both the computational cell width $\delta$ and the number of computational cells $J$ are scaled simultaneously. A proper formalization of this asymptotic limit may be helpful in understanding the effect of having thin computational cells in a thick domain, and to reconcile results from the spectral analysis for thin cells with results of the asymptotic structural analysis, in the limit as $J \rightarrow \infty$.

The study of the asymptotic properties of the integral transport matrix can prove useful in determining the accuracy of various spatial discretizations. In this respect, it is stressed that the overall effort in this research has been directed to the acceleration of iterative methods, regardless of accuracy of the spatial discretization considered. Even though the question of the exactness of the solution an iterative method would converge to, especially in the presence of very thick cells, has to be addressed, as far as the pure
acceleration issue is concerned, a method that would allow a fast rate of convergence regardless of solution accuracy, or lack thereof, is nonetheless highly valuable. It is noted that the discrete $S_N$–equivalent integral transport operator studied here is also WDD equivalent, from a spatial discretization point of view. Of course, the fully discretized $S_N$–equivalent integral transport operator is as accurate as the spatial discretization is accurate. WDD methods have been considered to ease the effort of setting up a formalism for the construction of the elements of the integral transport matrix. Fewer variables are involved with respect to higher-order nodal methods or to Finite Element Methods (FEM) and advantage can be taken of the continuity condition for the discrete ordinate angular fluxes across cell interfaces. But WDD methods, especially the AHOT-N0 considered in this research, are in general not accurate in problems with optically thick computational cells. For example, the AHOT-N0 does not possess the traditional Thick Diffusion Limit [24]. This can be verified by repeating the asymptotic analysis of the $A$ and $B$ matrices in the Thick Diffusion Limit and was verified by computing the cell-averaged scalar fluxes via Eq. (1.27) in this limit [45]. Hence, the construction and study of the asymptotic properties of the elements of the $S_N$–equivalent integral transport matrix corresponding to a certain spatial discretization can be a tool in the development and study of that spatial discretization. In this connection, it appears interesting to extend the construction effort for the integral transport matrix to other more accurate spatial discretizations, such as for example the Linear Discontinuous Finite Element Method (LDFEM) [21]. For the latter spatial discretization, the variables of interest are the projections of the scalar flux over
the basis functions defined for each computational cell. The continuity condition is no longer available, but “upwind” conditions are.

The interest in the extension of the $A$ and $B$ matrices formalism to other spatial discretizations is also due to the potential they offer to compute accurate benchmarking solutions. In fact, the availability of $A$ and $B$ (or, ultimately of the Jacobian $J$) allows the direct computation of the cell-averaged scalar fluxes via Eq. (1.27). The latter represents a useful tool as a means to build accurate solutions only affected by truncation and round-off errors, but no iteration errors, to test acceleration methods before developing such acceleration methods. Since a reference solution needs only be built once, the overhead related to building and storing the Jacobian matrix may be justified.

**Integral transport matrix in two-dimensional geometry:** a still open issue in two-dimensional geometry is obtaining general closed analytic expressions for all the element of the integral transport matrix. Further research is needed to solve this topological (individuation of all possible transport paths) and combinatorial (counting of the $\gamma$ coefficients) problem. We believe that the elements of the integral transport matrix can be obtained as some sort of multinomial distribution in the $\gamma$ coefficients.

For the AHOT-N0 spatial discretization it is desirable to extend the results of the asymptotic analysis to the case of non-uniform spatial meshes. What was pointed out for the case of one-dimensional geometry in terms of study of the accuracy of spatial discretization and computation of benchmark solutions via the integral transport matrix applies also to two-dimensional geometry. As far as the latter point is concerned, it is desirable to extend the formulation of the “No Sweep” algorithm to other types of spatial
discretization. The extension to higher-order nodal methods was already envisioned in [40]. The extension to FEM methods, such as the Bi-Linear Discontinuous Finite Element Method (BLDFEM) [46] appears also important due to the current interest in the application of FEM in the realm of computational particle transport. In this connection it is noted that, the availability of new computer architectures for massively parallel computations in the near future, may disclose new frontiers for transport methods based on direct solution techniques, possibly also based on the integral transport matrix.

**APB acceleration scheme:** as far as the APB acceleration scheme proposed in Ch. 7 is concerned, it will be necessary to ascertain its validity and the existence of potential limitations over a wider range of parameters than the model problem for the PHI configuration considered in Ch. 7. The testing will also need to explore other types of heterogeneous configurations. In the presence of possible limitations it is suggested to consider possible generalizations of the recipe that was proposed for the construction of the elements pertaining to cross-derivative coupling, or a new recipe altogether. It will also be necessary to derive in a rigorous fashion the vacuum (and other) boundary conditions for the nine-point stencil APB preconditioner. Even if the recipe proposed in Ch. 7 based on numerical testing is correct, still a rigorous justification is needed. It was noted that the APB preconditioner looks like a hybrid diffusion-transport operator. Is the incorporation of elements of the integral transport operator just an expedient approach or is there something more profound to be investigated from a theoretical point of view? Also, could this be the key to extend the current methodology to other diffusion-based acceleration schemes, notably DSA?
Development of other acceleration schemes that incorporate cross-derivative coupling: a Fourier analysis has been developed for the PHI configuration and coded in symbolic and numeric form using *Mathematica*, see Appendix B. Since the Fourier analysis allows obtaining the Jacobian matrix $J$, the $B$ matrix is also available. This opens the opportunity to build “from scratch” novel synthetic acceleration schemes based on a nine-point stencil matrix. For example, the eight elements of the preconditioner are all left unspecified in the Fourier analysis for PHI and expressions are sought for them that match the coefficients of as many powers as possible in a power expansion in $r$ and $s$ of the elements of $B$ centered around $r = s = 0$ (flat mode) or around $s = 0$ and $r = \pi / 2$ (high frequency longitudinal modes). Even better, again leaving the eight elements unspecified, the procedure that led to the AP formalism is repeated. Specifically, it can be tried to find an expression for the spectral radius for the novel acceleration scheme as a function of $r$ and $s$, and of the unspecified elements of the preconditioner. The spectral radius is then expanded in $r$ and $s$ and the elements of the preconditioner are determined to zero out as many coefficients in the frequency expansion as possible.

The objective of this analysis would be to ascertain if it is possible to obtain better spectral properties than the APB acceleration scheme in the asymptotic limit for the PHI configuration. In this connection, some fundamental questions arise. Is it possible to bring the spectral radius down to zero in the asymptotic limit for PHI, as it was for the homogeneous thick cell limit? Or is the long-range coupling characteristic of the PHI configuration an inherent limitation? Is it then possible to lump the elements coupling a cell with an entire layer of PHI in a single equivalent cell? If lumping is not possible, can sparse but non-local (non-banded) preconditioners be considered? Even in this case, the
wide availability of new computer architectures for massively parallel computations in the near future may disclose new frontiers for the construction, storage and inversion of such preconditioners.

