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ANALYSIS OF DETERMINISTIC AND STOCHASTIC IMPLICIT INTERFACE MODELS OF FLUID-INTERFACE INTERACTIONS

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ABSTRACT

The work presented in this thesis focuses on the analysis of fluid implicit interface interaction models.

Some rigorous theory is presented for a phase field Navier-Stokes vesicle-fluid interaction model in Chapter 2. The existence and uniqueness theorems of global weak solutions are proved.

In Chapter 3, a consistent and rigorous derivation of some stochastic fluid-structure interaction models based on an implicit interface formulation of the stochastic immersed boundary method is presented. As dictated by the fluctuation-dissipation theorem, a proper noise has been derived to be incorporated into the deterministic hydrodynamic fluid-structure interaction models in either the phase field or level-set framework. The resulting stochastic system is referred to as stochastic implicit interface model, which not only captures the fluctuation effect near equilibrium but also provides an effective tool to model the complex interfacial morphology. Furthermore, the stochastic implicit interface model is also considered with a quasi-steady

flow, which reduces the stochastic implicit interface model to a Langevin type equation of phase field (or level set) function with multiplicative noise.

The mathematical analysis of the stochastic implicit interface models is presented in Chapter 4. The well-posedness of pathwise solutions are established and also a uniform control over solutions in probability is provided.

Contents

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Chapter 1

Introduction

1.1 Overview

Fluid-structure interaction appears in many contexts in sciences and engineering, ranging from the studies of aerodynamics of aircraft, colloidal suspension in chemical reaction to cell migration in biological environment.

Many research efforts have been devoted to developing mathematical models for such interactions. For instance, the immersed boundary method in [66] models fluid-structure interaction by using discrete particles to represent the immersed structure. In [12, 13, 14], a level set method for fluid-structure interaction is discussed. Other relevant work includes the studies of complex fluids, for example, the modeling of liquid crystals [54].

The work presented in this thesis focuses on the analysis of the fluid elastic surface (or interface) interaction. It is largely motivated by the studies of flow deformation and the rheology of vesicle membranes and cells. The mechanical properties of vesicle membranes are known to play important roles in cell biology and physiology. Take the red blood cell (RBC) membrane for example, it consists of a mixed lipid-protein bilayer. Many blood flow properties are determined by the elastic character of RBC membrane. Such elastic character also enables RBCs to transverse capillaries. In fact, with the biconcave discoid shape the RBCs are capable of passing through capillaries with less than half of RBC diameter [58]. So it is important to understand the general mechanism that determines the shape of vesicle membrane when interacting with fluid and how such interaction impacts the flow properties in biological and physiological studies.

Considerable research efforts have been devoted to both experimental studies [1, 35, 43] and mathematical modeling and simulations of membrane properties and fluid constitution in recent years [5, 7, 8, 44, 41, 48, 49, 60, 61, 67, 68, 73, 74].

Particularly in [19, 20] a phase field model is introduced to study the static cell membrane deformation, in which the cell membrane is viewed as a closed elastic surface, represented implicitly by a so called phase field function. The equilibrium configuration of the elastic surface minimizes its elastic bending energy (will be discussed later). The simulations have successfully captured the typical shapes of cells found in natural biological environment[20]. To further include the interaction of vesicle membrane with background fluid, such as the RBCs passing in capillaries, a coupled phase field Navier-Stokes vesicle-fluid interaction (PFNS) model is proposed in [24]. The derivation of the coupled model is based on the least action principle. The resulting equations are similar to those used to model liquid crystals with director field [54]. As a part of this thesis, the existence and uniqueness of the weak solution to this coupled model is established in Chapter 2 with a modified Galerkin method.

Fluid-structure interaction may involve phenomena at many different length and time scales. While the microscopic fluctuations are generally very small on the macroscopic scale, they play essential roles in many important applications in materials sciences and fluid mechanics [50, 72, 56, 57], as well as in various biological processes and functions [72]. In fact, the small thermal fluctuation of RBC membranes has been observed in experiments [58]. This raises the question how to account for the small thermal fluctuation effects in the aforementioned PFNS model.

One approach to capture the microscopic fluctuation has been the introduction of stochastic noise in the macroscopic field equations. The resulting equations often are stochastic partial differential equations (SPDE). SPDEs have been intensively studied. The general theory on SPDE is discussed, for instance, in [69] by Da Prato and Zabczyk.

Many stochastic models have been developed for fluid-structure interactions. For instance the dissipative particle dynamics [37] and Stokesian dynamics [9]. Recently, a stochastic immersed boundary method (SIBM) has been proposed [4], which is a stochastic extension to the aforementioned immersed boundary method. Inherited from immersed boundary method, the representation of the immersed structure in SIBM is also discrete particles, which is different from the phase field formulation used in PFNS equation.

To capture the microscopic fluctuation in phase field or level set models, a stochastic implicit interface model (or SIIM) is derived based on SIBM in Chapter 3. SIIM provides a consistent treatment to fluid-interface interactions with fluctuation effects.

Some rigorous analysis of SIIM is carried out in Chapter 4. It has been showed when the phase field or level set function is transported via a mollified fluid velocity field, the pathwise solution of SIIM exists and is unique. Moreover, a uniform bound on solutions in probability has been derived.

In the rest of chapter, several important concepts will be briefly discussed to give an overview of this thesis work.

1.2 The Implicit Interface Formulation

In this thesis, the study of the fluid elastic surface interaction uses implicit interface formulations for elastic surface representation. Phase field functions are the primary implicit formulations considered.

A phase field function roughly speaking is a labeling function defined on computational domain Ω. The function takes value nearly $+1$ inside the closed surface and -1 outside, with a thin transition layer of width characterized by a small positive parameter. Its zero level set represents the surface (or interface) implicitly. This representation method is thus called implicit interface formulation. The advantage of using phase field function is that the dynamics of the elastic surface is implicitly encoded in the equation of phase field function. Hence it is unnecessary to explicitly track the surface.

Given a deformed surface, some types of interfacial energy associated with the surface could be expressed in terms of phase field function. Take the elastic bending energy for example. It is defined as [19]

$$E_b = \int_\Gamma \frac{\kappa}{2}(H - c_0)^2 dS, \tag{1.1}$$

where Γ represents the surface, H is the mean curvature of Γ, c_0 is the spontaneous curvature and κ is the bending modulus. Let ϕ denote the phase field function, then the corresponding phase field approximation for this energy is

$$E_b[\phi] = \frac{\kappa}{2\epsilon} \int_\Omega \left(\epsilon \triangle \phi + (\frac{1}{\epsilon}\phi + c_0\sqrt{2})(1-\phi^2) \right)^2 dx \ . \tag{1.2}$$

Such approximations have been extensively studied. A complete derivation of the above phase field energy approximation, and other relevant phase field formulations can be found in [19, 20].

Another implicit interface formulation is the level set method [12, 13]. The subsequent discussion on modeling and analysis is also applicable to the level set framework .

1.3 Fluid Implicit Interface Interaction Equations

Given an elastic surface in fluid represented by phase field function ϕ (or a level set function), the fluid elastic surface interaction could be characterized by three equations; a transport equation of ϕ, possibly looks like

$$\phi_t + u \cdot \nabla \phi = 0 \ , \tag{1.3}$$

which implies that the elastic surface is purely transported by fluid velocity field, and the fluid momentum equation,

$$u_t + u \cdot \nabla u = \mu \triangle u + \nabla p + \textit{force term} \ , \tag{1.4}$$

with incompressibility condition

$$\nabla \cdot u = 0 \ , \tag{1.5}$$

where *force term* represents the fluid elastic surface force interaction.

Given a potential energy $E[\phi]$, the derivation of the correct *force term* relies on the least action principle. The least action principle asserts that the actual flow particle trajectory $x(t, \alpha)$, for $0 \leq t \leq T_0$ minimizes the action functional [24, 17],

$$A[x(t,\alpha)] = \int_0^{T_0} \left(\int_\Omega \frac{1}{2} |u(t,x)|^2 dx - E[\phi] \right) dt \ ,$$

in which fluid velocity field $u(t, x)$ is implicitly defined by

$$\begin{cases} \dot{x}(t,\alpha) = u(t, x(t,\alpha)) \\ x(0,\alpha) = \alpha \ , \end{cases}$$

The action functional is the accumulation of the difference of fluid kinetic energy and potential energy $E[\phi]$ in time. So the fluid implicit interface interaction reflects the competition between fluid kinetic energy and potential energy $E[\phi]$.

Through proper variation, it turns out

$$\textit{force term} = \nabla E[\phi] \nabla \phi \ , \tag{1.6}$$

$\nabla E[\phi]$ here is a simple notation for the variational derivative of $E[\phi]$. Note that the form of *"force term"* is independent of the choice of energy $E[\phi]$.

For illustration, two examples are given here. The first example is the phase field approximation of surface tension energy of an interface, which has been used in the study of two-phase flow of complex fluids [79]. And the energy functional is written as

$$E[\phi] = \int_\Omega \frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{4\epsilon}(\phi^2 - 1)^2 dx \ ,$$

which represents the surface area of the interface. Then the *force term* is given by

$$\nabla E[\phi]\nabla\phi = \left\{ -\epsilon\triangle\phi + \frac{1}{\epsilon}(\phi^3 - \phi) \right\} \nabla\phi \ .$$

The second example is a level set formulation in [12, 13, 14] for modeling fluid-structure interaction. The corresponding energy functional with ϕ being the level set function is

$$E[\phi] = \int_\Omega E_d(|\nabla\phi|)\frac{1}{\epsilon}\eta(\frac{\phi}{\epsilon})dx,$$

where E_d is the energy density, ϵ is a small positive parameter, and cut-off function $\eta(r) = \frac{1}{2}(1 + \cos(\pi r))$ for $|r| \leq 1$ and $\eta(r) = 0$ otherwise. And the *force term* becomes

$$\begin{aligned} \nabla E[\phi]\nabla\phi &= \left\{ -\mathrm{div}\left(E_d'(|\nabla\phi|)\frac{1}{\epsilon}\eta(\frac{\phi}{\epsilon})\frac{\nabla\phi}{|\nabla\phi|} \right) \right. \\ &\quad \left. + E_d(|\nabla\phi|)\frac{1}{\epsilon^2}\eta'(\frac{\phi}{\epsilon}) \right\} \cdot \nabla\phi \end{aligned}$$

Since the derivation is via an energetic variational approach, there is a dissipative energy law for equations (1.3–1.5)

$$\frac{d}{dt}\left(\int_\Omega \frac{1}{2}|u(t,x)|^2 dx + E[\phi]\right) = -\mu \int_\Omega |\nabla u(t,x)|^2 dx.$$

In later chapters, the dissipative energy laws plays central role in the rigorous analysis of models.

1.4 Phase Field Navier-Stokes Vesicle-Fluid Interaction Model

The aforementioned phase field Navier-Stokes vesicle-fluid interaction model (PFNS) introduced in [24] is given by,

$$\begin{cases} u_t + u\cdot\nabla u = \nabla p + \mu\triangle u + \nabla E[\phi]\nabla\phi \ , \\ \nabla\cdot u = 0 \ , \\ \phi_t + u\cdot\nabla\phi = -\gamma\nabla E[\phi] \ . \end{cases} \tag{1.7}$$

where $E[\phi]$ is particularly set to the elastic bending energy (1.2) plus two additional penalty terms representing the constrains of surface area and volume enclosed by the surface. More precisely,

$$E[\phi] = E_b[\phi] + \frac{1}{2}M_1(A(\phi)-\alpha)^2 + \frac{1}{2}M_2(B(\phi)-\beta)^2 \ , \tag{1.8}$$

where

$$\text{Enclosed volume:} \qquad A(\phi) = \int_\Omega \phi dx \ ,$$

$$\text{Surface area:} \qquad B(\phi) = \int_\Omega \frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{4\epsilon}(\phi^2-1)^2 dx \ .$$

This model is modified from the fluid implicit interface interaction equations (1.3–1.5). Note that a damping term $-\gamma \nabla E[\phi]$ is added to the transport equation of ϕ.

The well-posedness of the coupled hydrodynamic equation (1.7) is established in Chapter 2. The main ingredient is applying two level Galerkin approximations, one for phase field function, the other for fluid velocity field. The challenge is to bound the energy change due to nonlinear force density term. With an additional assumption on the regularity of fluid velocity field the weak solution is unique.

1.5 Stochastic Implicit Interface Model (SIIM)

To capture the thermal fluctuation near both mechanical and thermal equilibrium, the deterministic hydrodynamic equations (1.3–1.5) is extended to the stochastic implicit interface model (SIIM) based on stochastic immersed boundary method [4, 66]. The main goal is to derive the proper form of noise to be incorporated in equations (1.3–1.5).

Assume ϕ_0 is a local minimizer of $E[\phi]$, and the Hessian of $E[\phi]$ at ϕ_0 is positive definite. Then $(u \equiv 0, \phi \equiv \phi_0)$ gives a stable steady state of the deterministic equation. Near equilibrium, the dynamics is governed by the linearized equation. Through the calculation of the correlation structure of the linearized equation, the proper form of the noise is derived by applying a version of fluctuation-dissipation theorem [30].

It turns out that the phase field or level set function should be purely transported via an incompressible velocity field, i.e.

$$\phi_t + u \cdot \nabla \phi = 0 \ , \tag{1.9}$$

and the velocity field u should satisfy the stochastic PDE

$$u_t + u \cdot \nabla u = \mu \triangle u + \nabla E[\phi] \nabla \phi + \nabla p + \text{“\textit{noise}”}, \tag{1.10}$$

where *“noise”* is delta correlated in time, and its strength is essentially determined by the dissipative term $\mu \triangle u$.

Given the nonlinear nature of the equations (1.9), (1.10) and the contributions due to the noise term, the model is considered in a low Reynolds number regime. Hence the full Navier-Stokes equation is simplified to a Stokes equation. Moreover a mollified flow with a smoothing kernel ζ is considered. Then the deterministic hydrodynamic equation is modified to

$$\begin{cases} u_t = \mu \triangle u + \nabla p + (\nabla E[\phi] \nabla \phi) * \zeta \ , \\ \phi_t + (u * \zeta) \cdot \nabla \phi = 0 \ , \\ \nabla \cdot u = 0 \ . \end{cases} \tag{1.11}$$

And the stochastic implicit interface model could be written in a general form as,

$$\text{(SIIM)} \quad \begin{cases} u_t = \mu \triangle u + \nabla p + (\nabla E[\phi] \nabla \phi) * \zeta + \sigma Q^{\frac{1}{2}} \frac{dW}{dt}, \\ \nabla \cdot u = 0, \\ \phi_t + (u * \zeta) \cdot \nabla \phi = 0, \end{cases} \tag{1.12}$$

where the noise term $\sigma Q^{\frac{1}{2}} \frac{dW}{dt}$ is solely determined by the dissipative character of the deterministic equation (1.11). Equation (1.12) is referred to as stochastic implicit interface model or SIIM for short. At the end of Chapter 3, SIIM with a quasi-steady flow is considered, which reduces (1.12) to a Langevin type of equation of phase field (or level set) function with multiplicative noise.

In Chapter 4, the well-posedness for the deterministic equation (1.11) and SIIM (1.12) will be established.

Chapter 2

Analysis of Phase Field Navier-Stokes Vesicle-Fluid Interaction Model

2.1 Background of Phase Field Navier-Stokes (PFNS) Equation

The flow deformation and rheology of vesicle membranes and cells are of many interests in biological and physiological applications. As motivated in the introduction chapter, it is a fundamental question to understand the shape of vesicle membranes when interacting with fluid in a biological environment.

Vesicle membrane is formed by lipid bilayer. It may be abstracted as an elastic surface. Its equilibrium shape is often characterized by the configuration that minimizes the elastic bending energy which is introduced in

(1.1) [36, 55, 63, 75]:

$$E_b = \int_\Gamma \frac{\kappa}{2}(H - c_0)^2 dS,$$

However, in fluid the resultant shape of vesicle membrane reflects the competition of the fluid kinetic energy and the membrane elastic bending energy.

To track the shape of vesicle membrane, it is convenient to use a phase field function. The phase field function, say ϕ, is a continuous labeling function defined on computational domain Ω. The function takes value nearly $+1$ inside the vesicle membrane and -1 outside. Across the vesicle membrane, ϕ has a thin transition layer of width characterized by a small positive parameter ϵ. The surface of vesicle membrane is represented by the zero level set of ϕ.

$$E_\epsilon[\phi] = \frac{k}{2\epsilon} \int_\Omega \left(\epsilon \triangle \phi + (\frac{1}{\epsilon}\phi + c_0\sqrt{2})(1 - \phi^2) \right)^2 dx$$

is an approximation to the elastic bending energy (1.1).

The fluid vesicle membrane interaction is subject to the constrains that the volume and surface area of the vesicle are preserved. To enforce the two constraints, a penalty method is used by defining a modified energy of vesicle membrane as,

$$E[\phi] = E_\epsilon[\phi] + \frac{1}{2}M_1(A(\phi) - \alpha)^2 + \frac{1}{2}M_2(B(\phi) - \beta)^2 \ , \tag{2.1}$$

where M_1, M_2 are two fixed large positive constants, and

$$\text{vesicle enclosed volume:} \qquad A(\phi) = \int_\Omega \phi dx \ ,$$
$$\text{vesicle surface area:} \qquad B(\phi) = \int_\Omega \frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{4\epsilon}(\phi^2-1)^2 dx \ .$$

The fluid-vesicle membrane interaction is governed by two equations, a momentum equation of fluid velocity field, and a transport equation of the vesicle membrane. As in (1.6), the vesicle membrane fluid force interaction in the momentum equation of fluid velocity field is given in terms of the elastic energy by $\nabla E[\phi]\nabla\phi$. However, the phase field function is transported via

$$\phi_t + u \cdot \nabla\phi = -\gamma\nabla E[\phi] \ .$$

An additional damping term $-\gamma\nabla E[\phi]$ with small positive parameter γ is added to provide some extra dissipation of energy. The resulting equation is the phase filed Navier-Stokes (PFNS) vesicle-fluid interaction model.

$$\text{(PFNS)} \quad \begin{cases} u_t + u\cdot\nabla u = \nabla p + \mu\triangle u + \nabla E[\phi]\nabla\phi & \text{in } [0,T]\times\Omega \\ \nabla\cdot u = 0 \quad \text{in } [0,T]\times\Omega \\ \phi_t + u\cdot\nabla\phi = -\gamma\nabla E[\phi] \quad \text{in } [0,T]\times\Omega \\ u(0,x) = \tilde{u}(x) \quad \text{in } \Omega \\ \phi(0,x) = \tilde{\phi}(x) \quad \text{in } \Omega \end{cases} \qquad (2.2)$$

As mentioned, $\nabla E[\phi]$ is a simple notation for the variational derivative of $E[\phi]$.

