A HYBRID NUDGING-ENSEMBLE KALMAN FILTER APPROACH TO DATA ASSIMILATION

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by

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ABSTRACT

A hybrid nudging-ensemble Kalman filter (HNEnKF) data assimilation approach that effectively combines the advantages of nudging and the EnKF is proposed and explored in this dissertation. It is first developed and tested in simplified models, the Lorenz three-variable system and a more realistic 2D shallow water model, with simulated observations, and then in a full-physics 3D mesoscale model, the Weather Research and Forecasting (WRF) model, using real observations.

The HNEnKF uses the EnKF to obtain a flow-dependent / time-dependent background error covariance matrix that can be used to compute a flow-dependent / time-varying nudging coefficient matrix. It also extends the nudging magnitude matrix to include the inter-variable influences of innovations via nonzero off-diagonal elements of the EnKF gain matrix. This additional coupling between the observations and the multivariate state may lead to a faster and more accurate adjustment of the background to observations than does traditional nudging. By use of nudging-type terms, the HNEnKF applies the EnKF gradually in time to achieve a more gradual data assimilation that greatly reduces the insertion noise common with intermittent methods such as the EnKF. Thus it combines the strengths of nudging and the EnKF while avoiding their individual weaknesses.

In the Lorenz three-variable system, the HNEnKF promotes a better fit of an analysis to data compared to that produced by nudging. When model error is introduced, it produces similar or better RMS errors compared to the EnKF while minimizing the error spikes / discontinuities created by the intermittent EnKF. It provides a continuous data assimilation with better inter-variable consistency and improved temporal smoothness than that of the EnKF. Compared to the ensemble Kalman smoother (EnKS), considered to be a “gold standard” in statistical data
assimilation methods, the HNEnKF has similar or better temporal smoothness with much smaller CPU time and data storage requirements.

In the 2D shallow water model, a quasi-stationary wave case and a moving vortex case are used to investigate the data assimilation methods. The HNEnKF generally produces smaller RMS errors in both the height and wind fields than the nudging and EnKF applied separately. The HNEnKF also has better temporal smoothness than the EnKF and the more practical and computationally efficient lagged EnKS used in the shallow water model. The HNEnKF takes advantage of the EnKF by effectively reducing the RMS errors through the flow-dependent background error covariances, and also retains the benefits of the continuous nudging by reducing the RMS errors gradually over time. Moreover, the HNEnKF produces a smoother evolution of the ageostrophic wind without any strong discontinuities / dynamic imbalances around the observation time, while the EnKF exhibits large bursts in the ageostrophic wind after the observations are assimilated.

The HNEnKF is further tested in the 3D WRF model with real observations using a Cross Appalachian Tracer Experiment case from September 1983 (CAPTEX-83). The HNEnKF generally has better posteriors of the wind and mass fields than the EnKF, although both HNEnKF and EnKF have larger posterior RMS errors than the observation-nudging four dimensional data assimilation (FDDA). The HNEnKF has similar or better priors of the wind and mass fields than the EnKF and FDDA in general. Moreover, the continuous HNEnKF has much lower noise levels as shown by the domain average absolute surface pressure tendency than the intermittent EnKF. Thus the ability of the HNEnKF to provide better temporal smoothness and dynamic consistency than the EnKF is further demonstrated. The HNEnKF analyses used in an atmospheric transport and dispersion (AT&D) model produce consistently better statistics of hits, misses and false alarms than the EnKF in the independent / indirect verification using the surface tracer data. Thus there appears to be some advantage in the WRF dynamic analyses produced by
the continuous HNEnKF compared to the intermittent EnKF, and proof-of-concept for this new hybrid data assimilation approach improving analyses and numerical predictions has been demonstrated.
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Chapter 1

Introduction

Numerical weather prediction (NWP) is an initial-value problem where a numerical model containing the tendency equations for the state variables predicts the future atmospheric state given an estimate of the present state of the atmosphere (initial conditions), and appropriate surface and upper boundary conditions. For a limited-area model, often used to obtain finer model resolutions over a mesoscale region, accurate lateral boundary conditions are also required. The model initial conditions at operational centers, for example, are often produced through a statistical combination of observations and short-range model forecasts (Kalnay 2003). This general approach of using a model background enhanced by observations to determine as accurately as possible the state of the atmospheric flow has become known as data assimilation.

Data assimilation techniques can be grouped into two general categories: intermittent and continuous data assimilation (e.g., Stauffer and Seaman 1990; Daley 1991). In an intermittent data assimilation method, observations can be processed in small batches intermittently in time. Optimal interpolation (OI, Gandin 1963), three-dimensional variational (3DVAR, Sasaki 1970; Lorenc 1986; Courtier et al. 1998), and the ensemble Kalman filter (EnKF, Evensen 1994; Houtekamer and Mitchell 1998) are examples of intermittent data assimilation methods. In comparison, a continuous data assimilation method uses observations continuously in time (every time step) over longer periods, so the correction to the analyzed state is smoother in time, which produces more physically realistic and dynamically consistent model data products (Bloom et al. 1996; Stauffer and Seaman 1990). The observations in continuous data assimilation can be assimilated at the same rate as that they are observed. Popular continuous data assimilation methods include nudging (Hoke and Anthes 1976; Stauffer and Seaman 1990), incremental
analysis update (IAU, Bloom et al. 1996; Ourmieres et al. 2006), four-dimensional variational (4DVAR, Lorenc 1986; Thepaut et al. 1993), and the ensemble Kalman smoother (EnKS, Cohn et al. 1994; Evensen and van Leeuwen 2000).

The EnKF uses the statistical properties of an ensemble model forecast to estimate the flow-dependent background error covariance in order to determine how an observation modifies the forecast background fields during the assimilation process (Evensen 1994). The EnKF is becoming increasingly popular compared to the 3DVAR and 4DVAR, because it is able to compute the flow-dependent background error covariance from an ensemble forecast and it has no requirement for a tangent linear model and adjoint model (e.g. Houtekamer and Mitchell 1998; Fujita et al. 2007). Numerous studies of the EnKF have been conducted for both global (e.g., Houtekamer and Mitchell 1998; Anderson 2001; Houtekamer and Mitchell 2001; Mitchell et al. 2002; Whitaker et al. 2004, 2008; Houtekamer et al. 2005, 2009) and limited-area NWP applications (e.g., Zhang et al. 2006; Fujita et al. 2007; Meng and Zhang 2008; Torn and Hakim 2008). The EnKF has also been applied for storm-scale studies not requiring any convective parameterization (e.g., Snyder and Zhang 2003; Zhang et al. 2004; Aksoy et al. 2009).

To take advantage of the flow-dependent background error covariance from the EnKF, hybrid EnKF and variational data assimilation methods have been proposed and tested. For example, a hybrid EnKF-3DVAR was discussed by Hamill and Snyder (2000), an ensemble-based 4DVAR (En4DVAR) was developed by Liu et al. (2008), and a hybrid ensemble transform Kalman filter (ETKF, Bishop et al. 2001 )-3DVAR was proposed by Wang et al. (2008a; 2008b).

However, the EnKF, as an intermittent data assimilation method, performs a data assimilation analysis at each observation time and then switches back to the standard model forecast process between analysis times. This cycle of a model integration period, analysis step, and then another model integration period often causes discontinuities / error spikes around the observation times (e.g., Hunt et al. 2004; Duane et al. 2006; Juckes and Lawrence 2009).
Moreover, these discontinuities can introduce a shock at the model restart stage and cause spurious high-frequency oscillations, and then possibly lead to data rejection (Bloom et al. 1996; Ourmieres et al. 2006). In the EnKF study of Fujita et al. (2007), the discontinuities of errors across the analysis step were shown to occur when hourly surface observations are assimilated into the model background. A logical question may be whether their reported RMS wind errors, increasing through the 6-h assimilation period, reflect in some way the enhanced divergence related to gravity-wave activity caused by the hourly updates. The high-frequency oscillations caused by intermittent data assimilation may result in spurious vertical motions triggering false convection, unrealistic precipitation, outflow boundaries and cold pools.

Thus because of the discontinuities, the ability of the EnKF to provide a time-continuous and seamless dynamic analysis is not guaranteed, although a continuous and seamless meteorological field is preferable in many applications, especially for use in driving air-quality and atmospheric transport and dispersion (AT&D) models (e.g., Stauffer et al. 2000; Tanrikulu et al. 2000; Otte 2008a, b). The discontinuities and dynamic imbalances in the meteorological fields may contaminate the AT&D and estimation of the source terms. Thus continuous and seamless meteorological background fields can improve the simulation of AT&D and hazard predictions (e.g., Deng et al. 2004; Deng and Stauffer 2006).

In contrast to the intermittent EnKF, nudging is a continuous data assimilation method. It relaxes the model state toward the observations by adding artificial terms to the prognostic equations (Hoke and Anthes 1976). The artificial terms are proportional to the difference between the observations and the model state. Nudging is designed to be applied every time step, allowing the corrections to be relatively small and applied gradually within a time window around the observation times (Stauffer and Seaman 1990; 1994). Nudging has been used in many data assimilation applications (e.g., Stauffer and Seaman 1990, 1994; Stauffer et al. 1991; Seaman et al. 1995; Leidner et al. 2001; Otte et al. 2001; Deng et al. 2004; Deng and Stauffer 2006;
Schroeder et al. 2006; Dixon et al. 2009; and Ballabrera-Poy et al. 2009). However, it is typically used with *ad hoc* nudging coefficients and spatial weighting functions based on past experience and experimentation. Adjoint parameter-estimation approaches have also been investigated using simplified models to determine the optimal coefficients (Zou et al. 1992; Stauffer and Bao 1993).

A hybrid nudging-EnKF (HNEnKF) approach is developed and tested in this dissertation. The HNEnKF directly combines the nudging and EnKF by using nudging-type terms to apply the EnKF gradually in time. The EnKF provides flow-dependent and time-dependent nudging coefficients to the nudging; the ensemble forecasts provide a more practical alternative for determining the nudging coefficients. It is hypothesized here that if the EnKF is applied gradually in time, a continuous and seamless analysis can be produced and the analysis will be improved by reducing the intermittent discontinuities or bursts. This hybrid combination of data assimilation methods should perform better than either method applied separately.

To investigate the hypothesis, the HNEnKF will be implemented for a dynamic analysis where the data assimilation is applied throughout a model integration period using increasingly complex and realistic models. The dynamic analysis focuses on the period in which the data assimilation is applied and the suitability of the generated datasets to be used for diagnostic studies or as inputs into other numerical models. The dynamic-analysis mode is very attractive for testing new data assimilation methods, because the effect of the data assimilation on the model fields between the observation times reflects the coupling of the data assimilation and the model, and the ability of the model to retain the observational information relative to losing valuable information from the observations and generating insertion noise / transients. A continuous, seamless meteorological analysis field with inter-variable consistency is very attractive for many studies, including air quality, wind energy, atmospheric chemistry and AT&D. Therefore, this dissertation focuses on improving the data assimilation method for dynamic analysis where data are assimilated throughout a model integration period.
As a proof-of-concept, this HNEnKF approach will be first tested in the Lorenz three-variable system (Lorenz 1963). The Lorenz three-variable model has served as a testbed for examining the properties of various data assimilation methods when used with strongly nonlinear dynamics (e.g., Evensen and van Leeuwen 2000; Yang et al. 2006; Chin et al. 2007; Auroux and Blum 2008; Pu and Hacker 2009).

Although encouraging results have been obtained by testing the HNEnKF in the Lorenz three-variable system, the Lorenz three-variable system does not have the basic atmospheric balances, such as geostrophic balance. Thus instead of jumping straight into a full-physics NWP model, we use a more realistic two-dimensional (2D) shallow water model next to test whether the HNEnKF has the ability to provide a continuous and improved analysis, and retain better intervariable consistency than the EnKF. The dynamic imbalance caused by the insertion noise common in the intermittent data assimilation method will be also explored in the shallow water model.

After the hypothesis has been tested in the Lorenz three-variable system and a shallow water model, a full-physics three-dimensional (3D) mesoscale model, the Weather Research and Forecasting (WRF, Skamarock et al. 2008) model, will be used to investigate the potential added value of the HNEnKF compared to the EnKF and nudging. The data assimilation component of the EnKF uses the Data Assimilation Research Testbed (DART, Anderson et al. 2009). With assimilation of real observations, the ability of the HNEnKF using a full-physics NWP model to show decreased spurious high-frequency oscillations compared to the intermittent EnKF will be explored. The dynamic analyses produced by the EnKF, nudging and the HNEnKF and used in an AT&D model, will be evaluated using independent surface tracer data.

In chapter 2, the HNEnKF approach is proposed and tested in the Lorenz three-variable system. In chapter 3, the HNEnKF approach is further tested in a 2D shallow water model for a quasi-stationary wave case and a moving vortex case. Chapters 2 and 3 are conditionally
accepted as a two-part study for publication in Tellus. The application of the HNEnKF in WRF/DART with real observations is explored in chapter 4, which will be published in a forthcoming paper in a peer-reviewed journal. Conclusions and future work are summarized in chapter 5.
Chapter 2

A Hybrid Nudging-Ensemble Kalman Filter Approach to Data Assimilation: Application in the Lorenz System

2.1. Introduction

Data assimilation combines the observations and the forecast by a numerical weather prediction model to produce an analysis. The analysis is considered as the best estimate of the current state of the atmosphere. Thus, an important objective of the data assimilation is to develop optimal methods to assimilate the observations to provide the best possible analysis and initialization for the forecast model.

The ensemble Kalman filter (EnKF) is currently a popular data assimilation method. The EnKF was first proposed by Evensen (1994) in an oceanographic application, and has subsequently been implemented in atmospheric applications (e.g., Houtekamer and Mitchell (1998), Anderson (2001), and Whitaker and Hamill (2002)). The EnKF uses the statistical properties of an ensemble forecast to estimate the flow-dependent background error covariances. These flow-dependent background error covariances determine how an observation affects the model variables. Then a new analysis ensemble with the statistics to minimize the analysis error is produced. By contrast, the three-dimensional variational method (3DVAR, Sasaki 1970; Lorenc 1986; Courtier et al. 1998), which assimilates observations sequentially and is computationally efficient, generally adopts a homogeneous and stationary background error covariance. The four-dimensional variational method (4DVAR, Lorenc 1986; Thepaut et al. 1993), which finds the trajectory that best fits the past and present observations, generally requires a tangent linear model and adjoint model to estimate the actual flow-dependent error
structure. Therefore, the EnKF is becoming increasingly popular compared to 3DVAR and 4DVAR methods, because it is able to efficiently compute the flow-dependent background error covariances from an ensemble forecast without requiring a tangent linear model and adjoint model (e.g., Houtekamer and Mitchell 1998; Fujita et al 2007).

To combine the advantages of EnKF and variational data assimilation methods, several hybrid data assimilation schemes have been studied. For example, a hybrid EnKF-3DVAR has been discussed by Hamill and Snyder (2000), in which the background error covariances are a linear combination of the stationary covariances used in 3DVAR and flow-dependent covariances computed from a short-range ensemble forecast. A hybrid ensemble transform Kalman filter (ETKF, Bishop et al. 2001)-3DVAR has been proposed by Wang et al. (2008a; 2008b). The hybrid ETKF-3DVAR combines the ensemble covariances with the static covariances used in 3DVAR, incorporates these covariances during the variational minimization by the extended control variable method, and maintains the ensemble perturbations by the ETKF. An ensemble-based 4DVAR (En4DVAR), developed by Liu et al. (2008), uses an ensemble forecast to provide the flow-dependent background error covariances and performs 4DVAR optimization without tangent linear and adjoint models.

However, the EnKF is an intermittent data assimilation approach, where observations are processed in small batches intermittently in time. The intermittent nature of the EnKF often causes discontinuities / error spikes around the observation times (e.g., Hunt et al. 2004; Fujita et al. 2007). Juckes and Lawrence (2009) reported similar “discontinuities” in the forward and backward Kalman filter analyses. Duane et al. (2006) also found that the Kalman filter algorithm has some “desynchronization bursts” at times of regime transitions between the Lorenz and “reversed Lorenz” phases. Thus the EnKF can produce discontinuities between the forecast and the analysis estimates. These discontinuities can introduce a shock at the model restart stage and cause spurious high-frequency oscillations and possibly lead to data rejection (Bloom et al. 1996;
Also because of the discontinuities, the ability of the EnKF to provide a time-continuous and seamless analysis is not guaranteed.

A time-continuous, seamless meteorological field is preferred in many applications, especially for use in driving air-quality and atmospheric-chemistry models (e.g., Stauffer et al. 2000; Tanrikulu et al. 2000; Otte 2008a, b). Improved meteorological conditions and seamless meteorological background fields can also improve the simulation of transport and dispersion (e.g., Deng et al. 2004; Deng and Stauffer 2006). Thus it is hypothesized here that if the EnKF could be applied gradually in time, a dynamic analysis where data assimilation is applied throughout a model integration period would be produced and the intermittent discontinuities and error bursts would be reduced.

The discontinuous nature of the analysis increments of the EnKF is recognized and discussed by Bergemann and Reich (2010) using a Lorenz system. They proposed a “mollified” EnKF, which is able to damp the spurious high-frequency adjustment processes caused by the discontinuous EnKF. They note that the term “mollification” introduced by Friedrichs (1944) denotes families of smooth functions that approach the Dirac delta function as the width of the time window approaches zero. In the “mollified” EnKF, each ensemble member assimilates the observations by the continuous EnKF with a mollified Dirac delta function at every time step within a time window.

A hybrid nudging-EnKF (HNEnKF) is proposed here with the same purpose as the mollified EnKF. The HNEnKF applies the EnKF gradually in time by directly combining the EnKF with nudging. Compared to the mollified EnKF that calculates the nudging coefficients from the background error covariance and observational cost function at every time step and updates each ensemble member gradually in time, the HNEnKF computes the EnKF gain matrix once at the observation time, and uses this EnKF gain matrix over the nudging time window within the nudging coefficients for one control member only. Therefore, the HNEnKF proposed
here is more computationally efficient and may be more practical than the mollified EnKF for more complex models.

Nudging, also known as Newtonian Relaxation, is a continuous data assimilation method that relaxes the model state toward the observations by adding artificial terms to the prognostic equations (Hoke and Anthes 1976). The artificial terms are proportional to the difference between the observations and the model state. Nudging is designed to be applied every time step, allowing the corrections to be relatively small and applied gradually within a time window around the observation times (Stauffer and Seaman 1990; 1994). Nudging has been used in many data assimilation applications (e.g., Stauffer and Seaman 1990, 1994; Stauffer et al. 1991; Seaman et al. 1995; Leidner et al. 2001; Otte et al. 2001; Deng et al. 2004; Deng and Stauffer 2006; Schroeder et al. 2006; Dixon et al. 2009; and Ballabrera-Poy et al. 2009). However, it is typically used with \textit{ad hoc} nudging coefficients and spatial weighting functions based on past experience and experimentation. Adjoint parameter-estimation approaches have also been investigated using simple models to determine the optimal coefficients (Zou et al. 1992; Stauffer and Bao 1993). When ensemble forecasts are available, the ensemble and the EnKF may provide a more practical alternative for determining the nudging coefficients.

Similar to nudging, the incremental analysis update (IAU, Bloom et al. 1996; Ourmieres et al. 2006; Lee et al. 2006) and the ensemble Kalman smoother (EnKS, Cohn et al. 1994; Evensen and van Leeuwen 2000) are also continuous data assimilation methods. The IAU method incorporates the analysis increments into the model integration in a gradual manner as a state-independent forcing term (Bloom et al. 1996). Comparatively, the nudging adds a state-dependent forcing term into the model integration, because the state variables used in the additional nudging terms vary with time. Therefore, IAU does not consider the changes to the difference between the observation and the model state (the innovation) during the model
integration. Thus nudging rather than IAU is chosen here as a means of applying the EnKF gradually in time.

The EnKS uses the EnKF solution as the first guess for the analysis, and applies future observations backward in time using the ensemble covariances. As an extension of EnKF, the EnKS is a continuous data assimilation method, and it uses an ensemble forecast to compute both the spatial and temporal error covariances. Thus we treat the EnKS (Evensen and van Leeuwen 2000; Whitaker and Compo 2002; Khare et al. 2008) as the “gold standard” against which to measure the success of other data assimilation methods as a benchmark.

The goal of this current study is to demonstrate that one can combine the advantages of the EnKF approach to data assimilation with the temporal smoothness of the continuous nudging approach. The HNEnKF proposed here uses nudging-type terms to apply the EnKF gradually in time in order to minimize the insertion shocks. The HNEnKF also has the ability to provide both the direction and the coupling strength from the EnKF to the nudging approach. Therefore, it is hypothesized that this hybrid combination of data assimilation methods should perform better than either method applied separately. To investigate the hypothesis that a continuous and seamless analysis can be produced if the EnKF is applied gradually in time, the proof-of-concept of this HNEnKF is first undertaken here using the Lorenz three-variable system (Lorenz 1963).