Finally it is recommended to extend the scope of this research to evaluate the potential of these novel extended preconditioners in multi-level preconditioning techniques, where Transport Synthetic Acceleration (TSA) [47] is typically used as a first preconditioning stage, employed in the realm of Krylov subspace techniques. As it was discussed in Ch. 2, Krylov iterative methods have been shown to improve convergence for heterogeneous multi-dimensional configurations in the presence of material discontinuities [9,34]. They are also currently investigated in the development of parallel algorithms for the solution of the transport equation [48].
Appendix A

Alternative Scaling for the PHI Configuration

A.1 Introduction

We perform an asymptotic analysis on the integral transport matrix in a limit of the Periodic Horizontal Interface (PHI) configuration wherein the cell height in both layers approaches 0 like $\Delta^{-2}$ while the total cross-section vanishes like $\Delta^{-1}$ in the thin (N) layer and diverges like $\Delta$ in the thick (K) layer, as $\Delta \to \infty$, see Fig. 7.1. In such limit we prove that the full integral transport operator acquires an asymptotically dominant diagonal matrix structure markedly different from a diffusive operator. We use this result to explain the apparent contradiction of earlier numerical results and analysis. Specifically, it will be shown that while the above limit of the PHI configuration, originally selected in [10], is conceptually acceptable for devising a neutral particle transport problem for which there exists no preconditioner with a cell-centered diffusion coupling stencil that is unconditionally stable and robust, it is not relevant from an application standpoint. As a matter of fact, the conclusion of the earlier Fourier analysis holds only for an infinite number of PHI layers where there is no leakage. For any finite extent configuration the height of the problem domain will become thinner as $\Delta \to \infty$, causing leakage losses to dominate the spectral properties thus producing rapid convergence of the SI or AP iterations.
An outline of the appendix follows. A summary of the results of the Fourier analysis for the alternative scaling of the PHI configuration is given in Sec. A.2. The results of the asymptotic analysis of the integral transport matrix obtained for this alternative scaling are presented in Sec. A.3. The apparent contradiction deriving from the comparison of the results from the asymptotic analysis with those from the Fourier analysis is reconciled in Secs. A.4 and A.5. Some concluding remarks are discussed in Sec. A.6.

A.2 Summary of Results of the Fourier Analysis

A Fourier analysis was performed in [10] for the scaling of the PHI configuration considered in this appendix. For brevity, in the remainder of the appendix this scaling will be referred to as the JCP scaling, since [10] originally appeared in the *Journal of Computational Physics*. The main findings of the Fourier analysis are summarized in the following.

It is an easy matter to implement the JCP scaling in the *Mathematica* notebook, see Appendix B, that was developed to perform the Fourier analysis for the AP acceleration scheme for the scaling of the PHI configuration studied in Ch. 7. It is in fact only necessary to scale $\Delta y$ as $\delta_y \Delta^{-2}$, in addition to the usual scaling for the total cross-sections. The result presented in Fig. A.1 refers to the case of the $S_0$ level symmetric quadrature of equal weights, and to the following choice of problem parameters: $\delta_x = \delta_y = 1$, $\sigma_\kappa = \sigma_N = 1$, $c_\kappa = c_N = 0.9999$. The plot in Fig. A.1 is similar to the one
presented in Fig. 7.5, and illustrates the loss of unconditional robustness of the AP scheme when applied to the JCP scaling of the PHI configuration. It is noted that the JCP scaling produces a steeper increase in the spectral radius than the scaling considered in Ch. 7. Therefore, the crisis of the AP formalism occurs at lower values of the scaling parameter $\Delta$ for the JCP scaling.

![Graph showing spectral radius of AP for the JCP scaling of the PHI configuration with $c_K = c_N = 0.9999$.]

Fig. A.1: Spectral radius of AP for the JCP scaling of the PHI configuration with $c_K = c_N = 0.9999$.

It was proven in [10] that the offending error modes that are responsible for the loss of robustness of the AP formalism for the JCP scaling are modes that are nearly flat in the $y$ direction, $s \sim 0$, and characterized by a high frequency in the $x$ direction, $r \sim \pi/2$. By way of comparison with the results presented in Fig. 7.7 and in Table 7.5
for the scaling of the PHI configuration considered in Ch. 7, similar results have been obtained for the JCP scaling in Fig. A.2 and in Table A.1, respectively.

The results in Fig. A.2 and in Table A.1 confirm that the JCP scaling of the PHI configuration is extremely effective in producing the crisis of the AP acceleration scheme, already for longitudinal modes of lower frequency than those required by the scaling considered in Ch. 7. This is evident comparing the maximum eigenvalue obtained for the 6×2 PHI configuration with periodic boundary conditions on all four sides for the two different scaling options, in Tables 7.5 and A.1, respectively.

Fig. A.2: Maximum eigenvalue of AP for a 6×6 and a 6×2 PHI configurations with periodic boundary conditions for the JCP scaling ($c_k = c_N = 0.9999$).
Table A.1: Maximum eigenvalue of $AP$ for longitudinal modes of increasing frequency for the JCP scaling of PHI.

<table>
<thead>
<tr>
<th></th>
<th>6×2</th>
<th>10×2</th>
<th>15×2</th>
<th>20×2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max</td>
<td>0.9996</td>
<td>0.9996</td>
<td>0.9996</td>
<td>0.9996</td>
</tr>
<tr>
<td>Eigenvalue</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

A.3 Asymptotic Analysis of the Integral Transport Matrix

Exact analytic expressions were derived in Sec. 6.3 for the elements of the $B$ matrix coupling a cell’s average flux in cell $(i, j)$ with the fluxes in its neighboring cells up to the second neighbors. With reference to the PHI configuration sketched in Fig. 7.1, for $j$ even the cell is in a K layer as indicated in Fig. 7.9.

The general expressions for the $B$ matrix elements in Eqs. (6.36) through (6.41) are evaluated for the material properties of the K and N layers in the PHI configuration, expressing them in terms of the configuration’s parameters, and studied in the limit as $\Delta \to \infty$ for the JCP scaling of the PHI configuration. The results of the asymptotic analysis obtained for the $B$ matrix elements pertaining to a cell $(i, j)$ in a K layer are summarized in Fig. A.3, for cell $(1, 2)$. As done in Chs. 6 and 7, the estimates of the strength of coupling of a thick cell’s average scalar flux with the neighbors beyond second are based on the leading order of the $\gamma$ coefficients for the two layers and on numerical studies.
In Fig. A.4 we present the behavior of the $B$ matrix elements pertaining to coupling of a K cell’s average flux with up to the second neighbors computed with the NS code, for an $S_6$ level symmetric quadrature with equal weights and the following choice of parameters: $\delta_x = \delta_y = 1$, $\sigma_K = \sigma_N = 1$, $c_K = c_N = 1$. The $B$ matrix elements approach the theoretically predicted asymptotes for values of $\Delta$ larger than ~10, thus verifying our asymptotic analysis.