The PFNS equation is complemented by boundary conditions (2.3). The particular boundary condition considered here is Dirichlet type for the phase field function ϕ and no-slip boundary condition for the velocity field u:

$$\text{(BC)} \quad \begin{cases} u = 0 \quad \text{on } \partial\Omega \\ \phi = -1, \ \triangle\phi = 0 \quad \text{on } \partial\Omega \, . \end{cases} \tag{2.3}$$

2.2 Main Results on Well-posedess of PFNS Equation

In the subsequent sections of this chapter, the rigorous proof of the existence and uniqueness of the solution to PFNS equation (2.2) will be discussed in detail. First, it is necessary to introduce several notations that will be used in the proof. Throughout this chapter,

1. $H_d(\Omega)$ denotes the space of divergence free vector fields in $H_0^1(\Omega)$, and $L_d^2(\Omega)$ is the divergence free subspace of $L^2(\Omega)$.

2. $H_d^{-1}(\Omega)$ is the dual space of $H_d(\Omega)$.

3. For any given time T, $L^p(0,T;L^q(\Omega))$ denotes the space of functions of both the time and space variables as defined in [70].

4. $< \cdot, \cdot >$ is the inner product in (and duality pairing with respect to) $L^2(\Omega)$.

5. For notational convenience, following trilinear form is defined

$$B(u,v,w) = \int_\Omega u \cdot \nabla v \cdot w \, dx \; . \tag{2.4}$$

The main results on the well-posedness of PFNS equation are the following existence and uniquess theorems.

Theorem 2.1. ***Existence of Weak Solution.*** *Let Ω be an open, bounded subset of $\mathbb{R}^3$ either having a smooth boundary or being a convex polyhedra. There exists a pair of functions ϕ and u with*

1. $u \in L^2(0,T;H_d(\Omega)) \cap W^{1,\frac{4}{3}}(0,T;H_d^{-1}(\Omega))$

2. $\phi \in L^2(0,T;H^2(\Omega)) \cap H^1(0,T;L^2(\Omega))$

which is a weak solution to equation (2.2) with boundary condition (2.3), that is,

1. *for any $\delta(x) \in H_d(\Omega)$, $\xi(x) \in L^2(\Omega)$, and a.e. $t \in [0,T]$,*

$$\left\{ \begin{array}{rcl} < u_t, \delta > + B(u,u,\delta) & = & -\mu < \nabla u, \nabla \delta > + \int_\Omega \nabla E[\phi] \nabla \phi \cdot \delta \, dx \\ < \phi_t, \xi > + B(u,\phi,\xi) & = & -\gamma < \nabla E[\phi], \xi > \end{array} \right. . \tag{2.5}$$

2. $u(0,x) = \tilde{u}(x)$, $\phi(0,x) = \tilde{\phi}(x)$ *where* $\tilde{u} \in L_d^2(\Omega)$ *and* $\tilde{\phi} + 1 \in H_0^2(\Omega)$.

Theorem 2.2. ***Uniqueness of Weak Solution.*** *For the weak solutions to equation (2.2) discussed in the previous existence theorem, if in addition the solution satisfies $u \in L^8(0,T;L^4(\Omega))$, then the weak solution is unique.*

2.3 Some Useful Formal Estimates

The dissipation of the kinetic energy is a basic property of the conventional incompressible Navier-Stokes equations. A similar energy law holds for the coupled PFNS equation, with the membrane bending elasticity energy being added to the kinetic energy to produce the total energy.

For convenience, denote

$$\begin{aligned} f(\phi) &= -\epsilon \triangle \phi + \frac{1}{\epsilon}(\phi^2 - 1)\phi \, , \\ g(\phi) &= -\triangle f(\phi) + \frac{1}{\epsilon^2}(3\phi^2 - 1) f(\phi) \, . \end{aligned}$$

Then, the energy is rewritten as

$$E[\phi] = \frac{k}{2\epsilon} \int_\Omega |f(\phi)|^2 dx + \frac{1}{2} M_1 (A(\phi) - \alpha)^2 + \frac{1}{2} M_2 (B(\phi) - \beta)^2 \, .$$

The direct computation shows

$$\nabla E[\phi] = k g(\phi) + M_1(A(\phi) - \alpha) + M_2(B(\phi) - \beta) f(\phi) \, . \tag{2.6}$$

Multiply u to the first equation in (2.2) and $\nabla E[\phi]$ to the second equation, then integrate over Ω, the following dissipative energy law is derived,

$$\frac{d}{dt}\left(\int_\Omega |u|^2 dx + E[\phi] \right) = -\mu \int_\Omega |\nabla u|^2 dx - \gamma \int_\Omega |\nabla E[\phi]|^2 \, dx \, . \tag{2.7}$$

Immediately one can conclude that if u and ϕ are the solutions of the PFNS, the uniform bounds (with respect to any $T > 0$) of the following types hold:

- $u \in L^\infty(0,T;L^2(\Omega)) \cap L^2(0,T;H_d(\Omega))$;
- $\phi \in L^\infty(0,T;H^2(\Omega))$;
- $f(\phi) \in L^\infty(0,T;L^2(\Omega))$;
- $\nabla E[\phi] \in L^2((0,T)\times(\Omega))$.

For weak solutions of (2.2), a weaker version of the energy law can be rigorously obtained via a Galerkin procedure outlined latter.

Based on the bounds from the energy law and the PFNS equation, a better estimates on the time derivatives can be obtained.

1. Let $v \in L^2(\Omega)$ and $\|v\|_{L^2(\Omega)} \le 1$, from equation (2.2),

$$\left| \int_\Omega \phi_t v \, dx \right| \le \left| \int_\Omega u \, \nabla\phi \, v \, dx \right| + \gamma \left| \int_\Omega \nabla E[\phi] v \, dx \right| .$$

   And,

$$\begin{aligned} \left| \int_\Omega u \, \nabla\phi \, v \, dx \right| &\le C\|v\|_{L^2(\Omega)}\|\nabla\phi\|_{L^3(\Omega)}\|u\|_{L^6(\Omega)} \\ &\le C'\|\phi\|_{H^2(\Omega)}\|u\|_{H_0^1(\Omega)}\|v\|_{L^2(\Omega)} , \end{aligned}$$

$$\left| \int_\Omega \nabla E[\phi] v dx \right| \le \|\nabla E[\phi]\|_{L^2(\Omega)}\|v\|_{L^2(\Omega)} .$$

   Therefore,

$$\|\phi_t\|_{L^2(\Omega)} \le C\left(\|\phi\|_{H^2(\Omega)}\|u\|_{H_0^1(\Omega)} + \|\nabla E[\phi]\|_{L^2(\Omega)}\right).$$

2. Take $v \in H_d(\Omega)$. Also from equation (2.2),

$$\begin{aligned} \left| \int_\Omega u_t \cdot v \, dx \right| &\leq \left| \int_\Omega u \cdot \nabla u \cdot v \, dx \right| + \left| \int_\Omega \nabla E[\phi] \nabla \phi \cdot v \, dx \right| \\ &\quad + \mu \|\nabla u\|_{L^2(\Omega)} \|\nabla v\|_{L^2(\Omega)} \,, \\ \|u_t\|_{H_d^{-1}(\Omega)} &\leq \|u \cdot \nabla u\|_{H^{-1}(\Omega)} + \mu \|\nabla u\|_{L^2(\Omega)} + \|\nabla E[\phi] \nabla \phi\|_{H^{-1}(\Omega)} \,. \end{aligned}$$

By the well known interpolation result [70],

$$\|u \cdot \nabla u\|_{H^{-1}(\Omega)} \leq C \|u\|_{L^2(\Omega)}^{\frac{1}{2}} \|\nabla u\|_{L^2(\Omega)}^{\frac{3}{2}} \,.$$

As for $\|\nabla E[\phi] \nabla \phi\|_{H^{-1}(\Omega)}$, now assume $v \in H_0^1(\Omega)$, with $\|v\|_{H_0^1(\Omega)} \leq 1$.

By the Sobolev inequality $\|v\|_{L^6(\Omega)} \leq C \|v\|_{H_0^1(\Omega)}$,

$$\begin{aligned} \left| \int_\Omega \nabla E[\phi] \nabla \phi \cdot v \, dx \right| &\leq \|\nabla E[\phi]\|_{L^2(\Omega)} \|\nabla \phi\|_{L^3(\Omega)} \|v\|_{L^6(\Omega)} \\ &\leq K_1 \|\nabla E[\phi]\|_{L^2(\Omega)} \|\nabla \phi\|_{L^3(\Omega)} \\ &\leq K_2 \|\nabla E[\phi]\|_{L^2(\Omega)} \|\phi\|_{H^2(\Omega)} \,. \end{aligned}$$

Hence,

$$\|u_t\|_{H_d^{-1}(\Omega)} \leq C \left(\|\nabla u\|_{L^2(\Omega)}^{\frac{3}{2}} \|u\|_{L^2(\Omega)}^{\frac{1}{2}} + \|\nabla u\|_{L^2(\Omega)} + \|\nabla E[\phi]\|_{L^2(\Omega)} \|\phi\|_{H^2(\Omega)} \right) \,.$$

2.4 Existence of Weak Solutions

This section is devoted to the proof of the existence of weak solutions to the coupled PFNS equation (2.2) with boundary condition (2.3). The existence theorem is established by first applying a modified Galerkin approximation to construct approximate solutions, then verifying their weak limit as a weak solution to (2.2).

2.4.1 A Modified Galerkin Approximation

Choose $\{\omega_n\} \subset L^2_d(\Omega)$ to be the eigenfunctions of Stokes operator, such that $\{\omega_n\}$ forms an orthonormal basis for $L^2_d(\Omega)$. Set $W_n = \text{Span}\{\omega_1, \omega_2, \dots, \omega_n\}$. Apply the Galerkin approximation to the velocity field u, one can get the approximate equation for $u \in W_n$ and $\phi \in H^2(\Omega)$:

$$\begin{cases} u_t + \mathcal{P}_n(u \cdot \nabla u) &= \mu \triangle u + \mathcal{P}_n(\nabla E[\phi] \nabla \phi) \\ \phi_t + u \cdot \nabla \phi &= -\gamma \nabla E[\phi] \\ u(0) = \mathcal{P}_n \tilde{u}(x) & \\ \phi(0) = \tilde{\phi}(x) & \end{cases} \tag{2.8}$$

where $\mathcal{P}_n$ is the L^2 projection operator to W_n. The following Lemma asserts the existence of solution to the approximate equation (2.8). It also provides a uniform energy estimate on the solution (with respect to the dimension n).

Lemma 2.1. ***Existence of Approximate Solution*** *There exists a pair of functions $u(t,x) \in W_n$, $\phi(t,x) \in H^2(\Omega)$ satisfying*

$$\begin{cases} < u_t, w > + B(u,u,w) &= -\mu < \nabla u, \nabla w > + \int_\Omega \nabla E[\phi] \nabla \phi \cdot w \, dx \\ < \phi_t, v > + B(u, \phi, v) &= -\gamma < \nabla E[\phi], v > \\ u(0) = \mathcal{P}_n \tilde{u}(x) & \\ \phi(0) = \tilde{\phi}(x) \ , & \end{cases} \tag{2.9}$$

$\forall w \in W_n$ and $v \in L^2(\Omega)$ for almost all $t \in [0,T]$. Furthermore, for a.e. $\hat{T} \in [0,T]$,

$$\int_0^{\hat{T}} \int_\Omega \mu|\nabla u|^2 + \gamma|\nabla E[\phi]|^2 dxdt + \int_\Omega \frac{1}{2}|u(\hat{T},x)|^2 dx + E[\phi(\hat{T},x)] \leq M \ ,$$

with a constant M independent of W_n.

Proof. 1. **Apply Galerkin approximation to ϕ**

Choose $\{\upsilon_1, \upsilon_2, \ldots\}$, the eigenfunctions of operator $\triangle$ under the homogeneous Dirichlet boundary condition such that they consist of an orthonormal basis of $L^2(\Omega)$. By the assumption on the domain Ω, the eigenfunctions of the Laplace operator have H^2 regularity. Set $V_m = \text{Span}\{\upsilon_1, \upsilon_2, \ldots, \upsilon_m\}$. Assume $u_m(x,t)$ and $\phi_m(x,t)$ are in the following form.

$$u_m(x,t) = \sum_{i=1}^{n} d_i(t)\omega_i(x),$$

and

$$\phi_m(x,t) = \sum_{j=1}^{m} h_j(t)\upsilon_j(x) - 1 \ .$$

Apply a modified Galerkin method to ϕ, then an approximate equation to equation (2.9) is derived,

$$\begin{cases} < u'_m, \omega_k > + B(u_m, u_m, \omega_k) &= -\mu < \nabla u_m, \nabla w_k > \\ & \quad + \int_\Omega \pi_m(\nabla E[\phi_m]) \nabla \phi_m \omega_k \, dx \ , \\ < \phi'_m, \upsilon_l > + B(u_m, \phi_m, \upsilon_l) &= -\gamma \int_\Omega \nabla E[\phi_m] \upsilon_l \ , \\ u_m(0,x) &= \mathcal{P}_n \tilde{u}(x) \ , \\ \phi_m(0,x) &= \pi_m(\tilde{\phi}(x) + 1) - 1 \ . \end{cases} \tag{2.10}$$

for $k = 1, 2, \ldots, n$, $l = 1, 2, \ldots, m$. Here, π_m denotes a L^2 (also H^2 if applicable) projection to V_m.

It is easy to see that the above finite dimensional ODE system has a solution local in time.

2. **Energy estimate**

In equation (2.10), replace w_k with u_m, v_l with $\pi_m(\nabla E[\phi_m])$, then,

$$\frac{d}{dt}\left(\frac{1}{2}\int_\Omega |u_m|^2 dx\right) = -\mu < \nabla u_m, \nabla u_m > + \int_\Omega \pi_m(\nabla E[\phi_m])\nabla\phi_m u_m \, dx$$

$$< \phi_m', \pi_m(\nabla E[\phi_m]) > + \int_\Omega \pi_m(\nabla E[\phi_m])\nabla\phi_m u_m \, dx$$

$$= -\gamma \int_\Omega \nabla E[\phi_m]\pi_m(\nabla E[\phi_m]) dx \, .$$

Since

$$< \phi_m', \pi_m(\nabla E[\phi_m]) >=< \pi_m(\phi_m'), \nabla E[\phi_m] >=< \phi_m', \nabla E[\phi_m] >= \frac{d}{dt}E[\phi_m],$$

the summation of the two expression above gives the energy law,

$$\frac{d}{dt}\left(\frac{1}{2}\int_\Omega |u_m|^2 dx + E[\phi_m]\right) = -\mu\int_\Omega |\nabla u_m|^2 dx - \gamma\int_\Omega |\pi_m(\nabla E[\phi_m])|^2 \, dx \, . \tag{2.11}$$

It implies,

$$\frac{1}{2}\int_\Omega |u_m(\hat{T}, x)|^2 dx + E[\phi_m(\hat{T}, x)] + \int_0^{\hat{T}}\int_\Omega \mu|\nabla u_m|^2 dx$$

$$+\gamma\,|\pi_m(\nabla E[\phi_m])|^2 \, dxdt \le \frac{1}{2}\int_\Omega |u_m(0, x)|^2 dx + E[\phi_m(0, x)] \, .$$

$\|u_m(0,x)\|_{L^2(\Omega)} \le \|\tilde{u}(x)\|_{L^2(\Omega)}$, and by the construction of $\phi_m(0,x)$, $\phi_m(0,x)$ converges to $\tilde{\phi}(x)$ in $H^2(\Omega)$ as $m \to \infty$. Hence there exists some constant M independent of W_n, such that,

$$\frac{1}{2}\int_\Omega |u_m(\hat{T},x)|^2 dx + E[\phi_m(\hat{T},x)] + \int_0^{\hat{T}} \int_\Omega \mu |\nabla u_m|^2 dx$$
$$+\gamma \left|\pi_m(\nabla E[\phi_m])\right|^2 dxdt \le M \ .$$

Note that such an energy law essentially gives the existence of local solutions for all time.

3. **Compactness of $\{u_m\}$ and $\{\phi_m\}$**

The energy law ensures that $\|u_m(t)\|_{L^2(\Omega)}$ and $\|\phi_m(t)\|_{L^2(\Omega)}$ are uniformly bounded in m and $t \in [0,T]$. Thus the solution of ODE (2.10) actually exists global in time. Furthermore, the energy law also indicates

- u_m is uniformly bounded in $L^\infty(0,T;L^2(\Omega)) \cap L^2(0,T;H_d(\Omega))$.
- ϕ_m is uniformly bounded in $L^\infty(0,T;H^2(\Omega))$ (thus in $L^2(0,T;H^2(\Omega))$)
- $\pi_m(\nabla E[\phi_m])$ is uniformly bounded in $L^2((0,T)\times\Omega)$.

Similar to the previous formal derivation, estimates on $\|u'_m\|_{H_d^{-1}(\Omega)}$ and $\|\phi'_m\|_{L^2(\Omega)}$ (here $'$ means differentiating in time) can be rigourously obtained:

- u'_m is uniformly bounded $L^{\frac{4}{3}}(0,T;H_d^{-1}(\Omega))$.

- ϕ'_m is uniformly bounded $L^2(0,T,L^2(\Omega))$.

Therefore, using the Aubin-Lions type compact embedding results [70], there exist some ϕ and u such that,

- u_m has a subsequence u_{m_k} converging to u weakly in $L^2(0,T,H_d(\Omega))$ and strongly in $L^2(0,T;L^2_d(\Omega))$.