The Lorenz three-variable model has served as a testbed for examining the properties of various data assimilation methods when used in systems with strongly nonlinear dynamics (e.g., Evensen and van Leeuwen 2000; Yang et al. 2006; Chin et al. 2007; Auroux and Blum 2008; Pu and Hacker 2009). The data assimilation techniques force a slave simulation towards a master simulation that represents the truth. This is similar to the approach taken by Yang et al. (2006), who extended the nudging approach from a single constant direction to a dynamically evolving direction given by either the bred vector or the singular vector when coupling the slave to the master. The coupling strength (nudging coefficient) necessary to achieve synchronization
between the slave and master simulations was tested over a wide range of values (1 to 100), but without any consideration of the relative size of the nudging term to the physical terms in the model equations and the potential creation of insertion noise. In this present study, several different data assimilation approaches are applied to the slave system. In addition to measuring the resulting error, the smoothness of the slave system is also measured using a new metric.

The general methodology of this HNEnKF is discussed in section 2.2. Section 2.3 describes the Lorenz three-variable model system and the application of the HNEnKF in this system. Section 2.4 introduces the evaluation plan and performance metrics, and the experimental design is discussed in section 2.5. Section 2.6 presents and discusses the results. Conclusions are summarized in section 2.7. The HNEnKF is further explored in a two-dimensional shallow water model in Chapter 3. The investigation of the HNEnKF in Chapters 2 and 3 will set the stage for the implementation of HNEnKF in the three-dimensional Weather Research and Forecasting (WRF) model: its results will be presented in Chapter 4.

2.2. General methodology for the HNEnKF approach

The evolution of a dynamical system can be represented as:

\[
\frac{d\mathbf{x}}{dt} = f(x),
\]

(2.1)

where \( \mathbf{x} \) and \( f \) are the state vector and dynamics function of the system respectively.

Given an observation \( y^a \), the analysis step of the EnKF consists of the following update (Evensen 1994):

\[
\mathbf{x}^a - x^f = \mathbf{K}(y^a - \mathbf{H}x^f),
\]

(2.2)
where \( x^f \) is the model forecast or background, \( x^a \) is the analysis, \( H \) is the observation operator that transforms or interpolates the model forecast variable to the observation variable and location, and \( K \) is the gain matrix of the EnKF. This gain matrix is defined as:

\[
K = BH^T \left( HBH^T + R \right)^{-1},
\]

(2.3)

where \( B \) is the covariance matrix of background errors and \( R \) is the covariance matrix of observation errors.

On the other hand, the basic form of a dynamical data assimilation system using traditional nudging can be written as:

\[
\frac{dx}{dt} = f(x) + G \cdot w \cdot (y^o - Hx),
\]

(2.4)

wherein the time derivative and model physics terms are as in Eq. (2.1) but a new term is added to relax or nudge the model background toward the observations. In Eq. (2.4), \( G \) is the nudging magnitude matrix and \( w \) is the nudging spatial-temporal weighting coefficient used to apply the innovation (observation minus the model background, \( y^o - Hx \)) in observation space and time to the model grid cell and time step. The product of \( G \) and \( w \) is defined here as the nudging coefficient matrix.

The traditional nudging data assimilation scheme uses a nudging coefficient matrix with nonzero diagonal elements and zero off-diagonal elements; thus innovations from one variable do not directly affect the others in the current time step. The nudging term is also kept small compared to the physical term, \( f(x) \), so that the model dynamics still play a major role in the data assimilation. The nudging coefficient matrix is often specified by past experience and experimentation (e.g., Stauffer and Seaman 1994) to emulate the error covariance, the correlation in the error at the observation location with that in a spatial region / temporal window about the observation site / observation time.
Compared to the intermittent data assimilation scheme EnKF, the HNEnKF method introduced here combines the continuous data assimilation of nudging with the flow-dependent weighting of EnKF to achieve a flow-dependent, continuous and gradual data assimilation. The HNEnKF builds the gain matrix of the EnKF into the nudging magnitude matrix (Kalata 1984; Painter et al. 1990), which provides flow-dependent / time-dependent nudging coefficients to the traditional nudging. In other words, the HNEnKF achieves the analysis of the EnKF gradually by combining it with nudging.

For the HNEnKF data assimilation scheme presented here, the nudging magnitude matrix \( G \) in Eq. (2.4) is a function of the EnKF gain matrix. Since the nudging assimilates the observed state gradually via the model tendency equations, the EnKF gain matrix should be modified to be applied to the nudging magnitude matrix. Thus, the nudging magnitude matrix in the HNEnKF method takes the form:

\[
G = t_w K, \tag{2.5}
\]

where \( t_w \) has the units of inverse time and must be made a function of the nudging weighting coefficient \( w \), in order to spread the magnitude of the EnKF gain matrix to every nudging time step. The specific form of \( t_w \) used in this chapter will be discussed in the following section.

Compared to traditional nudging, this HNEnKF takes advantage of ensemble forecasts to obtain a flow-dependent / time-dependent background error covariance matrix that can be used to compute a flow-dependent / time-varying nudging coefficient matrix. The HNEnKF approach can also be used to extend the nudging magnitude matrix to include the inter-variable influence of innovations via nonzero off-diagonal elements. This additional coupling between the observations and the multivariate state may lead to more accurate adjustment of the background to observations than the traditional nudging approach. Therefore, the HNEnKF is an advancement beyond the current capabilities of traditional nudging.
2.3. Model description and methodology for the Lorenz system

As a testbed for data assimilation, the nonlinear Lorenz three-variable model system offers the advantages of computational simplicity and strong nonlinear interactions among variables (Lorenz 1963). The model consists of three coupled and nonlinear ordinary differential equations:

$$\frac{dx}{dt} = \sigma(y - x)$$

$$\frac{dy}{dt} = rx - y - xz$$

$$\frac{dz}{dt} = xy - bz,$$

where the parameters are set to the standard values that produce a chaotic regime: $\sigma=10$, $r=28$, $b=8/3$ (Lorenz 1963).

For the HNEnKF approach, the system (Eq. (2.6)) becomes:

$$\frac{dx}{dt} = \sigma(y - x) + G_{xx} \cdot w \cdot (x^o - x) +$$

$$G_{xy} \cdot w \cdot (y^o - y) + G_{xz} \cdot w \cdot (z^o - z)$$

$$\frac{dy}{dt} = rx - y - xz + G_{yx} \cdot w \cdot (x^o - x) +$$

$$G_{yy} \cdot w \cdot (y^o - y) + G_{yz} \cdot w \cdot (z^o - z)$$

$$\frac{dz}{dt} = xy - bz + G_{zx} \cdot w \cdot (x^o - x) +$$

$$G_{zy} \cdot w \cdot (y^o - y) + G_{zz} \cdot w \cdot (z^o - z),$$

where each $G$ is an element in the nudging magnitude matrix $G$ in Eq. (2.4). In the traditional nudging approach, only the diagonal elements of the nudging magnitude matrix are nonzero. In contrast, for the HNEnKF, all elements of this matrix can be nonzero. Compared to the adaptive
nudging in Yang et al. (2006), here the EnKF gain matrix is used to provide both nudging direction and nudging strength.

For both the traditional nudging method and the HNEnKF methods as applied to the Lorenz three-variable model system, the nudging weighting coefficient \( w \) only varies in time because the model state has no spatial extent. The Stauffer and Seaman (1990) trapezoidal function, as shown in Figure 2.1, is used for this temporal weighting \( w \). In Figure 2.1, \( t \) is the model time, \( t^o \) is the observation time, and \( \tau_N \) is the half-period of the nudging time window. Given \( \tau_N \), \( w \), and the time step \( \Delta t \), the function \( t_w \) in Eq. (2.5) is defined as the inverse of the sum of the nudging temporal weighting coefficient in the half-period of the nudging time window:

\[
t_w = \frac{1}{\sum_{t^o - \tau_N}^{t^o + \tau_N} w \cdot \Delta t}.
\]  

Thus the nudging strength summed from the start of nudging to the observation time equals the EnKF gain. After the observation time, the nudging term usually becomes small and gradually decreases to 0, because the innovation is small due to the fact that nudging is accomplishing its task and the nudging temporal weighting coefficient is decreasing (Figure 2.1).

The general procedures of the HNEnKF are shown in Figure 2.2. The ensemble state contains ensemble members that are used to calculate the hybrid nudging magnitude matrix. The nudging state is a single member that assimilates observations by nudging with the hybrid nudging coefficients. The method for creating the initial conditions of the nudging state and ensemble state is described in section 2.5. Both the ensemble state and nudging state are integrated forward until an observation is available. The observations are denoted by the arrows. When an observation is available, the EnKF gain matrix \( K \) is first computed from the ensemble forecast of the ensemble state, and then the hybrid nudging magnitude matrix \( G(K, t_w) \) is
provided to the nudging state. The nudging state then assimilates the observation via Eq. (2.7) using these hybrid nudging coefficients. The trapezoid around the observation in the nudging state defines the nudging time window. Meanwhile the ensemble state assimilates the observation by the EnKF. After both the nudging state and ensemble state finish assimilating the observation at the observation time, the ensemble members are shifted by the difference between the ensemble mean and the nudging state. This results in a new ensemble state centered on the nudging state. Thus the ensemble spread of the ensemble state has been updated by the EnKF, and the ensemble mean of the ensemble state is defined to be the same as that of the nudging state at the observation time. Finally both the ensemble state and the nudging state are integrated forward simultaneously. This procedure cycles when the next observation becomes available.

2.4. Evaluation plan and performance metrics

We are not aware of any previous studies that provide a metric to quantitatively measure the discontinuities / error spikes resulting from the intermittent data assimilation method EnKF. It is suggested here that the average root-mean-square (RMS) error that is widely used in the data assimilation literature should not be the only measure of success because it may not reflect the model’s retention of data following the assimilation. Thus a new metric is proposed here to quantitatively measure the error spikes / discontinuities following data assimilation.

This metric, defined as the Discontinuity Parameter (DP), is the average absolute value of the RMS error difference between one time step before the observation time and the observation time:

\[ DP = \frac{1}{M} \sum_{i} |RMSE_{i-1} - RMSE_{i}|, \]  

(2.9)
where the RMSE denotes the RMS error, the subscript $i$ represents the time step when an observation is available, and $M$ is the total number of the observation times. Therefore, both the RMS error and DP will be used to evaluate the data assimilation methods, since the RMS error measures the success of a data assimilation method to fit the observations, and the DP measures the error spikes / discontinuities caused by a data assimilation method.

2.5. Experimental design

The truth state is obtained by integrating the equations in (2.6) from a true initial value $(1.508870, -1.531271, 25.46091)$. Observation errors chosen randomly from a Gaussian distribution with mean zero and variance 1.0, are added to the true state (the master) to obtain the simulated observations. The signal to noise ratios\(^1\) of variables $x$, $y$ and $z$ are 62.98, 81.38, and 72.75, respectively. The observations of all three variables are available. The observation frequency for data assimilation is one per 25 time steps by default, and then it is varied to one per 10 and one per 50 time steps as sensitivity experiments. Similarly, adding a random error to the true initial value produces a simulated initial value to emulate the real atmosphere, because the true initial value is unknown in the real atmosphere. This simulated initial value is used as the initial condition of the nudging state as shown in Figure 2.2. By adding random errors from a Gaussian distribution with mean zero and variance 1.0 to the simulated initial value, the initial values for an ensemble are derived. Similarly, these initial values are used as the initial conditions of the ensemble state as shown in Figure 2.2. The ensemble size is set to 100, because the performance of the EnKF saturates quickly as the ensemble size increases in the Lorenz three-variable model system (Chin et al. 2007), and 100 members is the maximum ensemble size used in the sensitivity study of EnKF to the ensemble size in Pu and Hacker (2009). Experiments are

\(^1\) The signal to noise ratio is the variance of the variable divided by its observation error variance.
first performed using a perfect model assumption. Then a stochastic process following Evensen (1997) is added to the model equations to simulate the model error. The model error covariance is defined to be diagonal with variances (2.00, 12.13, 12.31) for the three equations in (2.6) (Evensen 1997; Evensen and van Leeuwen 2000). Both the perfect and imperfect models are integrated in time using a fourth-order Runge-Kutta time difference scheme with a time step $\Delta t = 0.01$. We found that using a smaller time step of 0.001 does not change the results.

To eliminate the effects of start-up transients, the slave Lorenz system from the simulated initial value and the ensemble are integrated for 1000 time steps before beginning to assimilate the observations as in Yang et al. (2006). During the data assimilation phase, the EnKF, EnKS, traditional nudging, IAU and HNEnKF are each integrated for 3500 time steps. The first 500 time steps of the data assimilation cycle are discarded similar to Yang et al. (2006), and then the following 3000 time steps with data assimilation are used for analysis.

The results in the 3000-step period set-up may vary with initial conditions, so a set-up consisting of 100 random initial conditions has also been designed and performed. This set-up chooses 100 initial conditions randomly from the first 1000 time step integration of the true initial value, adds random errors with mean zero and variance 1.0 to the randomly chosen 100 initial conditions respectively, and then assimilates observations by the different data assimilation approaches for 1500 time steps following each initial condition. The first 500 time steps of data assimilation are again discarded, and then the following 1000 time steps of data assimilation are used for analysis.

The experimental design used for the 3000-step period set-up and the 100 random initial conditions set-up with both the perfect and imperfect models is shown in Table 2.1. The CTRL integrates the model forward without assimilating any observations. The following two experiments assimilate the observations by the EnKF and EnKS respectively. In the traditional nudging approach, the diagonal elements of $G$ are set to 10.0 (Yang et al. 2006). The IAU
method assimilates the observations using the traditional IAU, in which the IAU interval is the same as the analysis interval and the analysis increment is the difference between the observation and the model forecast (Bloom et al. 1996). The last two experiments assimilate the observations by the HNEnKF with diagonal elements (HNEnKF-D) and all elements of the hybrid nudging magnitude matrix (HNEnKF-A) respectively. Experiment HNEnKF-D is closer to the traditional nudging (Experiment Nudging), since neither of them have inter-variable influence of innovations via nonzero off-diagonal elements of the nudging magnitude matrix. The average RMS errors of the CTRL and the six data assimilation experiments compared to the truth in the 3000-step period set-up are calculated with all three variables at each time step. They are similarly computed for the 100 random initial conditions set-up that has a 1000-step period for each initial condition. Additionally, the new metric DP, which measures the error spikiness, is also computed for the two set-ups.

2.6. Results

2.6.1 Comparison of the HNEnKF with and without off-diagonal elements

The differences between the HNEnKF with only the diagonal elements of the hybrid nudging magnitude matrix and the HNEnKF with all elements of the hybrid nudging magnitude matrix are first explored. The average RMS errors of CTRL using no data assimilation, traditional nudging and the two HNEnKF approaches during the 3000-step period using both the perfect and imperfect model are shown in Figure 2.3. The traditional nudging and HNEnKF approaches produce much smaller average RMS errors than the CTRL. Thus the results of CTRL will not be shown in the following discussions. Compared to the HNEnKF with all elements of the hybrid nudging magnitude matrix (Experiment HNEnKF-A), the HNEnKF with only diagonal
elements of the hybrid nudging magnitude matrix (Experiment HNEnKF-D) produces results closer to the traditional nudging. Nonetheless, the HNEnKF-D has smaller average RMS errors than the traditional nudging. This suggests that there is some advantage to using flow-dependent / time-dependent background error covariance from the ensemble forecast to provide the nudging coefficients. Moreover, the HNEnKF-A has even lower average RMS errors than the HNEnKF-D. Thus the effectiveness of the HNEnKF-A to extend the nudging magnitude matrix to include inter-variable influences via nonzero off-diagonal elements is also demonstrated. This additional coupling from the inter-variable (off-diagonal) statistics leads to more accurate adjustment of background to the observation than does the traditional nudging method.

To further demonstrate the effectiveness of the HNEnKF using flow-dependent / time-dependent background error covariance from the ensemble forecast to provide the hybrid nudging coefficients, the average values of the hybrid nudging coefficients of the two HNEnKF approaches are shown in Figure 2.4. The diagonal hybrid nudging coefficients are smaller and within an order of magnitude of the traditional nudging coefficients. For Experiment HNEnKF-A (Figure 2.4b), the diagonal nudging coefficients are generally larger than the off-diagonal ones, and the off-diagonal coefficients relating to z are much smaller than those off-diagonal elements of x and y. These findings are consistent with the results of Yang et al. (2006). Also note that the off-diagonal terms can be negative because they are not really nudging terms because the off-diagonal corrections do not directly involve the predictive variable of the equation. Thus, the utility of the EnKF gain matrix to provide time-dependent information to the hybrid nudging coefficients has been demonstrated.

From the discussions above, the HNEnKF schemes have the flow-dependent / time-dependent hybrid nudging coefficients computed from the ensemble forecast. The HNEnKF-A experiment extends the nudging coefficients to non-zero off-diagonal elements and produces smaller average RMS error compared to HNEnKF-D. Therefore, the focus will be on HNEnKF-
2.6.2. Sensitivity of the data assimilation methods to observation frequency

In addition to comparing the results from Experiment HNEnKF to other data assimilation approaches in Experiments Nudging, IAU, EnKF and EnKS, the sensitivity of these data assimilation approaches to observation frequency is studied. The comparisons among these data assimilation approaches may vary due to different observation frequencies, since the ensemble spread has different time scales to grow given the different observation frequencies and the nudging may have difficulties adjusting to the evolving state with more frequent observations. The default observation frequency used in section 2.6.1 is one per 25 time steps. The other observation frequencies used here are one per 10 time steps and one per 50 time steps. The effects of the different data assimilation schemes (Table 2.1) with different observation frequencies are investigated here within the 3000-step period set-up.

Figure 2.5a shows the average RMS errors over all time steps for each data assimilation method with different observation frequencies under the perfect model assumption. As discussed earlier, the average RMS error is not the only measurement of success for a dynamic analysis, because it may not best reflect the error spikes or temporal smoothness of the data assimilation. As defined in section 2.4, the DP for this group of experiments is also computed, and it is shown in Figure 2.5b.

Experiment HNEnKF produces lower RMS errors than Experiment Nudging and IAU for all three observation frequencies, especially when the observation frequency is one per 50 time steps. Thus the use of flow-dependent / time-dependent nudging coefficients appears to be helpful in reducing the RMS error when the observations are sparse in time. Although
Experiment HNEnKF has somewhat larger RMS errors than Experiments EnKF and EnKS, Experiment HNEnKF has closer and similar values of DP to the EnKS and has much smaller values of DP than the intermittent EnKF. The continuous data assimilation experiments, EnKS, Nudging, IAU, and HNEnKF, have fewer / smaller discontinuities than the intermittent data assimilation experiment EnKF. Therefore, the HNEnKF combines the advantages of Nudging and EnKF, because it produces smaller RMS errors than the traditional nudging and has better values of DP than the EnKF.

Figure 2.6 shows the average RMS error and DP for each data assimilation method for the three different observation frequencies within the 3000-step period set-up using an imperfect model (see section 2.5). The IAU becomes unstable after adding model errors, so its results are not shown. Bergemann and Reich (2010) also report instability problems with their hybrid IAU method over long data assimilation cycles. Experiment HNEnKF produces lower average RMS errors than traditional nudging, which is similar to the result in the perfect model. The HNEnKF produces similar average RMS errors to the EnKF and EnKS when the observation frequency is one per 10 time steps and one per 25 time steps, but somewhat larger average RMS error for one per 50 steps. One reason that the HNEnKF has somewhat larger average RMS error than the EnKF and EnKS with observation frequency of one per 50 time steps may be: in this highly nonlinear Lorenz three-variable model system, the nudging may not perform well when the system is at transitions², since the model state may evolve too quickly to be corrected by the gradual nudging forcing within the nudging time window. However, as shown in Figure 2.6b, the HNEnKF has lower values of DP than the EnKF, suggesting smaller discontinuities than the EnKF. Moreover, the HNEnKF has similar or even better DP than the EnKS when the model is imperfect.

² The “transitions” mean the locations that are very sensitive to error, where a small amount of error may lead the model state to a different fixed point.
To ensure the EnKF and HNEnKF function properly, the ensemble spread is compared to the forecast error in the EnKF. The ensemble forecast spread and forecast RMS error of the ensemble mean are computed at the observation time but before assimilating the observation. When the observation frequency is one per 25 time steps, the ensemble spread and forecast error are computed every 25 time steps, and their comparisons are shown in Figure 2.7. For both perfect and imperfect models, the ensemble spread generally agrees with the forecast error, although the ensemble spread has more variance with the forecast error when the model error is introduced. Generally, the ensemble spread is linearly correlated with the forecast error and the slope of the “best-fit” line is approximately 1. Similar results are obtained for the other observation frequencies (not shown). We conclude that the ensemble spread provides a reasonable estimate of the forecast error in the EnKF and HNEnKF experiments, and therefore, the EnKF functions with proper ensemble spread.