The results of the asymptotic analysis obtained for the $B$ matrix elements pertaining to a cell $(i,j)$ in an N layer, as depicted in Fig. 7.12, are summarized in Fig. A.5, for cell (1,1). In Fig. A.6 we present the behavior of the $B$ matrix elements pertaining to coupling of an N cell’s average flux with up to the second neighbors computed with the NS code, for the same choice of parameters as in Fig. A.4. In this case also, the $B$ matrix elements approach the theoretically predicted asymptotes for values of $\Delta$ larger than ~10, thus verifying our asymptotic analysis.

The results presented in the figures contained in this section indicate that the diagonal elements of the $B$ matrix are, to leading order, equal to 1 independent of a layer’s material properties. It is noted that, in contrast to the results obtained in Figs. 7.10 and 7.13, the results summarized in Figs. A.3 and A.5, for the JCP scaling, are independent of the cells’ aspect ratio. This circumstance is due to the fact that the leading terms in the asymptotic expressions for the $\gamma$ coefficients for the JCP scaling are not subject to any cancellation, as opposed to the negative sign present in the numerator of the $\gamma_{m,N}^{\mu}$ coefficients, where $\mu = x$ or $y$, for the scaling of the PHI configuration considered in Ch. 7.
Fig. A.3: Strength of coupling of a thick cell’s average flux with its neighbors for the JCP scaling of PHI.

Fig. A.4: Numerical verification of B asymptotic behavior predicted in Fig. A.3.
Fig. A.5: Strength of coupling of a thin cell’s average flux with its neighbors for the JCP scaling of PHI.

Fig. A.6: Numerical verification of B asymptotic behavior predicted in Fig. A.5.
Similar to what was observed for the scaling considered in Ch. 7, for the JCP scaling also the asymptotic behavior of the $\gamma$ coefficients, both for the case of a cell in an N layer and in a K layer, points to long-range coupling of a cell’s average flux with those in other cells, independent of the distance of the cells in the mesh. In particular, the elements coupling a cell in layer N or K to all layer K cells in the same column are $O\left(\Delta^{-1}\right)$, while all the other elements in the matrix are higher order in $\Delta$. Also, as far as the coupling of the cells in two adjacent layers is concerned, it is noted that the $O\left(\Delta^{-3}\right)$ elements of the $B$ matrix coupling a thin cell to a diagonal neighbor in the adjacent thick layer are as many as the diagonal neighbors contained in that layer. In other words, no decay is observed, along the $x$ direction, in the strength of coupling of a thin cell’s average flux with the diagonal neighbors in the adjacent thick layer. The latter observations are important for the ensuing discussion in the next section.

A.4 An Apparent Paradox Resolved

The results obtained in the previous section are summarized by the expression $B = I + O\left(\Delta^{-1}\right)$, namely $B$ acquires the diagonally dominated structure of the identity matrix $I$ in the JCP asymptotic limit for the PHI configuration. Since the $O\left(\Delta^{-1}\right)$ elements effect the coupling of a cell with all the other cells in the same column belonging to any layer containing material K, it is evident that the structure acquired by the discrete integral operator is non-diffusive.
It is pointed out that the integral transport matrix $B$ appears to approach the identity matrix $I$ in all asymptotic limits in which the computational cells in the spatial mesh are made thinner and thinner. In fact, this asymptotic behavior was also observed in Sec. 3.4.3, studying the thin cell limit for a homogeneous slab, and in Sec. 6.7, investigating the thin cell limit for a homogeneous two-dimensional configuration. In this connection, it is noted that the JCP scaling of PHI is such that the K cells are made thicker and thicker in the $x$ direction but do become thinner and thinner in the $y$ direction in the asymptotic limit, as a consequence of the $\Delta^{-2}$ scaling of $\Delta y$. Therefore, both the N and K layers are optically thin in the $y$ direction in the JCP scaling.

In order to discuss the implications of $B$ approaching $I$ from a synthetic acceleration scheme’s point of view, it is convenient to write Eqs. (1.12) and Eq. (1.18) in fully discretized form in terms of the Jacobian matrix $J$:

$$\phi^{(t+1/2)}_{i} = J \left( \phi^{(t)}_{i} + s \right) \quad \text{(A.1)}$$

$$\phi^{\infty} = \phi^{(t+1/2)} + B^{-1} J \left( \phi^{(t+1/2)} - \phi^{(t)} \right) \quad \text{(A.2)}$$

In case $I$ is used to approximate $B$ in Eq. (A.2), the resulting acceleration scheme is nothing else but SI. More specifically, in the limit $\Delta \to \infty$ in which $B$ and $I$ are coincident, Eqs. (A.1) and (A.2) state that it would be possible to obtain the limit solution $\phi^{\infty}$ in two mesh-sweeps, one for the cell-averaged scalar fluxes and one for their residuals. Therefore, immediate convergence could be obtained using SI without any need for preconditioning.
This conjecture has been verified by solving a test problem similar to the one considered in Table I of [10] but with a uniform fixed source distribution and vacuum boundary conditions on all four sides, consistent with the analysis performed in this work. Also, a wider range of values is considered for the $\Delta$ parameter to investigate the JCP asymptotic limit. Note that the scaling parameter $\Delta$ used in this work corresponds to $\sigma^{-1}$ used in [10]. The $L_2$ norm estimates of the spectral radius obtained for SI are reported in Table A.2 as a function of $\Delta$ and the number of cells in the Cartesian mesh $I \times J$, for the same choice of problem parameters as in Fig. A.1. As in Table 7.3, the last row in Table A.2 contains the results of the Fourier analysis for SI obtained for the JCP scaling of the PHI configuration. The convergence criterion for the spectral radius is $\varepsilon_\phi = 1 \times 10^{-5}$ and the pre-set maximum number of iterations is 500.