- ϕ_m has a subsequence ϕ_{m_l} converging to ϕ weakly in $L^2(0,T;H^2(\Omega))$ and strongly in $L^2(0,T;W^{1,p}(\Omega))$ for $1 \le p < 6$.

For convenience, if there is no ambiguity, u_m and ϕ_m will be identified with their subsequences.

4. **Passing weak limits of $\{u_m\}$ and $\{\phi_m\}$**

   Choose $w(t,x) = \alpha(t)\delta(x)$, $v(t,x) = \alpha(t)\xi(x)$ where $\alpha \in C([0,T])$, $\delta \in W_n$, and $\xi \in V_m$, then

$$\int_0^T < u'_m, w > + B(u_m,u_m,w)\,dt = -\int_0^T \mu < \nabla u_m, \nabla w > \,dt \\ + \int_0^T \int_\Omega \pi_m(\nabla E[\phi_m])\nabla\phi_m \cdot w\,dx\,dt\ ,$$

$$\int_0^T < \phi'_m, v > + B(u_m,\phi_m,v) = -\gamma \int_0^T < \nabla E[\phi_m], v > \,dt\ .$$

In which,

$$\begin{aligned}
\nabla E[\phi_m] &= k\{-\triangle f(\phi_m) + \frac{1}{\epsilon^2}(3\phi_m^2 - 1)f(\phi_m)\} \\
&\quad +M_1(A(\phi_m) - \alpha) + M_2(B(\phi_m) - \beta)f(\phi_m) \\
&= k\{-\triangle[-\epsilon\triangle\phi_m + \frac{1}{\epsilon}(\phi_m^2 - 1)\phi_m] + \frac{1}{\epsilon^2}(3\phi_m^2 - 1)f(\phi_m)\} \\
&\quad +M_1(A(\phi_m) - \alpha) + M_2(B(\phi_m) - \beta)f(\phi_m) \qquad (2.12) \\
&= \epsilon k\triangle^2\phi_m + L(\phi_m)
\end{aligned}$$

where $L(\phi_m)$ denotes the lower order term. Note that the $\|L(\phi_m)\|_{L^2((0,T)\times\Omega)}$ is uniformly bounded by the uniform bound on ϕ_m in $L^\infty(0,T;H^2(\Omega))$.

Then,

$$\begin{aligned}
\pi_m(\nabla E[\phi_m]) &= \pi_m(\epsilon k\triangle^2\phi_m) + \pi_m(L(\phi_m)) \\
&= \epsilon k\triangle^2\phi_m + \pi_m(L(\phi_m)) .
\end{aligned}$$

Together with the energy estimate (2.11),

$$\begin{aligned}
&\|\epsilon k\triangle^2\phi_m\|_{L^2((0,T)\times\Omega)} \\
&\quad \leq \|\pi_m(\nabla E[\phi_m])\|_{L^2((0,T)\times\Omega)} + \|\pi_m(L(\phi_m))\|_{L^2((0,T)\times\Omega)} \\
&\quad \leq \|\pi_m(\nabla E[\phi_m])\|_{L^2((0,T)\times\Omega)} + \|L(\phi_m)\|_{L^2((0,T)\times\Omega)} .
\end{aligned}$$

Therefore,

$$\|\nabla E[\phi_m]\|_{L^2((0,T)\times\Omega)} \leq \|\pi_m(\nabla E[\phi_m])\|_{L^2((0,T)\times\Omega)} + 2\|L(\phi_m)\|_{L^2((0,T)\times\Omega)} .$$

(a) **Weak limit of $\{\nabla E[\phi_m]\}$.**

Claim that (a subsequence of) $\{\nabla E[\phi_m]\}$ converges to $\nabla E[\phi]$ weakly in $L^2((0,T)\times\Omega)$. By the energy law (2.11), $f(\phi_m)$ is uniformly bounded in $L^\infty(0,T;L^2(\Omega))$, hence uniformly bounded in $L^2((0,T)\times\Omega)$. It is enough to show for $\forall g\in C_0^\infty([0,T]\times\Omega)$,

$$\lim_{m\to\infty}\int_0^T\int_\Omega f(\phi_m)g\,dxdt=\int_0^T\int_\Omega f(\phi)g\,dxdt\ .$$

$$\int_0^T\int_\Omega f(\phi_m)g\,dxdt=\int_0^T\int_\Omega[-\epsilon\triangle\phi_m+\frac{1}{\epsilon}(\phi_m^2-1)\phi_m]g\,dxdt\ .$$

It is sufficient to check on the nonlinear terms only. Since ϕ_m is uniformly bounded in $L^\infty(0,T;H^2(\Omega))$,

$$\|\phi_m(t)\|_{C^{0,\tau}(\Omega)}\le C\|\phi_m(t)\|_{H^2(\Omega)}\le M$$

for $t\in[0,T]$. Hence, $\phi_m(t,x)$ is uniformly bounded in $[0,T]\times\Omega$. Furthermore, ϕ_m has as subsequence converging to ϕ strongly in $L^2(0,T,W^{1,p})$ for $1\le p<6$. Then a subsequence of ϕ_m converges to ϕ almost everywhere in $[0,T]\times\Omega$. By the Lebesgue-Dominated Theorem,

$$\lim_{n\to\infty}\int_0^T\int_\Omega\phi_m^3g\,dxdt=\int_0^T\int_\Omega\phi^3g\,dxdt\ .$$

Similarly, It is needed to verify that

$$\lim_{m\to\infty}\int_0^T\int_\Omega\nabla E[\phi_m]g\,dxdt=\int_0^T\int_\Omega\nabla E[\phi]g\,dxdt\ . \qquad (2.13)$$

To give more details, follow (2.12) term by term. First,

$$\int_0^T \int_\Omega \triangle^2 \phi_m g \, dxdt = \int_0^T \int_\Omega \triangle \phi_m \triangle g \, dxdt$$
$$\to \int_0^T \int_\Omega \triangle \phi \triangle g \, dxdt = \int_0^T \int_\Omega \triangle^2 \phi g \, dxdt$$

as $m \to \infty$.

Next,

$$\left| \int_0^T \int_\Omega \triangle(\phi_m^3 - \phi^3) g \, dxdt \right| = 3 \left| \int_0^T \int_\Omega (\phi_m^2 \nabla \phi_m - \phi^2 \nabla \phi) \cdot \nabla g \, dxdt \right|$$
$$\leq C \left| \int_0^T \int_\Omega (\phi_m^2 - \phi^2) \nabla \phi_m \nabla g \, dxdt \right| + C \left| \int_0^T \int_\Omega \phi^2 (\nabla \phi - \nabla \phi_m) \nabla g \, dxdt \right|$$
$$\leq C' \|\phi_m^2 - \phi^2\|_{L^2((0,T)\times\Omega)} \|\nabla \phi_m\|_{L^2((0,T)\times\Omega)} + C' \|\nabla \phi - \nabla \phi_m\|_{L^1((0,T)\times\Omega)} .$$

Hence, as $m \to \infty$,

$$\left| \int_0^T \int_\Omega \triangle(\phi_m^3 - \phi^3) g \, dxdt \right| \to 0 .$$

Now, consider

$$\left| \int_0^T \int_\Omega (\phi_m^2 f(\phi_m) - \phi^2 f(\phi)) g \, dxdt \right| \leq \left| \int_0^T \int_\Omega (f(\phi_m) - f(\phi)) \phi^2 g \, dxdt \right|$$
$$+ \left| \int_0^T \int_\Omega (\phi^2 - \phi_m^2) g f(\phi_m) dxdt \right| = I_1 + I_2 .$$

Then $I_1 \to 0$ since $f(\phi_m) \rightharpoonup f(\phi)$ weakly in $L^2((0,T)\times\Omega)$. In addition,

$$I_2 \leq \|g\|_{L^\infty((0,T)\times\Omega)} \|f(\phi_m)\|_{L^2((0,T)\times\Omega)} \|\phi_m^2 - \phi_m^2\|_{L^2((0,T)\times\Omega)} \to 0 .$$

It is also easy to show,

$$\lim_{n\to\infty}\int_0^T\int_\Omega B(\phi_m)f(\phi_m)g\,dxdt=\int_0^T\int_\Omega B(\phi)f(\phi)g\,dxdt\ .$$

(b) **Verifying the approximate equation**.

Choose $g\in L^2((0,T)\times\Omega)$. Since $\nabla E[\phi_m]$ weakly converges to $\nabla E[\phi]$ and $\pi_m(g)$ converges strongly to g in $L^2((0,T)\times\Omega)$,

$$\begin{aligned}&\left|\int_0^T <\pi_m(\nabla E[\phi_m])-\nabla E[\phi],g> dt\right|\\ &\quad=\left|\int_0^T <\nabla E[\phi_m],\pi_m(g)>-<\nabla E[\phi],g>)\,dt\right|\\ &\quad\le\left|\int_0^T <\nabla E[\phi_m]-\nabla E[\phi],g>\ dt\right|+\left|\int_0^T <\nabla E[\phi_m],\pi_m(g)-g>\ dt\right|\\ &\quad\to 0\ ,\end{aligned}$$

as $m\to\infty$. Therefor $\pi_m(\nabla E[\phi_m])$ converges to $\nabla E[\phi]$ weakly in $L^2((0,T)\times\Omega)$.

Now, one can let $m\to\infty$ to recover

$$\begin{aligned}\int_0^T <u_t,w>+B(u,u,w)\,dt &= -\int_0^T\mu<\nabla u,\nabla w>\ dt\\ &\quad+\int_0^T\int_\Omega\nabla E[\phi]\nabla\phi\cdot w\,dx\,dt\\ \int_0^T <\phi_t,v>+B(u,\phi,v) &= -\gamma\int_0^T <\nabla E[\phi],v>\ dt\ .\end{aligned}$$

And,

$$\begin{aligned}&\frac{1}{2}\int_\Omega|u(\hat{T},x)|^2dx+E[\phi(\hat{T},x)]+\int_0^{\hat{T}}\int_\Omega\mu|\nabla u|^2dx+\gamma\,|\nabla E[\phi]|^2\,dxdt\\ &\qquad\le M\ .\end{aligned}$$

Since $\alpha = \alpha(t)$ is arbitrarily chosen in $C([0,T])$, one can conclude for any $\delta \in W_n$ and $\xi \in V_m$,

$$\left\{ \begin{array}{rcl} < u_t, \delta > + B(u,u,\delta) & = & -\mu < \nabla u, \nabla \delta > + \int_\Omega \nabla E[\phi] \nabla \phi \cdot \delta \, dx \\ < \phi_t, \xi > + B(u,\phi,\xi) & = & -\gamma \int_\Omega \nabla E[\phi] \xi \, dx \; . \end{array} \right. \tag{2.14}$$

By density argument, it is also true for any $\delta \in W_n$ and $\xi \in L^2(\Omega)$.

Set $\alpha(0) = 1$ and $\alpha(T) = 0$, one can show $u(0,x) = \mathcal{P}_n \tilde{u}(x)$ and $\phi(0,x) = \tilde{\phi}(x)$.

Finally, since for $i > n$

$$\int_0^T \int_\Omega u_m(t,x) \zeta(t) \omega_i(x) \, dx \, dt = 0$$

for any $\zeta(t) \in C([0,T])$, by taking $m \to \infty$,

$$\int_\Omega u(t,x) \omega_i(x) \, dx = 0$$

for almost all $t \in [0,T]$ when $i > n$. Therefore $u \in W_n$. This completes the proof of this lemma.

□

2.4.2 Proof of the Existence Theorem

It is time to wrap up the proof of the existence theorem. According to Lemma 2.1, for any positive time $\hat{T} \in (0,T)$, and for each W_n, the equation

(2.8) has a solution u_n and ϕ_n, such that

$$\int_0^{\hat{T}} \int_\Omega \mu|\nabla u_n|^2 + \gamma|\nabla E[\phi_n]|^2 dxdt + \int_\Omega \frac{1}{2}|u_n(\hat{T},x)|^2 dx + E[\phi_n(\hat{T},x)] \leq M \tag{2.15}$$

where M is independent of W_n. Hence,

- u_n is uniformly bounded in $L^\infty(0,T;L^2(\Omega)) \cap L^2(0,T;H_d(\Omega))$.
- ϕ_n is uniformly bounded in $L^\infty(0,T;H^2(\Omega))$(particularly in $L^2(0,T;H^2(\Omega))$)
- $\nabla E[\phi_n]$ is uniformly bounded in $L^2((0,T)\times\Omega)$.

Also,

- u_n' is uniformly bounded $L^{\frac{4}{3}}(0,T;H_d^{-1}(\Omega))$.
- ϕ_n' is uniformly bounded $L^2((0,T)\times\Omega)$.

Therefore, there exist some ϕ and u, such that,

- u_n has a subsequence u_{n_k} converging to u weakly in $L^2(0,T,H_d(\Omega))$ and strongly in $L^2((0,T)\times\Omega)$.
- ϕ_n has a subsequence ϕ_{n_l} converging to ϕ weakly in $L^2(0,T;H^2(\Omega))$ and strongly in $L^2(0,T;W^{1,p}(\Omega))$ for $1 \leq p < 6$.

Similar to the claim in Lemma 2.1, (a subsequence of) $\nabla E[\phi_n]$ converges weakly to $\nabla E[\phi]$ in $L^2((0,T)\times\Omega)$.

Choose $w(t,x) = \alpha(t)\delta(x),\ v(t,x) = \alpha(t)\xi(x)$ where $\alpha \in C([0,T]),\ \delta \in W_n$, and $\xi \in C(\Omega)$, then consider

$$\int_0^T < u_n', w > + B(u_n, u_n, w)\, dt = -\int_0^T \mu < \nabla u_n, \nabla w > \ dt$$
$$+ \int_0^T \int_\Omega \nabla E[\phi_n]\phi_n w \, dx\, dt \ ,$$
$$\int_0^T < \phi_n', v > + B(u_n, \phi_n, v) = -\gamma \int_0^T < \nabla E[\phi], v > \ dt \ .$$

Let $n \to \infty$,

$$\int_0^T < u_t, w > + B(u, u, w)\, dt = -\int_0^T \mu < \nabla u, \nabla w > \ dt$$
$$+ \int_0^T \int_\Omega \nabla E[\phi]\phi w \, dx\, dt \ ,$$
$$\int_0^T < \phi_t, v > + B(u_n, \phi, v)\, dt = -\gamma \int_0^T < \nabla E[\phi], v > \ dt \ .$$

Because $\alpha(t)$ is an arbitrarily chosen function in $C([0,T])$, one can conclude for any $\delta \in W_n$, $\xi \in C(\Omega)$,

$$\begin{cases} < u_t, \delta > + B(u, u, \delta) & = & -\mu < \nabla u, \nabla \delta > + \int_\Omega \nabla E[\phi] \nabla \phi \cdot \delta \, dx \\ < \phi_t, \xi > + B(u, \phi, \xi) & = & -\gamma < \nabla E[\phi], \xi > \end{cases}$$

By density argument, it is also true for any $\delta \in H_0^1(\Omega)$ and $\xi \in L^2(\Omega)$. Set $\alpha(0) = 1$ and $\alpha(T) = 0$, one can show $u(0,x) = \tilde{u}(x)$, and $\phi(0,x) = \tilde{\phi}(x)$. This concludes the proof of the main existence theorem.□

2.5 Uniqueness of Weak Solution

Under some additional regularity assumption on the velocity field, one can show the weak solution is indeed unique.

First introduce a few notations to simplify the later discussion. Define

$$G(\phi) = \frac{1}{2}\int_\Omega \left(k\epsilon|\triangle\phi|^2 + \frac{k}{\epsilon}|\nabla\phi|^2 + |\phi|^2 \right) dx,$$

then it is easy to check that $\frac{1}{C}\|\phi\|^2_{H^2(\Omega)} \le G(\phi) \le C\|\phi\|^2_{H^2(\Omega)}$.

Define also

$$\begin{aligned} M(\phi) &= \frac{\delta G(\phi)}{\delta\phi} = k\epsilon\triangle^2\phi - \frac{k}{\epsilon}\triangle\phi + \phi \\ N(\phi) &= \nabla E[\phi] - M(\phi) \ . \end{aligned}$$

Assume u_i, ϕ_i and p_i $(i = 1, 2)$ are two weak solutions to equation (2.2) satisfying the assumptions given in the uniqueness theorem. Let $\hat{u} = u_1 - u_2$, $\hat{\phi} = \phi_1 - \phi_2$ and $\hat{p} = p_1 - p_2$. A Gronwall type inequality for $\hat{u}$ and $\hat{\phi}$ will be derived to prove the uniqueness.

1. **Derivation of a Gronwall inequality**

   First,

$$\left\{ \begin{array}{lcl} \hat{u}' + \hat{u}\nabla u_1 + u_2\nabla\hat{u} &=& \nabla\hat{p} + \mu\triangle\hat{u} + (M(\phi_1) + N(\phi_1))\nabla\phi_1 \\ && \quad -(M(\phi_2) + N(\phi_2))\nabla\phi_2 \ , \\ \hat{\phi}' + u_1\nabla\phi_1 - u_2\nabla\phi_2 &=& -\gamma(M(\hat{\phi}) + N(\phi_1) - N(\phi_2)) \ . \end{array} \right. \tag{2.16}$$

   Multiply $\hat{u}$ to the first equation in (2.16) and $M(\hat{\phi})$ to the second one, integrate in space,

$$\begin{aligned} &\frac{d}{dt}\int_\Omega \frac{1}{2}|\hat{u}|^2 dx + \int_\Omega \hat{u}\nabla u_1 \hat{u} dx = -\mu\int_\Omega |\nabla\hat{u}|^2 dx \\ &\quad + \int_\Omega (M(\phi_1)\nabla\phi_1 - M(\phi_2)\nabla\phi_2)\hat{u} + \int_\Omega (N(\phi_1)\nabla\phi_1 - N(\phi_2)\nabla\phi_2)\hat{u} dx \ , \end{aligned}$$

$$\frac{d}{dt}G(\hat{\phi}) + \int_\Omega (u_1\nabla\phi_1 - u_2\nabla\phi_2)M(\hat{\phi})dx = -\gamma\int_\Omega |M(\hat{\phi})|^2 dx$$
$$-\gamma\int_\Omega M(\hat{\phi})(N(\phi_1) - N(\phi_2))dx$$

Hence,

$$\begin{aligned}
&\frac{d}{dt}\left(\int_\Omega \frac{1}{2}|\hat{u}|^2 dx + G(\hat{\phi})\right) + \gamma\int_\Omega |M(\hat{\phi})|^2 dx + \mu\int_\Omega |\nabla\hat{u}|^2 dx + B(\hat{u}, u_1, \hat{u}) \\
&= \int_\Omega (M(\phi_1)\nabla\phi_1 - M(\phi_2)\nabla\phi_2)\hat{u} - (u_1\nabla\phi_1 - u_2\nabla\phi_2)M(\hat{\phi})dx \\
&\quad + \int_\Omega (N(\phi_1)\nabla\phi_1 - N(\phi_2)\nabla\phi_2)\hat{u}dx - \gamma\int_\Omega M(\hat{\phi})(N(\phi_1) - N(\phi_2))dx
\end{aligned}$$

Recall $B(u, v, w) = \int_\Omega u\cdot\nabla v\cdot w dx$.