As discussed in this section, with a perfect model the HNEnKF produces smaller RMS errors than the traditional nudging, although it has somewhat larger RMS errors than the EnKF. Moreover, the HNEnKF has much smaller values of DP than the EnKF, and closer values of DP to the EnKS. When model error is introduced, the HNEnKF produces similar RMS errors to the EnKF except when the observation frequency is one per 50 time steps, and it also has much lower values of DP than the EnKF. Therefore, the HNEnKF is able to retain the advantages of the EnKF and produce better temporal smoothness, although it sometimes has somewhat larger RMS errors than the EnKF.

2.6.3. Sensitivity of the data assimilation methods to initial conditions

Results in sections 2.6.1 and 2.6.2 are based on a 3000-step period set-up as in Yang et al. (2006). However, the results may vary over different periods and different initial conditions. So
a statistical set-up with 100 random initial conditions is performed for both perfect and imperfect
models in this section as described in section 2.5.

Table 2.2 and Table 2.3 show the average RMS error and DP of the different data
assimilation schemes with the default observation frequency in the 100 random initial conditions
set-up for the perfect model experiment. As shown by Table 2.2, Experiment HNEnKF under the
perfect model assumption produces smaller average RMS errors than traditional nudging and
IAU, but larger average RMS errors than the EnKF and the EnKS. A paired Student t-test is
performed to examine if the average RMS errors are significantly different among the data
assimilation methods. The null hypothesis is that the two data assimilation methods produce the
same average RMS error. A p-value, which is the probability of observing a value at least as
extreme as the test statistic under the null hypothesis, less than 0.05 rejects the null hypothesis,
indicating that the average RMS error of the data assimilation method in the row is significantly
different from that of the data assimilation method in the column. The results of the paired
Student t-test of the average RMS error are also shown in Table 2.2. The differences among the
data assimilation methods are all significant. The Nudging, IAU, HNEnKF and EnKS
experiments have significantly better DP than the intermittent data assimilation method EnKF
(Table 2.3). Moreover, the HNEnKF has slightly better, but significantly different DP, than the
EnKS as shown in Table 2.3.

Table 2.4 and Table 2.5 are the same as Table 2.2 and Table 2.3 except that the results are
for the imperfect model. As mentioned in section 2.6.2, the IAU becomes numerically unstable
when model error is introduced, so its results are not shown. The HNEnKF produces slightly
smaller but significantly different average RMS error than either Nudging or EnKF, although it
has larger average RMS error than the EnKS (Table 2.4). Moreover, Table 2.5 indicates that the
HNEnKF has much smaller values of DP than the EnKF and slightly smaller but significantly
different values of DP than the EnKS, while the traditional nudging experiment (Nudging)
produces the best values of DP. Therefore, the results obtained in the 100 random initial conditions set-up are generally consistent with those in the 3000-step period set-up. Moreover, the results from this section based on the paired Student t-test with a 95% confidence level demonstrate that the conclusions from the 3000-step period set-up are generally valid.

### 2.6.4. Nudging coefficients constraints

The underlying assumption for nudging, as stated by Stauffer and Seaman (1990; 1994), is that the nudging terms should be constrained to be smaller than the model’s physical terms in order to retain the physical properties and dynamic balance / inter-variable consistency of the system. For this highly nonlinear Lorenz three-variable model system, the nudging terms may need to be larger when the system is at transitions. The synchronization of the master (truth run) with the slave (model with coupling / nudging terms) in Yang et al. (2006), using a coupling strength that varies from 1 to 100, may violate this assumption. Thus the nudging coefficient constraints for the HNEnKF are investigated further here.

Figure 2.8 shows the average ratios of the nudging terms over the sum of the physical terms in each equation in the 3000-step period set-up of HNEnKF under the perfect model assumption. The ratio of the y nudging term in the y-equation is 0.13 which is slightly larger than 0.1 (an order of magnitude difference in the magnitudes of the nudging term and physical terms). The other nudging terms have ratios smaller than 0.1.

Thus Experiment HNEnKF is generally able to make small and effective innovations to the model background to correct the model trajectory, as shown by the smaller average RMS errors compared to the Experiment Nudging. It can also minimize the insertion noise and produce smaller (better) DP compared to the EnKF. Any nudging-type approach, including our HNEnKF should consider the magnitude of the nudging terms relative to the physical forcing.
terms, so that dynamic balance and consistency are retained in addition to reducing the RMS errors compared to the truth state. Hollingsworth et al. (1986) discussed a similar criterion, which requires the magnitude of the analysis increment to be smaller than that of the forecast increment.

2.6.5. Computational efficiency

The HNEnKF experiment is shown to produce similar or slightly better average RMS errors to the EnKF for the imperfect model but better DP than the EnKF in general. It also produces similar or even better values of DP compared to the gold standard EnKS. However, the EnKS is much more CPU-intensive than the HNEnKF, and also requires greater storage proportional to the total number of analysis times over which the statistics are to be applied. Although all the EnKF, HNEnKF and EnKS experiments have an ensemble forecast that is more expensive than a single model run as used in Experiments Nudging and IAU, the EnKS applies future observations backward to the initial time, which adds even more computational cost for calculating the temporal error correlations compared with the EnKF and HNEnKF. This is also the reason that the EnKS requires greater storage than the EnKF and HNEnKF - the ensemble spread at each analysis time (here every time step) needs to be stored and is used to compute the temporal error correlations.

Table 2.6 shows the CPU time cost of the various data assimilation schemes with the default observation frequency in the 100 random initial conditions set-up. The Nudging and IAU experiments have the smallest CPU time cost, because they do not include an ensemble forecast. The HNEnKF has similar CPU time cost to the EnKF, but the EnKS has a CPU time cost more than 200 times that of the EnKF and HNEnKF. Thus the HNEnKF produces somewhat larger average RMS error than the EnKS and similar or better DP to the EnKS, but with substantially reduced CPU time and storage costs.
2.7. Conclusions

A new hybrid nudging-EnKF (HNEnKF) data assimilation approach that produces time-continuous, seamless dynamic analyses over a fixed period is explored here using the Lorenz three-variable system with both perfect and imperfect models. The HNEnKF approach allows the EnKF to be applied gradually in time via nudging-type terms. The flow-dependent, time-varying error covariance matrix is used to compute the nudging coefficients rather than using ad hoc values derived from theory and experience. The HNEnKF using all elements of the nudging magnitude matrix produces better results than the HNEnKF using only the diagonal elements of the nudging magnitude matrix, because it allows for greater inter-variable influences from the data assimilation via the nonzero off-diagonal elements of the nudging magnitude matrix.

The HNEnKF approach promotes a better fit to the data compared to traditional nudging or IAU while also minimizing the error spikes or bursts created by intermittent assimilation methods such as the EnKF. When model error is introduced, the HNEnKF still produces lower average RMS errors than the traditional nudging and closer or better average RMS errors compared to the EnKS and EnKF respectively. The ensemble spread provides a reasonable estimate of the forecast error in the EnKF and HNEnKF experiments. The HNEnKF also produces better DP than the EnKF and even better DP than the EnKS. The EnKS, as the gold standard, is much more computationally expensive and has larger storage requirements. The EnKS requires more than 200 times more CPU time than the EnKF and HNEnKF used in this study.

Although the HNEnKF is comparable in cost to the EnKF, it offers a gradual, continuous assimilation of the data with better inter-variable consistency, improved temporal smoothness, and reduced noise levels between the observation times compared to the EnKF. The hybrid nudging terms in the HNEnKF are on average an order of magnitude smaller than the physical
terms in all three equations. Any nudging-type approach should not use nudging terms that are relatively large compared to the physical forcing terms, so that dynamic balance and consistency are retained in addition to reducing the RMS errors compared to the truth state.

The advantages of the HNEnKF demonstrated in the Lorenz three-variable system motivated us to further explore this HNEnKF approach in a more realistic two-dimensional shallow-water model system in Chapter 3. Building on the encouraging results obtained from Chapters 2 and 3 using simplified models, we will apply the HNEnKF to the three-dimensional WRF model. The results will be presented in Chapter 4.
Table 2.1. Experimental design.

<table>
<thead>
<tr>
<th>Exp. Name</th>
<th>Exp. Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CTRL</td>
<td>Assimilate no observations</td>
</tr>
<tr>
<td>EnKF</td>
<td>Assimilate observations by ensemble Kalman filter</td>
</tr>
<tr>
<td>EnKS</td>
<td>Assimilate observations by ensemble Kalman smoother</td>
</tr>
<tr>
<td>Nudging</td>
<td>Assimilate observations by traditional nudging (diagonal terms only in Eq. (2.7) with nudging coefficients of 10)</td>
</tr>
<tr>
<td>IAU</td>
<td>Assimilate observations by incremental analysis update</td>
</tr>
<tr>
<td>HNEEnKF-D</td>
<td>Assimilate observations by hybrid nudging-EnKF with diagonal elements only of the hybrid nudging magnitude matrix</td>
</tr>
<tr>
<td>HNEEnKF-A</td>
<td>Assimilate observations by hybrid nudging-EnKF with all elements of the hybrid (HNEEnKF) nudging magnitude matrix</td>
</tr>
</tbody>
</table>
Table 2.2. The average RMS error in the 100 random initial conditions set-up for the data assimilation methods described in Table 2.1 with the default observation frequency (one per 25 time steps) for the perfect model. + denotes there is significant difference; - denotes there is no significant difference.

<table>
<thead>
<tr>
<th></th>
<th>EnKF</th>
<th>EnKS</th>
<th>Nudging</th>
<th>IAU</th>
<th>HNEnKF</th>
</tr>
</thead>
<tbody>
<tr>
<td>EnKF</td>
<td>0.84</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
</tr>
<tr>
<td>EnKS</td>
<td>0.48</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
</tr>
<tr>
<td>Nudging</td>
<td>2.70</td>
<td>+</td>
<td>+</td>
<td></td>
<td></td>
</tr>
<tr>
<td>IAU</td>
<td></td>
<td></td>
<td></td>
<td>1.66</td>
<td>+</td>
</tr>
<tr>
<td>HNEnKF</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1.54</td>
</tr>
</tbody>
</table>
Table 2.3. The same as Table 2.2, except for the DP.

<table>
<thead>
<tr>
<th></th>
<th>EnKF</th>
<th>EnKS</th>
<th>Nudging</th>
<th>IAU</th>
<th>HNEnKF</th>
</tr>
</thead>
<tbody>
<tr>
<td>EnKF</td>
<td>0.74</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
</tr>
<tr>
<td>EnKS</td>
<td>0.20</td>
<td>+</td>
<td>-</td>
<td>+</td>
<td></td>
</tr>
<tr>
<td>Nudging</td>
<td>0.22</td>
<td>-</td>
<td></td>
<td>+</td>
<td></td>
</tr>
<tr>
<td>IAU</td>
<td></td>
<td></td>
<td></td>
<td>0.20</td>
<td>+</td>
</tr>
<tr>
<td>HNEnKF</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.16</td>
</tr>
</tbody>
</table>
Table 2.4. The same as Table 2.2, except for the imperfect model.

<table>
<thead>
<tr>
<th></th>
<th>EnKF</th>
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<th>Nudging</th>
<th>IAU</th>
<th>HNEEnKF</th>
</tr>
</thead>
<tbody>
<tr>
<td>EnKF</td>
<td>2.73</td>
<td>+</td>
<td>-</td>
<td></td>
<td>+</td>
</tr>
<tr>
<td>EnKS</td>
<td>1.87</td>
<td>+</td>
<td></td>
<td></td>
<td>+</td>
</tr>
<tr>
<td>Nudging</td>
<td>3.01</td>
<td>+</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>IAU</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HNEEnKF</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2.64</td>
</tr>
</tbody>
</table>
Table 2.5. The same as Table 2.4, except for the DP.

<table>
<thead>
<tr>
<th></th>
<th>EnKF</th>
<th>EnKS</th>
<th>Nudging</th>
<th>IAU</th>
<th>HNEEnKF</th>
</tr>
</thead>
<tbody>
<tr>
<td>EnKF</td>
<td>2.96</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td></td>
</tr>
<tr>
<td>EnKS</td>
<td>0.58</td>
<td>+</td>
<td></td>
<td>+</td>
<td></td>
</tr>
<tr>
<td>Nudging</td>
<td>0.36</td>
<td></td>
<td></td>
<td></td>
<td>+</td>
</tr>
<tr>
<td>IAU</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HNEEnKF</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.50</td>
</tr>
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</table>
Table 2.6. Total CPU time cost of different data assimilation schemes with the default observation frequency in the 100 initial conditions set-up.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>EnKF</th>
<th>EnKS</th>
<th>Nudging</th>
<th>IAU</th>
<th>HNEEnKF</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU Time</td>
<td>16</td>
<td>3414</td>
<td>4</td>
<td>5</td>
<td>16</td>
</tr>
</tbody>
</table>

(see)
Figure 2.1. The temporal weighting function $w$ of nudging, where $t$ is the model time, $t^o$ is the observation time and $\tau_N$ is the half period of nudging time window (after Stauffer and Seaman 1990).
Figure 2.2. Schematic showing the procedures of the hybrid nudging-EnKF approach. The trapezoid around the observation denotes the temporal nudging weighting function over the nudging time window.
Figure 2.3. The average RMS errors for the 3000-step dynamic-analysis period set-up for the control run without data assimilation, traditional nudging, and two kinds of hybrid nudging-EnKF approaches described in Table 2.1 for (a) perfect model and (b) imperfect model.
Figure 2.4. The average hybrid nudging coefficients in the 3000-step period set-up in each equation for (a) Experiment HNEnKF-D, (b) Experiment HNEnKF-A. The dashed line denotes the magnitude of the nudging coefficient used in the traditional nudging approach.
Figure 2.5. The average performance metrics over the 3000-step dynamic-analysis period set-up for the different data assimilation methods described in Table 2.1 with various observation frequencies of one per 10 time steps (OF10), one per 25 time steps (OF25), and one per 50 time steps (OF50), under a perfect model assumption for (a) RMS error and (b) DP. Smaller values are more desirable for both metrics.
Figure 2.6. Same as Figure 2.5, except for the imperfect model.
Figure 2.7. The ensemble spread and error of the 3000-step period setup using an observation frequency one per 25 time steps. (a) perfect model and (b) imperfect model.
Figure 2.8. The average ratios of the hybrid nudging terms in each equation compared to the sum of the physical terms for the 3000-step period set-up for Experiment HNEnKF. The dashed line denotes a ratio of 0.1, where the nudging term is an order of magnitude smaller than the sum of the physical forcing terms.
Chapter 3

A Hybrid Nudging-Ensemble Kalman Filter Approach to Data Assimilation: Application in a Shallow Water Model

3.1. INTRODUCTION

Data assimilation is critical for providing the best possible analysis and improving model forecasts. The ensemble Kalman filter (EnKF), first proposed by Evensen (1994), has become a popular data assimilation method for atmospheric applications (e.g., Houtekamer and Mitchell 1998; Anderson 2001; and Whitaker and Hamill 2002), where it is able to provide a flow-dependent estimate of the background error covariances used to determine the weights of the observations within a data-assimilation analysis. However, the EnKF, an intermittent data assimilation scheme, performs a data-assimilation analysis at each observation time and switches back to a standard model integration between analysis times. This cycle of a model integration period, analysis step, and then another model integration period often causes discontinuities / error spikes around the observation times (e.g., Hunt et al. 2004).

Discontinuities in the analyses produced by intermittent data assimilation approaches may be related to dynamic imbalances caused by intermittent insertion of observations into the model background. In the EnKF study of Fujita et al. (2007), the discontinuities of errors across the analysis step are shown to occur when hourly surface observations are assimilated into the model background. A logical question is whether their reported RMS wind errors, increasing through the 6-h assimilation period, reflect in some way the enhanced divergence related to gravity-wave activity caused by the hourly updates. There are also discontinuities reported in the forward and backward Kalman filter analyses as discussed in Juckes and Lawrence (2009).
Duane et al. (2006) also found the Kalman filter algorithm to have some “desynchronization bursts” at times of regime transitions between the Lorenz and “reversed Lorenz” phases.

The intermittent spikes or bursts within a dynamic analysis caused by the EnKF can have negative consequences when the analyses are used for subsequent numerical weather prediction (NWP) or other model-data applications. Time-continuous, seamless meteorological fields are important for diagnostic dynamic studies (e.g., Rife et al. 2010; Monaghan et al. 2010) and especially for air-quality and atmospheric-chemistry modeling (e.g., Stauffer et al. 2000; Tanrikulu et al. 2000; Otte 2008a, b). The accumulated errors and discontinuities in the meteorological fields may adversely affect atmospheric transport and dispersion and source characterization. Improved and seamless meteorological conditions (wind, stability, convective processes, boundary layer depth, etc.) can improve the accuracy of atmospheric transport and dispersion simulations (e.g., Deng et al. 2004).

To take advantage of the flow-dependent and time-dependent error covariances of the EnKF while reducing its intermittent assimilation noise, a hybrid nudging-EnKF (HNEnKF) approach was proposed and tested in the Lorenz three-variable system (Chapter 2). Our hypothesis is that if the EnKF is applied gradually in time, a continuous and seamless dynamic analysis can be produced. The HNEnKF effectively combines the ensemble data assimilation characteristics of the EnKF and the gradual, continuous adjustments towards observations of the nudging to achieve a temporally smoother data assimilation, resulting in dynamic analyses with better inter-variable consistency and dynamic balance.

Nudging, which has been widely used in NWP applications (e.g., Colle and Mass 2000a, b; Schroeder et al. 2006; Deng et al. 2004; Otte 2008a, b; Dixon et al. 2009; Ballabrera-Poy et al. 2009), is a continuous data assimilation scheme designed to be applied every time step of an assimilation cycle, allowing corrections to be made gradually within a time window around the observation times (Stauffer and Seaman 1990, 1994). Thus, all data can have their maximum
impact at their individual observation times, rather than being artificially collected to a single synoptic time. In addition to directly modifying model fields towards observations, nudging is also being used to modulate the model fields according to the observations in an indirect way. Pleim and Gillian (2009) nudged soil moisture and deep soil temperature according to the biases in 2-m air temperature and relative humidity between the model and observation-based analyses. Dixon et al. (2009) used latent heat nudging to assimilate radar-derived surface precipitation rates and cloud nudging to assimilate moisture fields derived from satellite, radar and surface observations. Ballabrera-Poy et al. (2009) used nudging to constrain the evolution of the fast variables to their observations and the local ensemble transform Kalman filter to initialize the slow variables, since the spurious covariances from the fast variables degrade the performance of the data assimilation. However, nudging is often used with ad hoc nudging coefficients and spatial weighting functions based on past experience and experimentation (e.g., Stauffer and Seaman 1990, 1994). To overcome this drawback, parameter-estimation approaches have been explored to optimally determine the nudging coefficients (Zou et al. 1992; Stauffer and Bao 1993), but they have not been developed adequately for real-case applications. We hypothesize that the HNEnKF offers a more practical nudging-type solution for shallow water and more complex mesoscale models by using the flow-dependent and time-dependent weighting functions computed from the gain matrix of the EnKF.

As introduced in Chapter 2, the HNEnKF approach takes advantage of the ensemble forecast to obtain a flow-dependent / time-dependent background error covariance matrix that can be used to compute flow-dependent and time-varying nudging coefficients. The HNEnKF can also extend the nudging magnitude matrix to include the inter-variable influence of innovations via nonzero off-diagonal matrix elements. This additional coupling between the observations and the multivariate state is able to lead to more accurate adjustment of the background to observations than the traditional nudging approach. Moreover, the HNEnKF, using nudging-type
terms to apply the EnKF gradually in time, provides an analysis with better temporal smoothness than that from the EnKF.

The HNEnKF data assimilation approach was first evaluated in the Lorenz three-variable system in Chapter 2, because this model often has served as a testbed for examining the properties of various data assimilation methods in simple yet strongly nonlinear dynamical systems (e.g., Evensen and van Leeuwen 2000; Yang et al. 2006; Chin et al. 2007; Auroux and Blum 2008; Pu and Hacker 2009). It was found that the HNEnKF promoted a better fit of an analysis to data compared to that produced solely by nudging. The HNEnKF provided a continuous data assimilation with better inter-variable consistency and improved temporal smoothness than that of the EnKF, since it minimized the error spikes / discontinuities created by the intermittent EnKF. Because the HNEnKF showed encouraging results in the Lorenz system as presented in Chapter 2, its effectiveness is evaluated in a more physically realistic model. Thus the HNEnKF is applied here in a two-dimensional (2D) shallow water model where the dynamic imbalances caused by the insertion noise common in intermittent data assimilation methods can be assessed more thoroughly. This work serves as a logical next step for the HNEnKF before its application to real data in a full-physics, three-dimensional mesoscale model such as the Weather Research and Forecasting (WRF) model (Skamarock et al. 2008).