*Table A.2: Spectral radius of SI for the JCP scaling of PHI ($c_K = c_N = 0.9999$).*

<table>
<thead>
<tr>
<th>$I \times J$</th>
<th>$10^0$</th>
<th>$10^1$</th>
<th>$10^2$</th>
<th>$10^3$</th>
<th>$10^4$</th>
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<td>6.45x10^-3</td>
<td>6.48x10^-4</td>
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<tr>
<td>20x20</td>
<td>0.983</td>
<td>0.607</td>
<td>0.117</td>
<td>1.28x10^-2</td>
<td>1.30x10^-3</td>
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<tr>
<td>40x40</td>
<td>0.995</td>
<td>0.780</td>
<td>0.213</td>
<td>2.54x10^-2</td>
<td>2.59x10^-3</td>
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<tr>
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<td>0.901</td>
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<tr>
<td>160x160</td>
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<td>0.964</td>
<td>0.544</td>
<td>9.55x10^-2</td>
<td>1.03x10^-2</td>
<td>1.04x10^-3</td>
</tr>
<tr>
<td>Fourier</td>
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<td>0.999</td>
<td>0.999</td>
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</tbody>
</table>

The number of iterations consumed to reach convergence of the scalar fluxes, for the same problem driven by a unit fixed source scaled as $\Delta$ in all computational cells, is reported in Table A.3. The scalar fluxes are converged with a convergence criterion $\varepsilon_\phi = 10^{-5}$ and a pre-set maximum number of iterations equal to 50.
Notice that, for any given mesh, the spectral radius and the number of iterations decrease as \( \Delta \) increases, and eventually convergence in a few source iterations is obtained as predicted by the asymptotic analysis. The same test problem has also been solved by SI preconditioned with AP building similar tables. Again, for any given mesh, the spectral radius and number of iterations do decrease as \( \Delta \) increases and AP also converges in a few iterations in the asymptotic regime.

Table A.3: Number of SI iterations for the JCP scaling of PHI \((c_K = c_N = 0.9999)\).

<table>
<thead>
<tr>
<th>IxJ</th>
<th>(10^0)</th>
<th>(10^1)</th>
<th>(10^2)</th>
<th>(10^3)</th>
<th>(10^4)</th>
<th>(10^5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10x10</td>
<td>&gt;50</td>
<td>14</td>
<td>6</td>
<td>4</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>20x20</td>
<td>&gt;50</td>
<td>23</td>
<td>7</td>
<td>4</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>40x40</td>
<td>&gt;50</td>
<td>42</td>
<td>9</td>
<td>5</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>80x80</td>
<td>&gt;50</td>
<td>&gt;50</td>
<td>12</td>
<td>5</td>
<td>4</td>
<td>3</td>
</tr>
<tr>
<td>160x160</td>
<td>&gt;50</td>
<td>&gt;50</td>
<td>19</td>
<td>6</td>
<td>4</td>
<td>3</td>
</tr>
</tbody>
</table>

These numerical results indicate that the asymptotic limit considered in [10] for the PHI configuration, while conceptually important in devising a particle transport problem for which there exists no preconditioner with a cell-centered diffusion coupling stencil that is unconditionally stable and robust, is not relevant from an application standpoint. Since the cell height in both layers is scaled as \( \Delta^{-2} \), the entire problem height will decrease as \( \Delta \to \infty \) for any \( J < \infty \), hence the transport problem becomes leakage dominated in the \( y \) direction. This explains the decreasing spectral radius and number of iterations in each row of the SI and AP tables in spite of the analytic results obtained in [10], and summarized in Sec. A.2, indicating lack of robustness for AP in this limit. The latter observations have led to devising the new scaling for the PHI configuration.
considered in Ch. 7. As evident from the results in Tables 7.3 and 7.4, the spectral radius and the number of iterations do not decrease as $\Delta$ increases for the new scaling since the K layer is made thicker and thicker both in the $x$ and in the $y$ direction. Therefore, the new scaling does not favor leakage for any finite manifestation of the PHI configuration in the asymptotic limit of interest.

It is important to note that even though the numerical results in Tables A.2 and A.3 do not serve the purpose of numerically substantiating the thesis proved in [10], they cannot be invoked to contradict it. The proof conducted in [10] is based on an infinite medium Fourier analysis of the error modes for SI and SI preconditioned with AP. In the case of an infinite medium, the scaling considered for the PHI configuration cannot introduce any leakage in the transport problem, and the conclusions drawn in [10] hold. In particular, the spectral radius of SI for a PHI configuration with $c_K = c = c_N$ approaches $c$ and the spectral properties of SI preconditioned with AP approach those of SI, in the limit $\Delta \to \infty$. Notice that, once leakage is suppressed via the periodic boundary conditions as in the 6×6 case considered in Sec. A.2, the spectral radius (hence the number of iterations) increases as $\Delta$ is increased, consistent with the results of the Fourier analysis. Notwithstanding, an open question remains: How is it possible to reconcile the apparent paradox arising from a comparison of the results from the asymptotic analysis for the integral transport matrix in the JCP limit with those from the Fourier analysis of SI for the infinite PHI configuration?

In order to answer this question it is observed that the conclusion drawn from the asymptotic analysis of the $B$ matrix, namely that $B = I + O(\Delta^{-1})$ as $\Delta \to \infty$, is true both
for a finite and an infinite mesh. However, in the case of an infinite mesh, hence of an infinite-dimensional $B$ matrix, the approximation $B = I$ is no longer valid. As pointed out previously, the $O(\Delta^{-1})$ elements in matrix $B$ are spread out throughout the matrix due to the long-range coupling, to $O(\Delta^{-1})$, of a cell in the PHI configuration with all the other cells in the same column belonging to any layer containing material $K$. In other words, $B$ is sparse and local to $O(\Delta^0)$, while it is sparse but non-local to $O(\Delta^{-1})$. Due to this non-locality the $O(\Delta^{-1})$ terms may not be overlooked in the case of an infinite mesh, even if $\Delta \to \infty$. The role played by the $O(\Delta^{-1})$ terms in the case of an infinite mesh will be further illustrated in the next section by analyzing the similar conceptual problem of solving the linear system $[I - \Delta^{-1}F]x = r$, where $I$ is the $J \times J$ identity matrix, $F$ is the $J \times J$ matrix whose elements are all 1 and $r$ is the $J \times 1$ vector whose elements are all 1, in the double limit $\Delta, J \to \infty$.

Similar arguments can be invoked to justify why high frequency longitudinal modes are still the offending error modes for the AP acceleration scheme also for the JCP scaling of the PHI configuration. We believe that the same conjecture on the role of cross-derivative coupling that was illustrated in Sec. 7.5 holds true for the JCP scaling, in the case of an infinite medium/mesh. In this case, the sum on the right hand side of Eq. (7.89) becomes a series and though each of the terms corresponding to coupling of a thin cell’s average flux to its diagonal neighbors in the adjacent thick layer is only $O(\Delta^{-3})$ while coupling with the first Cartesian neighbor is $O(\Delta^{-1})$, the cumulative
effect of an infinite superposition of such $O\left(\Delta^{-3}\right)$ terms, resulting from long-range coupling in the $x$ direction, cannot be overlooked in the asymptotic limit and determines a strong dependence of $B_{nk}$ on $r$.

A.5 Solution of the $J$-Dimensional System $[I - \Delta^{-1}F]x = r$ in the Limit $\Delta, J \to \infty$

The solution to the linear algebraic system:

$$Hx \equiv [I - \Delta^{-1}F]x = r,$$  \hspace{1cm} (A.3)

where $I$ is the $J \times J$ identity matrix, $F$ is the $J \times J$ matrix whose elements are all 1 and $r$ is the $J \times 1$ vector whose elements are all 1, is investigated in the double limit $\Delta, J \to \infty$.