Since $B(\hat{u}, u_1, \hat{u}) = -B(\hat{u}, \hat{u}, u_1)$,

$$\begin{aligned}
|B(\hat{u}, u_1, \hat{u})| &= |B(\hat{u}, \hat{u}, u_1)| \\
&\leq \|\hat{u}\|_{L^4(\Omega)}\|\nabla\hat{u}\|_{L^2(\Omega)}\|u_1\|_{L^4(\Omega)} \\
&\leq \|\hat{u}\|_{L^2(\Omega)}^{1/4}\|\nabla\hat{u}\|_{L^2(\Omega)}^{7/4}\|u_1\|_{L^4(\Omega)} \\
&\leq \varrho\|\nabla\hat{u}\|_{L^2(\Omega)}^2 + C(\varrho)\|\hat{u}\|_{L^2(\Omega)}^2\|u_1\|_{L^4(\Omega)}^8
\end{aligned}$$

where ϱ is an arbitrary small positive number.

Direct calculation shows,

$$\begin{aligned}
&\int_\Omega (M(\phi_1)\nabla\phi_1 - M(\phi_2)\nabla\phi_2)\hat{u} - (u_1\nabla\phi_1 - u_2\nabla\phi_2)M(\hat{\phi})dx \\
&\qquad = \int_\Omega (M(\phi_1)\nabla\hat{\phi} + M(\hat{\phi})\nabla\phi_2)\hat{u} - (u_1\nabla\hat{\phi} + \hat{u}\nabla\phi_2)M(\hat{\phi})dx \\
&\qquad = \int_\Omega M(\phi_1)\nabla\hat{\phi}\,\hat{u}dx - \int_\Omega u_1\nabla\hat{\phi}\,M(\hat{\phi})dx = J_1 - J_2\ ,
\end{aligned}$$

and

$$\begin{aligned}|J_1| &\leq \|M(\phi_1)\|_{L^2(\Omega)}\|\nabla\hat{\phi}\|_{L^4(\Omega)}\|\hat{u}\|_{L^4(\Omega)} \\ &\leq \varrho\|\hat{u}\|^2_{H^1_0(\Omega)} + \frac{C}{\varrho}\|M(\phi_1)\|^2_{L^2(\Omega)}\|\hat{\phi}\|^2_{H^2(\Omega)} \ ,\end{aligned}$$

$$\begin{aligned}|J_2| &\leq \|M(\hat{\phi})\|_{L^2(\Omega)}\|u_1\|_{L^4(\Omega)}\|\nabla\hat{\phi}\|_{L^4(\Omega)} \\ &\leq \varrho\|M(\hat{\phi})\|_{L^2(\Omega)} + \frac{C}{\varrho}\|u_1\|^2_{H^1_0(\Omega)}\|\phi\|^2_{H^2(\Omega)} \ .\end{aligned}$$

Moreover,

$$\begin{aligned}&\int_\Omega (N(\phi_1)\nabla\phi_1 - N(\phi_2)\nabla\phi_2)\hat{u}dx \\ &= \int_\Omega (N(\phi_1)\nabla\hat{\phi}\,\hat{u}dx + \int_\Omega (N(\phi_1) - N(\phi_2))\nabla\phi_2)\,\hat{u}dx \\ &= K_1 + K_2 \ ,\end{aligned}$$

with

$$\begin{aligned}|K_1| &\leq \|N(\phi_1)\|_{L^2(\Omega)}\|\nabla\hat{\phi}\|_{L^4(\Omega)}\|\hat{u}\|_{L^4(\Omega)} \\ &\leq C\|N(\phi_1)\|_{L^2(\Omega)}\|\hat{\phi}\|_{H^2(\Omega)}\|\hat{u}\|_{H^1_0(\Omega)} \\ &\leq \varrho\|\hat{u}\|^2_{H^1_0(\Omega)} + \frac{C'}{\varrho}\|N(\phi_1)\|^2_{L^2(\Omega)}\|\hat{\phi}\|^2_{H^2(\Omega)} \ ,\end{aligned}$$

and

$$
\begin{aligned}
|K_2| &\leq \|N(\phi_1) - N(\phi_2)\|_{L^2(\Omega)} \|\nabla \phi_2\|_{L^4(\Omega)} \|\hat{u}\|_{L^4(\Omega)} \\
&\leq C\|N(\phi_1) - N(\phi_2)\|_{L^2(\Omega)} \|\nabla \phi_2\|_{H^2(\Omega)} \|\hat{u}\|_{H_0^1(\Omega)} \\
&\leq \varrho \|\hat{u}\|^2_{H_0^1(\Omega)} + \frac{C'}{\varrho} \|N(\phi_1) - N(\phi_2)\|^2_{L^2(\Omega)} \|\phi_2\|^2_{H^2(\Omega)} \\
&\leq \varrho \|\hat{u}\|^2_{H_0^1(\Omega)} + \frac{C'}{\varrho} \|N(\phi_1) - N(\phi_2)\|^2_{L^2(\Omega)} \, .
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
\left| \int_\Omega M(\hat{\phi})(N(\phi_1) - N(\phi_2)) dx \right| &\leq \|M(\hat{\phi})\|_{L^2(\Omega)} \|N(\phi_1) - N(\phi_2)\|_{L^2(\Omega)} \\
&\leq \varrho \|M(\hat{\phi})\|^2_{L^2(\Omega)} + \frac{1}{4\varrho} \|N(\phi_1) - N(\phi_2)\|^2_{L^2(\Omega)} \, .
\end{aligned}
$$

Now claim (to be verified later):

$$
\|N(\phi_1) - N(\phi_2)\|_{L^2(\Omega)} \leq C\|\phi_1 - \phi_2\|_{H^2(\Omega)} = C\|\hat{\phi}\|_{H^2(\Omega)} \, . \tag{2.17}
$$

Recall that $\|\hat{\phi}\|^2_{H^2(\Omega)} \leq CG(\hat{\phi})$. Using (2.17) and putting everything together,

$$
\begin{aligned}
\frac{d}{dt} \int_\Omega \frac{1}{2} |\hat{u}|^2 dx + G(\hat{\phi}) &\leq C \left(\int_\Omega \frac{1}{2} |\hat{u}|^2 dx + G(\hat{\phi}) \right) \\
&\quad \cdot \left(\|M(\phi_1)\|^2_{L^2(\Omega)} + \|u_1\|^2_{H_0^1(\Omega)} + \|u_1\|^8_{L^4(\Omega)} + \|N(\phi_1)\|^2_{L^2(\Omega)} + 1 \right) \, .
\end{aligned}
$$

Using the estimates already derived and the extra assumption on the velocity field,

$$
\left(\|M(\phi_1)\|^2_{L^2(\Omega)} + \|u_1\|^2_{H_0^1(\Omega)} + \|u_1\|^8_{L^4(\Omega)} + \|N(\phi_1)\|^2_{L^2(\Omega)} \right)
$$

is integrable in time. This implies if $\hat{u}(t) = 0$ and $\hat{\phi}(t) = 0$ at $t = 0$, then $\hat{u} = 0$ and $\hat{\phi} = 0$ for all time, which proves the uniqueness theorem.

2. **Proof of claim (2.17)**

It is only left to verify the claim (2.17) used in the above proof. By (2.6) and the definitions of M and N,

$$\begin{aligned} N(\phi) &= -\frac{k}{\epsilon}\triangle\phi^3 + \frac{2k}{\epsilon}\triangle\phi + \frac{3k}{\epsilon^2}\phi^2 f(\phi) - \frac{k}{\epsilon^2} f(\phi) - \phi \\ &\quad + M_1(A(\phi) - \alpha) + M_2(B(\phi) - \beta) f(\phi)\ . \end{aligned}$$

This leads to

$$\begin{aligned} \|N(\phi_1) - N(\phi_2)\|_{L^2(\Omega)} &\leq C\{\|\triangle\phi_1^3 - \triangle\phi_2^3\|_{L^2(\Omega)} + \|\triangle\phi_1 - \triangle\phi_2\|_{L^2(\Omega)} \\ &\quad + \|\hat{\phi}\|_{L^2(\Omega)} + \|\phi_1^2 f(\phi_1) - \phi_2^2 f(\phi_2)\|_{L^2(\Omega)} + \|f(\phi_1) - f(\phi_2)\|_{L^2(\Omega)} \\ &\quad + \|A(\hat{\phi})\|_{L^2(\Omega)} + \|B(\phi_1) f(\phi_1) - B(\phi_2) f(\phi_2)\|_{L^2(\Omega)}\} \end{aligned}$$

According to the energy estimate derived in the proof of existence theorem, $\phi_i \in L^\infty(0, T; H^2(\Omega))$, $i = 1, 2$. Therefore, for $i, j = 1, 2$,

$$\begin{aligned} &\|\phi_i(t, x)\|_{L^\infty([0,T]\times\Omega)} \leq M\ , \\ &\|\nabla(\phi_i(t, x)\phi_j(t, x))\|_{L^\infty([0,T], L^6(\Omega))} \leq M\ , \\ &\|\Delta(\phi_i(t, x)\phi_j(t, x))\|_{L^\infty([0,T], L^2(\Omega))} \leq M \end{aligned}$$

for some constant M. Now it is sufficient to carefully estimate the individual terms respectively. A generic time-independent constant C is used.

$$\|\triangle\phi_1^3 - \triangle\phi_2^3\|_{L^2(\Omega)} \leq \|\triangle\hat{\phi}(\phi_1^2 + \phi_1\phi_2 + \phi_2^2)\|_{L^2(\Omega)} + \|\hat{\phi}\triangle(\phi_1^2 + \phi_1\phi_2 + \phi_2^2))\|_{L^2(\Omega)}$$
$$+2\|\nabla\hat{\phi}\cdot\nabla(\phi_1^2 + \phi_1\phi_2 + \phi_2^2)\|_{L^2(\Omega)} \leq C\|\hat{\phi}\|_{H^2(\Omega)} .$$

$$\begin{aligned}\|f(\phi_1) - f(\phi_2)\|_{L^2(\Omega)} &\leq C(\|\triangle\hat{\phi}\|_{L^2(\Omega)} + \|\hat{\phi}\|_{L^2(\Omega)} + \|\phi_1^3 - \phi_2^3\|_{L^2(\Omega)}) \\ &\leq C\|\hat{\phi}\|_{H^2(\Omega)} .\end{aligned}$$

$$\begin{aligned}\|\phi_1^2 f(\phi_1) - \phi_2^2 f(\phi_2)\|_{L^2(\Omega)} &\leq \|(\phi_1^2 - \phi_2^2)f(\phi_1)\|_{L^2(\Omega)} + \|\phi_2^2(f(\phi_1) - f(\phi_2))\|_{L^2(\Omega)} \\ &\leq C\|\hat{\phi}\|_{H^2(\Omega)} .\end{aligned}$$

$$|B(\phi_1) - B(\phi_2)| \leq C(\|\nabla(\phi_1 + \phi_2)\|_{L^2(\Omega)})\|\nabla\hat{\phi}\|_{L^2(\Omega)}$$
$$+C\left|\int_\Omega (\phi_1^2 + \phi_2^2 - 2)(\phi_1 + \phi_2)\hat{\phi}dx\right| \leq C\|\hat{\phi}\|_{H^2(\Omega)} .$$

$$\|B(\phi_1)f(\phi_1) - B(\phi_2)f(\phi_2)\|_{L^2(\Omega)} \leq \|B(\phi_1)(f(\phi_1) - f(\phi_2))\|_{L^2(\Omega)}$$
$$+\|(B(\phi_1) - B(\phi_2))f(\phi_2)\|_{L^2(\Omega)} \leq C\|\hat{\phi}\|_{H^2(\Omega)} .$$

Summing together, the claim (2.17) is verified.

2.6 Some Final Remarks about the Proof

At the end of this Chapter, several remarks on the proofs are stated here to provide a better understanding.

Remark 2.1. The assumption on the domain ensures that H^2 regularity for the Laplace operator with homogeneous boundary condition can be obtained. $\square$

Remark 2.2. Due to the standard theory for the conventional Navier-Stokes equations without the membrane stress [70] and the simple L^2 gradient flow of the elastic bending energy without the fluid transport [78], it is easy to see that the main task at hands is to analyze the coupling terms in the PFNS equation, which has similar spirits as that in the study of coupled systems for fluid and liquid crystal director [52]. Therefore, it is necessary to consider (control) the contribution to the momentum equation of the additional stress tensor due to the membrane deformation. With the energy law established below, it turns out that the solution space $L^2(0,T,H_d(\Omega)) \cap W^{1,\frac{4}{3}}(0,T,H_d^{-1}(\Omega))$ for the velocity field u remains the same as that for the conventional three dimensional incompressible Navier-Stokes equations. This reflects the fact that the membrane stress tensor does not pose any extra limitation on the regularity of the weak solution of the velocity field. Meanwhile, the solution space $L^2(0,T,H^2(\Omega)) \cap H^1(0,T;L^2(\Omega))$ for ϕ also coincides with the natural space for the solution of the simple L^2 gradient flow of the elastic bending energy, again showing that the effect of fluid transport on the phase field function can also be properly controlled.

□

Remark 2.3. Due to the limited regularity in u, the issue of uniqueness of the weak solution remains open even for the conventional Navier-Stokes equations in three dimension without the membrane effect. Hence there is no proof for uniqueness of the global weak solutions for the coupled PFNS equation in general. However, with a better regularity assumption on the weak solutions, as in the case of the conventional Navier-Stokes equations [70], the uniqueness can be assured. □

Remark 2.4. The analysis largely relies on the damping term in the evolution of the phase field function and can not be readily extended to the case of a pure transport. Such cases were treated in [53] for the systems for viscoelastic materials. However, the nonlinear coupling terms involve higher derivatives in this discussion. □

Chapter 3

Stochastic Implicit Interface Model

In the last chapter, the PFNS model, a special fluid-structure interaction model, is analyzed. In real world, fluid-structure interaction may involve phenomena at many different length scales and time scales. Although the microscopic fluctuations are generally small, they play essential roles in many applications in materials science and biological science. Particularly, it is widely known that the effects of thermal fluctuations are important for various biological processes and functions in the biological system where the lipid bilayer vesicles interact with surrounding fluid. Then this raises the question on how to properly incorporate the fluctuations effects in the PFNS model discussed in Chapter 2, or in more general fluid implicit interface interaction equation briefly described in Section 1.3.

In this Chapter, the detailed derivation of the fluid implict interface interaction equation will be given first. Then the issue of capturing the fluctuation effects will be addressed based on the stochastic immersed boundary method [4, 46] with an implicit interface. The resulting equations are systems of stochastic partial differential equations involving the fluid variables (velocity and pressure in the primitive variable formulation) and the phase field or level set variables characterizing the motion of the immersed interface.

3.1 The Derivation of Fluid Implicit Interface Interaction Equation

Let a phase field function (or level set function) ϕ represent the interface (or surface) immersed in a fluid environment. $E[\phi]$ is the elastic energy corresponding to the interface configuration. The fluid implicit interface interaction is characterized by the competition of the fluid kinetic energy and interfacial energy $E[\phi]$.