An observation system simulation experiment (OSSE) is conducted here to explore the performance of the HNEnKF in the 2D shallow water model. A quasi-stationary wave case and a moving vortex case are used to compare nudging, EnKF and HNEnKF. Their sensitivities to observation frequency, observation network (data density) and ensemble size are explored, because these attributes vary across the real data atmospheric applications. An investigation of the dynamic balance following data insertion is conducted by calculating the evolution of the ageostrophic wind in the analyses from the different data assimilation methods. In this way, we
are also able to quantitatively assess the dynamic imbalance / discontinuities caused by intermittent data insertion compared to continuous data assimilation methods.

A fourth data assimilation method, the ensemble Kalman smoother (EnKS), which was considered the “gold standard” in Chapter 2, is also applied here. The EnKS, an extension of EnKF, uses the solution of the EnKF as a first guess analysis, and then applies later observations backward in time using the ensemble variances (Evensen and van Leeuwen 2000). However, as discussed in Chapter 2, the EnKS is much more CPU-intensive than the EnKF and HNEnKF, and also requires much greater storage proportional to the total number of analysis times over which the statistics are to be applied. Thus, to reduce the CPU and storage requirements of the EnKS, we use a lagged version of the EnKS that assumes the time correlation in the ensemble statistics approaches zero over a certain time interval. While still impractical for most realistic meteorological applications, the EnKS provides a benchmark for the methods described here.

The methodology of the HNEnKF is reviewed in section 3.2. Section 3.3 describes the model setup and experiment design, in which the model description, initial conditions, simulated observations, verification data and metrics, and ensemble error covariance inflation and localization are presented. The results are discussed in section 3.4. Section 3.5 explores the dynamic balance and temporal smoothness of the HNEnKF and EnKF analyses. The computational efficiency of the data assimilation methods is discussed in section 3.6. Conclusions are summarized in section 3.7.

3.2. Methodology for the HNEnKF approach

To apply the EnKF continuously rather than only at the analysis times, the HNEnKF approach combines the EnKF (Evensen 1994; Houtekamer and Mitchell 1998) and observation nudging (Stauffer and Seaman 1990; 1994). A schematic of the HNEnKF approach is shown
in Figure 2.2 of Chapter 2. We start with an ensemble of N background forecasts that will be updated by the EnKF (called the “ensemble state”), and a single forecast that will be updated by the hybrid nudging-type terms (called the “nudging state”). The following five steps are repeated for each data assimilation cycle: 1) Compute the hybrid nudging coefficients using the ensemble forecast via the EnKF algorithm. 2) Integrate the nudging state by continuously applying nudging with the hybrid nudging coefficients. 3) Update each ensemble member of the ensemble state using the EnKF. 4) Re-define the ensemble mean to be the analysis of the nudging state by re-centering the ensemble around the nudging state at the observation time while retaining the ensemble spread. 5) Integrate the ensemble state and the nudging state forward to the next observation time.

The nudging scheme adds non-physical relaxation terms into the governing model equations. The full set of model equations is then used to nudge the model state towards the observation state gradually, as shown by Eq. (3.1):

\[
\frac{dx}{dt} = f(x) + G \cdot w_s \cdot w_t \cdot (y^o - Hx),
\]  

(3.1)

where \(x\) and \(f\) are the state vector and standard forcing function of the system, \(y^o\) is the observation vector, \(H\) is the observation operator that transforms or interpolates the model variable to the observation variable and location, \(G\) is the nudging magnitude matrix, and \(w_s\) and \(w_t\) are the spatial and temporal nudging weighting coefficients. The difference between the observed and modeled states, \(y^o - Hx\), is called the innovation. The coefficients \(w_s\) and \(w_t\) are used to map the innovation, defined in observation space and time, to the model grid cell and time step. The nudging coefficient is defined here as the product of \(G\), \(w_s\) and \(w_t\).

The relative intensity with which an innovation of a given variable affects the tendencies of the model’s predictive variables is controlled by the elements of the nudging magnitude matrix.
In most nudging applications the innovation of a particular variable can influence only the tendency of that variable; hence only the diagonal matrix elements are nonzero while all off-diagonal elements are zero. The nonzero diagonal elements are usually specified by past experience and experimentation (e.g., Stauffer and Seaman 1994). Here, the flow-dependent hybrid nudging coefficients, computed from the ensemble forecast, are elements of the EnKF gain matrix multiplied by a function of the temporal nudging weighting coefficient. The flow-dependent hybrid nudging coefficient is then described by Eq. (3.2):

\[ G \cdot w_s = t_{w_t} \cdot K, \]

(3.2)

where \( t_{w_t} \) is a function of the temporal nudging weighting coefficient and \( K \) is the EnKF gain matrix.

The function \( t_{w_t} \) in Eq. (3.2) has the units of inverse time to make the units of the hybrid nudging coefficient inverse time as required for nudging. The magnitude of the EnKF gain matrix is applied every time step within the nudging time window to the innovation terms in the model tendency equations. The function \( t_{w_t} \) used here is defined as the sum of the temporal nudging weighting coefficient over half of the assimilation time window, as described by:

\[ t_w = 1/\left( \sum_{t^o - \tau_N}^{t^o} w_t \cdot \Delta t \right). \]

(3.3)

In Eq. (3.3), \( \Delta t \) is the time step, \( t \) is the model time, \( t^o \) is the observation time, and \( \tau_N \) is the half-period of the nudging time window. The temporal nudging weighting coefficient \( w_t \) is the same as that used in Chapter 2, following the trapezoidal function defined by Stauffer and Seaman (1990).

As stated above, the \( K \) in Eq. (3.2) is the EnKF gain matrix, defined as:

\[ K = B H^T \left( H B H^T + R \right)^{-1}, \]

(3.4)
where $B$ is the covariance matrix of background errors, $H$ is the transformation or interpolation operator, and $R$ is covariance matrix of observation errors.

Thus the HNEnKF method takes advantage of ensemble forecasts and its flow-dependent background error covariances to provide flow-dependent nudging coefficients. It also extends the nudging magnitude matrix from having nonzero diagonal elements and zero off-diagonal elements to being a full nonzero matrix. The effectiveness and added value of the HNEnKF with nonzero off-diagonal elements compared to the HNEnKF with diagonal elements only was demonstrated in Chapter 2. Therefore, the HNEnKF using the full nonzero matrix from the EnKF will be applied and investigated further here in the more realistic shallow water model.

3.3. Model setup and experimental design

The shallow water model system is described in this section, followed by a description of the initial conditions for the wave case and vortex case used to investigate the HNEnKF approach. The so-called truth states and simulated observations for both cases are also presented, along with the verification data and evaluation metrics. A summary of the experiments and their design details including the ensemble design, number of ensemble members, and data assimilation parameter settings such as traditional nudging weights, radius of influence, and EnKF error covariance localization and inflation are also presented.

3.3.1. Model description

The barotropic nonlinear shallow-water equations with the hybrid nudging-EnKF terms take the following form:
\[
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} - f v = -g \frac{\partial h}{\partial x} + \kappa \nabla^2 u + \\
G_{uu} \cdot w_t \cdot (u^o - u) + G_{uv} \cdot w_t \cdot (v^o - v) + G_{uh} \cdot w_t \cdot (h^o - h)
\]

\[
\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + f u = -g \frac{\partial h}{\partial y} + \kappa \nabla^2 v + \\
G_{vu} \cdot w_t \cdot (u^o - u) + G_{vv} \cdot w_t \cdot (v^o - v) + G_{vh} \cdot w_t \cdot (h^o - h) \tag{3.5}
\]

\[
\frac{\partial h}{\partial t} + u \frac{\partial h}{\partial x} + v \frac{\partial h}{\partial y} = -h \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) + \kappa \nabla^2 h + \\
G_{hu} \cdot w_t \cdot (u^o - u) + G_{hv} \cdot w_t \cdot (v^o - v) + G_{hh} \cdot w_t \cdot (h^o - h)
\]

\[0 \leq x \leq L, \quad 0 \leq y \leq D,\]

where \( u \) and \( v \) are the velocity components in the \( x \) and \( y \) directions, \( h \) is the depth of the fluid, \( g \) is the acceleration of gravity, \( f \) is the Coriolis parameter, \( \kappa \) is the diffusion coefficient, \( L \) and \( D \) are the dimensions of the rectangular domain of integration, and each \( G \) with subscripts \( u, v, \) or \( h \) is an element in the product of the nudging magnitude matrix \( G \) and spatial nudging weighting coefficient \( W_s \) in Eq. (3.1). The Coriolis parameter \( f \) is defined as constant \( 10^{-4} \text{ s}^{-1} \) in an \( f \)-plane approximation. The diffusion coefficient \( \kappa \) is specified as \( 10^4 \text{ m}^2\text{s}^{-1} \).

The shallow water model equations (3.5) are integrated forward on a C-grid (Arakawa and Lamb 1977), which is used by many mesoscale models including the WRF model (Skamarock et al. 2008). The domain dimensions \( L \) and \( D \) are set to 500 km and 300 km in the \( x \) and \( y \) directions respectively. The grid dimensions are \( 52 \times 31 \) using 10 km grid spacing in both directions. A leapfrog scheme with a time step of 30 s is used to integrate the model forward in time. Model initial and lateral boundary conditions are defined in the following section.
In the traditional nudging approach, only the diagonal elements of the nudging magnitude matrix $G$ (i.e., $G_{uu}$, $G_{vv}$ and $G_{hh}$) in Eq. (3.5) are nonzero. For the HNEnKF tested here, all elements of this $G$ matrix are nonzero as discussed in section 3.2 and as demonstrated in the Lorenz three-variable model in Chapter 2.

3.3.2. Case descriptions, initial conditions and lateral boundary conditions

The HNEnKF is tested in 24-h simulations for two cases: a quasi-stationary wave (Case I) and a moving vortex (Case II). Reduced acceleration of gravity $g$ is used in the quasi-stationary wave case, and defined as 0.5 ms$^{-2}$. The true initial condition of Case I follows Grammeltvedt (1969) and Zhu et al. (1994). The true initial height is given by:

$$h(x, y) = H_0 + H_1 \tanh \left( \frac{9(D/2 - y)}{2D} \right) + H_2 \text{sech}^2 \left( \frac{9(D/2 - y)}{D} \right) \sin \left( \frac{2\pi}{L} \right),$$

(3.6)

where $H_0$, $H_1$ and $H_2$ are set to 50.0 m, 5.5 m, and 3.325 m respectively. The true initial wind field is derived from the initial height field assuming geostrophy. The true initial height and wind fields are shown in Figure 3.1a. A large phase error ($\pi/4$) is added into Eq. (3.6) to create the initial height field of the nudging state. The phase errors of the ensemble members are created by adding random errors with Gaussian distribution having zero mean and a variance of $\pi/4$ added onto the phase error ($\pi/4$) of the initial height of the nudging state. The initial winds of the nudging state and the ensemble members are derived from the initial height fields through the geostrophic relationship.

Figure 3.1b shows the true initial condition of Case II. The background mean height is 200 m, and the background uniform wind speed in the $x$ direction is 10 ms$^{-1}$ and there is no mean
flow in the y direction. A parabolic-shaped height perturbation with a maximum value of 20 m and a length scale of ~100 km, is introduced in the center of the domain. The wind and height truth fields are also geostrophically balanced initially.

The initial height fields of the nudging state and the ensemble state are based on shape-preserving perturbations to the truth state. For the nudging state, the true perturbation center is moved westward one grid point and southward two grid points, and a random error of Gaussian distribution with mean zero and variance 2.0 is added onto the maximum value of the truth and is used to scale the parabolic-shaped height perturbation. The initial height fields of the ensemble members have random errors with Gaussian distribution with zero mean and a variance of 2.0 multiplied by the grid spacing, placed onto the perturbation center of the initial nudging state. Random errors with Gaussian distribution mean zero and variance 2.0 are also superimposed on the maximum value used to define the amplitude of the initial nudging height perturbation field. The initial wind fields are also derived from the initial height fields using the geostrophic relationship in both the nudging and the ensemble state.

Periodic lateral boundary conditions are used at the west-east boundaries in both cases. Case I has a free-slip rigid wall boundary condition at the southern and northern boundaries where the height and u-component are defined from the values one point inside the boundary. For Case II, the tendencies of height and wind components are set to zero at the south-north boundaries.

3.3.3 The truth state and simulated observations

Truth states for each case are generated by first integrating a finer-scale model with grid spacing of 1 km, grid dimensions of 511 x 301 and a time step of 1 s. For this purpose the model initial fields have no random or phase errors. The simulated observations are then produced by
adding random errors with a Gaussian distribution with zero mean and assumed variances onto the 1-km truth fields. The simulated observations for Case I have variances $\sigma_u^2 = 0.5 \ m^2 \ s^{-2}$, $\sigma_v^2 = 0.5 \ m^2 \ s^{-2}$ and $\sigma_h^2 = 2.5 \ m^2$. The variances of the simulated observations in Case II are given by $\sigma_u^2 = 2.0 \ m^2 \ s^{-2}$, $\sigma_v^2 = 2.0 \ m^2 \ s^{-2}$ and $\sigma_h^2 = 20.0 \ m^2$. These variances are around 10% of their mean values.

Four types of observation networks are tested in this study. The first observation network (OBSN I) has only one observation site, which is shown by the gray solid square near the domain center in Figure 3.1a. Instead of having the observation located right in the domain center, random displacements within one coarse grid cell are added to the domain center to produce the observation site. The second observation network (OBSN II) consists of 19 observations spaced 25 km apart along the center latitude of the domain ($y = 150$ km), and shown by the gray diamonds in Figure 3.1a. This OBSN II is chosen as the default or baseline observation network. The gray circles in Figure 3.1a represent the third observation network (OBSN III), which has 11 observations spaced 25 km apart in the north-south direction off-center and at $x = 150$ km. The last observation network (OBSN IV) combines the OBSN II and OBSN III networks. The baseline configuration observations are available every three hours.

3.3.4. Verification data and metrics

The verification data, based on the 1-km truth model simulation, is available at every grid point of the 10-km coarse domain. For a given grid point on the coarse domain, the verification value is the average of the surrounding $10 \times 10$ grid points on the 1-km fine-scale truth domain. The root-mean-square (RMS) errors of height and wind are computed separately every minute. Because the signal (amplitude) of the unforced wave or vortex is decreased gradually over time
by diffusion, the actual model RMS error computed versus the truth field decreases with time. Thus a normalized RMS error is used here, which is defined as the actual RMS error divided by the domain standard deviation of the truth field.

However, as discussed in Chapter 2, the RMS error is not the only measure of success of a data assimilation technique, because it may not reflect discontinuities or noise generation in the analysis caused by the data assimilation method. Thus, a discontinuity parameter (DP) defined in Chapter 2 is also used here. The DP is the average absolute value of the RMS error difference in the analysis one time step (30 s) before the observation time and that at the observation time. Therefore this measure is able to quantitatively assess the magnitude of error spikes / discontinuities induced following the data insertion.

3.3.5. Summary of experiments

As shown in Table 3.1, five basic experiments are conducted in this study: 1) CTRL, assimilating no observations; 2) Nudging, using traditional observation nudging to relax the model state to the observations gradually with a fixed nudging strength $10^{-4}$ s$^{-1}$ and an isotropic Cressman-type influence function defined by a radius of influence (Stauffer and Seaman 1994); 3) EnKF, assimilating the observations using the EnKF; 4) HNEnKF, assimilating the observations by the HNEnKF approach; and 5) EnKS, assimilating the observations by the lagged EnKS. Experiments CTRL and Nudging are single model experiments, while Experiments EnKF, HNEnKF and EnKS use an ensemble of model forecasts. Experiments are conducted first for a baseline configuration using 20 ensemble members, 3-hourly observations and an observation network consisting of an east-west line of observations spaced 25 km apart at the central latitude (OBSN II). Ensemble sizes of 10 and 40 members, and observation
frequencies of hourly and 6-hourly and three other observation networks (OBSN I, OBSN III and OBSN IV) are also applied as sensitivity tests to the above baseline experiments.

The radius of influence for the observation nudging used in Experiment Nudging is specified to be the same as the error covariance localization length scale of Experiment EnKF and HNEnKF defined further below. Both the Nudging and HNEnKF experiments have a 2-h nudging time window extending 1 h on each side of the observations. The trapezoidal temporal nudging coefficient function is defined by Stauffer and Seaman (1990) and applied as in Chapter 2. It has a maximum weight of 1.0 within the center half of the 2-h window, decreasing linearly to 0.0 at the ends of the window.

For the ensemble-based data assimilation experiments, to avoid filter divergence, the method suggested by Hamill et al. (2001) is used to increase the background error covariances somewhat by inflating the deviation of the background members with respect to their mean by a small amount (i.e. an inflation factor of 1.1 is used here). In addition, an error covariance localization method is used following Houtekamer and Mitchell (2001), where a fifth-order piecewise rational function (Gaspari and Cohn 1999) is used to scale the background error covariance. The error covariance localization parameter 2c (see Eq. (4.10) of Gaspari and Cohn (1999)) is set to 500 km, which is the wavelength in Case I. Similarly, Case II has the error covariance localization parameter 2c set to 100 km, which is the scale of the initial vortex.

Following Khare et al. (2008), error covariance inflation is applied in the EnKS only to the prior estimates of the EnKF, and it is also set to 1.1. For efficiency, a lagged EnKS is applied here, which applies each observation backward only to the previous observation time every 30 minutes.
3.4. Results

We begin by applying a baseline 24-h model dynamic analysis assimilating 3-hourly observations from OBSN II (east-west line of observations at central latitude) using an ensemble size 20 to the wave case (Case I) and the moving vortex case (Case II) described in section 3.3.2. The performance of the HNEnKF method is compared to that of the observation nudging and EnKF applied separately, and also to the EnKS.

In subsequent subsections, we further investigate the HNEnKF using a set of sensitivity tests changing only one factor at a time (the observation frequency, observation network or ensemble size) from the baseline configuration. The observation frequency (OBSF) varies from 3-hourly observations (OBSF 3) in the baseline to hourly observations (OBSF 1) and 6-hourly observations (OBSF 6). The four types of observation networks (OBSN) described in section 3.3.3 are then tested. Finally, the ensemble size (ENS) varies from 20 (ENS 20), to 10 (ENS 10) and 40 (ENS 40).

3.4.1. Baseline results

Figure 3.2 shows the normalized RMS errors of height and wind for the set of experiments in Table 3.1 for the wave Case I. Experiment Nudging fails to reduce the RMS error of either the height or wind fields (see discussion further below) while Experiment EnKF shows a significant error reduction every 3 h when observations are assimilated as evidenced by the strong RMS error decreases at the observation times. However a rapid increase in error is evident soon after the observations are assimilated. This pattern is consistent with the 6-h assimilation period results in Figure 1 of Fujita et al. (2007) using MM5 (Grell et al. 1994). It is also consistent with the presence of error spikes around the observation times shown in the Lorenz system results in
Chapter 2. By comparison, Experiment HNEnKF combining the EnKF and the continuous nudging approach shows the RMS error decreasing smoothly in time. The RMS errors of the HNEnKF experiment are lower than those of the EnKF experiment almost continuously after the first time the observations are assimilated. The dark gray dash-dotted vertical lines 30 minutes apart from Experiment EnKS denote the improvement in RMS error obtained by applying the next available observation back to the previous observation time. Since the next observation is applied backward only to the previous observation time every 30 minutes, the normalized RMS error of the EnKS is very similar to that of the EnKF, where large error corrections are made when observations are assimilated. Thus the HNEnKF applied here produces smaller RMS errors throughout the assimilation period than either the EnKF or EnKS, and it also produces smoother analyses in time than both the EnKF and EnKS.

The normalized RMS errors of height and wind for the moving vortex Case II are shown in Figure 3.3. It is interesting that the CTRL (using no data assimilation) performs best for the height field from the first observation time to the third observation time (Figure 3.3a), followed by Experiments Nudging and HNEnKF. Note that the values for Experiments CTRL, Nudging and HNEnKF are from single-model experiments while EnKF and EnKS represent ensemble averages. Following the third observation time (9 h), Experiment HNEnKF shows a clear RMS error improvement in the height field over all the other data assimilation schemes. The wind field (Figure 3.3b), on the other hand, responds more rapidly and decisively early in the simulation period to the data assimilation methods. These results suggest that the height field in Figure 3.3a is likely to be adjusting more to the wind-field forcing than to the height observations directly. Unlike in Figure 3.2b, Experiment Nudging is able to reduce the wind RMS error gradually in time compared to CTRL. As in the wave case of Figure 3.2, strong adjustments by the EnKF at the observation times in Case II are seen in the wind field, and Experiment EnKS has strong error corrections when observations are assimilated. Similar to the wave case shown in Figure 3.2b,
the HNEnKF approach has smaller wind RMS error than the EnKF and EnKS, and it reduces the wind RMS error smoothly in time with fewer and weaker discontinuities compared to the EnKF and EnKS.