Even though the present investigation is of a conceptual nature, not necessarily related to a specific asymptotic structure acquired by the integral transport matrix, it is worthwhile to observe that a matrix structure very similar to the one under consideration is approached, to leading order, by the integral transport matrix in the thin cell limit for a homogeneous, uniform-mesh slab that was investigated in Sec. 3.4.3.

Specifically, the following error is formed:

$$\text{err} = \max \left(\text{abs}[\bar{x} - r]\right),$$  \hspace{1cm} (A.4)

where $\bar{x} = H^{-1}r$ is the exact solution to the system in Eq. (A.3). Since $r$ would be the solution to the latter system in case $H \equiv I$, the double limit, $J, \Delta \to \infty$, is a measure of how good $I$ is an asymptotic approximation to $H$. For a fixed $J$ the error is expected to tend to zero in the limit as $\Delta \to \infty$, confirming that the identity matrix is a good low-
order approximation to the full $H$ matrix in that limit. In the following though, it will be shown that the latter expectation can no longer be true if the dimensions of the matrix are also scaled, via the $J$ parameter.

Reasoning as in Sec. 3.6, it is possible to show that for a generic $J$:

$$\det(H) = 1 - \frac{J}{\Delta}$$  \hspace{1cm} (A.5)

$$H^{-1} = \frac{1}{1 - \frac{J}{\Delta}} \begin{bmatrix}
1 - \frac{(J-1)}{\Delta} & \frac{1}{\Delta} & \frac{1}{\Delta} & \cdots & \frac{1}{\Delta} \\
\frac{1}{\Delta} & 1 - \frac{(J-1)}{\Delta} & \frac{1}{\Delta} & \cdots & \frac{1}{\Delta} \\
\frac{1}{\Delta} & \frac{1}{\Delta} & 1 - \frac{(J-1)}{\Delta} & \cdots & \frac{1}{\Delta} \\
\cdots & \cdots & \cdots & \cdots & \cdots \\
\frac{1}{\Delta} & \frac{1}{\Delta} & \frac{1}{\Delta} & \cdots & 1 - \frac{(J-1)}{\Delta}
\end{bmatrix}$$  \hspace{1cm} (A.6)

The error is the same for all the elements of vector $\bar{x} - r$:

$$err = \max\left(\text{abs}\left[\bar{x} - r\right]\right) = \left|\frac{1}{1 - \frac{J}{\Delta}} \left[1 - \frac{(J-1)}{\Delta}\right] + (J-1)\frac{1}{\Delta}\right|^{-1}$$  \hspace{1cm} (A.7)

Performing the due simplifications:

$$err = \left|\frac{1}{1 - \frac{J}{\Delta}}\right|^{-1} = \left|\frac{J}{\Delta}\right|^{-1} = \left|\frac{J}{-J + \Delta}\right|$$  \hspace{1cm} (A.8)
This general closed-form analytic expression can be analyzed considering various limits for both $J$ and $\Delta$. These limits can be grouped according to the following three possible scenarios: 1) If $\lim_{J,\Delta \to \infty} \left( \frac{J}{\Delta} \right) \to 0$, equivalent to saying that $J \to \infty$ slower than $\Delta \to \infty$, then $err \to 0$. It is noted that the case in which $J$ is a fixed integer and $\Delta \to \infty$, is a particular instance of this scenario; 2) If $\lim_{J,\Delta \to \infty} \left( \frac{J}{\Delta} \right) \to const \neq 0$, equivalent to saying that $J \to \infty$ as fast as $\Delta \to \infty$, then $err \to \left| \frac{const}{1 - const} \right|$. In particular, if $\lim_{J,\Delta \to \infty} \left( \frac{J}{\Delta} \right) \to 1$, then $err \to \infty$. Note, in fact, that in this case $\det(H) = 1 - \frac{J}{\Delta} \to 0$, since an infinite number $J$ of infinitesimal contributions $\frac{1}{\Delta}$ is accumulated in the difference; 3) If $\lim_{J,\Delta \to \infty} \left( \frac{J}{\Delta} \right) \to \infty$, equivalent to saying that $J \to \infty$ faster than $\Delta \to \infty$, then $err \to 1$.

While in scenario 1 the identity matrix is a good approximation of the full $H$ matrix, in both scenarios 2 and 3, $I$ is no longer a good approximation of $H$.

A numerical verification of the results expected in 1, 2 and 3 has been carried out using MATLAB [49] considering three cases, each representing an instance of 1, 2 and 3, respectively. The sequence $J = [10, 50, 100, 500, 1000, 5000]$, with $\Delta = J^2$, represents an instance of 1. The resulting error is plotted in Fig. A.7. The numerical results verify the prediction that the error approaches zero as the dimension of the problem is increased.
Fig. A.7: Error as a function of $J$ for the case $\Delta = J^2$.

The sequence $J = [10, 50, 100, 500, 1000, 5000]$, with $\Delta = J$, represents an instance of 2. The resulting error is plotted in Fig. A.8 and, as predicted, corresponds to an infinite error in the double precision arithmetic employed in the numerical computation. The random large magnitude of the error is due to the fact that, for $\Delta = J$, the $H$ matrix is close to singular in double numerical precision. Therefore, $\text{det}(H)$ oscillates around the machine epsilon $\left(2.22 \times 10^{-16}\right)$ and consequently the error, which is
proportional to the inverse of \( \det(H) \), as evident from Eq. (A.8), oscillates around the inverse of the machine epsilon \( (4.50 \times 10^{15}) \).

Finally, the sequence \( J = [10, 50, 100, 500, 1000, 5000] \), with \( \Delta = \sqrt{J} \), represents an instance of 3. The resulting error is plotted in Fig. A.9. The numerical results verify the prediction that the error approaches a unit value as the dimension of the problem is increased.

*Fig. A.8: Error as a function of \( J \) for the case \( \Delta = J \).*
Since, as noted at the beginning of this section, the integral transport matrix $B$ acquires an asymptotic structure similar to matrix $H$ in the thin cell limit for a homogeneous, uniform-mesh slab, a few concluding remarks deriving from the conceptual study conducted in this section are discussed in the following for a slab.

The asymptotic analysis performed in Sec. 3.4.3 in the thin cell limit $\delta \to 0$ represents an instance of scenario 1, assuming $\Delta = \frac{1}{\delta}$ and $J$ fixed. From a physical point of view this situation corresponds to a case in which the computational cells are
becoming thin because the overall size of the problem, namely the width of the slab, \( L = J \delta \), where \( J \) is fixed, is becoming thin, \( L \to 0 \). In this asymptotic limit the transport problem is therefore dominated by leakage at the edges of the “vanishing” slab. In particular, the results obtained in Sec. 3.6 manipulating the integral transport matrix to leading order were derived explicitly assuming a fixed \( J \) and are true under this assumption, as it was stressed in Sec. 3.6.