Consider the description of incompressible fluid velocity field in Lagrange coordinate. Let $x(t, \alpha)$ denote the fluid particle trajectory, then velocity field is implicitly defined by

$$\begin{cases} \dot{x}(t, \alpha) = u(t, x(t, \alpha)) \ , \\ x(0, \alpha) = \alpha \ . \end{cases} \tag{3.1}$$

Furthermore, the phase field function ϕ is assumed to be purely transported via fluid velocity field with initial value ϕ_0, then

$$\begin{cases} \phi_t + u \cdot \nabla \phi = 0 \ , \\ \phi(0,x) = \phi_0(x) \ . \end{cases} \tag{3.2}$$

For a fixed time T_0, the least action principle asserts that the actual fluid particle trajectory $x(t, \alpha)$ minimizes the action functional [24, 17],

$$A[x(t,\alpha)] = \int_0^{T_0} \left(\int_\Omega \frac{1}{2} |u(t,x)|^2 dx - E[\phi] \right) dt \ .$$

Therefore, the variation with respect to the fluid particle trajectory gives

$$\delta A[x(t,\alpha)] = \int_0^{T_0} \int_\Omega \nabla p \, \delta x \, dx \, dt \ ,$$

with ∇p being the pressure, the Lagrange multiplier due to incompressibility of the fluid. To be more precise about the variation, let $\{x^\varepsilon(t,\alpha)\}$ be a family of impressible fluid particle trajectories, where ε is the index. The variation δ means,

$$\delta A[x(t,\alpha)] = \frac{d}{d\varepsilon}|_{\varepsilon=0} A[x^\varepsilon(t,\alpha)] \ . \tag{3.3}$$

In the Lagrange coordinate

$$\begin{aligned} \delta A[x(t,\alpha)] &= \int_0^{T_0} \int_\Omega (\delta \dot{x}(t,\alpha) \, u(t, x(t,\alpha)) - \nabla E[\phi] \cdot \delta\phi) \, d\alpha \, dt \\ &= \int_0^{T_0} \int_\Omega (-(u_t + u \cdot \nabla u) \cdot \delta x - \nabla E[\phi] \, \delta\phi) \; d\alpha \, dt \end{aligned}$$

Later in Lemma 3.1, it will be shown that

$$\delta\phi = -\nabla\phi \cdot \delta x \ .$$

Therefore,

$$\delta A[x(t,\alpha)] = \int_0^{T_0} \int_\Omega (-(u_t + u \cdot \nabla u) + \nabla E[\phi]\nabla\phi)\, \delta x\, dx\, dt\ .$$

It implies the Euler equation

$$u_t + u \cdot \nabla u = \nabla p + \nabla E[\phi]\nabla\phi\ .$$

Add the viscosity term $\mu\triangle u$, then the momentum equation is derived

$$u_t + u \cdot \nabla u = \mu\triangle u + \nabla p + \nabla E[\phi]\nabla\phi\ .$$

To sum up, the fluid implicit interface interaction could be described by

$$\begin{cases} u_t + u \cdot \nabla u = \mu\triangle u + \nabla p + \nabla E[\phi]\nabla\phi\ , \\ \phi_t + u \cdot \nabla\phi = 0\ , \\ \nabla \cdot u = 0\ . \end{cases} \tag{3.4}$$

3.2 Stochastic Immersed Boundary Method

To capture the fluctuation effects, the stochastic immersed boundary method is used with the implicit interface formation to derive the proper form of noise to be incorporated into equation (3.4). The immersed boundary method can be formulated to model the interaction between an incompressible viscous fluid and an immersed structure represented by discrete particles. The typical equation of immersed boundary method [66] is given by

$$\begin{cases} u_t + u \cdot \nabla u = \mu \triangle u + \nabla p + \sum_i f_i \cdot \zeta_r(x - X_i) \ , \\ \dot{X}_i(t) = \int u(t,x) \zeta_r(X_i - x) dx \ , \\ \nabla \cdot u = 0 \ , \end{cases} \tag{3.5}$$

where X_i is the position of the i^{th} particle, f_i is the force interaction between the i^{th} particle and the fluid, and ζ_r is a delta function for $r = 0$ or a regularized version parameterized by some positive constant $r > 0$. Typically, r may represent the size of a blob around the particle position in the latter case. In the derivation of the stochastic immersed boundary method (SIBM)[4, 46], a potential energy $V(\{X_i\})$ is defined as a function of the particle position vectors $\{X_i\}$, and the forces are given by $\{f_i = -\nabla_i V(\{X_i\})\}$. For fluids in the low Reynolds number regime, the Navier-Stokes equations may be simply replaced by the Stokes equation. To model the stochastic effects, noise terms f and $\{g_i\}$ are first added into the equations to get:

$$\begin{cases} u_t = \mu \triangle u + \nabla p + \sum_i f_i \cdot \zeta_r(x - X_i) + f \ , \\ \dot{X}_i(t) = \int u(t,x) \zeta_r(X_i - x) dx + g_i \ , \\ \nabla \cdot u = 0 \ . \end{cases} \tag{3.6}$$

Then, the equation (3.6) is linearized around the equilibrium solution of the corresponding deterministic equation and the resulting linear system is subsequently expanded in the Fourier space. The correlation structure of the solution to the linearized equation in Fourier space can be explicitly computed. By imposing that the solution obeys Boltzmann distribution as the dynamics reaches the thermal equilibrium, the proper forms of noises f and $\{g_i\}$ are obtained. If one views the index i as a continuous parameter, then the particles forms an immersed interface and the summation in the momentum equation can be simply replaced by an integration over the interface.

3.3 Stochastic Immersed Boundary Method with Implicit Interface Representation

In the immersed boundary method, the immersed structure is explicitly described by the positions of particles $\{X_i\}$. And the potential energy is a function of $\{X_i\}$. In the implicit interface model, a continuous labeling function is used to characterize the interface configuration, hence the potential energy is in functional form.

The deterministic equation (3.4) formally has a dissipative energy law,

$$\frac{d}{dt}\left(\int_\Omega \frac{1}{2}|u(t,x)|^2 dx + E[\phi]\right) = -\mu \int_\Omega |\nabla u|^2 dx.$$

Assume ϕ_0 is a local minimizer of $E[\phi]$, and the Hessian of $E[\phi]$ at ϕ_0 is positive definite. Then $(u \equiv 0, \phi \equiv \phi_0)$ gives a stable steady state of the deterministic equation (3.4).

Through the calculation of the correlation structure of the linearized equation, the proper form of the noise to be incorporated in the stochastic system can be derived. For the sake of illustration, a periodic boundary condition is assumed for both the flow variables and the interface marker. And the computational domain Ω is set to a unit cell of periodic domain.

Let L_0 be the linearized operator of ∇E at ϕ_0. As an illustrative example, if

$$E[\phi] = \int \frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{4\epsilon}(\phi^2 - 1)^2 d\Omega \ ,$$

then the linearized operator

$$L_0[\psi] = -\epsilon\triangle\psi + \frac{1}{\epsilon}(3\phi_0^2 - 1)\psi \ .$$

By linearizing the equation and introducing the noise terms f and g, the following coupled stochastic system is formally obtained,

$$\begin{cases} u_t = \mu\triangle u + \nabla p + L_0[\psi]\cdot\nabla\phi_0 + f \ , \\ \psi_t + u\cdot\nabla\phi_0 = g \ , \\ \nabla\cdot u = 0 \ , \end{cases} \tag{3.7}$$

where $\psi = \phi - \phi_0$, f and g are two Gaussian noises. f and g are assumed to be delta correlated in time.

Expand (3.7) in Fourier space with k denoting the wave number, then

$$\begin{cases} \frac{d}{dt}\hat{u}_k = -4\pi^2\mu|k|^2 P_k\hat{u}_k + P_k\sum_{l,k'}\pi_{k,l}\sigma_{l,k'}\hat{\psi}_{k'} + P_k\hat{f}_k \\ \frac{d}{dt}\hat{\psi}_k = -\sum_{k'}\tilde{\pi}_{k,k'}\hat{u}_{k'} + \hat{g}_k \end{cases} \tag{3.8}$$

where $P_k = I - \frac{k\otimes k}{|k|^2}$ is the projection to ensure incompressibility of fluids [71]. In the Fourier variables,

$$\widehat{L_0[\psi]}_l = \sum_{k'} \sigma_{l,k'} \hat{\psi}_{k'} \ ,$$

with $\{\sigma_{l,k'}\}$ determined by the linearized operator L_0. And,

$$\pi_{k,l} = \int_\Omega \nabla\phi_0 e^{-i2\pi(k-l)x} dx \,, \qquad \text{and} \qquad \tilde{\pi}_{k,l} = \int_\Omega [\nabla\phi_0]^T e^{-i2\pi(k-l)x} dx \,.$$

Moreover, $\hat{f}_k$ and $\hat{g}_k$ are Fourier coefficients of noises f and g, i.e.

$$f(t) = \sum \hat{f}_k(t) \cdot e^{i2\pi kx} \quad \text{and} \quad g(t) = \sum \hat{g}_k(t) \cdot e^{i2\pi kx} \ .$$

$\hat{f}_k$ and $\hat{g}_k$ are finite dimensional Gaussian white noises. Their correlations are to be determined in Proposition 3.1 and 3.4 later.

Let $a(t) = (\hat{u}, \hat{\psi})^T$. The linearized equation (3.8) can be abbreviated as an infinite system of ODEs,

$$\frac{d}{dt} a(t) = Da(t) + n(t), \tag{3.9}$$

where $n(t) = (P_k \hat{f}_k, \hat{g}_k)^T$ and the matrix operator D has the form

$$D = \begin{bmatrix} D_{11} & D_{12} \\ D_{21} & 0 \end{bmatrix}$$

with its entries defined by:

$$\begin{aligned} (D_{11})_{k,k'} &= -4\pi^2 \mu |k|^2 \delta_{k,k'} P_k \ , \\ (D_{12})_{k,k'} &= \textstyle\sum_l P_k \pi_{k,l} \sigma_{l,k'} \ , \\ (D_{21})_{k,k'} &= -\tilde{\pi}_{k,k'} \ , \end{aligned}$$

where the notation $\delta_{k,k'} = \begin{cases} 1 & \text{if } k = k' \, , \\ 0 & \text{otherwise} \, . \end{cases}$

Now, let

$$\Pi = (\pi_{k,l}), \quad \tilde{\Pi} = (\tilde{\pi}_{k,k'}) \, , \quad \Sigma = (\sigma_{l,k'}),$$

and define

$$P = \begin{bmatrix} \ddots & & \\ & P_k & \\ & & \ddots \end{bmatrix} .$$

Then $D_{12} = P \cdot \Pi \cdot \Sigma$ and $D_{21} = -\tilde{\Pi}$.

It follows from the fluctuation-dissipation theorem [46, 30] that the equilibrium solution obeys Boltzmann distribution. The probability density formally is given by

$$\frac{1}{Z} \exp[-\frac{1}{2K_bT}(\sum_k |\hat{u}_k|^2 + \sum_{k,k'} \sigma_{k,k'} \hat{\psi}_{k'} \overline{\hat{\psi}}_k)],$$

where Z is a normalization constant, K_b is Boltzmann constant and T denotes the temperature. To be more precise,

1. The velocity field is real, thus $\hat{u}_k = \overline{\hat{u}}_{-k}$. Moreover, due to the incompressibility of the fluid, $\hat{u}_k \cdot k = 0$. It implies that the probability distribution of $\hat{u}_k$ lives on the orthogonal complement of the vector k, rather than the whole space.

2. ψ is also a real function, hence $\hat{\psi}_k = \overline{\hat{\psi}}_{-k}$.

It is clear that $\hat{u}$ and $\hat{\psi}$ are independent. Therefore, when the dynamics reaches the thermal equilibrium, it can be assumed that the correlation matrix of the solution is given by

$$\lim_{t\to\infty} < a(t) \otimes \overline{a(t)} >= K_b T \cdot \begin{bmatrix} C_{11} & 0 \\ 0 & C_{22} \end{bmatrix}$$

where $< \cdot >$ represents the expectation,

$$< \hat{u} \otimes \overline{\hat{u}} >= K_b T \cdot C_{11} \quad \text{and} \quad < \hat{\psi} \otimes \overline{\hat{\psi}} >= K_b T \cdot C_{22} \; .$$

Direct calculation shows that $(C_{11})_{k,k'} = \delta_{k,k'} P_k$ and $C_{22} = \Sigma^{-1}$. For illustrative purposes, consider the case of two space dimension though the derivation works in three dimension as well. Let r_k and s_k represent the real and imaginary parts of $\hat{u}_k$ respectively. Because of the independence implied by Boltzmann distribution and $\hat{u}_k = \overline{\hat{u}}_{-k}$,

$$\begin{aligned} < \hat{u}_k \otimes \overline{\hat{u}}_{k'} > &= < r_k \otimes r_{k'} > \\ &\quad + < s_k \otimes s_{k'} > + i[< s_k \otimes r_{k'} > - < r_k \otimes s_{k'} >] \\ &= < r_k \otimes r_{k'} > + < s_k \otimes s_{k'} > \\ &= \delta_{k,k'} \left(< r_k \otimes r_k > + < s_k \otimes s_k >\right) \; . \end{aligned}$$

For $k \neq 0$, let $|r_k| = r$ and $\frac{k}{|k|} = (\cos\theta, \sin\theta)$, then,

$$\begin{aligned}
< r_k \otimes r_k > &= \left\langle r \begin{pmatrix} \sin\theta \\ -\cos\theta \end{pmatrix} \cdot r(\sin\theta, -\cos\theta) \right\rangle \\
&= < r^2 > \cdot \begin{pmatrix} \sin^2\theta & -\sin\theta\cos\theta \\ -\cos\theta\sin\theta & \cos^2\theta \end{pmatrix} \\
&= < r^2 > \cdot \left(I - \begin{pmatrix} \cos^2\theta & \sin\theta\cos\theta \\ \cos\theta\sin\theta & \sin^2\theta \end{pmatrix} \right) \\
&= < r^2 > \cdot (I - \frac{k \otimes k}{|k|^2}) \\
&= < r^2 > \cdot P_k
\end{aligned}$$

Since $\hat{u}_k = \overline{\hat{u}}_{-k}$, r satisfies the distribution $\frac{1}{Z}\exp(-\frac{r^2}{K_b T})$. Hence

$$< r^2 > = \frac{K_b T}{2} \text{ and } < r_k \otimes r_k > = \frac{K_b T}{2} \cdot P_k \, .$$

Similarly $< s_k \otimes s_k > = \frac{K_b T}{2} \cdot P_k$. Therefore

$$< \hat{u}_k \otimes \overline{\hat{u}}_{k'} > = K_b T \cdot \delta_{k,k'} P_k \, .$$

That is, $(C_{11})_{k,k'} = \delta_{k,k'} P_k$. For C_{22}, it can be computed similarly without much difficulty.

While the derivation uses a two dimensional form, one can extend the calculation to three dimension as well. The detail is omitted here.

It follows from (3.9) that,

$$\frac{d}{dt} < a \otimes \overline{a} > = D < a \otimes \overline{a} > + < a \otimes \overline{a} > D^* + N$$

where $\{\cdot\}^*$ denotes the adjoint operation (transpose of the complex conjugate) and the last term N is the Ito's correction. Recall the assumption that the noise is delta correlated in time, N satisfies $< n(t) \otimes \overline{n(t')} >= N\delta(t-t')$.

Setting $t \to \infty$, follow from the equilibrium distribution

$$N = -K_b T(DC + CD^*) \ .$$

Taking N in block matrix form,

$$N = \begin{bmatrix} N_{11}, N_{12} \\ N_{21}, N_{22} \end{bmatrix} \ ,$$

then

$$\begin{aligned} &N_{11} = 8\pi^2 \mu K_b T |k|^2 P_k \delta_{k,k'}, \\ &N_{22} = 0, \\ &N_{12} = -K_b T(D_{12}C_{22} + C_{11}D_{21}^*) = K_b T[P\Pi\Sigma\Sigma^{-1} - P\tilde{\Pi}^*] = 0 \ , \end{aligned}$$

and $N_{21} = 0$.

Now, $N_{22} = 0$ implies that the noise $g = 0$. A proposition is summarized below to highlight the conclusion of the above derivation.

Proposition 3.1. *The coupled system of equations*

$$\begin{cases} u_t + u \cdot \nabla u = \mu \triangle u + \nabla p + \nabla E[\phi]\nabla\phi + f \ , \\ \phi_t + u \cdot \nabla\phi = 0 \ , \\ \nabla \cdot u = 0 \end{cases} \tag{3.10}$$

describes the dynamics near the mechanical and thermal equilibrium. That is, ϕ should be purely transported via velocity field without any noise perturbation, and a proper noise f should be added to the fluid momentum equation. When expanding in Fourier space of the spatial variables, the Fourier *coefficients* $\{\hat{f}_k\}$ *of* f *satisfy*

$$< P_k\hat{f}_k(t) \otimes \overline{P_{k'}\hat{f}_{k'}(t')} >= 8\pi^2\mu K_b T|k|^2 P_k \delta_{k,k'}\delta(t-t') \tag{3.11}$$

for any k, k' *and* t, t'.

The simplest way to construct the Gaussian noise that satisfies (3.11) is to let

$$f = \sqrt{8\pi^2\mu K_b T} \cdot \sum_k |k| \frac{dW_k}{dt} \cdot e^{i2\pi kx} \ ,$$

where $\{W_k\}$ are independent standard complex Wiener processes.

The random force derived here is body force. But it also can be written as stress. Without losing generality, consider the 2D case. Let $\varpi^{(1)}(t,x)$, $\varpi^{(2)}(t,x)$ be two independent standard Wiener processes, defined by

$$\varpi^{(1)}(t,x) = \sum_k \varpi_k^{(1)}(t) \cdot e^{i2\pi kx}$$
$$\varpi^{(2)}(t,x) = \sum_k \varpi_k^{(2)}(t) \cdot e^{i2\pi kx}$$

where $\{\varpi_k^{(i)}(t)\}$ with $i = 1, 2$ are independent complex valued Wiener processes.

Construct the stress S as,

$$S = \begin{pmatrix} \frac{d\varpi^{(1)}}{dt} & \frac{d\varpi^{(2)}}{dt} \\ \frac{d\varpi^{(2)}}{dt} & -\frac{d\varpi^{(1)}}{dt} \end{pmatrix} .$$

Direct calculation shows

$$\nabla \cdot S = \sum_k 2\pi|k| \cdot i \begin{pmatrix} \frac{k_1}{|k|} \cdot \frac{d\varpi_k^{(1)}}{dt} + \frac{k_2}{|k|} \cdot \frac{d\varpi_k^{(2)}}{dt} \\ \frac{k_1}{|k|} \cdot \frac{d\varpi_k^{(2)}}{dt} - \frac{k_2}{|k|} \cdot \frac{d\varpi_k^{(1)}}{dt} \end{pmatrix} \cdot e^{i2\pi kx} \ .$$

Redefine

$$\frac{dW_k}{dt} = i \begin{pmatrix} \frac{k_1}{|k|} \cdot \frac{d\varpi_k^{(1)}}{dt} + \frac{k_2}{|k|} \cdot \frac{d\varpi_k^{(2)}}{dt} \\ \frac{k_1}{|k|} \cdot \frac{d\varpi_k^{(2)}}{dt} - \frac{k_2}{|k|} \cdot \frac{d\varpi_k^{(1)}}{dt} \end{pmatrix} \ .$$

It is easy to show $\{W_k(t)\}$ are 2D complex vector valued Wiener processes. That is,

$$\nabla \cdot S = \sum_k 2\pi|k| \frac{dW_k}{dt} \cdot e^{i2\pi kx} \ .$$

Note that the stress is not unique. For instance, let

$$\varpi^{(3)} = \sum_k \varpi_k^{(3)}(t) \cdot e^{i2\pi kx}$$

be another standard complex Wiener process independent of $\varpi^{(1)}(t,x)$ and $\varpi^{(2)}(t,x)$. Construct

$$S' = S + \frac{d\varpi^{(3)}(t,x)}{dt} \cdot \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \ .$$

It is readily checked that

$$\nabla \cdot S' = \nabla \cdot S + \textit{gradient term}$$

and the *gradient term* could be absorbed in pressure. The correlation of S' is

$$< S'_{i,j}(t,x), S'_{l,m}(t',x') >= \delta(t-t')\delta(x-x') \cdot (\delta_{il}\delta_{jm} + \delta_{im}\delta_{jl}) \ . \quad (3.12)$$

Random stress has been used in many physical models. For instance, in [76] a stress with the same correlation as S' has been incorporated into a steady Stokes equation to derive a Langevin type equation of vesicle motion.