To explain why the observation nudging does not reduce the RMS error in Case I (Figure 3.2), but does decrease the error in Case II (Figure 3.3), the sums of nudging tendency terms in each equation of Eq. (3.5) are shown on the whole domain for Experiments Nudging and HNEnKF at the first observation time (3 hours) for both Case I and Case II (Figure 3.4). Figure 3.4a indicates that the sums of nudging tendency terms from Experiment Nudging are quite different from those of Experiment HNEnKF in Case I. For instance, the sums in the u equation for Nudging are positive on every grid point, but those of HNEnKF show dipole patterns with positive and negative values. As discussed before, HNEnKF reduces the RMS error successfully while Nudging does not. Thus the specified nudging coefficients in Nudging do not appear to represent the error correlations realistically in Case I. In Figure 3.4b, the sums of the nudging tendency terms in Nudging are more similar to those of the HNEnKF in Case II. For example, the sums of nudging tendency terms of Nudging in the v equation have a negative maximum around grid point (30, 15) and positive maximum around grid point (40, 14), which are located close to those of the HNEnKF. Figure 3.3b shows both the Nudging and HNEnKF reducing the wind RMS error, although HNEnKF has lower wind RMS error than Nudging. Thus the specified nudging coefficients in Case II for Experiment Nudging are better able to capture the more realistic error correlations computed by HNEnKF. This demonstrates that nudging, used alone with simple isotropic weighting, may have difficulty adapting to the non-isotropic error structure often encountered in a simulation.

For the moving vortex Case II, the analyses of the Truth, CTRL and the data assimilation experiments at the end of simulation are shown in Figure 3.5. The analysis of the EnKS is not shown, since it is the same as that of the EnKF at the end of simulation. Instead of having a
trough at around $x=70\text{km}$, the CTRL for Case II has a ridge there. The trough produced by the CTRL is further east than the Truth and strengthens towards the south. The HNEnKF produces the closest result to the Truth regarding the phase, orientation and strength of the trough, followed by the Nudging. The trough produced by the EnKF is further east and meanders from north to south rather than having a spatially coherent north-south orientation as in the Truth. These results are qualitatively consistent with those of the normalized RMS error comparison shown by Figure 3.3.

In both the wave Case I and the vortex Case II, the baseline HNEnKF is able to produce smaller RMS errors throughout the 24-h period than the other data assimilation experiments (Nudging, EnKF and EnKS). It also produces a smoother analysis in time than either the EnKF or EnKS, because it has smaller discontinuities around the observation times than the EnKF and EnKS. Thus, the hybrid combination of nudging and the EnKF produces a dynamic analysis with lower errors than the nudging and EnKF applied separately.

3.4.2. Sensitivity to observation frequency

In this section the data assimilation methods are explored with various observation frequencies or intervals using the baseline OBSN II and ensemble size of 20 in both Case I and Case II, since the performances of the data assimilation methods may vary with different observation frequencies and real observations typically have different frequencies. The baseline observation frequency is every three hours (OBSF 3), and observation frequencies of every one hour (OBSF 1) and every six hours (OBSF 6) are now tested. In Figure 3.6 the average RMS error computed every minute and the DP computed at every observation time for the height and wind fields for wave Case I are shown. For each observation frequency, Experiments HNEnKF, EnKF, and EnKS have lower average RMS errors than Experiment Nudging in both the height
and wind fields, since the specified constant nudging coefficients poorly represent the error correlations as discussed in section 3.4.1. Experiment HNEnKF has the lowest average height and wind RMS errors for all three observation frequencies. Experiments HNEnKF and Nudging have much smaller values of DP (fewer / smaller discontinuities) than Experiments EnKF and EnKS in both the height and wind fields for all three observation frequencies, especially when observation frequencies are every three hours and every six hours.

The RMS error and DP for vortex Case II are shown in Figure 3.7. As discussed in section 3.4.1, the specified nudging coefficients for this case appear to better represent the error correlations than those for Case I. Thus the Nudging experiment has similar average height RMS errors to the HNEnKF (Figure 3.7a), and similar or larger average wind RMS errors than the HNEnKF (Figure 3.7c). Experiment HNEnKF produces lower average height RMS errors than the EnKF and EnKS for the three observation frequencies. The HNEnKF has similar average wind RMS errors to the EnKF and EnKS when observation frequencies are every three hours and every six hours, although it has larger average wind RMS error than the EnKF and EnKS when the observation frequency is increased to one hour. From Figure 3.3b, the EnKF and EnKS were found to have an advantage in their average RMS errors through the first three hours because of the ensemble averaging compared to the single-model used by Nudging and HNEnKF, and this affects the average statistics over the entire model period shown in Figure 3.7. As in Figure 3.7b and Figure 3.7d, the HNEnKF and Nudging show much smaller values of DP (fewer / smaller discontinuities) than the EnKF and EnKS in the height field (Figure 3.7b) and wind field (Figure 3.7d). These characteristics of the HNEnKF are attractive for the diagnostic dynamic studies and research studies using air-quality and atmospheric-transport and dispersion modeling.

As mentioned in section 3.3.5, the EnKS applies each observation backward to the previous observation time every 30 minutes. Then, to give the EnKS the greatest advantage, the average RMS errors of the height and wind fields can also be computed every 30 minutes.
However, the 30-minute EnKS results are still similar to those presented above (not shown). Thus generally the HNEnKF is able to produce lower average RMS error and improved (smaller) values of DP than the EnKF and EnKS in Case I and Case II regardless of the observation frequency.

The analyses of the Nudging, EnKF and HNEnKF of Case II with OBSF 1 at the end of simulation are shown by Figure 3.8. Both the HNEnKF and Nudging produce similar analyses to the Truth, while the trough produced by the HNEnKF is closer in the north-south gradient to the Truth than the Nudging. The height field from the ensemble mean of the EnKF exhibits more short wave energy than that of the Truth, HNEnKF and Nudging. The EnKF produces a weaker trough somewhat west than that of the Truth. Comparison with Figure 3.5 reveals that all data assimilation experiments have improved analyses at the end of simulation due to more frequent observations being assimilated.

### 3.4.3. Sensitivity to observation network

With the baseline 3-hourly observation frequency and ensemble size 20, the data assimilation methods are now applied with the various observation networks discussed in section 3.3.3, in order to simulate the real observation networks that have sparse and dense data-density regions. Figure 3.9 shows the average values of RMS error and DP over the 24-h period for Case I using the different observation networks for the data assimilation experiments. Figure 3.9a and Figure 3.9c show that Experiment HNEnKF produces the smallest average RMS error in both the height and wind fields for all four observation networks. Figure 3.9b and Figure 3.9d indicate that the HNEnKF has the smallest values of DP, which means the best temporal smoothness of the dynamic analyses. The EnKF and EnKS have much larger values of DP than both the Nudging and HNEnKF. The EnKS usually has slightly smaller RMS errors than the EnKF at the
analysis steps due to future observations being applied backward, and the lagged EnKS applies the next observation backward every 30 minutes instead of every time step. This explains why the EnKS has even larger values of DP than the EnKF. The HNEnKF retains the benefits of the EnKF by using flow-dependent and time-dependent error covariances that effectively reduce the RMS error, and it also yields a more seamless analysis by producing a smoother solution in time with smaller / fewer discontinuities than the EnKF by using nudging-type terms to apply the EnKF corrections continuously in time.

Figure 3.10 shows the average values of RMS error and DP for the moving vortex Case II when assimilating observations from the different observation networks. The HNEnKF produces the smallest average height and wind RMS errors in OBSN II and OBSN IV. However in OBSN I (for height and wind) and OBSN III (for wind), the HNEnKF produces larger average RMS error than the EnKF and EnKS. This is likely because the error reduction in the EnKF and EnKS mainly comes from ensemble averaging, as shown in Figure 3.3b in the first three hours when no observations are assimilated. In addition, the observations in OBSN I and OBSN III play a much reduced role compared to the larger number of observations along the direction of the mean flow in OBSN II and OBSN IV. Obviously, the OBSN I and OBSN III networks cannot detect the eastward moving vortex sufficiently. Nonetheless, as shown by Figure 3.10b and Figure 3.10d, the HNEnKF still has lower, more desirable DP than the EnKF and EnKS, even with OBSN I and OBSN III.

The analyses of the Nudging, EnKF and HNEnKF of Case II with OBSN IV at the end of simulation are shown by Figure 3.11. Regarding the phase, orientation and strength of the trough, the HNEnKF produces the closest results to the Truth, followed by the Nudging. The EnKF is unable to produce a trough with coherent structure and orientation similar to that of the Truth. Comparison to Figure 3.5 indicates that all data assimilation experiments have generally similar analyses to those with OBSN II, while the HNEnKF has better trough amplitude than that with
OBSN II. This is because the OBSN III added to OBSN II to define OBSN IV cannot detect the eastward moving vortex sufficiently; thus the north-south line of observations in OBSN III does not provide much useful information and there is greater benefit from adding more observations in time to the OBSN II east-west distribution of observations (Figure 3.8).

### 3.4.4. Sensitivity to ensemble size

The ensemble-based data assimilation methods, EnKF and HNEnKF, may perform differently with different ensemble size. Thus in order to investigate the sensitivity of the data assimilation methods to ensemble size, the results of the data assimilation methods using 20 members for Case I and Case II are compared to those for 40 ensemble members and 10 ensemble members. The baseline 3-hourly observation frequency and OBSN II are used.

The average values of RMS error and DP over the 24-h period for wave Case I with the different ensemble sizes are shown in Figure 3.12. Naturally, the results for the single-model Experiment Nudging do not vary with ensemble size, and the RMS errors are much larger than the other data assimilation experiments for both height and wind. When ensemble size is decreased to 10, Experiment HNEnKF has similar average RMS errors to those of Experiments EnKF and EnKS in both the height and wind fields. However, when ensemble size is increased to 20 and then to 40, the HNEnKF produces smaller average RMS errors than the EnKF and EnKS in both the height and wind fields. Apparently the HNEnKF is able to take advantage of the EnKF background error covariances within its continuous assimilation framework when ensemble size is larger. As shown by Figure 3.12b and Figure 3.12d, the HNEnKF always has much smaller values of DP than the EnKF and EnKS.

Figure 3.13 shows the average RMS error and DP for the set of data assimilation experiments for vortex Case II with the three different ensemble sizes. For all three ensemble
sizes, Experiment HNEnKF has smaller average height RMS errors than the Experiments EnKF and EnKS. The HNEnKF approach has similar average wind RMS errors to the EnKF and EnKS when ensemble size is 10 and 20, and it has smaller average wind RMS error than the EnKF and EnKS when ensemble size increases to 40. Similar to the results for Case I, Experiment HNEnKF also has much smaller values of DP than the EnKF and EnKS for all three ensemble sizes. Although the small DP of HNEnKF is similar to that of Nudging, the RMS errors for HNEnKF are generally lower than those for Nudging for the two cases.

The analyses of the EnKF and HNEnKF of Case II with ENS 40 at the end of simulation are shown by Figure 3.14. The HNEnKF again produces a trough with better phase, orientation and strength than the EnKF. The EnKF does not have a spatially coherent trough with north-south orientation. However, comparison of Figure 3.14 to Figure 3.5 suggests that the HNEnKF and EnKF with ENS 40 produce generally similar analyses to those with ENS 20. Thus adding ensemble members for case II appears to have little effect on the analysis at the end of the simulation. Possible reasons why the fit of the analyses to the data vary over the sets of experiments are investigated further in the next section that presents spread-error relationships of the EnKF.

3.4.5. Relationship between ensemble spread and forecast error

To ensure the EnKF and HNEnKF function properly, the ensemble forecast spread is compared to the forecast error of the ensemble mean. Instead of using scatterplots as in Chapter 2, we plot the range of the ensemble spread and forecast error following Wang and Bishop (2003), because the larger number of points and overplots for these 2D model results make interpretation of scatterplots more difficult. We start from a scatterplot of points for which the abscissa of each point is given by the ensemble spread and the ordinate by the forecast error for
each grid point at every analysis time. These points are then sorted in order of increasing ensemble spread, and then divided into four equally populated bins. Then the average values of the ensemble spread and forecast error in each bin are computed and plotted.

Figure 3.15 presents the plots of each group of sensitivity experiments as discussed in sections 3.4.2-3.4.4 of Case I for the height and wind fields. Given different observation frequencies (Figure 3.15a and Figure 3.15b) and observation networks (Figure 3.15c and Figure 3.15d), we find that the ensemble spread has an approximately linear correlation to the forecast error with a slope somewhat larger than 1. With the different ensemble sizes (Figure 3.15e and Figure 3.15f), the relationships between the ensemble spread and forecast error are also approximately linear, while the slopes of ENS 40 and ENS 10 are closer to 1 than that of ENS 20. This may help explain the smaller average RMS errors of EnKF with ENS 40 and ENS 10 compared to those of ENS 20 (Figure 3.12a and Figure 3.12c). Thus the ensemble spreads of ENS 40 and ENS 10 for this single case provide a better estimate of the forecast error than that of ENS 20 for this one case.

The relationships between the ensemble spread and forecast error of each group of sensitivity experiments of Case II are shown in Figure 3.16. Given different observation frequencies (Figure 3.16a and Figure 3.16b) and observation networks (Figure 3.16c and Figure 3.16d), we again see the ensemble spread having an approximately linear correlation to the forecast error. The slopes of the height field are close to 1, while those of the wind field are somewhat larger than 1. With different ensemble sizes (Figure 3.16e and Figure 3.16f), the relationships between the ensemble spread and forecast error are also approximately linear. The slopes for the height field with different ensemble sizes are similar to each other and close to 1, which may explain the similar average height RMS errors of the EnKF with different ensemble sizes (Figure 3.13a). The slope for the wind field with ENS 20 is closer to 1 than those of ENS
40 and ENS 20, which may explain the slightly smaller average wind RMS error of EnKF with ENS 20 compared to those with ENS 40 and ENS 10 (Figure 3.13c).

Therefore, for the three groups of sensitivity experiments, the ensemble spread generally provides a reasonable estimate of the forecast error and possible explanations for some of the differences among the experiments. We emphasize that these results are based on only two cases, and many more cases are needed to truly assess the spread-error relationship of an ensemble.

3.5. Analysis of dynamic balance following data insertion

The motivation for developing the HNEnKF method is that an improved analysis with greater temporal smoothness and inter-variable consistency can be obtained if the data are applied gradually and continuously within a model using nudging-type terms that have been conditioned using the error covariance matrix of the EnKF. These terms can reduce dynamic imbalances and insertion shocks caused by intermittent data assimilation approaches. A calculation of the magnitude of the pressure tendencies or vertical motions in a mesoscale model is often performed to analyze the dynamic imbalances or noise introduced by the data insertion (e.g., Chen and Huang 2006). Here in the shallow water model, the evolution of the ageostrophic winds is used to quantify the effects of data insertion on the model balance.

To better investigate the impact of the data insertion on the dynamic balance that takes place through the model adjustment and induction processes due to few observation systems providing both mass and wind data, we evaluate the impact of assimilating only height observations or only wind observations at the third hour. The baseline model configuration using 20 ensemble members (ENS 20) and an east-west line of observations along the mean flow (OBSN II) is applied here to both cases. The magnitude of the ageostrophic winds is computed
every time step at each grid point for the truth state at 1-km horizontal grid spacing and the data assimilation experiments at 10-km grid spacing. The verification data obtained by simply averaging the neighboring 10 × 10 1-km grid points from the truth to the 10-km grid are also used to compute the ageostrophic winds (10km_VER). The ageostrophic wind is the difference between the geostrophic wind computed from the model (or verification data) height field and the model (or verification data) wind field. Then the magnitude of the ageostrophic wind is averaged over the domain.

Figure 3.17a shows the evolution of domain-averaged ageostrophic wind speed in wave Case I when only height observations are assimilated at the third hour. It is clearly shown that the ensemble members using the EnKF (gray lines) have dynamic imbalances / strong ageostrophic winds following the data assimilation. The ensemble mean (black line) also shows a discontinuity or noise burst after 3 h. By comparison, Experiment HNEnKF (green line) has the ageostrophic wind gradually evolving in time following the data insertion, which qualitatively follows the truth (blue line) and the 10km_VER but has a higher magnitude (red line). The time evolution of the ageostrophic wind following the data insertion represents the dynamic balance effects of the data assimilation. The larger magnitudes of the domain-averaged ageostrophic wind from the data assimilation experiments, compared to the 1-km truth are mainly caused by coarser resolution effects, as seen by comparing the truth (blue) to the 10km_VER (red).

Figure 3.17b shows that when only wind observations are assimilated at the third hour in the wave Case I, a few ensemble members have a strong discontinuity in the ageostrophic wind, but the noise burst in the ensemble mean is not as obvious as when only height observations are assimilated. By comparison of Figure 3.17b to Figure 3.17a, the model adjustments appear to come more from the height field observations at this time for this case than the wind field observations. The HNEnKF still shows the ageostrophic wind varying smoothly in time, similar to when only height observations were assimilated.
The domain-averaged ageostrophic wind in the vortex Case II is shown in Figure 3.18. When only height observations are assimilated (Figure 3.18a), the ensemble members of EnKF and their ensemble mean again have a strong discontinuity in the ageostrophic wind. By comparison, the HNEnKF shows a much smaller effect: the ageostrophic wind decreases gradually following the data insertion, very similar to that of the truth and 10km_VER. Similar to Case I, the difference in the ageostrophic wind magnitude between the data assimilation experiments and the truth mainly comes from the grid resolution. When only wind observations are assimilated (Figure 3.18b), there are also ageostrophic wind bursts in the ensemble members and their ensemble mean, although the magnitudes of the discontinuities are not as large as those obtained when assimilating height observations only. The HNEnKF again performs similarly to the truth and 10km_VER that have the ageostrophic wind evolving gradually in time without any large discontinuities.

Thus the EnKF, an intermittent data assimilation method, experiences larger dynamic imbalances and ageostrophic wind tendencies in the model state following the observation time compared to the continuous HNEnKF method. The HNEnKF is able to better maintain the dynamic balance by gradually applying nudging-type terms that have been computed using the error covariance matrix of the EnKF, thus producing a more continuous and seamless analysis in time.

3.6. Computational efficiency

As discussed in Chapter 2, the EnKF, HNEnKF and EnKS experiments utilize an ensemble forecast that is more computationally expensive than a single model run as used in Experiment Nudging. The EnKS is even more CPU-intensive than the EnKF and HNEnKF, and also requires greater storage proportional to the total number of analysis times over which the
statistics are used. Similar to Chapter 2, the computational efficiency of these data assimilation methods is discussed in this section.

Table 3.2 shows the CPU time cost of the various data assimilation schemes using the baseline configuration. The Nudging has the smallest CPU time cost, because it does not require an ensemble of forecasts. The HNEnKF has similar CPU time cost to the EnKF, since both involve an ensemble forecast. These results are consistent with those of Chapter 2. The EnKS has a CPU time cost around 2.5 times that of the EnKF and HNEnKF. We would expect smaller RMS error and DP of the EnKS if it is operated as in Chapter 2 by applying future observations backward to the initial time every time step. The relative CPU time cost of EnKS is much smaller here than that of Chapter 2, because the more practical, lagged EnKS used here only applies each observation backward to the previous observation time every 30 minutes. The HNEnKF produces similar or better RMS error and DP than the lagged EnKS, but with reduced CPU time and storage costs.

3.7. Conclusions

The hybrid nudging-EnKF (HNEnKF) data assimilation approach, introduced in Chapter 2 for the three-variable Lorenz system, is further investigated here using a 2D shallow water model. The HNEnKF combines the advantages of both the EnKF and nudging by applying the EnKF gradually in time via nudging-type terms. The HNEnKF uses the EnKF to provide flow-dependent and time-dependent nudging coefficients and also includes nonzero off-diagonal elements for better inter-variable influences from the innovations.

A quasi-stationary wave case (Case I) and a moving vortex case (Case II) are used to test the HNEnKF method for dynamic analysis and NWP-type applications. The HNEnKF in the baseline configuration (3-hourly observations, observation network OBSN II and 20 ensemble
members) generally reduces the RMS errors through the 24-h period more than the nudging and EnKF applied separately. Moreover, the HNEnKF retains the benefits from the EnKF while using a continuous assimilation to improve the model state gradually rather than making strong corrections and discontinuities at the analysis steps as with the intermittent EnKF assimilation. Thus it has smaller (better) values of the discontinuity parameter (DP) than the EnKF. The HNEnKF also produces lower DP (better temporal smoothness) than the reduced-cost lagged EnKS. Moreover, the average RMS errors in the 24-h HNEnKF simulations are comparable or lower than those of the EnKS used in this study. The HNEnKF is comparable in cost to the EnKF, and both the HNEnKF and EnKF yield smaller CPU time and storage costs than the EnKS.