Scenario 2 has not been considered in this work. Nevertheless, it is of potential interest, since it could be used to model a mesh refinement problem. In this case, the width of the slab is fixed, e.g. \( L = 1 \), and the computational cells are becoming thinner and thinner as the number \( J \) of computational cells in the spatial mesh is increased:

\[
\Delta = \frac{1}{\delta} = \frac{1}{J} = J, \quad J \to \infty
\]  
(A.9)

It is noted that the results of the asymptotic analysis for the elements of the integral transport matrix obtained in Sec. 3.4.3 would be the same for this case, since they only depend on \( \delta \to 0 \), no matter how the limit is obtained. In this case though, the impact of the increasing size of the integral transport matrix, as \( J \) is increased, on any indication coming from the structural analysis of the matrix elements must also be considered. This is in particular true because of the long-range coupling of the cell-averaged scalar fluxes that is characteristic of thin-cell problems. In the end, the failure of approximating the full matrix structure with the identity matrix in scenario 2 is due to the fact that a number \( J \to \infty \) of “small” \( (1/J) \to 0 \) elements is ignored in each row of the matrix, while \( J(1/J) \to 1 \) is not negligible.
In general, it should be recognized that the quantity typically scaled in any asymptotic structural analysis of the integral transport matrix is \( \sigma L = \sigma J \), and either \( \sigma \) or \( L \) or \( J \) can be separately or simultaneously scaled in the analysis depending on the problem under consideration. Reasoning only in terms of a limit in which \( \sigma L \rightarrow 0 \) can be misleading, if one ignores the parameter that is actually scaled to produce a vanishing number of MFPs in the computational cells. In other words, one must clearly identify the numerical experiment that is being analyzed in interpreting the results of the structural analysis. In particular, if \( J \) is scaled and the overall scaling considered leads to long-range coupling, then the impact of the size of the integral transport matrix on the results of the structural analysis cannot be ignored. The same reasoning can of course be extended to two-dimensional problems, considering both \( \sigma L \) and \( \sigma J \).

Similar considerations apply to scenario 3 that eventually could represent a means to approach the infinite medium assumed in the Fourier analysis. In this connection, the discussion presented in this section reconciles the apparent contradiction between the results of the asymptotic structural analysis and those of the Fourier analysis for the JCP scaling of the PHI configuration.

In closing this section it is observed that the previous discussion also points to the fact that, if a certain low-order approximation (preconditioner) to the full transport operator breaks down for a certain problem due to long-range coupling, then resorting to mesh refinement could potentially be of no use to improve the spectral properties.
A.6 Conclusion

A study of the asymptotic properties of the integral transport matrix has been carried out for the Periodic Horizontal Interface (PHI) configuration in the asymptotic limit originally introduced in [10]. In this limit the full integral transport matrix acquires a diagonally dominated non-diffusive structure. This result has been used to show that the asymptotic limit for the PHI configuration considered in [10], while conceptually useful in devising a particle transport problem for which there exists no preconditioner with a cell-centered diffusion coupling stencil that is unconditionally stable and robust, is not relevant from an application standpoint since it favors particle leakage at the boundaries of any finite-domain transport problem. The experience gained from the study of this asymptotic limit has been used to devise the new scaling of the PHI configuration that was considered in Ch. 7 and that was shown to avoid the drawback of introducing excessive leakage in finite problem configurations.
Appendix B

Mathematica Notebook for the Fourier Analysis of PHI

The following commands illustrate the process used to perform the Fourier analysis of SI and of the APB acceleration scheme for the PHI configuration. Inserting these commands into a Mathematica notebook and evaluating them produces plots of the spectral radii of SI and APB as a function of the scaling parameter $\Delta$. In case $P_{N_{Kx}}$ and $P_{K_{Ny}}$ are set equal to zero, the same notebook can be used to perform the Fourier analysis for the traditional AP acceleration scheme.

```mathematica
<<Utilities`CleanSlate`
Off[General::spell]

Nq = 6;
Pr = 128;
parametri = {\delta_x \rightarrow \text{SetPrecision}[1, Pr], \delta_y \rightarrow \text{SetPrecision}[1, Pr],
             \sigma_N \rightarrow \text{SetPrecision}[1, Pr], \sigma_K \rightarrow \text{SetPrecision}[1, Pr]}
scattering = {c_N \rightarrow \text{SetPrecision}[0.99999999, Pr],
             c_K \rightarrow \text{SetPrecision}[0.99999999, Pr]}

if[Nq == 1, angoli = {\mu_1 \rightarrow \text{SetPrecision}[0.5773503, Pr],
                    \eta_1 \rightarrow \text{SetPrecision}[0.5773503, Pr]}]
if[Nq == 1, pesi = {p \rightarrow \text{SetPrecision}[1/4, Pr]}]
if[Nq == 1, w = {p}, w = w /. pesi];
if[Nq == 1, \mu = {\mu_1}];
if[Nq == 1, \eta = {\eta_1}];

if[Nq == 3, angoli = {\mu_1 \rightarrow \text{SetPrecision}[0.3500212, Pr],
                    \eta_1 \rightarrow \text{SetPrecision}[0.3500212, Pr],
                    \mu_2 \rightarrow \text{SetPrecision}[0.3500212, Pr],
                    \eta_2 \rightarrow \text{SetPrecision}[0.8688903, Pr],
                    \mu_3 \rightarrow \text{SetPrecision}[0.8688903, Pr],
                    \eta_3 \rightarrow \text{SetPrecision}[0.3500212, Pr]}]
```
if[Nq == 3, pesi = {p -> SetPrecision[1/12, Pr]}]
if[Nq == 3, w = {p, p, p}, w = w /. pesi];
if[Nq == 3, μ = {μ1, μ2, μ3}];
if[Nq == 3, η = {η1, η2, η3}];

if[Nq == 6, angoli = {μ1 -> SetPrecision[0.256143, Pr],
η1 -> SetPrecision[0.256143, Pr],
μ2 -> SetPrecision[0.266344, Pr],
η2 -> SetPrecision[0.681565, Pr],
μ3 -> SetPrecision[0.256143, Pr],
η3 -> SetPrecision[0.932085, Pr],
μ4 -> SetPrecision[0.681565, Pr],
η4 -> SetPrecision[0.266344, Pr],
μ5 -> SetPrecision[0.681565, Pr],
η5 -> SetPrecision[0.681565, Pr],
μ6 -> SetPrecision[0.932085, Pr],
η6 -> SetPrecision[0.256143, Pr]}]
if[Nq == 6, pesi = {p -> SetPrecision[1/24, Pr]}]
if[Nq == 6, w = {p, p, p, p, p, p}, w = w /. pesi];
if[Nq == 6, μ = {μ1, μ2, μ3, μ4, μ5, μ6}];
if[Nq == 6, η = {η1, η2, η3, η4, η5, η6}];