In all the discussion, the energy functional can take on a very general form. Several examples are given here as illustration.

Example 1. First consider a stochastic model for fluid interface interaction under the surface tension.

In the study of the surface tension based on a phase field function, when a constant surface tension is assumed, the corresponding energy $E[\phi]$ is defined as [19]

$$E[\phi] = \int_\Omega \frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{4\epsilon}(\phi^2-1)^2 dx \ ,$$

which represents the surface area of the interface. The corresponding force density term is given by

$$\nabla E[\phi]\nabla\phi = \left\{-\epsilon\triangle\phi + \frac{1}{\epsilon}(\phi^3-\phi)\right\}\nabla\phi \ . \tag{3.13}$$

Substituting the above into the system (3.10), a stochastic phase field fluid interface interaction model with the interfacial energy being governed by the surface tension is derived. While written formally as a force term, $\nabla E[\phi]\nabla\phi$ should be best interpreted as an approximation to the extra stress due to the interface deformation. Notice that the momentum equation can also be rewritten as

$$u_t + u \cdot \nabla u = \mu \triangle u + \nabla p - \epsilon \Delta\phi \nabla\phi + f \ ,$$

where the nonlinear term $\epsilon^{-1}(\phi^3 - \phi)\nabla\phi$ is absorbed into the pressure term.

Example 2. The phase field approximation of the bending elastic energy in the studies of vesicle membranes [24] is explained in Chapter 2. Recall the corresponding phase field energy is given by

$$\begin{aligned} E[\phi] &= \frac{k}{2\epsilon}\int_\Omega \left(\epsilon\triangle\phi + (\frac{1}{\epsilon}\phi + c_0\sqrt{2})(1-\phi^2)\right)^2 dx \\ &+ \frac{M_1}{2}\left(\int_\Omega [\frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{4\epsilon}(\phi^2-1)^2]\, dx - A_0\right)^2 \\ &+ \frac{M_2}{2}\left(\int_\Omega \phi\, dx - V_0\right)^2 . \end{aligned}$$

where the first penalty term involving M_1 is used for preserving the surface area of the interface and the second penalty term involving M_2 is for the volume conservation. For simplicity, the spontaneous curvature c_0 is set to 0. The force density $\nabla E[\phi]\nabla\phi$ calculated in [18, 24] is given by

$$\begin{aligned} \nabla E[\phi]\nabla\phi &= kg(\phi)\nabla\phi \\ &+ M_1\left(\int_\Omega \frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{4\epsilon}(\phi^2-1)^2\, dx - A_0\right) f(\phi)\nabla\phi \\ &+ M_2\left(\int_\Omega \phi\, dx - V_0\right)\nabla\phi \ , \end{aligned} \tag{3.14}$$

where

$$f(\phi) = -\epsilon \triangle \phi + \frac{1}{\epsilon}(\phi^2 - 1)\phi \ ,$$

$$g(\phi) = -\triangle f(\phi) + \frac{1}{\epsilon^2}(3\phi^2 - 1) f(\phi) \ .$$

Substituting into the momentum equation, the stochastic phase field fluid structure interaction model with bending elastic energy is obtained. Note that with the incompressibility condition satisfied by u, M_2 can be set to 0 in the last term of the force expression (3.14), since the volume constraint is automatically satisfied by the transport equation for ϕ. Similar to the previous example, the first term in the force $\nabla E[\phi]\nabla\phi$ corresponds to the diffuse interface approximation to the extra Willmore stress due to the bending elastic energy (see [24] for a derivation of the consistency with the sharp interface model). The penalty term for the area constraint can also be formulated via introducing a Lagrange multiplier. Effectively, its contribution is then similar to that derived from the variation of the surface tension (3.13).

Example 3. In [12, 13, 14], a level set model for incompressible fluid-structure interaction is discussed. Similar to the phase field approach, a level set function ϕ is used to represent the elastic material in fluid. The energy is defined as

$$E[\phi] = \int_\Omega E_d(|\nabla\phi|)\frac{1}{\epsilon}\eta(\frac{\phi}{\epsilon})dx,$$

where E_d is the energy density, ϵ is a small positive parameter, and cut-off function $\eta(r) = \frac{1}{2}(1+\cos(\pi r))$ for $|r| \le 1$ and $\eta(r) = 0$ otherwise. The force density is

$$\begin{aligned} \nabla E[\phi]\nabla\phi &= \left\{-\text{div}\left(E_d'(|\nabla\phi|)\frac{1}{\epsilon}\eta(\frac{\phi}{\epsilon})\frac{\nabla\phi}{|\nabla\phi|}\right)\right. \\ &\quad \left. + E_d(|\nabla\phi|)\frac{1}{\epsilon^2}\eta'(\frac{\phi}{\epsilon})\right\}\cdot\nabla\phi \end{aligned} \tag{3.15}$$

The force density in [14] is derived through the principle of virtual work. That is the force density, say F, is derived from

$$\frac{d}{dt}E[\phi] = -\int_\Omega F\cdot u\,dx\ .$$

The expression of $\nabla E[\phi]\nabla\phi$ in (3.15) differs from F up to a gradient term, which is absorbed into the pressure term. By substituting the force density (3.15) into the system (3.10), a stochastic level-set fluid-interface model is derived. Depending on how the energy density E_d is chosen, it can be used to model interfacial energies of various kinds, just like the phase field counterpart.

All the above three examples are special cases of the SIIM given in (3.10). Naturally other variations can be considered in the future.

Before the end this section, a couple of remarks need to be stated.

Remark 3.1. Recall that the noise form is derived from the linearized the equation around an equilibrium state of the deterministic dynamics. However, the only noise contribution appears in the coupled stochastic model is in the momentum equation. Moreover, the noise is independent of the choice of equilibrium state. This means that potentially this model could be adopted to study the case when the deterministic dynamics may have multiple equilibrium states (even though the steady state velocity field should always be zero due to the dissipative energy law). □

Remark 3.2. The noise derived for the stochastic implicit interface model is very much the same as the noise derived in stochastic immersed boundary method [46]. In fact, the noise is determined by the dissipative character of the deterministic system. The dissipation of implicit interface fluid interaction and stochastic immersed boundary method is due to the viscosity (or Stokes operator). So it is not surprising to get the same noise. This matter will be further commented in the next section. □

3.4 General Stochastic Implicit Interface Model for a Mollified Flow

The proper form of the noise for phase field-fluid interaction equation is derived in the previous section. It turns out the noise term only appears in the fluid momentum equation. Generally speaking, the presence of the noise term weakens the regularity of the fluid velocity field, which leads to the difficulty of interpreting transport equation of the phase field or level set function in a suitable functional setting. As a possible remedy, a mollified fluid velocity field is considered. This technique has been used widely in the literature, including the setting of the Immersed Boundary Methods and SIBM [46].

For simplicity, consider a symmetric kernel ζ, i.e. $\zeta(x) = \zeta(|x|)$, and define ϕ via the mollified transport equation,

$$\begin{cases} \phi_t + (u * \zeta) \cdot \nabla\phi = 0 \ , \\ \phi(0) = \phi_0 \ . \end{cases} \tag{3.16}$$

Here $*$ denotes the standard convolution operator.

Despite of this change, it is still possible to derive the corresponding deterministic equation through the least action principle on a periodic domain. And the mollification does not affect the noise form derived in section 3.3.

Define the mollified flow map $z(t, \alpha)$ by

$$\begin{cases} \dot{z}(t, \alpha) = \displaystyle\int_\Omega u(t, y)\zeta(z(t, \alpha) - y)dy \ , \\ z(0, \alpha) = \alpha \ . \end{cases}$$

Since u is divergence free, $z(t, \alpha)$ is a volume preserving map. The transport equation (3.16) implies that $\phi(t, x) = \phi_0(z^{-1}(t, x))$. The change of the transport equation of ϕ results in corresponding change to the momentum equation of the fluid velocity. Before obtaining the new equation, a technical lemma is needed.

Lemma 3.1. *The variation* $\delta\phi = -\nabla\phi \cdot \delta z$. *And* $\delta z = \delta x * \zeta$, *thereby* $\delta\phi = -\nabla\phi \cdot (\delta x * \zeta)$.

Proof. $\phi(t,x) = \phi_0(z^{-1}(t,x))$ implies

$$\delta\phi = \nabla\phi_0(z^{-1}(t,x)) \cdot \delta z^{-1}(t,x)\ .$$

Since $z^{-1}(t, z(t,\alpha)) = \alpha$, $\delta z^{-1}(t, z(t,\alpha)) + \nabla_x z^{-1}(t, z(t,\alpha))\delta z(t,\alpha) = 0$. Immediately,

$$\delta z^{-1}(t,x) = -\nabla_x z^{-1}(t,x)\delta z\ .$$

Therefore,

$$\begin{aligned} \delta\phi &= -\nabla\phi_0(z^{-1}(t,x))\,\nabla_x z^{-1}(t,x)\,\delta z \\ &= -\nabla_x\phi(t,x)\delta z\ . \end{aligned}$$

In $\dot{z}(t,\alpha) = \int_\Omega u(t,y)\zeta(z(t,\alpha) - y)dy$, fix $\alpha = \alpha_0$. We carry out the computation in Lagrange coordinate.

$$\begin{aligned} \frac{d}{dt}\delta z(t,\alpha_0) &= \int_\Omega \frac{d}{dt}\delta x(t,\alpha) \cdot \zeta(z(t,\alpha_0) - x(t,\alpha))d\alpha \\ &\quad + \int_\Omega \dot{x}(t,\alpha)\nabla\zeta(z(t,\alpha_0) - x(t,\alpha))(\delta z(t,\alpha_0) - \delta x(t,\alpha))d\alpha \\ &= \frac{d}{dt}\left(\int_\Omega \delta x(t,\alpha)\zeta(z(t,\alpha_0) - x(t,\alpha))d\alpha\right) \\ &\quad + \int_\Omega [\delta z(t,\alpha_0)\dot{x}(t,\alpha) - \dot{z}(t,\alpha_0)\delta x(t,\alpha)] \cdot \nabla\zeta(z(t,\alpha_0) - x(t,\alpha))d\alpha \end{aligned}$$

Convert back to Eulerian coordinate. Note that div$\delta x = 0$,

$$
\begin{aligned}
& \int_\Omega [\delta z(t,\alpha_0)\dot{x}(t,\alpha) - \dot{z}(t,\alpha_0)\delta x(t,\alpha)] \cdot \nabla\zeta(z(t,\alpha_0) - x(t,\alpha))d\alpha \\
= & \int_\Omega [\dot{z}(t,\alpha_0)\delta x(t,y) - \delta z(t,\alpha_0)u(t,y)] \cdot \nabla_y\zeta(z(t,\alpha_0) - y)dy \\
= & \ 0 \, .
\end{aligned}
$$

Since $\delta z(0) = \delta x(0) = 0$, we conclude that

$$\delta z(t,\alpha_0) = \int_\Omega \delta x(t,\alpha)\zeta(z(t,\alpha_0) - x(t,\alpha))d\alpha \, .$$

holds for any α_0. That is

$$\delta z = \delta x * \zeta \text{ and } \delta\phi = -\nabla\phi \cdot (\delta x * \zeta) \, .$$

□

Proposition 3.2. *When ϕ is transported via the mollified flow, the fluid particle trajectory that minimizes the action functional (3.3) defines a fluid velocity field u which satisfies*

$$u_t + u \cdot \nabla u = (\nabla E[\phi]\nabla\phi) * \zeta + \nabla p \, .$$

Proof. we start with

$$\delta A[x(t,\alpha)] = \int_0^{T_0} \left(\int_\Omega \delta\dot{x}(t,\alpha)\, u(t,x(t,\alpha)) - \nabla E[\phi]\, \delta\phi \, d\alpha \right) dt \, .$$

Integrate by part and enforce the condition $\delta x(0) = \delta x(T_0) = 0$,

$$\delta A[x(t,\alpha)] = \int_0^{T_0} \int_\Omega (-(u_t + u \cdot \nabla u)\delta x - \nabla E[\phi]\delta\phi) \, dxdt \, .$$

By Lemma 3.1, $\delta\phi = -\nabla\phi \cdot (\delta x * \zeta)$,

$$\delta A[x(t,\alpha)] = \int_0^{T_0} \int_\Omega \{-(u_t + u \cdot \nabla u)\delta x + \nabla E[\phi]\nabla\phi \cdot (\delta x * \zeta)\}\, dxdt\ .$$

Recall the assumption that ζ is a symmetric kernel, i.e. $\zeta(x-y) = \zeta(y-x)$,

$$\delta A[x(t,\alpha)] = \int_0^{T_0} \int_\Omega \{-(u_t + u \cdot \nabla u) + (\nabla E[\phi]\nabla\phi) * \zeta\} \cdot \delta x\, dxdt\ .$$

Therefore,

$$u_t + u \cdot \nabla u = (\nabla E[\phi]\nabla\phi) * \zeta + \nabla p\ ,$$

where ∇p is the Lagrange multiplier due to $\text{div}\delta x = 0$. □

Again, this version of the least action principle used above does not provide the term $\mu\triangle u$ for the viscous effect. The viscous term is normally added back to the equation to provide the energy dissipation. For the low Reynolds number case, it is reasonable to ignore the nonlinear term $u \cdot \nabla u$ in the momentum equation and simply consider the linear Stokes equation with the suitable modification. Taking all these into account, the following proposition is summarized.

Proposition 3.3. *Consider the level set or phase field function ϕ being transported via the mollified flow and fluid in the low Reynolds number regime, then the fluid velocity field and ϕ satisfy the coupled system of equa-*

tions,

$$\begin{cases} u_t = \mu \triangle u + (\nabla E[\phi]\nabla\phi) * \zeta + \nabla p \ , \\ \phi_t + (u * \zeta)\cdot \nabla \phi = 0 \ , \\ \nabla \cdot u = 0 \ . \end{cases} \tag{3.17}$$

The deterministic Immersed Boundary Method can also be derived within the framework of the least action principle, with or without considering mollification of the fluid velocity. The corresponding action functional is

$$A[x(t,\alpha)] = \int_0^{T_0} \left(\int_\Omega \frac{1}{2}|u(t,x)|^2 dx - V(\{X_i\}) \right) dt \ ,$$

so that

$$\delta A[x(t,\alpha)] = \int_0^{T_0} \left(\int_\Omega -(u_t + u\cdot\nabla u)\delta x d\alpha - \sum_i \nabla_i V \delta X_i(t) \right) dt \ .$$

By Lemma 3.1, $\delta X_i = \int_\Omega \delta x(t,\alpha)\zeta_r(x(t,\alpha) - X_i)d\alpha$,

$$\begin{aligned} \delta A[x(t,\alpha)] &= \int_0^{T_0} \left(\int_\Omega -(u_t + u\cdot\nabla u)\delta x d\alpha - \sum_i \nabla_i V \delta X_i \right) dt \\ &= \int_0^{T_0} \int_\Omega \left(-(u_t + u\cdot\nabla u) - \sum_i \nabla_i V \, \zeta_r(x(t,\alpha) - X_i(t)) \right) \cdot \delta x(t,\alpha) d\alpha dt \ . \end{aligned}$$

This then leads to

$$u_t + u\cdot\nabla u = -\sum_i \nabla_i V \cdot \zeta_r(x - X_i(t)) + \nabla p \ .$$

After adding the viscosity term $\mu\triangle u$, the Immerse Boundary Method is recovered.

Note that formally the following dissipative energy law can be derived by multiplying u to the first equation in (3.17) and $\nabla E[\phi]$ to the second equation, then integrating over the spatial domain:

$$\frac{d}{dt}\left(\int_\Omega \frac{1}{2}|u|^2 dx + E[\phi]\right) = -\mu \int_\Omega |\nabla u|^2 dx.$$

Assume that ϕ_0 is a non-degenerated local minimum of $E[\phi]$. Linearizing (3.17) around ($u \equiv 0$, $\phi = \phi_0$) and incorporating the noises f and g to the dynamics equations,

$$\begin{cases} u_t = \mu \triangle u + \nabla p + (L_0[\psi] \cdot \nabla \phi_0) * \zeta + f \ , \\ \psi_t + (u * \zeta) \cdot \nabla \phi_0 = g \ . \end{cases}$$

Expand the linearized equations in the Fourier space, using the same notation as in section 3.3. Recall $a(t) = (\hat{u}, \hat{\psi})^T$, so

$$\frac{d}{dt} a(t) = Da(t) + n(t) \ ,$$

and

$$D = \begin{bmatrix} D_{11} & D_{12} \\ D_{21} & 0 \end{bmatrix} \ .$$

The only differences from the terms in the equation (3.9) are

1. $D_{12} = P \cdot Y \cdot \Pi \cdot \Sigma$, where diagonal block matrix

$$Y = \begin{bmatrix} \ddots & & \\ & \hat{\zeta}_k \cdot I & \\ & & \ddots \end{bmatrix} ,$$

   where I is an identity matrix, and

2. $D_{21} = -\tilde{\Pi} \cdot Y$.

Then further computation shows $N = -K_b T(DC + CD^*)$ with N being the same as before except that

$$N_{12} = -K_b T(D_{12}C_{22} + C_{11}D_{21}^*) = K_b T[PY\Pi\Sigma\Sigma^{-1} - PY^*\tilde{\Pi}^*] \ .$$

Since ζ is symmetric, $Y^* = Y$, and

$$N_{12} = 0 \ .$$

So the same conclusion is reached that the noise g should vanish too and f remains the same as the case without the velocity mollification. Again, the discussion here is summarized as a proposition.