Sensitivity experiments using different observation frequencies (OBSF 1, OBSF 3 and OBSF 6), observation networks (OBSN I, OBSN II, OBSN III and OBSN IV) and ensemble sizes (ENS 10, ENS 20 and ENS 40) are also performed. In general, the results found in the baseline HNEnKF simulations for producing comparable or smaller average RMS errors throughout the 24-h period and smaller (better) values of DP than the EnKF and EnKS around the analysis times are confirmed.

To ensure that the EnKF and HNEnKF function properly, the ensemble spread is compared to the forecast error for each group of sensitivity experiments. The relationship between the ensemble spread and forecast error of the ensemble mean is approximately linear with slopes close to or somewhat larger than 1. Thus the ensemble spread provides a reasonable estimate of the forecast error, and the difference in the spread-error relationship may help to explain some of the differences among the experimental results (e.g., Figure 3.12 and Figure 3.13). For example, use of ensemble size 40 in Experiment EnKF produces somewhat better RMS errors and spread-error relationships than the ensemble size 20 in Case I, while Case II results show little added value or worse results between 20 and 40 members and the spread-error
relationship appears to be slightly better for 20 members compared to 40 members. Note that the HNEnKF still produces somewhat better results with increasing ensemble size (Figure 3.12 and Figure 3.13) for both cases likely due to its use of ensemble spread within its continuous assimilation framework and the smaller insertion noise as measured by DP. Again we emphasize that many more cases are needed to truly assess the spread-error relationship for an ensemble and its effect on the ensemble-based data assimilation methods, and calibration of the spread-error relationship may also be needed (e.g., Kolczynski et al. 2009; Kolczynski et al. 2011).

The added value of the HNEnKF over the EnKF is further investigated by analyzing the effects of the data assimilation methods on the model dynamic balance (i.e., evolution of the ageostrophic winds) following the assimilation of only wind data or only mass data. The EnKF, as an intermittent data assimilation approach, has strong discontinuities in the model state at the analysis times, as shown by the bursts in the domain-averaged ageostrophic winds. By comparison, the HNEnKF, which applies the error covariance information of the EnKF gradually in time, produces a smooth evolution of the ageostrophic wind, without any strong discontinuities following the data insertion, more like the ageostrophic wind in the truth and 10-km verification data. Thus it is demonstrated that the continuous HNEnKF produces seamless analyses with a greater degree of dynamic balance compared to the EnKF. Building on these encouraging results in Chapters 2 and 3, we are now applying this HNEnKF approach to real data in the three-dimensional WRF model and these results will be reported in Chapter 4.
<table>
<thead>
<tr>
<th>Exp. Name</th>
<th>Exp. Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CTRL</td>
<td>Assimilate no observations</td>
</tr>
<tr>
<td>Nudging</td>
<td>Assimilate observations by observation nudging with nudging coefficients of $10^{-4}$ s$^{-1}$</td>
</tr>
<tr>
<td>EnKF</td>
<td>Assimilate observations by ensemble Kalman filter</td>
</tr>
<tr>
<td>HNEEnKF</td>
<td>Assimilate observations by hybrid nudging-EnKF</td>
</tr>
<tr>
<td>EnKS</td>
<td>Assimilate observations by lagged ensemble Kalman smoother</td>
</tr>
</tbody>
</table>
Table 3.2. Total CPU time cost of different data assimilation schemes with baseline configuration.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Nudging</th>
<th>EnKF</th>
<th>HNEnKF</th>
<th>EnKS</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU Time (sec)</td>
<td>47</td>
<td>298</td>
<td>299</td>
<td>732</td>
</tr>
</tbody>
</table>
Figure 3.1. The truth initial height and wind fields. (a) Case I and observation networks, and (b) Case II. The gray solid square in (a) denotes the observation site of OBSN I ($x=25.3$, $y=15.7$), the gray diamonds show the observation sites of OBSN II ($y=15$), and the gray circles indicate the observation sites of OBSN III ($x=15$). The OBSN IV includes both the gray diamonds (OBSN II) and gray circles (OBSN III).
Figure 3.2. The normalized RMS error of Case I for Experiments CTRL (thin light gray solid line), Nudging (thick light gray solid line), EnKF (dark gray solid line), HNEEnKF (black dash-dotted line) and EnKS (dark gray dash-dotted line). The baseline configuration (OBSF 3, OBSN II, ENS 20) is used for all of the data assimilation experiments. (a) height field and (b) wind field.
Figure 3.3. Same as Figure 3.2, except for Case II.
Figure 3.4. The sums of nudging tendency terms from Eq. (3.5) at every grid point at the first observation time (3 hours) of the baseline simulation. (a) Case I and (b) Case II. The left column shows the sums of the nudging terms for each equation $u$, $v$ and $h$ from Experiment Nudging, and the right column shows the sums of the three hybrid nudging terms for each equation $u$, $v$ and $h$ from Experiment HNEnKF.
Figure 3.5. The height and wind fields of Case II at the end of the dynamic analysis using the baseline configuration. (a) Truth, (b) CTRL, (c) Nudging, (d) EnKF and (e) HNEnKF.
Figure 3.6. Height and wind RMS error and DP for Case I and Experiments Nudging, EnKF, HNEnKF and EnKS with different observation frequencies. (a) the average height RMS error, (b) the average height DP, (c) the average wind RMS error and (d) the average wind DP. Smaller values are better values for both average RMS error and DP.
Figure 3.7. Same as Figure 3.6, except for Case II.
Figure 3.8. The height and wind fields of Case II at the end of the dynamic analysis for baseline configuration except using OBSF 1. (a) Nudging, (b) EnKF and (c) HNEEnKF.
Figure 3.9. Height and wind RMS error and DP for Case I and Experiments Nudging, EnKF, HNEnKF and EnKS with different observation networks. (a) the average height RMS error, (b) the average height DP, (c) the average wind RMS error and (d) the average wind DP.
Figure 3.10. Same as Figure 3.9, except for Case II.
Figure 3.11. The height and wind fields of Case II at the end of the dynamic analysis for baseline configuration except using OBSN IV. (a) Nudging, (b) EnKF and (c) HNEnKF.
Figure 3.12. Height and wind RMS error and DP for Case I and Experiments Nudging, EnKF, HNEEnKF and EnKS with different ensemble sizes. (a) the average height RMS error, (b) the average height DP, (c) the average wind RMS error and (d) the average wind DP.
Figure 3.13. Same as Figure 3.12, except for Case II.
Figure 3.14. The height and wind fields of Case II at the end of the dynamic analysis for baseline configuration except using ENS 40. (a) EnKF and (b) HNEnKF.
Figure 3.15. The range of ensemble spread and forecast error for the height and wind fields of the EnKF in Case I. (a) height field with different observation frequencies, (b) wind field with different observation frequencies, (c) height field with different observation networks, (d) wind field with different observation networks, (e) height field with different ensemble sizes, and (d) wind field with different ensemble sizes.
Figure 3.16. The same as Figure 3.15, except for Case II.
Figure 3.17. The domain-averaged ageostrophic wind computed for Case I for Experiments EnKF (each ensemble member in light gray, and the ensemble mean in black), HNEnKF (green), and the 1-km Truth (blue) and the 10-km_VER (red). (a) assimilating height observations only and (b) assimilating wind observations only.
Figure 3.18. Same as Figure 3.17, except for Case II.
Chapter 4

A Hybrid Nudging-Ensemble Kalman Filter Approach to Data Assimilation in WRF/DART

4.1. Introduction

A hybrid nudging-EnKF (HNEnKF) approach has been developed and tested in the Lorenz three-variable model (Chapter 2) and a two-dimensional (2D) shallow water model (Chapter 3) for dynamic analysis and numerical weather prediction. Building on the positive results obtained using the HNEnKF in these simple models, we apply it here to a full-physics three-dimensional mesoscale model using real data.

The HNEnKF combines the EnKF (Evensen 1994; Houtekamer and Mitchell 1998) and observation nudging (Stauffer and Seaman 1990; Stauffer and Seaman 1994) to take advantage of the strengths of both methods while avoiding their individual weaknesses. It applies the EnKF gradually in time via nudging-type terms to achieve better temporal smoothness and inter-variable consistency and reduce the data insertion shocks that often occur with intermittent data assimilation methods. The HNEnKF uses flow-dependent and time-dependent hybrid nudging coefficients based on the gain matrix of the EnKF rather than ad hoc nudging coefficients based largely on scaling arguments and past experience (e.g., Stauffer and Seaman 1994; Schroeder et al. 2006). It also extends the traditional observation nudging coefficients (Stauffer and Seaman 1994) to include zero off-diagonal elements in the nudging magnitude matrix to improve the inter-variable influences of the innovations and the dynamic consistency.

The HNEnKF was first tested in the Lorenz three-variable system (Lorenz 1963) using an observation system simulation experiment (OSSE), as discussed in Chapter 2. The HNEnKF
using all elements of the nudging magnitude matrix produced better results than the HNEnKF using only the diagonal elements of the nudging magnitude matrix, because it allowed for greater inter-variable influences via the nonzero off-diagonal elements of the nudging magnitude matrix from the data assimilation. Thus the HNEnKF using all elements of the nudging magnitude matrix was then adopted for further use and evaluation. It promoted a better fit of an analysis to data compared to that produced by nudging. It provided a continuous data assimilation with better inter-variable consistency and improved temporal smoothness compared to the EnKF.

To further investigate the performance of the HNEnKF in a more realistic model and explore the dynamic imbalance caused by the intermittent EnKF, the HNEnKF was tested in a two-dimensional (2D) shallow water model study where OSSEs were conducted (Chapter 3). In a quasi-stationary wave case and a moving vortex case, the HNEnKF generally produced smaller RMS errors in both the height and wind fields than the nudging and EnKF applied separately. It retained the benefits of the continuous nudging by reducing the RMS errors gradually in time, while the intermittent EnKF had strong corrections and discontinuities at the analysis steps that were consistent with the results of Fujita et al. (2007) and Chapter 2. Moreover, the HNEnKF produced a smoother evolution of the ageostrophic wind without any strong discontinuities around the observation time, while the EnKF had large bursts in the ageostrophic wind after the observations were assimilated. Thus the HNEnKF was able to produce a continuous, seamless and more dynamically balanced analysis compared to the EnKF.

Building on the encouraging idealized model results using OSSEs in Chapters 2 and 3, here we apply the HNEnKF to real surface and rawinsonde data in the three-dimensional Weather Research and Forecasting (WRF) model (Skamarock et al. 2008). The EnKF calculations are performed within the Data Assimilation Research Testbed (DART, Anderson et al. 2009). As in Chapters 2 and 3, the HNEnKF is again compared to the EnKF and nudging applied separately,
but here we perform a real-data study with truly independent / indirect verification of the data assimilation results against surface tracer observations.

Both nudging and the EnKF have been widely applied in atmospheric modeling studies using real observations. In nudging FDDA, the model state is relaxed continuously toward the observed state at each time step by adding an artificial tendency term, which is based on the difference between the two states, to the prognostic equations. Data assimilation can be accomplished by nudging the model solutions toward gridded analyses based on observations (analysis nudging), or directly toward the individual observations (observation nudging) (Stauffer and Seaman 1990; Stauffer et al. 1991; Stauffer and Seaman 1994). Nudging is attractive since it is a continuous and gradual assimilation method that can effectively and efficiently reduce model errors over multiple scales (e.g., Stauffer and Seaman 1994; Seaman et al. 1995; Colle and Mass 2000a, b; Leidner et al. 2001; Deng et al. 2004; Garvert et al. 2005; Deng and Stauffer 2006; Schroeder et al. 2006; Otte 2008a, b; Dixon et al. 2009; Ballabrera-Poy et al. 2009). Observation nudging is especially attractive for asynoptic data and fine-scale applications (e.g., Schroeder et al. 2006), and it is the nudging method used within the HNEnKF. The EnKF, on the other hand, is an intermittent data assimilation method that requires a set or ensemble of model forecasts, and provides flow-dependent statistics based on the ensemble for the assimilation of observations. The method is growing in popularity as computing power and the use of ensembles continue to increase. Numerous studies of the EnKF have been conducted with real observations (e.g., Houtekamer et al. 2005; Fujita et al. 2007; Szunyogh et al. 2008; Torn and Hakim 2008; Zhang et al. 2011). The EnKF has been shown to outperform the three-dimensional variational (3DVAR) data assimilation in both global (e.g., Whitaker et al. 2008) and limited-area numerical weather prediction applications (e.g., Meng and Zhang 2008; Zhang et al. 2011). Encouraging results were obtained by using the EnKF to assimilate real surface observations in Fujita et al. (2007).
New data assimilation methods are needed to exploit the strengths of the various data assimilation methods while avoiding their individual weaknesses. Thus combinations of data assimilation methods, i.e., hybrid approaches, merit further investigation. Although the studies of hybrid data assimilation methods for assimilating real observations in real atmospheric models are on the increase, they are still rather limited. Buehner (2005) developed a hybrid system based on the operational 3DVAR at the Canadian Meteorological Centre and tested it with the full set of operational observations. Small forecast improvements were found by using the hybrid system, and it was suggested that the ensemble size be increased. Buehner et al. (2010b) compared the hybrid methods, the 3DVAR and the four-dimensional variational (4DVAR) data assimilation methods with flow-dependent covariances computed from the EnKF and the Ensemble-4D-Var (En-4D-Var) (Buehner et al. 2010a), with real observations in a one-month period experiment. It was found that the use of the EnKF flow-dependent background error covariances in the 3DVAR and 4DVAR led to a large forecast improvement in the southern extratropics and small forecast improvement in the tropics. The En-4D-Var method had slightly worse forecasts compared to the 4DVAR with EnKF background error covariances. Wang et al. (2008b) tested the hybrid ensemble transform Kalman filter–three-dimensional variational data assimilation (ETKF-3DVAR, Wang et al. 2008a) with real observations. The hybrid ETKF-3DVAR method improved the 12-h forecasts compared to the 3DVAR technique.

Given the encouraging but limited real-data results of hybrid methods and the effective use of nudging and EnKF separately, the hybrid method combining nudging and the EnKF is further tested here in WRF/DART using real observations. The HNEnKF allows the use of the EnKF flow-dependent error covariances within a continuous and more gradual data assimilation framework for reduction of the insertion noise common with intermittent method EnKF (Duane et al. 2006; Fujita et al. 2007; Juckes and Lawrence 2009). A 48-h simulation of the Cross Appalachian Tracer Experiment (CAPTEX-83, Deng et al. 2004) case from 1200 UTC 18
September 1983 to 1200 UTC 20 September 1983 is conducted to demonstrate the proof of concept of the HNEnKF. Both surface and rawinsonde observations are assimilated. The hourly meteorological model outputs (analyses) are then used to drive the Second-Order Closure Integrated Puff (SCIPUFF, Sykes et al. 2004) atmospheric transport and dispersion (AT&D) model. The observed surface tracer concentration data is then used as an independent/indirect verification of the data assimilation approaches. The SCIPUFF-predicted surface tracer concentrations driven by the hourly dynamic analyses from the set of data assimilation experiments are compared statistically to the observed surface tracer data.

In section 4.2, the methodology of the HNEnKF approach is briefly described. Section 4.3 presents the details of the experimental design, including description of the model, observations, and the parameters used in the data assimilation experiments. An overview of the CAPTEX case and tracer study is presented in section 4.4. Section 4.5 discusses the results from the different data assimilation experiments for the meteorology, insertion noise and surface tracer verification. The conclusions of the study are summarized in section 4.6.

4.2. Methodology for the HNEnKF approach in WRF/DART

The procedures of the HNEnKF approach follow Chapter 3. A schematic of the HNEnKF approach is shown in Figure 2.2. We start with an ensemble of N background forecasts that will be updated by the EnKF (called the “ensemble state”), and a single forecast that will be updated by the hybrid nudging-type terms (called the “nudging state”). The following five steps are repeated for each data assimilation cycle: 1) Compute the hybrid nudging coefficients using the ensemble forecast via the EnKF algorithm. 2) Integrate the nudging state by continuously applying nudging with the hybrid nudging coefficients. 3) Update each ensemble member of the ensemble state using the EnKF. 4) Re-define the ensemble mean to be the analysis of the
nudging state by re-centering the ensemble around the nudging state at the observation time while retaining the ensemble spread. 5) Integrate the ensemble state and the nudging state forward to the next observation time.

Equation (4.1) shows the full set of model equations having the additional nudging terms that are used to gradually relax the model state towards the observation state.

\[
\frac{dx}{dt} = f(x) + G \cdot w_s \cdot w_t \cdot (y^o - x),
\]

where \( x \) and \( f \) are the state vector and standard forcing function of the system, \( y^o \) is the observation vector, \( G \) is the nudging magnitude matrix, and \( w_s \) and \( w_t \) are the spatial and temporal nudging weighting coefficients. The spatial and temporal nudging weighting coefficients are used to map the innovation in observation space and time to the model grid cell and time step. The product of \( G, w_s \) and \( w_t \) is defined as the nudging coefficient. While the \( w_s \) in the shallow water model in Chapter 3 was two-dimensional (i.e., no vertical dimension), the \( w_s \) in WRF is three-dimensional with variations in both the horizontal and vertical directions.

The flow-dependent hybrid nudging coefficients used in the HNEnKF approach are computed from the ensemble forecast, and are elements of the EnKF gain matrix normalized by the sum of the temporal nudging weighting coefficient over half of the assimilation time window. The flow-dependent hybrid nudging coefficient is then described by Eq. (4.2):

\[
G \cdot w_s = \frac{1}{\sum_{t=t_e-t_{am}} w_t \cdot \Delta t} \cdot K,
\]
where $K$ is the EnKF gain matrix, $\Delta t$ is the time step, $t$ is the model time, $t^0$ is the observation time, and $\tau_N$ is the half-period of the nudging time window. The temporal nudging weighting coefficient $w_t$ follows the trapezoidal function defined by Stauffer and Seaman (1990).

It is important to note that the hybrid nudging coefficients are computed from Eq. (4.2); that is, they come directly from the EnKF in DART (see section 4.3.1) that contains information from the flow-dependent background error covariances. Thus there is no need to specify the nudging strength (i.e., elements in the nudging magnitude matrix $G$) or the spatial nudging weighting coefficient $w_s$ in either the horizontal or vertical directions. Substituting the state vector $x$ by a vector comprised of $u$- and $v$- wind components, potential temperature and mixing ratio on every model grid point, Eq. (4.1) becomes the governing equations of WRF including the hybrid nudging terms with their coefficients defined by Eq. (4.2). It is also important to note that the hybrid nudging terms include not only the standard diagonal terms (i.e., the innovations in $u$ in the $u$-equation, and the innovations in $v$ in the $v$-equation, etc.), but also the off-diagonal terms (i.e., innovations in $u$ in the $v$-equation, and the innovations in $v$ in the $u$-equation, etc.). This statistical inter-variable influence of the innovations from the EnKF is included in the model’s dynamic relaxation terms to gradually and continuously force the model towards the observations, thereby reducing the error spikes and dynamic imbalances often produced by intermittent assimilation methods (e.g., Chapters 2 and 3).
4.3. Model configurations and experimental design

4.3.1 WRF/DART model description

In this study, the WRF-ARW version 3.1.1 (Skamarock et al. 2008) is used to test the HNEnKF approach. The model simulation has horizontal grid-spacing of 12 km on a 208×190 horizontal grid with 33 vertical levels and a model top at 100 hPa. The WRF model domain is shown in Figure 4.1. The model is configured to use the longwave Rapid Radiative Transfer Model (RRTM: Mlawer et al. 1997), the shortwave Dudhia radiation scheme (Dudhia 1989), and the 5-layer thermal diffusion land-surface scheme. Several options are used for model microphysics, convective parameterization and planetary boundary layer (PBL) turbulence, as outlined in Table 4.1 and discussed in section 4.3.3.

The simulation starts at 1200 UTC 18 September 1983, and continues for 48 hours. The NCEP / NCAR Global Reanalyses are used to generate the initial conditions (ICs) and lateral boundary conditions (LBCs) for the WRF model. Because the NCEP / NCAR Global Reanalyses have a coarse resolution of 2.5°×2.5°, the ICs and LBCs generated by the reanalyses are enhanced by a modified Cressman objective analysis (Benjamin and Seaman 1985; Deng et al. 2009) in the WRF modeling system.