Nc = 2;
IM = IdentityMatrix[Nc];
JM = 0 * IM;
FMI = IM - i * Sin[r/2] *
    
    (2 * χN / (Cos[r/2] + i * αN * Sin[r/2]) +
    0 2 * χK / (Cos[r/2] + i * αK * Sin[r/2]))^* +
    
    (2 * νN * (Cos[s] + i * βK * Sin[s]) - 2 * νN
    -2 * νK 2 * νK * (Cos[s] + i * βN * Sin[s]))^* +
    
    (1/((βN + βK) * Cos[s] + i * (1 + βN * βK) * Sin[s]));

FMII = IM - i * Sin[r/2] *
    
    (2 * χN / (Cos[r/2] + i * αN * Sin[r/2]) +
    0 2 * χK / (Cos[r/2] - i * αK * Sin[r/2]))^* +
    
    (2 * νN * (Cos[s] + i * βK * Sin[s]) - 2 * νN
    -2 * νK 2 * νK * (Cos[s] + i * βN * Sin[s]))^* +
    
    (1/((βN + βK) * Cos[s] + i * (1 + βN * βK) * Sin[s]));

FMIII = IM - i * Sin[r/2] *
    
    (2 * χN / (Cos[r/2] - i * αN * Sin[r/2]) +
    0 2 * χK / (Cos[r/2] - i * αK * Sin[r/2]))^* +
    
    (2 * νN * (Cos[s] - i * βK * Sin[s]) - 2 * νN
    -2 * νK 2 * νK * (Cos[s] - i * βN * Sin[s]))^* +
    
    (1/((βN + βK) * Cos[s] - i * (1 + βN * βK) * Sin[s]));
\[
\begin{align*}
\text{FMIV} &= \text{IM} \times \exp(i \times \sin(x/2)) \\
&= \left( \\
&\begin{pmatrix}
2 \times \nu / (\cos(x/2) + i \times \alpha \times \sin(x/2)) & 0 \\
0 & 2 \times \nu / (\cos(x/2) + i \times \alpha \times \sin(x/2))
\end{pmatrix} + \\
&\begin{pmatrix}
2 \times \nu \times (\cos(s) - i \times \beta \times \sin(s)) & -2 \times \nu \\
-2 \times \nu \times (\cos(s) - i \times \beta \times \sin(s)) & 2 \times \nu \times (\cos(s) - i \times \beta \times \sin(s))
\end{pmatrix} \\
&\times (1 / ((\beta s + \beta e) \times \cos(s) - i \times (1 + \beta s \times \beta e) \times \sin(s)))
\end{align*}
\]

\[
\text{GM} = \left( \begin{array}{cc}
1 / c_s & 0 \\
0 & 1 / c_s
\end{array} \right);
\]
\[ S_K = \sigma_K / \varepsilon; \]
\[ K_K = \mu / (S_K \Delta x) \quad \text{. Join}[\text{parametri}, \text{angoli}]; \]
\[ N_K = \eta / (S_K \Delta y) \quad \text{. Join}[\text{parametri}, \text{angoli}]; \]
\[ A_K = \text{Coth}(1 / (2 * K_P) - 2 * K_K); \]
\[ B_K = \text{Coth}(1 / (2 * N_P) - 2 * N_K); \]
\[ \gamma_{\text{MK}} = C_K \times 1 / (1 + (2 * K_K / (1 + A_K)) + (2 * N_K / (1 + B_K))) \quad \text{. scattering}; \]
\[ \gamma_{\text{NK}} = (2 * N_K / (1 + B_K)) / (1 + (2 * K_K / (1 + A_K)) + (2 * N_K / (1 + B_K))); \]
\[ \gamma_{\text{SK}} = (2 * K_K / (1 + A_K)) / (1 + (2 * K_K / (1 + A_K)) + (2 * N_K / (1 + B_K))); \]
\[ \gamma_{\text{SY}} = C_K \times (2 / (1 + B_K)) / (1 + (2 * K_K / (1 + A_K)) + (2 * N_K / (1 + B_K))) \quad \text{. scattering}; \]
\[ \gamma_{\text{SY}} = ((2 * N_K / (1 + B_K)) + ((2 * N_K + A_K + 1) / (1 + A_K)) * ((B_K - 1) / (1 + B_K))) / \]
\[ (1 + (2 * K_K / (1 + A_K)) + (2 * N_K / (1 + B_K))); \]
\[ \frac{d}{dx} x_k = -s_k \Delta x \Delta x * \]
\[ \sum_{k=1}^{N_k} \frac{w[[k]] * (2 * K_K[[k]] + A_K[[k]]) \times (2 * K_K[[k]] + B_K[[k]])}{\text{parametri}}; \]
\[ \frac{d}{dy} x_k = -s_k \Delta y \Delta y * \]
\[ \sum_{k=1}^{N_k} \frac{w[[k]] * (2 * N_K[[k]] + B_K[[k]]) \times (2 * N_K[[k]] + A_K[[k]])}{\text{parametri}}; \]
For \[ k = 1, \quad k < N_k + 1, \]
\[ \text{Valorik} = \text{Join}[[x_K \rightarrow K_K[[k]], \quad \nu_N \rightarrow K_N[[k]], \quad A_N \rightarrow A_K[[k]], \quad B_N \rightarrow B_K[[k]], \quad K_N \rightarrow K_K[[k]], \quad \nu_K \rightarrow N_K[[k]], \quad A_K \rightarrow A_K[[k]], \quad B_K \rightarrow B_K[[k]]], \text{scattering}]; \]
\[ \text{JMInvI} = \text{JMInvII} / \text{Valorik}; \]
\[ \text{JMInvII} = \text{JMInvIII} / \text{Valorik}; \]
\[ \text{JMInvIII} = \text{JMInvIV} / \text{Valorik}; \]
\[ \text{JMInvIV} = \text{JMInvI}; \]
\[ \text{JMInvI} = \text{Inverse}[\text{JMInvII}]; \]
\[ \text{JMInvII} = \text{Inverse}[\text{JMInvIII}]; \]
\[ \text{JMInvIII} = \text{Inverse}[\text{JMInvIV}]; \]
\[ \text{JMInvIV} = \text{Inverse}[\text{JMInvI}]; \]
For \[ i = 1, \quad i < N_i + 1, \]
For \[ j = 1, \quad j < N_j + 1, \]
\[ \text{JM}[[i, j]] = \text{JM}[[i, j]] + w[[k]] \times (\text{JM}[[i, j]] + \text{JM}[[i, j]] + \text{JM}[[i, j]] + \text{JM}[[i, j]] + \text{JM}[[i, j]]); \]
\[ j++; \]
\[ i++; \]
\[ k++; \]
\[ P_{\text{MKX}} = -\left(\text{Abs}[S_K - S_N] / S_K\right) * S_K \Delta x \Delta y * \]
\[ \sum_{k=1}^{N_k} \left( w[[k]] * (\gamma_{\text{MK}}[[k]] \times (\gamma_{\text{MK}}[[k]] + \gamma_{\text{MK}}[[k]] + \gamma_{\text{MK}}[[k]] + \gamma_{\text{MK}}[[k]] + \gamma_{\text{MK}}[[k]])) \right) \quad \text{. parametri}; \]
\[ P_{\text{MKY}} = -\left(\text{Abs}[S_K - S_N] / S_K\right) * S_N \Delta x \Delta y * \]
\[
\sum_{k=1}^{N} \left( w[k] \times (\gamma_{\text{L}}[k]) \times (\gamma_{\text{R}}[k]) \times (\gamma_{\text{S}}[k]) \times (\gamma_{\text{P}}[k]) \right) / \text{parametri;}
\]