Proposition 3.4 (Stochastic implicit interface model (SIIM))**.** *To capture the near equilibrium fluctuation effect in the structure-fluid interaction model with an implicit interface representation, the following system of equations can be used.*

1. *The phase field or level set function is transported via a mollified velocity field, i.e.*

$$\phi_t + (u * \zeta) \cdot \nabla\phi = 0 \ , \tag{3.18}$$

where ζ is a symmetric kernel.

2. The velocity field u is incompressible

$$\nabla \cdot u = 0 \ , \tag{3.19}$$

and satisfies the stochastic equation

$$u_t = \mu \triangle u + (\nabla E[\phi] \nabla \phi) * \zeta + \nabla p + f, \tag{3.20}$$

where the noise f is delta correlated in time, and in Fourier expansion of the spatial variables, it satisfies (3.11).

So far the noise has been expressed in Fourier space. However, it is the dissipative character of the deterministic system that determines the form of noise. And the dissipation comes from the Stokes operator. The effective noise is the projection of noise f in (3.20) in the divergence free subspace, which is spanned by the eigenfunctions of Stokes operator. In fact, the noise can be expressed in terms of the eigenvalues and eigenfunctions of Stokes operator. To be more precise, if $\{\lambda_k, \, \omega_k(x)\}$ are the eigenvalues and normalized eigenfunctions of Stokes operator, then the noise is

$$\sigma \sum_k \sqrt{\lambda_k} \frac{dW_k}{dt} \cdot \omega_k(x) \ , \ \text{or in an abstract form } \sigma Q^{\frac{1}{2}} \frac{dW}{dt} \tag{3.21}$$

where all relevant constants are absorbed into constant σ, and Q indeed is the Stokes operator. The noise (3.21) can be obtained by expanding the fluid momentum equation in terms of the eigenfunctions of Stokes operator instead of Fourier modes, then computing the correlation structure of the linearized equation. The procedure is exactly the same as using Fourier modes.

In the last section, it has been showed on periodic domain when the noise is expressed in terms of Fourier modes, it is equivalent to consider a random stress, with the correlation defined by (3.12). In fact, the equivalence is not limited to periodic domain.

Consider a general domain Ω in $\mathbb{R}^2$, let $\{e_1(x), e_2(x), \ldots\}$ be an orthonormal basis of $L^2(\Omega)$, from the same discussion in last section, the stress

$$S = \begin{pmatrix} \sum_k e_k(x)\dfrac{d\beta_k(t)}{dt} & \sum_k e_k(x)\dfrac{d\vartheta_k(t)}{dt} \\ \sum_k e_k(x)\dfrac{d\vartheta_k(t)}{dt} & -\sum_k e_k(x)\dfrac{d\beta_k(t)}{dt} \end{pmatrix} .$$

is equivalent to a stress S' with correlation defined by (3.12), where $\{\beta_k(t)\}$, $\{\vartheta_k(t)\}$ are standard Wiener processes in $\mathbb{R}$. And it turns out when projected in divergence free subspace $\operatorname{div} S$ is equivalent to $\sum_k \sqrt{\lambda_k}\dfrac{dW_k}{dt} \cdot \omega_k(x)$.

It is sufficient to verify

$$\left\langle \int_\Omega \operatorname{div} S(t,x) \cdot \omega_m(x)dx, \int_\Omega \operatorname{div} S(t',x) \cdot \omega_n(x)dx \right\rangle = \delta(t-t')\delta_{mn}\lambda_m .$$

Write $\omega_m(x) = (\omega_{1m}(x), \omega_{2m}(x))^T$, then

$$\begin{aligned}
\int_\Omega \operatorname{div} S \cdot \omega_m \, dx &= \left(\int_\Omega \partial_1 e_k \omega_{1m} - \partial_2 e_k \omega_{2m} \, dx \right) \cdot \frac{d\beta_k}{dt} \\
&\quad + \left(\int_\Omega \partial_2 e_k \omega_{1m} + \partial_1 e_k \omega_{2m} \, dx \right) \cdot \frac{d\vartheta_k}{dt} \\
&= \left(\int_\Omega e_k \cdot (-\partial_1 \omega_{1m} + \partial_2 \omega_{2m}) \, dx \right) \cdot \frac{d\beta_k}{dt} \\
&\quad + \left(\int_\Omega e_k \cdot (-\partial_2 \omega_{1m} - \partial_1 \omega_{2m}) \, dx \right) \cdot \frac{d\vartheta_k}{dt} \ ,
\end{aligned}$$

in which there is a summation over index k omitted for a cleaner notation. Such notation will be used afterwards without mention if it does not cause confusing. By Parseval identity,

$$\begin{aligned}
&\left\langle \int_\Omega \operatorname{div} S(t,x) \cdot \omega_m(x) dx, \int_\Omega \operatorname{div} S(t',x) \cdot \omega_n(x) dx \right\rangle \\
&= \delta(t-t') \cdot \int_\Omega (-\partial_1 \omega_{1m} + \partial_2 \omega_{2m}) \cdot (-\partial_1 \omega_{1n} + \partial_2 \omega_{2n}) \\
&\qquad + (-\partial_2 w_{1m} - \partial_1 \omega_{2m}) \cdot (-\partial_2 w_{1n} - \partial_1 \omega_{2n}) \, dx \\
&= \delta(t-t') \cdot \int_\Omega -\triangle w_m \cdot w_n \, dx \\
&= \delta(t-t') \delta_{mn} \lambda_m \ .
\end{aligned}$$

At end of this section, several comments are stated here.

Remark 3.3. If the mollifying kernel ζ, in limiting case, is a delta function, then the SIIM equation (3.18, 3.19, 3.20) goes back to the case discussed in section 3.3 with the same form of noise satisfying the same equation (3.11).

□

Remark 3.4. While the striking similarity in the SIIM with and without the mollification is not surprising as seen from the derivation, the assumption on the periodic boundary conditions simplifies much of the technical discussion. For other boundary conditions, one may consider deriving similar stochastic models, but special care near the boundary needs to be taken when a mollification is introduced. □

Remark 3.5. A simplified linear Stokes equation is considered in Proposition 3.3 and 3.4. The derivation of the noise through the linearized equation is identical for both the full Navier-Stokes and linear Stokes equations. In practice though, the simplified Stokes equation can be often utilized to describe the bulk fluid motion in the low Reynolds number regime. Computationally, simulations based on the SIIM corresponding to the Stokes equation may also be more efficient to carry out than the full Navier-Stokes counterpart. □

3.5 The Consistence of SIIM with Boltzmann Distribution at Equilibrium

The derivation of SIIM is through the explicit calculation of the correlation structure of the linearized hydrodynamic equation. The form of noise is obtained under the assumption that the equilibrium probability distribution of the solution to the linearized equation is Bolzmann distribution. The raises the question whether Boltzmann distribution corresponds to an invariant measure induced by SIIM (not only the linearized equation). The heuristic analysis shows it is reasonable to expect such consistence of SIIM with Boltzmann distribution at equilibrium.

To show this consistence, a finite dimension truncation of SIIM equations (3.18-3.20) is considered, that is, the SIIM equation is projected to a finite dimensional space. Then it is equivalent to an stochastic ODE system. Formally a Fokker-Planck equation can be derived. It will be shown Boltzmann distribution is an equilibrium solution to the Fokker-Planck equation.

Without losing generality, set the smoothing kernel ζ to a delta function and remove unnecessary constants in SIIM. The essence of SIIM is the following stripped equation.

$$\begin{cases} u_t = \triangle u + \nabla p + \nabla E[\phi]\nabla\phi + \sqrt{2}Q^{\frac{1}{2}}\dfrac{dW}{dt}, \\ \nabla\cdot u = 0, \\ \phi_t + u\cdot\nabla\phi = 0, \end{cases} \tag{3.22}$$

Let Ω be a unit cell of periodic domain. Assume $\{\lambda_k,\, \omega_k(x)\}$ are eigenvalues and eigenfunctions of Stokes operator with periodic boundary condition on Ω. (Similar argument is also applicable to bounded open domain and Stokes operator with zero boundary condition.) Then the noise term

$$Q^{\frac{1}{2}}\frac{dW}{dt} = \sum_k \sqrt{\lambda_k}\frac{d\beta_k}{dt}\cdot\omega_k(x)\ ,$$

where $\{\beta_k\}$ are standard Wiener processes.

Let $\{\nu_k\}$ an orthonormal basis of $L^2(\Omega)$. Then the finite dimensional spaces

$$W_N = span\{\omega_1, \omega_2, \ldots, \omega_N\} \quad \text{and} \quad V_N = span\{\nu_1, \nu_2, \ldots, \nu_N\}$$

will serve the solution space for the truncated finite dimension equation (3.22).

Write $u_N(t,x) = \sum_{k \le N} u_k(t) \cdot \omega_k(x)$, $\phi_N(t) = \sum_{k \le N} \phi_k(t) \cdot \nu_k(x)$. Construct the following stochastic ODE system,

$$\begin{cases} u_k' = -\lambda_k u_k + \displaystyle\int_\Omega (\Lambda_N \nabla E[\phi_N]) \nabla \phi_N \cdot \omega_k(x) dx + \sqrt{2\lambda_k} \frac{d\beta_k}{dt} \\ \phi_k' = - \displaystyle\int_\Omega u_N \nabla \phi_N \cdot \nu_k \, dx \, . \end{cases} \tag{3.23}$$

where $k \le N$ and Λ_N is the L^2 projection to space V_N. This construction has the same spirit as the modified Galerkin method in Chapter 2. The stochastic ODE system can be regarded as a finite dimension approximation to the stochastic PDE (3.22). It is easy to check when the noise is removed from the resulting finite dimensional system, the following dissipative energy law holds

$$\frac{d}{dt}\left(\frac{1}{2}\|u_N(t,x)\|^2_{L^2(\Omega)} + E[\phi_N(t,x)]\right) = -\|\nabla u_N\|^2_{L^2(\Omega)} \, . \tag{3.24}$$

The corresponding Fokker-Planck equation of probability density function

$\eta(\{u_k\},\{\phi_k\})$ is

$$\eta_t + \sum_{k\le N} \nabla_{u_k}((-\lambda_k u_k + l_k)\cdot\eta) + \sum_{k\le N} \nabla_{\phi_k}(-h_k\cdot\eta) = \sum_{k\le N} \lambda_k \eta_{u_k u_k}$$

where $l_k = \int_\Omega (\Lambda_N \nabla E[\phi_N])\nabla\phi_N \omega_k(x)\,dx$, and $h_k = \int_\Omega u_N \nabla\phi_N \nu_k\,dx$. Thus it is left to verify that the Bolztmann distribution

$$\eta_0(\{u_k\},\{\phi_k\}) = \frac{1}{Z}\exp\left\{-\left(\frac{1}{2}\sum_{k\le N} u_k^2 + E[\sum_{k\le N}\phi_k\nu_k(x)]\right)\right\}$$

is a solution to

$$\sum_{k\le N} \nabla_{u_k}((-\lambda_k u_k + l_k)\cdot\eta) + \sum_{k\le N} \nabla_{\phi_k}(-h_k\cdot\eta) = \sum_{k\le N} \lambda_k \cdot \eta_{u_k u_k}\ .$$

Proceed with the calculation term by term

- $\nabla_{u_k}((-\lambda_k u_k + l_k)\cdot\eta_0) = -\lambda_k\eta_0 + (-\lambda_k u_k + l_k)\cdot\partial_{u_k}\eta_0$.

- $\nabla_{\phi_k}(-h_k\cdot\eta_0) = -\partial_{\phi_k} h_k\cdot\eta_0 - h_k\cdot\partial_{\phi_k}\eta_0$.

- $\lambda_k\eta_{u_k u_k} = -\lambda_k(\eta_0 + u_k\cdot\partial_{u_k}\eta_0)$.

After the simplification, it is sufficient to verify

$$\sum_{k\le N} \left(l_k\cdot\partial_{u_k}\eta_0 - \partial_{\phi_k} h_k\cdot\eta_0 - h_k\cdot\partial_{\phi_k}\eta_0\right) = 0\ . \qquad (3.25)$$

Note that

- $$\partial_{\phi_k} h_k = \partial_{\phi_k}\int_\Omega u_N \nabla(\sum_{k\le N}\phi_k\nu_k)\cdot\nu_k\,dx = \int_\Omega u_N\nabla\nu_k\nu_k\,dx = 0\ .$$

- $$\sum_{k\le N} l_k\cdot\partial_{u_k}\eta_0 = -\left(\sum_{k\le N} l_k u_k\right)\cdot\eta_0 = -\sum_{k\le N}\left(\int_\Omega (\Lambda_N\nabla E[\phi_N])\nabla\phi_N u_N\,dx\right)\cdot\eta_0\ .$$

- $$\begin{aligned}\sum_{k\le N} h_k\cdot\partial_{\phi_k}\eta_0 &= -\left(\sum_{k\le N}\int_\Omega (u_N\cdot\nabla\phi_N)\nu_k(x)\,dx\cdot\int_\Omega \nabla E[\phi_N]\nu_k\,dx\right)\cdot\eta_0\\ &= -\left(\int_\Omega (\Lambda_N\nabla E[\phi_N])\nabla\phi_N u_N\,dx\right)\cdot\eta_0\end{aligned}$$

Then equation (3.25) is verified.

Since Boltzmann distribution is a probability density function of an invariant measure induced by every finite dimension approximate equation. It is reasonable to expect that such property remains true as the space dimension $N\to\infty$. This work will be put to future exploration.

Another related question is whether probability measure induced by the SIIM will converge to the invariant measure corresponding to Boltzmann distribution when SIIM starts at a given initial value. Such problem of similar stochastic ODEs has been studied in [59]. An archetypal dynamics often discussed is the following Langevin equation,

$$\begin{cases}\dfrac{dp}{dt} = -\gamma\,p - F'(q) + \sqrt{2\gamma}\dfrac{dW}{dt}\ ,\\ \dfrac{dq}{dt} = p\end{cases} \tag{3.26}$$

where $p\,,q\in\mathbb{R}$, W is a standard Brownian motion, and γ is a positive constant. The equation represents a randomly perturbed dissipative Hamiltonian system with p being the momentum and q being the displacement.

This system is similar to the truncated finite dimension equation (3.23) in the following sense,

1. The random noise is only incorporated in the momentum equation, and the other equation represents a transport.

2. When the noise $\sqrt{2\gamma}\frac{dW}{dt}$ is removed from (3.26), the deterministic equation has the dissipative energy law,

$$\frac{d}{dt}\left(\frac{1}{2}p^2 + F(q)\right) = -\gamma\, p^2 \tag{3.27}$$

   which is similar to (3.24). And the term $-\gamma p$ plays the role of $-\lambda_k u_k$ in (3.23).

3. There is a known invariant measure for (3.26) with Boltzmann distribution

$$\frac{1}{Z}\exp\{-(\frac{1}{2}p^2 + F(q))\}\ ,$$

   as its probability density.

The sufficient conditions of convergence of the probability measure to the invariant measure are minorization condition and the existence of Lyapunov function (see Theorem 2.5 in [59]). The Lyapunov function $V(p,q)$ satisfies that $V(p,q)$ goes to infinity as $p \to \infty$, $q \to \infty$, and

$$\mathbb{E}[V(p(t),q(t))|\mathcal{F}_s] \leq \alpha V(p(s),q(s)) + \beta$$

with $0 < \alpha < 1$ and $\beta \geq 0$.

It is possible to construct the Lyapunov function with desired property for certain types of energy. For instance, consider $E[\phi] = \int \frac{1}{2}|\nabla\phi|^2\,dx$. The total energy is a natural Lyapunov function for the truncated finite dimensional system (3.23) with a given initial value $\phi_N(0,x) = \phi_0(x) \in V_N$.

Define Lyapunov function

$$V(u_N,\phi_N) = \frac{1}{2}\|u_N\|^2_{L^2} + \frac{1}{2}\|\nabla\phi_N\|^2_{L^2}\ .$$

By straightforward computation,

$$d\,V(u_N(t),\phi_N(t)) = -\|\nabla u_N\|^2_{L^2}\,dt + (\sum_{k\leq N}\lambda_k)dt + \text{martingale}\ .$$

Then there exist some positive constants C_1 and C_2,

$$\begin{aligned}\frac{d}{dt}\mathbb{E}(V(u_N,\phi_N)) &= -\mathbb{E}(\|\nabla u_N\|^2_{L^2}) + \sum_{k\leq N}\lambda_k \\ &\leq -C_1\cdot\mathbb{E}(V(u_N,\phi_N)) + C_1\cdot\mathbb{E}(\frac{1}{2}\|\nabla\phi_N\|^2_{L^2}) + \cdot C_2\end{aligned}$$

In finite dimensional space, $\|\nabla\phi_N\|^2_{L^2} \leq C_3\|\phi_N\|^2_{L^2}$ for some constant C_3.

Note that

$$\begin{aligned}
\frac{d}{dt}\int_\Omega |\phi_N|^2\,dx &= 2\sum_{k\le N}\phi_k(t)\cdot\phi_k'(t)\\
&= -2\sum_{k\le N}\phi_k\cdot\int_\Omega u_N\cdot\nabla\phi_N\,\nu_k\,dx\\
&= -2\int_\Omega u_N\cdot\nabla\frac{1}{2}|\phi_N|^2dx\\
&= 0\,.
\end{aligned}$$

Hence, $\|\phi_N\|_{L^2}^2 = \|\phi_0\|_{L^2}^2$, which implies $\|\nabla\phi_N\|_{L^2}^2 \le C_3\|\phi_0\|_{L^2}^2$. Then for some positive constant C_4

$$\frac{d}{dt}\mathbb{E}(V(u_N,\phi_N)) \le -C_1\cdot\mathbb{E}(V(u_N,\phi_N)) + C_4\,.$$

Therefore,

$$\mathbb{E}(V(u_N(t),\phi_N(t))|\mathcal{F}_s) \le e^{-C_1(t-s)}V(u_N(s),\phi_N(s)) + \frac{C_4}{C_1}(1-e^{-C_1(t-s)})\,.$$

Then it is reasonable to expect the probability measure induced by the system converges to the invariant measure corresponding to Boltzmann distribution, though the sufficient condition is only partially checked. Also note that the inverse inequality $\|\nabla\phi_N\|_{L^2}^2 \le C_3\|\phi_N\|_{L^2}^2$ cannot be extended to infinite dimension case. The rigorous discussion will be considered in future work.