The DART (Anderson et al. 2009) is used to perform the data assimilation calculations of the EnKF, and it is able to interface directly with WRF. The DART has a variety of algorithms for the ensemble filters, such as ensemble adjustment Kalman filter (EAKF; Anderson 2001), ensemble Kalman filter with perturbed observations (Evensen 1994), and particle filter (Snyder et al. 2008), to name a few. The EAKF, the default filter in DART, is chosen here. The EAKF is a deterministic ensemble square root filter, which updates the probability distribution of a model state given the prior estimate of the model state’s probability distribution, the observations and
their associated errors. The prior probability distribution of the model state is obtained from the statistics of an ensemble that incorporates flow-dependent background error covariance information. For simplicity, the EAKF is called EnKF in the following discussions, since the EAKF is one kind of EnKF. We also modified the WRF/DART code to apply the new HNEnKF approach. The parameters used in DART will be discussed in section 4.3.4.

4.3.2 Observations and verification techniques

Three-hourly surface observations and twelve-hourly rawinsonde observations from the World Meteorological Organization (WMO) are assimilated from 1200 UTC 18 September 1983 to 1200 UTC 20 September 1983. For the ensemble-based experiments, the observation error variances of wind and temperature are adapted from WRF 3DVAR (Baker et al. 2004). The observation error variance for relative humidity is set to 10% of the saturated specific humidity.

Ideally we would want to withhold some of the observations for independent verification of the data assimilation methods. However, this case had no special additional meteorological observations. Thus to evaluate and compare the performance of the different data assimilation methods on the meteorology, the analysis (posteriors) closeness-of-fit statistics to the assimilated observations are first computed. Then three-hourly forecasts (priors) of each data assimilation method are verified against the observations that will be assimilated during the next data assimilation cycle.

Moreover, an independent verification of the data assimilation approaches is performed by using the hourly output of each WRF experiment to drive the SCIPUFF AT&D model (Sykes et al. 2004) to predict surface tracer concentrations that are then verified against the observed surface tracer concentration data. In this way, the quality of the analyses produced by each data assimilation method is assessed using the SCIPUFF predictions. The 12-km SCIPUFF domain is
shown as the inner black frame within the 12-km WRF domain in Figure 4.1. The SCIPUFF simulation starts at 1700 UTC 18 September 1983, and continues for 24 hours. The observed surface tracer concentration data is available at 2200 UTC 18 September 1983, 0400 UTC 19 September 1983, 1000 UTC 19 September 1983, and 1600 UTC 19 September 1983. The surface tracer sampling sites and the measurements at the four observation times are shown in Figure 4.2.

4.3.3 Ensemble configurations

Two types of ensembles are configured for the ensemble-based data assimilation experiments. The first ensemble, which is called the IC ensemble, is produced by adding perturbations to the ICs and LBCs interpolated from the NCEP / NCAR global reanalyses and enhanced by the WMO observations in the objective analysis. The perturbations are drawn from a multivariate normal distribution by use of the WRF-3DVAR (Baker et al. 2004). This ensemble uses the first model physics configuration in Table 4.1: the WSM 3-class microphysics scheme (Hong et al. 2004), the Kain-Fritsch cumulus parameterization scheme (Kain and Fritsch 1990) and the Mellor-Yamada-Janjić (MYJ) turbulent kinetic energy (TKE) PBL scheme (Janjić 1994). This type of ensemble is then constructed using both 24 and 48 members.

The second type of ensemble also explores the sensitivities of the ensemble-based data assimilation methods to the physics (PH) configuration, and it is called the ICPH ensemble. The eight different physics configurations shown in Table 4.1 are applied. Besides the physics schemes used in the IC ensemble, the Lin et al. microphysics scheme (Lin et al. 1983), Betts-Miller-Janjić convective scheme (Betts and Miller 1986; Janjić 1994), and the Yonsei University (YSU) PBL scheme (Hong et al. 2006) are also used. Three IC ensemble members are generated the same way as in the IC ensemble for each physics configuration to produce the 24-member
ICPH ensemble. For the 48-member ICPH ensemble, six IC ensemble members are generated the same way as in the IC ensemble for each of the eight physics configurations.

### 4.3.4 Experimental design

The complete set of data assimilation experiments is defined in Table 4.2. Experiment CTRL has no data assimilation throughout the 48-h period. The FDDA experiment uses observation nudging (Stauffer and Seaman 1994; Deng et al. 2009) throughout the WRF simulation period to gradually relax the model state u-component and v-component winds, potential temperature and mixing ratio towards the observations. The major parameters used by FDDA are summarized in Table 4.3. The nudging strength is specified to be $4 \times 10^{-4}$ s$^{-1}$. Standard spatial and temporal weighting functions (Stauffer and Seaman 1994; Schroeder et al. 2006) are used for the observation nudging. The horizontal radius of influence varies from 67 km at the surface, to 100 km above the surface, to 200 km at 500 hPa and levels higher than 500 hPa (Schroeder et al. 2006). The horizontal weighting function also varies with the difference between terrain elevation at the observation site and that at the surrounding grid points (e.g., Stauffer and Seaman 1994). The vertical weighting function used to spread surface data above the surface follows Rogers et al. (2011). For the stable PBL model regimes, the vertical weighting function is 1.0 from surface to 50 m above ground level (AGL), and then it linearly decreases to 0.0 from 50 m to 100 m AGL. For the unstable PBL regimes, the vertical weighting function is 1.0 from the surface through the model PBL depth, and then it linearly decreases to 0.0 from the PBL top to 50 m above the PBL top. The half-period of the time window is 1 hour for the surface data and 2 hours for the rawinsonde data.

The EnKF experiments use the default EnKF in DART to assimilate the wind, temperature and mixing ratio observations. Experiments EnKFIC24 and EnKFIC48 use the 24-
member and 48-member IC ensembles, respectively. Experiments EnKFICPH24 and EnKFICPH48 use the 24-member and 48-member ICPH ensembles, respectively. The HNEnKF experiments use the HNEnKF approach to assimilate the wind, temperature and mixing ratio observations. The HNEnKFIC24 and HNEnKFIC48 use the 24-member and 48-member IC ensemble, and HNEnKFICPH24 and HNEnKFICPH48 use the 24-member and 48-member ICPH ensemble.

The major data assimilation parameters for Experiments EnKF and HNEnKF are also summarized in Table 4.3. As discussed above, the hybrid nudging coefficients of HNEnKF, which are the product of G and \( w_s \), are computed directly from the EnKF; thus there is no need to specify the nudging strength and spatial weighting function for the HNEnKF. The half-period nudging time window of HNEnKF is specified the same as that in the FDDA. Both the EnKF and HNEnKF experiments use error covariance localization to avoid the unrealistic error correlations at larger distance scales and filter divergence. The ensemble error covariance localization is applied by use of the piecewise rational fifth-order polynomial function following Gaspari and Cohn (1999) in the three-dimensional physical space. Two parameters, one for the horizontal cutoff distance and the other for the vertical cutoff distance, are used to control the error covariance localization scale. The horizontal cutoff distance is defined to be 533 km, which is the same radius as the first scan used in the modified Cressman objective analysis based on the rawinsonde spacing in the United States. The vertical cutoff distance is set to 150 hPa. Finally, adaptive error covariance inflation (Anderson 2007) is also used to reduce filter error and avoid filter divergence for the ensemble-based data assimilation experiments. The values of the adaptive error covariance inflation are computed by using a hierarchical Bayesian approach (Anderson 2007) and the same assimilated observations.
4.4. Overview of the 18-20 September 1983 CAPTEX-83 case

The 18-20 September 1983 episode from CAPTEX is chosen as the test case for the HNEnKF in WRF/DART, because it had the most complete tracer measurements of the CAPTEX cases. This mid-latitude cyclone case is widely used for air-quality and regional transport studies (e.g., Deng et al. 2004; Deng and Stauffer 2006). It had a large anticyclone centered over the Mid-Atlantic coast. To the northwest of the high pressure system, a cold front and a warm front (see Figure 4.2) propagated quickly through the western Great Lakes with areas of showers and thunderstorms varying in intensity and location through the period. For the 18-19 September episode, 208 kg of the perfluorocarbon tracer gas (C₇F₁₄) was released at ground level at Dayton, Ohio (OH), denoted by R in Figure 4.2. The release period was 1700-2000 UTC 18 September. The cold front is especially important since it tends to define the western edge of the tracer plume through the period.

By 2200 UTC 18 September (Figure 4.2a), the cold front is crossing Michigan (MI) and the warm front extends from Lake Huron to western New York (NY). The tracer plume shown by the observed tracer concentration data was advected northeastward to northern OH, which is consistent with the southwesterly wind flow ahead of the cold front. Six hours later, the cold front is passing through Detroit MI, and the warm front has propagated to eastern NY. The low-level jet (LLJ) at 850 hPa, which was located around Niagara Falls (not shown), led to rapid transport of the tracer plume from the Midwest to northern New England during the nocturnal period, as shown in Figure 4.2b. By 1000 UTC 19 September (Figure 4.2c), the cold front is advancing towards northern NY through Lake Ontario, while the warm front moved eastward into Maine. The tracer plume also continued to race eastward into northern New England. By 1600 UTC 19 September (Figure 4.2d), the cold front is located across northern NY, and the tracer plume begins to exit the monitoring network.
The standard surface weather observations at 1200 UTC 18 September (not shown) indicate some thunderstorm activity close to the warm front that extended from eastern Wisconsin (WI) to southern MI, with widespread showers throughout the rest of MI. By 1800 UTC 18 September when the warm front propagated eastward, the thunderstorms were located mostly near Lake Ontario, and they had weakened at 0000 UTC 19 September. By 0600 UTC 19 September, some thunderstorms were active along the frontal boundaries but weakened again by 1800 UTC 19 September. So this case featured a typical eastward moving mid-latitude weather system with both cold and warm frontal boundaries with some areas of convective precipitation during the period.

4.5. WRF/DART Results

In this section, we first perform a statistical evaluation of the dynamic analyses and three-hourly forecasts produced by the set of data assimilation experiments (Table 4.2) using the meteorological data for wind speed, wind direction, temperature and relative humidity. Then we assess the results of the various data assimilation methods for temporal smoothness and the creation of insertion noise within the model. Finally, we perform an independent verification of the dynamic analyses using the AT&D model and the observed surface concentration tracer data.

4.5.1 Evaluation using meteorological data

The dynamic analyses created by the set of data assimilation experiments for the CAPTEX case use standard three-hourly surface data and twelve-hourly rawinsonde data. The fit-to-observation statistics (postersiors) at each analysis time will be discussed first. Then the three-hourly forecasts (priors) launched from each analysis following data assimilation will be
verified against the observations available for the next three-hour cycle of data assimilation. Examination of the priors will indicate the ability of the model to retain the assimilated information from the previous cycle.

Figure 4.3 shows the average RMS errors of the posteriors for the set of experiments for all model layers over the 48-h period for wind speed, wind direction, temperature and relative humidity. The levels of statistical significance of the comparisons among the average RMS errors of the posteriors for the set of experiments are shown in Table 4.4 for the same meteorological variables. The statistical significance is obtained using a bootstrap resampling procedure that is applied to the observations and the model-interpolated values during the data assimilation period. The average RMS error of the bootstrapped sample is then computed. This procedure is repeated for 10000 random samples. Following Buehner et al. (2010b), the relative frequency that one experiment has lower average RMS error than another experiment is computed. A significance level is then obtained from this relative frequency that represents the probability that two experiments have different average RMS errors. The relative frequencies and significance levels of the posteriors of the set of experiments are presented by Table 4.4. The relative frequencies in Table 4.4 give the probability of the experiment in the column having smaller average RMS error than the experiment in the row. The situations with a significance level above 90% (95%) are denoted by underline (boldface font).

As shown by Figure 4.3, all data assimilation experiments produce smaller average RMS errors of the posteriors for the wind speed, wind direction, temperature and relative humidity than the CTRL. Table 4.4 confirms that the average RMS errors of the data assimilation experiments are significantly smaller than those of the CTRL at the 95% significance level. Note that Experiments CRTL and FDDA do not use an ensemble and thus their statistics are the same for each ensemble group.
For the IC24 experiments (IC ensemble with 24 members), Experiment FDDA has the smallest RMS errors for all four variables; that is, the WRF simulation using observation nudging FDDA shows the closest fit to the assimilated observations of all the experiments. This is confirmed by Table 4.4, which shows that the Experiment FDDA has significantly smaller average RMS errors for all four variables than the EnKFIC24 and HNEnKFIC24 at the 95% significance level. The HNEnKFIC24 has larger RMS errors than the FDDA, but smaller RMS errors than the EnKFIC24 for all four variables. Table 4.4 shows that the HNEnKFIC24 has significantly smaller average RMS errors of wind direction (at the 95% level), temperature (at the 90% level) and relative humidity (at the 95% level) than the EnKFIC24, although the difference of wind speed between HNEnKFIC24 and EnKFIC24 is not significant. Thus the HNEnKFIC24 improves the fit-to-observation statistics compared to the EnKFIC24 in general, although it has larger RMS errors compared to the FDDA.

The average RMS errors of the posteriors for the experiments including multi-physics ensemble members are shown by the group ICPH24 in Figure 4.3. For the wind speed and wind direction, the FDDA has smaller average RMS errors than the EnKFICPH24 and HNEnKFICPH24, which are significant at the 95% level (Table 4.4). The HNEnKFICPH24 has lower average RMS errors of wind speed and wind direction than the EnKFICPH24; however, the differences are not statistically significant. For the temperature and relative humidity, the EnKFICPH24 has similar average RMS errors to the FDDA, which are consistent with the significance levels. Both the FDDA and EnKFICPH24 have lower average RMS errors of temperature and relative humidity than the HNEnKFICPH24, which are significant at the 95% level.

Comparing the average RMS errors of the group ICPH24 to the group of IC24, we see that EnKFICPH24 and HNEnKFICPH24 have similar average RMS errors for wind speed and wind direction to the EnKFIC24 and HNEnKFIC24, respectively. For temperature and relative
humidity, the EnKFICPH24 and HNEnKFICPH24 have smaller RMS errors than the respective IC ensemble experiments, which are confirmed by the 95% significance levels presented in Table 4.4. Moreover, the reduction of the average RMS error of the EnKFICPH24 is larger than that of the HNEnKFICPH24. Thus the addition of the multi-physics ensemble members in the ICPH ensemble improves the fit-to-observation statistics for the mass fields in the EnKF and HNEnKF compared to the IC ensemble, and especially so for the EnKF.

To understand why the ICPH ensemble improves the posteriors of the mass field compared to the IC ensemble, we examined the ensemble spreads of 2-m temperature from IC and ICPH ensembles. The spread from the IC ensemble is introduced by the perturbations of ICs and LBCs, and it is often associated with the location of baroclinic systems. Thus large spread from the IC ensemble is found near the low pressure system and along the frontal boundaries for this case (not shown). Besides the spread introduced by the perturbations of ICs and LBCs, the spread from the ICPH ensemble is affected by the use of different model physics and parameterization schemes, and it is increased by as much as a factor of two compared to that from the IC ensemble. This conclusion is consistent with the finding of Fujita et al. (2007) that the physics ensemble tended to give larger spread in thermodynamic variables than in dynamic variables, because the thermodynamic variables were more directly associated with the physical processes than the dynamic variables. Thus it is not surprising that the ICPH ensemble, which has the characteristics of both IC ensemble and physics ensemble, generates larger spread of the thermodynamics variables than the IC ensemble only (not shown). The algorithm of the EnKF shows that the correction of a variable from an observation is larger at the locations with larger spread (Evensen 1994). Therefore, the larger ensemble spread of the mass field from the ICPH ensemble helps to explain why the multi-physics ensemble further improves the analysis of the mass field of the EnKF and HNEnKF, as shown in Figure 4.3.
The average RMS errors of the posteriors of the experiments with the increased ensemble size of 48 members are shown by the groups IC48 and ICPH48 in Figure 4.3. The corresponding significance levels are presented in Table 4.4. The relative results comparing EnKF and HNEnKF are very similar to those reported using the 24 ensemble members. The HNEnKF has an advantage in the fit-to-observations over the EnKF, and the inclusion of the multi-physics ensemble members improves the posteriors of the mass fields in both EnKF and HNEnKF, with a larger improvement in the EnKF. The increase of ensemble size from 24 to 48 slightly improves the average RMS errors of the EnKF and HNEnKF for both the IC and ICPH ensembles. However, only EnKFIC48 has significantly smaller RMS errors than its 24-member EnKF counterpart (EnKFIC24) and only for relative humidity (at the 90% level). The HNEnKFIC48 and HNEnKFICPH48 have significantly smaller average RMS errors of the wind speed compared to HNEnKFIC24 (at the 90% level) and HNEnKFICPH24 (at the 95% level), respectively.

Next we examine the average RMS errors of the priors of the set of experiments for wind speed, wind direction, temperature and relative humidity. All data assimilation experiments produce smaller average RMS errors of wind speed, temperature and relative humidity in the priors than does the CTRL (Figure 4.4). Table 4.5 shows the details on the levels of statistical significance of the comparisons among the average RMS errors of the priors for the set of experiments, and it confirms that all data assimilation experiments have significantly smaller average RMS errors of wind speed, temperature and relative humidity than the CTRL. For the wind direction, the FDDA and HNEnKF experiments have smaller average RMS errors than the CTRL, but the differences are not statistically significant. The EnKF experiments have even larger average RMS errors of wind direction than the CTRL, although only EnKFIC24 has significantly larger average RMS error of wind direction than the CTRL.

For the IC24 group of experiments, the three data assimilation experiments produce very similar average RMS errors for wind speed, which are consistent with the significance levels.
The HNEnKFIC24 and FDDA have similar average RMS errors of wind direction, and both of them have smaller average RMS errors of wind direction than the EnKFIC24. Table 4.5 confirms that the FDDA and HNEnKFIC24 have significantly smaller average RMS error of wind direction than the EnKFIC24. The HNEnKFIC24 and EnKFIC24 have similar average RMS errors for temperature, and they both have significantly smaller average temperature RMS errors than the FDDA. The HNEnKFIC24 has smaller average RMS errors of relative humidity than both EnKFIC24 and FDDA, while the EnKFIC24 has smaller average RMS error of relative humidity than the FDDA. Table 4.5 shows that these differences are statistically significant. Therefore, the HNEnKFIC24 produces similar or better three-hourly forecasts than EnKFIC24 for the wind and mass fields. The HNEnKFIC24 also improves the three-hourly forecast of the mass fields compared to the FDDA, and has similar RMS errors to the FDDA for the wind field.

For the group of ICPH24 experiments, the wind field average RMS error comparisons among the three data assimilation experiments are consistent with those from the group of IC24 experiments. For the mass fields, the EnKFICPH24 has slightly smaller average RMS errors than the HNEnKFICPH24, while both of them have smaller average RMS errors than the FDDA. Table 4.5 shows that both the EnKFICPH24 and HNEnKFICPH24 have significantly smaller average RMS errors of temperature and relative humidity than the FDDA. The EnKFICPH24 has significantly smaller average RMS error of temperature than the HNEnKFICPH24, while it has statistically similar average RMS error of relative humidity to the HNEnKFICPH24. Compared to the IC ensemble, the addition of multi-physics ensemble members in the ICPH ensemble slightly improves the three-hourly forecast of the temperature and relative humidity of the EnKF, although only the improvement of relative humidity is statistically significant.

When the ensemble size increases from 24 to 48 members, the comparative results of the priors from the 48 ensemble member experiments are generally the same as those for the 24
ensemble member experiments. The increase of ensemble size slightly improves the average RMS errors of the priors of the EnKF and HNEnKF for both the IC and ICPH ensembles, although the improvements are not statistically significant as shown in Table 4.5.

4.5.2 Evaluation of temporal smoothness and insertion noise

To explore the temporal smoothness and potential for insertion noise and dynamic imbalance related to intermittent data assimilation methods, the domain average absolute surface pressure tendency is examined here. The magnitude of the surface pressure tendency is often used to quantify model noise in a mesoscale model following data insertion or model initialization (e.g., Chen and Huang 2006). Figure 4.5 shows the evolutions of the domain average absolute surface pressure tendency for Experiments FDDA, HNEnKFIC24, and each ensemble member of Experiment EnKFIC24 and the ensemble mean. It is clear that the EnKF has much higher noise levels than both the FDDA and HNEnKF when the observations are assimilated, as shown by both the individual ensemble members and the ensemble mean. The noise levels of the EnKF are even higher at the twelve-hourly times when both surface observations and rawinsonde data are assimilated than the other three-hourly times when only surface observations are assimilated. Therefore, the more observations assimilated by the EnKF, the higher the noise level produced by the intermittent EnKF. These spurious high-frequency oscillations decrease quickly with time, but the noise levels of the EnKF are still higher through the 48-h period than those of the FDDA and HNEnKF.