\[
C_N = S_N \times \Delta x \times \Delta y \times C_N / \text{Join[parametri, scattering]};
\]

\[
C_K = S_K \times \Delta x \times \Delta y \times C_K / \text{Join[parametri, scattering]};
\]

\[
\text{CM} = \left( \begin{array}{cc}
C_N & 0 \\
0 & C_K
\end{array} \right);
\]

\[
\text{APoxNN} = (2 \times \Delta y) / ((\Delta x / \text{daxN}) + (\Delta x / \text{daxN})) / \text{parametri;}
\]

\[
\text{APoyNK} = (2 \times \Delta x) / ((\Delta y / \text{dayN}) + (\Delta y / \text{dayN})) / \text{parametri;}
\]

\[
PdN = (S_N \times \Delta x \times \Delta y \times (1 - c_N) - 2 \times \text{APoxNN} - 2 \times \text{APoyNK} - 4 \times F_{\text{PKG}}) / \text{Join[parametri, scattering]};
\]

\[
\text{APoxKK} = (2 \times \Delta y) / ((\Delta x / \text{daxK}) + (\Delta x / \text{daxK})) / \text{parametri;}
\]

\[
\text{APoyKN} = (2 \times \Delta x) / ((\Delta y / \text{dayK}) + (\Delta y / \text{dayK})) / \text{parametri;}
\]

\[
PdK = (S_K \times \Delta x \times \Delta y \times (1 - c_K) - 2 \times \text{APoxKK} - 2 \times \text{APoyKN} - 4 \times F_{\text{PKG}}) / \text{Join[parametri, scattering]};
\]

\[
\text{PM} = \left( \begin{array}{cc}
2 \times \text{APoyKN} \times \text{Cos}[s] + 4 \times F_{\text{PKG}} \times \text{Cos}[r] \times \text{Cos}[s] & PdK + 2 \times \text{APoxKK} \times \text{Cos}[r]
\end{array} \right);
\]

\[
\text{RoSI} = 0;
\]

\[
\text{RoP} = 0;
\]

\[
\text{For}[i = 1, i < \text{NF} + 1,
\text{For}[j = 1, j < \text{NF} + 1,
R = 0.1 \times \pi \times (i - 1);
S = 0.1 \times \pi \times (j - 1);
\text{EigSI} = \text{Eigenvalues}[[\text{JM} /. \{r \rightarrow R, s \rightarrow S\}]];
\text{EigSI1} = \text{Abs}[\text{Extract}[\text{EigSI}, \{1\}]];
\text{EigSI2} = \text{Abs}[\text{Extract}[\text{EigSI}, \{2\}]];
\text{MaxESI} = \text{Max}[\text{EigSI1}, \text{EigSI2}];
\text{RoSI} = \text{Max}[\text{RoSI}, \text{MaxESI}];
\text{PinvM} = \text{Inverse}[\text{PM} /. \{r \rightarrow R, s \rightarrow S\}];
\text{TPM} = \text{JM} + \text{PinvM} \cdot \text{CM} \cdot (\text{JM} - \text{IM}) /. \{r \rightarrow R, s \rightarrow S\};
\text{EigP} = \text{Eigenvalues}[\text{TPM}];
\text{EigP1} = \text{Abs}[\text{Extract}[\text{EigP}, \{1\}]];
\text{EigP2} = \text{Abs}[\text{Extract}[\text{EigP}, \{2\}]];
\text{MaxEP} = \text{Max}[\text{EigP1}, \text{EigP2}];
\text{RoP} = \text{Max}[\text{RoP}, \text{MaxEP}];
\text{j++;}
\text{i++;}
\text{SrSI}[t] = \text{RoSI};
\text{SrP}[t] = \text{RoP};
\text{PlotsSI}[t, 1] = \text{Delta}[t];
\text{PlotsSI}[t, 2] = \text{SrSI}[t];
\text{PlotP}[t, 1] = \text{Delta}[t];
\text{PlotP}[t, 2] = \text{SrP}[t];
\text{JM} = 0 \times \text{IM};
\text{Print}[\text{SetPrecision}[\text{RoP}, 3]];
t++;]
<< Graphics`Graphics`
LogLinearListPlot[PLOTSI, AxesOrigin → {1, 0}, PlotRange → {0, 1.1},
PlotJoined → True, PlotStyle → Hue[.6], AxesLabel → {Δ, SR}]

<< Graphics`Graphics`
LogLinearListPlot[PLOTSI, AxesOrigin → {1, 0}, PlotRange → {0, 1.1},
PlotJoined → True, PlotStyle → Hue[.6], AxesLabel → {Δ, SR}]

SetPrecision[DELTA, 8]
SetPrecision[SRSI, 8]
SetPrecision[DELTA, 8]
SetPrecision[SRP, 8]
CleanSlate[]


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VITA

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Massimiliano Rosa was born on October 14, 1971 in Como, Italy. He pursued his studies at Ce.S.N.E.F, Centro Studi Nucleari Enrico Fermi, the nuclear engineering department of the Polytechnic Institute of Milan. He received his Laurea degree (5 year degree) in Nuclear Engineering with first class honors in June of 2002. During the spring semester of 2004 he enrolled in the nuclear engineering graduate program at The Pennsylvania State University as a doctoral student under the supervision of Professor Yousry Y. Azmy. He spent the summers of 2005 and 2006 at Los Alamos National Laboratory as a graduate student intern working with the Transport Methods Section of the Computational Physics and Methods Group (CCS-2). His professional interests lie in the area of nuclear computational science with a particular focus on synthetic acceleration methods for the iterative solution of neutral particle transport problems in deterministic transport theory. He completed his doctoral degree in August of 2007.