It is important to note that the HNEnKF, similar to the FDDA but using flow-dependent and time-dependent error covariances from the EnKF, does not show large spikes or discontinuities in surface pressure tendency as the EnKF. These spikes can be greatly reduced by using a digital filter (e.g., Lynch and Huang 1992), but the digital filter can also smooth out
physically realistic model-generated high-frequency motions. The HNEnKF does not require any
digital filtering and shows temporally smooth and better balanced model solutions following the
data insertions, which is consistent with the results of applying the HNEnKF in the shallow water
model (Chapter 3).

A comparison of the data insertion noise levels for the EnKF and HNEnKF when using
the 24-member IC ensemble versus the 24-member ICPH ensemble is shown in Figure 4.6. The
evolution of the ensemble mean of the domain average absolute surface pressure tendencies from
Experiment EnKFICPH24 is compared to that of EnKFIC24 in Figure 4.6a. The noise levels of
the EnKFICPH24 at the three-hourly observation times are even higher than those of the
EnKFIC24. However, the noise levels of the HNEnKFICPH24 are very similar to those of the
HNEnKFIC24, as shown by Figure 4.6b. Thus adding multi-physics ensemble members increases
the already high noise levels of the EnKF, while it has very little impact on the low noise levels of
the HNEnKF. Similar results are obtained when the ensemble size is increased from 24 to 48
(not shown). Therefore, the advantages shown in the previous section for the meteorological
fields from the HNEnKF compared to the EnKF are also generally accompanied by much lower
noise levels following the data assimilation of the HNEnKF compared to the EnKF. When the
EnKF with the ICPH ensemble produces smaller average RMS errors of the mass field than the
HNEnKF with the ICPH ensemble, the noise levels of the EnKF are even higher.

4.5.3 Evaluation using independent surface tracer data

An independent verification of the dynamic analyses produced by the set of data
assimilation experiments (Table 4.2) is performed here by comparing the predicted SCIPUFF
surface tracer concentrations to the observed CAPTEX-83 surface concentration data. The
minimum threshold used for defining “nonzero” concentrations for the predicted and observed
surface tracer concentration field is set to 3.0 fl/l (e.g., Lee et al. 2009). This threshold value is three times the minimum value detected by the sensor.

The total numbers of hits, misses and false alarms composited over the 24-h tracer study period for the set experiments are shown in Figure 4.7. Overall, the use of Experiment FDDA meteorology fields in SCIPUFF produces the largest number of hits (29) and smallest number of misses (7), while its false alarms were neither the largest nor smallest from the set of experiments. By comparison, Experiment CTRL produces five fewer hits (24) and five more misses (12) than FDDA. Please note that the sum of hits and misses is a constant (one more miss means one fewer hit). Thus for brevity only the number of hits and false alarms will be discussed, because we want to maximize the number of hits and minimize the number of misses and false alarms. Experiment CTRL had 19 false alarms compared to 13 false alarms for FDDA. Please note that the statistics for CTRL and FDDA are independent of the ensemble data assimilation experiments group.

For the group of IC24 experiments, Experiment FDDA has six more hits than EnKFIC24, and HNEEnKFIC24 has three more hits than the EnKFIC24, while EnKFIC24 has one fewer hit than the CTRL. All three data assimilation experiments have fewer false alarms than the CTRL, while the HNEEnKFIC24 produces the smallest number of false alarms. The better temporal smoothness (better dynamic balance) of the HNEEnKF dynamic analyses compared to that of the EnKF, as discussed in the previous section, may help explain why SCIPUFF using the HNEEnKF meteorology fields has better statistics of the independent tracer concentration data than the EnKF. This may also contribute to why the FDDA experiment performs better than the other experiments.

When the additional multi-physics ensemble members are used, the HNEEnKFICPH24 has five more hits and five fewer false alarms than the EnKFICPH24, while the FDDA has two more hits and one more false alarm than the HNEEnKFICPH24. The EnKFICPH24 has one fewer hit
and three more false alarms than the EnKFIC24. The HNEnKFICPH24 has one more hit than the HNEnKFIC24, while HNEnKFICPH24 has the same number of false alarms as the HNEnKFIC24. Therefore, the ICPH ensemble increases the hits (and decreases the misses) with no change of the false alarms for the HNEnKF. But the ICPH ensemble degrades all three tracer statistics for the EnKF. The increase in the noise levels in the EnKF caused by the inclusion of the multi-physics ensemble members, as discussed in the previous section, may contribute to the degradation of the statistics verified against the surface concentration data, because the increased noise levels indicate degraded dynamic consistency.

When the ensemble size is increased from 24 to 48 members, the EnKFIC48 has one more hit than the EnKFIC24, while it has the same number of false alarms as EnKFIC24. The EnKFICPH48 has one fewer hit and one fewer false alarm than the EnKFICPH24. The HNEnKFIC48 has one fewer hit and one more false alarm than the HNEnKFIC24. The HNEnKFICPH48 has one fewer hit and one fewer false alarm than the HNEnKFICPH24. Thus there is no clear improvement or degradation for either the EnKF or HNEnKF when the ensemble size is increased from 24 to 48. This is consistent with the meteorology statistics and the noise levels that are fairly similar for the same ensemble data assimilation experiments using 24 versus 48 ensemble members. The differences in the meteorological statistics and the noise levels are larger between the IC and ICPH ensembles than those between 24 and 48 ensemble members. The 48-member ICPH ensemble again degrades all three tracer statistics for the EnKF compared to the IC ensemble, which is consistent with the results with 24 ensemble members. However, the ICPH ensemble with 48 members increases the hits, and decreases the false alarms for the HNEnKF compared to the IC ensemble.

To assess the overall performance of each data assimilation method verified against the observed surface tracer data, we assign an ordinal ranking to the set of experiments in Table 4.6. The rank is based on the sum of misses and false alarms in the 24-h tracer study period. Since the
sum of hits and misses is a constant, the hits are already represented by the value of misses. By looking for smaller values of the sum of misses and false alarms, we can define the better performing experiments in terms of the tracer verification. Experiment FDDA has the smallest value of the sum (20), while Experiment HNEnKF with the 24-member or 48-member ICPF ensemble (HNEnKFICPH24 or HNEnKFICPH48) has a value only one larger than that of the FDDA. The HNEnKF with the 24-member and 48-member IC ensemble (HNEnKFIC24 and HNEnKFIC48) has values of 22 and 24, respectively. All HNEnKF experiments produce smaller values of the sum than the EnKF experiments. The best EnKF experiment, EnKFIC48, shows a value of 26, followed by EnKFIC24 with 27, and these sums are five or six larger than that of the best HNEnKF experiment (HNEnKFICPH24 or HNEnKFICPH48). Finally, Experiments EnKFICPH24, EnKFICPH48 and CTRL show a value of 31, and this value is at least 10 larger than those at or near the top of the list, Experiments FDDA and HNEnKFICPH24 / HNEnKFICPH48.

Although this independent verification is for only one case with a limited sample, the results are consistent. The experiments having good posteriors and priors along with low insertion noise scored higher with the independent tracer data. There appears to be some advantage in the hourly fields produced by the continuous HNEnKF compared to the intermittent EnKF. This is also consistent with the lower noise levels of Experiment HNEnKF compared to the Experiment EnKF in the previous section. Therefore, the added value of the HNEnKF, which applies the EnKF gradually in time via nudging-type terms and produces better temporal smoothness, has been demonstrated.
4.6. Conclusions

A hybrid nudging-EnKF (HNEnKF) data assimilation approach was proposed and tested in the Lorenz and shallow water model systems in Chapters 2 and 3, and it is investigated here using WRF/DART with real observations from the CAPTEX-83 case. The HNEnKF effectively combines the strengths of the EnKF and nudging while avoiding their individual weaknesses. It applies the EnKF gradually in time via nudging-type terms, and provides flow-dependent and time-dependent nudging coefficients by using the EnKF. The HNEnKF also extends the nudging coefficients to include nonzero off-diagonal elements, which improves the inter-variable influences of the innovations and dynamic consistency.

The set of data assimilation methods is first verified against the meteorological data. The levels of statistical significance of the comparisons among the data assimilation methods are produced by a bootstrap resampling procedure. For the 24-member IC ensemble based on perturbations of the ICs and LBCs, the HNEnKF dynamic analyses (posteriors) have significantly better fit-to-observation statistics than the EnKF for both wind and mass fields in general, although both HNEnKF and EnKF have larger posterior RMS errors than the FDDA. The HNEnKF has similar or better three-hourly forecast (prior) statistics than the EnKF and FDDA. The 24-member ICPH ensemble significantly improves the posteriors of the mass field compared to the IC ensemble for both the EnKF and HNEnKF, with larger improvements for the EnKF. The 24-member ICPH ensemble also significantly improves the priors of the relative humidity compared to the IC ensemble for the EnKF. The wind field posteriors and priors are very similar for the IC and ICPH ensembles with 24 ensemble members. The increase of ensemble size from 24 to 48 slightly improves the posteriors and priors of the EnKF and HNEnKF for wind and mass for both the IC and ICPH ensembles, but only the posteriors of relative humidity of the EnKF with the IC ensemble and the posteriors of wind speed of the HNEnKF with both the IC and
ICPH ensemble are significantly improved when ensemble size increases from 24 to 48. The comparisons between EnKF and HNEnKF for both the IC and ICPH ensembles of 48 ensemble members are consistent with those of the 24 ensemble members.

The analyses of the domain average absolute surface pressure tendency shows that the intermittent EnKF has much higher noise levels than the continuous HNEnKF and FDDA approaches when three-hourly observations are assimilated. The noise levels in the EnKF are even higher at the twelve-hourly times when rawinsonde data are also assimilated and when multi-physics ensemble members are included, while the HNEnKF shows little sensitivity to these factors. This demonstrates that the HNEnKF is able to provide better temporal smoothness and dynamic consistency in the hourly analyses than the EnKF while retaining its advantages by using the flow-dependent and time-dependent background error covariances to spread the innovations in the horizontal and vertical directions.

Finally, the set of data assimilation methods is verified against the independent surface tracer data. The FDDA has the best overall statistics, as represented by the smallest value of the sum of misses and false alarms, followed by the HNEnKF using the ICPH ensemble and having a value only one larger than that of the FDDA. The HNEnKF produces consistently better statistics than the EnKF. Compared to the IC ensemble, the ICPH ensemble decreases the misses without increasing the false alarms for the HNEnKF, but the ICPH ensemble degrades all tracer data statistics for the EnKF. Because the HNEnKF analyses used to drive the SCIPUFF produce consistently better tracer data verification statistics than the EnKF, there appears to be some advantage in the dynamic analyses produced by the continuous HNEnKF compared to the intermittent EnKF, as we hypothesized using simple models and OSSEs in Chapters 2 and 3.

This real-data, full-physics WRF mesoscale model application of the HNEnKF using the CAPTEX-83 meteorological and tracer data further demonstrates the proof-of-concept of the HNEnKF for its potential added value for fitting the observations and improving meteorological
analyses while reducing the insertion noise and increasing dynamic consistency and temporal smoothness. In the future, both the EnKF and HNEnKF will be attractive methods for data assimilation especially over complex terrain with fine model resolution. For complex terrain, where observations are often more sparse, the flow-dependent background error covariances may be able to better capture the terrain influences and maximize their effect. Moreover, the HNEnKF may have some added advantage over the EnKF with complex terrain and fine resolution due to its lower noise levels and continuous data assimilation. Over complex terrain, where noise levels are naturally higher, the insertion noise can more easily stimulate false convection resulting in unrealistic precipitation.
Table 4.1. Eight different physics configurations for the ICPH ensemble. The first physics configuration is the default physics configuration used in the IC ensemble.

<table>
<thead>
<tr>
<th>Physics configuration</th>
<th>Microphysics</th>
<th>Convective</th>
<th>PBL</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>WSM-3</td>
<td>Kain-Fritsch</td>
<td>MYJ</td>
</tr>
<tr>
<td>2</td>
<td>Lin et al.</td>
<td>Kain-Fritsch</td>
<td>MYJ</td>
</tr>
<tr>
<td>3</td>
<td>WSM-3</td>
<td>Betts-Miller-Janic</td>
<td>MYJ</td>
</tr>
<tr>
<td>4</td>
<td>WSM-3</td>
<td>Kain-Fritsch</td>
<td>YSU</td>
</tr>
<tr>
<td>5</td>
<td>Lin et al.</td>
<td>Betts-Miller-Janic</td>
<td>MYJ</td>
</tr>
<tr>
<td>6</td>
<td>Lin et al.</td>
<td>Kain-Fritsch</td>
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</tr>
<tr>
<td>7</td>
<td>WSM-3</td>
<td>Betts-Miller-Janic</td>
<td>YSU</td>
</tr>
<tr>
<td>8</td>
<td>Lin et al.</td>
<td>Betts-Miller-Janic</td>
<td>YSU</td>
</tr>
</tbody>
</table>
Table 4.2. Experimental design of the HNEnKF in WRF/DART.

<table>
<thead>
<tr>
<th>Exp. Name</th>
<th>Exp. Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CTRL</td>
<td>Assimilate no observations</td>
</tr>
<tr>
<td>FDDA</td>
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Table 4.3. Major data assimilation parameters for the set of experiments. See section 4.3.4 for details.

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<th>Experiment</th>
<th>Nudging strength</th>
<th>Horizontal radius of influence</th>
<th>Surface data vertical radius of influence (stable PBL)</th>
<th>Surface data vertical radius of influence (unstable PBL)</th>
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<th>Horizontal error covariance localization</th>
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<td>PBL top plus 50m</td>
<td>1-2 h</td>
<td>---</td>
<td>---</td>
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<tr>
<td>EnKF</td>
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<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>533 km</td>
<td>150 hPa</td>
<td>Adaptive inflation</td>
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<tr>
<td>HNEEnKF</td>
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<td>---</td>
<td>---</td>
<td>---</td>
<td>1-2 h</td>
<td>533 km</td>
<td>150 hPa</td>
<td>Adaptive inflation</td>
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Table 4.4. Relative frequencies and significance levels of the bootstrapped average RMS errors of the posteriors of the set of experiments. The values are the relative frequencies that give the probability of the experiment in the column having smaller average RMS error than the experiment in the row. Boldface font denotes the significance level higher than 95%, and underline denotes the significance level higher than 90%.

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Table 4.5. Same as Table 4.4, except for the priors.

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Table 4.6. Ordinal ranking of the set of experiments by the sum of misses and false alarms from the independent tracer data verification.

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Figure 4.1. The WRF 12-km domain (outer domain) and the 12-km SCIPUFF domain (inner domain).
Figure 4.2. Surface cold and warm fronts and observed tracer concentrations (parts of perfluorocarbon per $10^{15}$ parts of air by volume, or femtoliters/liter) over the surface sampling network during CAPTEX-83 at (a) 2200 UTC 18 September, (b) 0400 UTC 19 September, (c) 1000 UTC 19 September, and (d) 1600 UTC 19 September 1983 (After Deng et al. 2004). "R" is the release point at Dayton, OH.
Figure 4.2. (Continued)
Figure 4.3. The average RMS errors of the posteriors for Experiments CTRL and FDDA, and Experiments EnKF and HNEEnKF for both IC and ICPH ensembles with 24 or 48 ensemble members through the 48-h simulation period. (a) wind speed (ms$^{-1}$), (b) wind direction (degrees), (c) temperature (K) and (d) relative humidity (percent).
Figure 4.4. The same as Figure 4.3, except for the priors.
Figure 4.5. The evolutions of the domain average absolute surface pressure tendency of Experiment FDDA, each ensemble member of Experiment EnKFIC24 and their ensemble mean, and Experiment HNEnKFIC24.
Figure 4.6. The evolutions of the domain average surface pressure tendencies. (a) ensemble mean of Experiments EnKFIC24 and EnKFICPH24, and (b) Experiments HNEnKFIC24 and HNEnKFICPH24.
Figure 4.7. The composite statistics (hits, misses and false alarms) of the predicted surface tracer concentration through the 24-h period from each experiment from Table 2 verified against the observed surface tracer concentration data.
Chapter 5
Conclusions and Future Work

A hybrid nudging-EnKF (HNEnKF) data assimilation approach is proposed and explored in this dissertation. It effectively combines the strengths of the nudging and EnKF while avoiding their individual weaknesses. The HNEnKF provides flow-dependent and time-dependent nudging coefficients by using the EnKF, and improves the inter-variable influences and dynamic consistency by also including the nonzero off-diagonal elements of the EnKF gain matrix in the nudging coefficients. It applies the EnKF gradually in time via nudging-type terms, and achieves a more gradual data assimilation that greatly reduces the insertion noise.

The HNEnKF is first tested in the Lorenz three-variable system with different observation frequencies and initial conditions. It promotes a better fit of an analysis to data compared to that produced by nudging. It provides a continuous data assimilation with better inter-variable consistency and improved temporal smoothness than that of the EnKF. Compared to the “gold standard” EnKS, the HNEnKF has similar or better temporal smoothness than that of the EnKS, and with much smaller CPU time and data storage requirements.

To further investigate the performance of the HNEnKF in a more realistic model and explore the dynamic imbalance caused by the intermittent EnKF, we test the HNEnKF in a 2D shallow water model. In a quasi-stationary wave case and a moving vortex case, the HNEnKF generally produces smaller RMS errors in both the height and wind fields than the nudging and EnKF applied separately. It retains the benefits of the continuous nudging by reducing the RMS errors gradually in time, compared to the intermittent EnKF that has strong corrections and discontinuities at the analysis steps. The EnKF produces somewhat better (worse) RMS errors and spread-error relationships in Case I (Case II) when ensemble size increases from 20 to 40.
However, the HNEnKF produces somewhat better results for both Case I and II with increasing ensemble size. This is likely due to the use of ensemble spread within the continuous assimilation framework and the smaller insertion noise of the HNEnKF. Moreover, the HNEnKF produces smoother evolution of the ageostrophic wind without any strong discontinuities / dynamic imbalances around the observation time, while the EnKF has large bursts in the ageostrophic wind after the observations are assimilated.

Building on the encouraging results from the idealized models, we further test the HNEnKF in the 3D WRF model with real observations using the CAPTEX-83 case. The HNEnKF generally has better posteriors than the EnKF for both wind and mass fields, although both HNEnKF and EnKF have larger posterior RMS errors than the observation-nudging FDDA. The HNEnKF has similar or better priors than the EnKF and FDDA in general. Moreover, the intermittent EnKF has much higher noise levels of the domain average absolute surface pressure tendency than the continuous HNEnKF and FDDA, especially around the observation or analysis times. Thus the ability of the HNEnKF to provide better temporal smoothness and dynamic consistency than the EnKF is demonstrated. When the independent surface tracer data is used for verification, the HNEnKF produces consistently better statistics of hits, misses and false alarms than the EnKF. Thus there appears to be some advantage in the dynamic analyses produced by the continuous HNEnKF compared to the intermittent EnKF.

The HNEnKF has been explored using idealized models with simulated observations and a full-physics atmospheric mesoscale model with real observations. For the application of the HNEnKF to current atmospheric models with real observations, more cases are needed. Only one case is used here to test the proof-of-concept of the HNEnKF in WRF/DART. Although a bootstrap resampling procedure is adopted to build the statistical significance, more cases are needed to sufficiently establish statistical significance. Moreover, slight improvements of the fit-to-observation statistics and three-hourly forecasts of the HNEnKF are obtained with the
ensemble size increasing from 24 to 48, when the HNEnKF is applied to WRF/DART. In order to produce statistically significant improvements of the fit-to-observation statistics and three-hourly forecasts resulting from the variations in ensemble size, a sufficiently larger ensemble size may be required.

In the future, both the EnKF and HNEnKF will be attractive methods for data assimilation over complex terrain with fine model resolution. The EnKF is able to provide a flow-dependent estimate of the background error covariances for use in data assimilation through the use of an ensemble forecast, and the HNEnKF provides flow-dependent nudging coefficients by using the EnKF. For complex terrain, where observations are often more sparse, the flow-dependent background error covariances may be able to better capture the terrain influences and maximize their effect. Moreover, the HNEnKF may have some added advantage over the EnKF with complex terrain and fine resolution due to its lower noise levels and continuous data assimilation. Over complex terrain, where noise levels are naturally higher, the insertion noise can more easily stimulate false convection resulting in unrealistic precipitation.

The HNEnKF has been investigated in dynamic-analysis mode where the data assimilation is applied throughout the model integration. The investigation of the HNEnKF for dynamic initialization is also needed, since improved forecasts from data assimilation are very important for many applications. For the forecast problem, a data assimilation method is used during a pre-forecast period to generate spun-up and better balanced initial conditions to produce an improved subsequent forecast. Because the HNEnKF is able to produce better temporal smoothness and dynamic consistency in the dynamic analysis and lower RMS errors in the 3-hourly priors at the next observation times compared to the EnKF as tested in WRF/DART, it is hypothesized that the HNEnKF will provide better balanced initial conditions and then improved subsequent forecasts than the EnKF.
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VITA

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