3.6 Stochastic Implicit Interface Model with a Quasi-Steady Flow

Continuing with the discussion of SIIM, in this section SIIM with a quasi-steady flow will be considered. Without the loss of generality, set the smoothing kernel ζ to the delta function. For convenience, let A represent the Stokes operator. Then the SIIM equation is rewritten as

$$\begin{cases} u_t = -Au + \nabla E[\phi]\nabla\phi + \sqrt{2}A^{\frac{1}{2}}\dfrac{dW}{dt} \ , \\ \nabla u = 0 \ , \\ \phi_t + u \cdot \nabla\phi = 0 \ . \end{cases} \tag{3.28}$$

To consider the SIIM with a quasi-steady flow, u_t is dropped from the momentum equation. The resultant equation is a steady Stokes equation coupled with the transport equation of implicit interface.

$$\begin{cases} 0 = -Au + \nabla E[\phi]\nabla\phi + \sqrt{2}A^{\frac{1}{2}}\dfrac{dW}{dt} \ , \\ \nabla u = 0 \ , \\ \phi_t + u \cdot \nabla\phi = 0 \ . \end{cases} \tag{3.29}$$

Physically, this means fluctuation is only considered on time scales on which the inertial term can be neglected in fluid momentum equation. There is relevant discussion on fluid-vesicle interaction with fluctuation effect in [76], in which random force appears as stress in Stokes equation. But the model is simplified such that only random force on the vesicle accounts for the motion of vesicle and random force elsewhere is neglected.

Formally, one can solve the velocity field from the steady Stokes equation, and substitute into the transport equation of ϕ, i.e.

$$u = A^{-1}[\nabla E[\phi]\nabla\phi] + \sqrt{2}A^{-\frac{1}{2}}\frac{dW}{dt} ,$$

$$\phi_t = -A^{-1}[\nabla E[\phi]\nabla\phi]\cdot\nabla\phi + \nabla\phi\cdot\sqrt{2}A^{-\frac{1}{2}}\frac{d\widetilde{W}}{dt} , \tag{3.30}$$

where $\frac{d\widetilde{W}}{dt} = -\frac{dW}{dt}$. Without causing any confusing, $\frac{d\widetilde{W}}{dt}$ will be simply written as $\frac{dW}{dt}$. First look at the deterministic part,

$$\phi_t = -A^{-1}[\nabla E[\phi]\nabla\phi]\cdot\nabla\phi ,$$

which is a dissipative dynamics, in fact,

$$\frac{d}{dt}E[\phi] = -\int A^{-\frac{1}{2}}[\nabla E[\phi]\nabla\phi]\cdot A^{-\frac{1}{2}}[\nabla E[\phi]\nabla\phi]\,dx \le 0 . \tag{3.31}$$

For a better understanding, the infinite dimensional system (3.30) is projected to the finite dimensional space as in the previous section. Let $\{\omega_n\}$ be the normalized eigenfunctions of Stokes operator A, and $\{\nu_n\}$ be an orthonormal basis of $L^2(\Omega)$ space. Define finite dimensional spaces

$$W_N = \mathrm{span}\{\omega_1,\omega_2,\ldots,\omega_N\} \quad \text{and} \quad V_N = \mathrm{span}\{\nu_1,\nu_2,\ldots,\nu_N\} .$$

Construct the approximate equation in finite dimensional space V_N as,

$$\phi_t = \Lambda_N[-A^{-1}[(\Lambda_N\nabla E[\phi])\,\nabla\phi]\cdot\nabla\phi + \sqrt{2}\nabla\phi\cdot A^{-\frac{1}{2}}\frac{dW}{dt}] . \tag{3.32}$$

Λ_N represents the L^2 projection to V_N. ϕ is restricted to V_N, thus $\phi = \sum_{k\le N}\phi_k\nu_k(x)$. ϕ is then identified with vector $(\phi_1,\phi_2,\ldots,\phi_N)^T$. And $\frac{dW}{dt} = \sum_{k\le N}\frac{dW_k}{dt}\cdot\omega_k(x)$.

In V_N, the approximate equation is equivalent to a system of ODEs,

$$\int_\Omega \phi_t \cdot \nu_s \, dx = -\int_\Omega A^{-1}(\Lambda_N \nabla E[\phi] \cdot \nabla \phi) \nabla \phi \cdot \nu_s \, dx + \sqrt{2} \int_\Omega \nabla \phi \, A^{-\frac{1}{2}} \frac{dW}{dt} \cdot v_s \, dx \ , \ \forall s \leq N$$

$$\begin{aligned}
&\int_\Omega \nabla \phi \, A^{-\frac{1}{2}} \frac{dW}{dt} \cdot v_s \, dx \\
&\quad = \int_\Omega \left(\sum_l \phi_l \nabla \nu_l \right) \cdot \left(\sum_k \frac{1}{\sqrt{\lambda_k}} \omega_k \frac{dW_k}{dt} \right) \cdot v_s \, dx \\
&\quad = \sum_k \left(\sum_l \frac{\phi_l}{\sqrt{\lambda_k}} b_{k,l,s} \right) \cdot \frac{dW_k}{dt} \\
&\quad = \sum_k L_{sk} \cdot \frac{dW_k}{dt} \\
&\quad = L \cdot \frac{dW}{dt} \ ,
\end{aligned}$$

where $b_{k,l,s} = \int_\Omega \omega_k \cdot \nabla \nu_l \cdot \nu_s \, dx$, and $L_{sk} = \sum_l \frac{\phi_l}{\sqrt{\lambda_k}} b_{k,l,s}$. Similarly,

$$\int_\Omega A^{-1}(\Lambda_N \nabla E[\phi] \cdot \nabla \phi) \nabla \phi \cdot \nu_s \, dx = \sum_i \sum_k L_{sk} L_{ik} \frac{\partial E[\phi]}{\partial \phi_i} = L L^T \nabla_\phi E[\phi] \ ,$$

Therefore,

$$\phi_t = -L L^T \nabla_\phi E[\phi] + \sqrt{2} L \cdot \frac{dW}{dt} \ . \tag{3.33}$$

It turns out if the stochastic integral $L \cdot \frac{dW}{dt}$ is interpreted as Stratonovich integral[26, 64] $L \circ \frac{dW}{dt}$, Boltzmann distribution

$$\eta_0(\phi) = \frac{1}{Z} e^{-E[\phi]}$$

is an equilibrium solution to the Fokker-Planck equation induced by (3.33). The Stochastic ODE (3.33) in Stratonovich sense written componentwise is equivalent to

$$\dot{\phi}_s = -L_{sk}L_{ik}\nabla_i E[\phi] + \nabla_i L_{sk} \cdot L_{ik} + \sqrt{2}L_{sk}\frac{dW_k}{dt} \text{ ,for } s \le N$$

in Ito sense, where ∇_i means ∂_{ϕ_i}, and the summation over index i, k is omitted for a cleaner notation. The corresponding Fokker-Planck equation is

$$\eta_t + \nabla_s(-L_{sk}L_{ik}\nabla_i E[\phi]\eta) + \nabla_s(\nabla_i L_{sk} \cdot L_{ik}\eta) = \nabla_s\nabla_i(L_{sk}L_{ik}\eta) \ .$$

Again there is implied summation over index s, k, i. The same notation will be used later in this section without further mention. To verify Boltzmann distribution η_0 as the equilibrium distribution, it is sufficient to check

$$\nabla_s(-L_{sk}L_{ik}\nabla_i E[\phi]\eta_0) + \nabla_s(\nabla_i L_{sk} \cdot L_{ik}\eta_0) = \nabla_s\nabla_i(L_{sk}L_{ik}\eta_0) \ . \tag{3.34}$$

By straightforward calculation,

$$\nabla_s\nabla_i(L_{sk}L_{ik}\eta_0) = \nabla_s(\nabla_i L_{sk} \cdot L_{ik}\eta_0 + L_{sk} \cdot \nabla_i L_{ik}\eta_0 + L_{sk}L_{ik}\nabla_i\eta_0)$$

Note that

$$\begin{aligned} \nabla_i L_{ik} &= \frac{1}{\sqrt{\lambda_k}} b_{k,i,i} = 0 \\ L_{sk}L_{ik}\nabla_i\eta_0 &= -L_{sk}L_{ik}\nabla_i E[\phi]\eta_0 \ . \end{aligned}$$

Then (3.34) is verified. To highlight the result, the discussion is wrapped up as the following proposition.

Proposition 3.5 (SIIM with Quasi-Steady Flow)**.** *When a quasi-steady flow considered, SIIM is reduced to*

$$\phi_t = -A^{-1}[\nabla E[\phi]\nabla\phi]\cdot\nabla\phi + \nabla\phi\cdot\sqrt{2}A^{-\frac{1}{2}}\frac{dW}{dt}\ ,$$

Moreover, if the above stochastic PDE is understood in Stratonovich sense, Boltzmann distribution is the probability density function of an invariant probability measure induced by the finite dimensional system (3.33) .

Similar results can be derived for stochastic immersed boundary method. Drop u_t in stochastic immersed boundary method equation (3.6),

$$\begin{cases} 0 = -Au + \sum_i (-\nabla V(X)\zeta_r(x-X_i)) + \sqrt{2}A^{\frac{1}{2}}\frac{dW}{dt}\ , \\ \nabla u = 0\ , \\ \dot{X}_k = \int_\Omega u(t,x)\zeta_r(x-X_k)\,dx\ . \end{cases} \tag{3.35}$$

Solve u from the steady Stokes equation, and substitute into the transport equation of particles $\{X_s\}$, then

$$\dot{X}_s = -\sum_i \int_\Omega A^{-1}[\nabla_i V(X)\zeta_r(x-X_i)]\zeta_r(x-X_s)\,dx + \sqrt{2}\int_\Omega A^{-\frac{1}{2}}\frac{dW}{dt}\cdot\zeta_r(x-X_s)\,dx\ . \tag{3.36}$$

Follow the discussion of implicit interface model above,

$$\begin{aligned} &\int_\Omega A^{-\frac{1}{2}}\frac{dW}{dt}\cdot\zeta_r(x-X_s)\,dx \\ &\qquad = \sum_l \frac{1}{\sqrt{\lambda_l}}\int_\Omega \omega_l(x)\zeta_r(x-X_s)\,dx\cdot\frac{dW_l}{dt} \\ &\qquad = \sum_l M_{sl}\frac{dW_l}{dt}\ , \end{aligned}$$

where $M_{sl} = \frac{1}{\sqrt{\lambda_l}} \int_\Omega \omega_l(x) \zeta_r(x - X_s)$. And,

$$-\sum_i \int_\Omega A^{-1}[\nabla_i V(X) \zeta_r(x - X_i)] \zeta_r(x - X_k)\, dx$$
$$= -\sum_l \sum_i M_{sl} M_{il}^T \nabla_i V \ .$$

Therefore,

$$\dot{X} = -MM^T \nabla V(X) + \sqrt{2} M \frac{dW}{dt} \ . \tag{3.37}$$

If (3.37) is understood in Stratonovich sense, the equivalent equation interpreted in Ito sense is written componentwise as

$$\dot{X}_s = -M_{sl} M_{il}^T \cdot \nabla_i V(X) + \nabla_i M_{sl} \cdot M_{il} + \sqrt{2} M_{sl} \frac{dW_l}{dt} \ .$$

The induced Fokker-Planck equation is

$$\eta_t + \nabla_s \cdot (-M_{sl} M_{il}^T \nabla_i V \eta) + \nabla_s \cdot (\nabla_i M_{sl} \cdot M_{il} \eta) = \nabla_s \cdot \left(\nabla_i \cdot (M_{sl} M_{il}^T \eta) \right) \ .$$

To verify Boltzmann distribution

$$\eta_0 = \frac{1}{Z} e^{-V(X)}$$

as an equilibrium solution to the Fokker-Planck equation, it is sufficient to verify,

$$\nabla_s \cdot (-M_{sl} M_{il}^T \nabla_i V \eta_0) + \nabla_s \cdot (\nabla_i M_{sl} \cdot M_{il} \eta_0) = \nabla_s \cdot \left(\nabla_i \cdot (M_{sl} M_{il}^T \eta_0) \right) \ .$$

Direct calculation shows,

$$\nabla_s \cdot (\nabla_i \cdot (M_{sl} M_{il}^T \eta_0)) = \nabla_s \cdot (\nabla_i M_{sl} M_{il}^T \eta_0 + M_{sl} \nabla_i \cdot M_{il}^T \eta + M_{sl} M_{il}^T \nabla_i \eta_0) \ .$$

Note that,

$$\nabla_i \cdot M_{il} = \frac{1}{\sqrt{\lambda_l}} \nabla_i \cdot \int_\Omega \omega_l(x) \zeta_r(x - X_i)\, dx = 0 \ ,$$

$$M_{sl} M_{il}^T \nabla_i \eta_0 = -M_{sl} M_{il}^T \nabla_i V(X) \eta_0 \ .$$

Then Boltzmann distribution indeed is an equilibrium solution to the Fokker-Planck equation.

It is worth pointing on a 2D periodic domain, the eigenfunctions of Stokes operator could be expressed in terms of Fourier modes. And Stratonovich interpretation of (3.37) coincides with its Ito interpretation. Then eigenfunctions of Stokes operator are $\omega_l(x) = \frac{l^\perp}{|l|} e^{i2\pi l x}$ with eigenvalues $4\pi^2 |l|^2$, where $l = (l_1, l_2)^T$ and $l^\perp = (-l_2, l_1)^T$. In fact the extra term $\sum_{i,l} \nabla_i M_{sl} \cdot M_{i\ -l}$ due to Stratonovich interpretation of stochastic integral is 0.

$$\begin{aligned}
&\sum_{i,l} \nabla_i M_{sl} \cdot M_{i\ -l} \\
&\quad = \sum_{i,l} \nabla_i \Big(\frac{1}{2\pi |l|} \int_\Omega \omega_l(x) \zeta_r(x - X_s)\, dx \Big) \cdot \frac{1}{2\pi |l|} \int_\Omega \omega_{-l}(x) \zeta_r(x - X_s)\, dx \\
&\quad = \sum_{l} \nabla_s \Big(\frac{1}{2\pi |l|} \int_\Omega \omega_l(x) \zeta_r(x - X_s)\, dx \Big) \cdot \frac{1}{2\pi |l|} \int_\Omega \omega_{-l}(x) \zeta_r(x - X_s)\, dx
\end{aligned}$$

$$\begin{aligned}
&\nabla_s \left(\int_\Omega \omega_l(x) \zeta_r(x - X_s)\, dx \right) \cdot \int_\Omega \omega_{-l}(x) \zeta_r(x - X_s)\, dx \\
&\quad = \frac{i2\pi}{|l|} l^\perp \cdot l^T \int_\Omega e^{i2\pi l (x - X_s)} \zeta_r(x)\, dx \cdot \frac{(-l)^\perp}{|l|} \int_\Omega e^{-i2\pi l (x - X_s)} \zeta_r(x)\, dx
\end{aligned}$$

$l^T \cdot (-l)^{\perp} = 0$ implies

$$\sum_{i,l} \nabla_i M_{sl} \cdot M_{i\ -l} = 0 \ .$$

3.7 Summary of Stochastic Implicit Interface Model

In this Chapter, the stochastic implicit interface model (SIIM) is discussed in detail. SIIM incorporates the random noise into deterministic hydrodynamic equations to capture the thermal fluctuation.

The derivation of SIIM is based on stochastic immersed boundary method with implicit interface representation. By computing the correlation structure of the linearized hydrodynamic equation, and with the assumption that Boltzmann distribution is the equilibrium distribution, the proper form of noise is derived in Fourier space. And the noise should only appear in the fluid momentum equation and is independent of the choice of interfacial energy functional, and the steady state around which the linearized equation is derived. In fact, the noise is solely determined by the dissipative character of the deterministic hydrodynamic equation. Such dissipative character is due to the viscosity (or Stokes operator). Provided the contribution of noise and the nonlinear nature of the derived equation, a mollified velocity field is considered in the transport equation of the implicit interface. Moreover, in low Reynolds number regime, the full Navier-Stokes is simplified to linear Stokes equation. The resulting equations (3.18–3.20) are referred to as stochastic implicit interface model (SIIM).

Although the noise is derived from a linearized dynamics, heuristic analysis has verified that Boltzmann distribution in fact corresponds to an invariant probability measure induced by the the nonlinear stochastic hydrodynamics proposed.

Finally, SIIM with a quasi-steady flow is discussed. When inertial is neglected in the fluid momentum equation, the original stochastic hydrodynamic equation is reduced to a dissipative Langevin type equation of phase field (or level set) function with multiplicative noise. It has been discovered that if such stochastic equation is interpreted in Stratonovich sense, Boltzmann distribution corresponds to an invariant probability measure as well.

Chapter 4

Analysis of the Stochastic Implicit Interface Model

In the previous chapter, a stochastic implicit interface model is presented in Proposition 3.3 and 3.4 to capture the fluctuation in fluid-structure interaction. The SIIM model has the advantage that the form of equation is independent of the choice of energy functional of phase field (or level set) function. In this chapter, the well-posedness of SIIM and its deterministic counterpart will be established for some types of energy for illustration, though the technique used in the proof is also applicable for other forms of energy. This matter will be commented later in this chapter.

4.1 Analysis of the Deterministic Model

The deterministic model will be rigorously analyzed first. The approach is again based on Galerkin approximation. And the key is to derive proper a priori estimates of solutions. Such estimates depend on the nonlinear force density $\nabla E[\phi]\nabla\phi$ and the regularity of kernel ζ. For convenience, the notation $f_\zeta \triangleq f * \zeta$ is used to represent the convolution when there is no ambiguity.

To illustrate the idea, an energy with a relatively simpler form is chosen, that is,

$$E[\phi] = \int_\Omega \frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{4\epsilon}(\phi^2-1)^2 dx \; . \tag{4.1}$$

Such an energy is often used to model the surface tension of immersed structure. The corresponding force density is

$$(\nabla E[\phi]\nabla\phi) * \zeta = (-\epsilon\triangle\phi\nabla\phi + \frac{1}{\epsilon}(\phi^3-\phi)\nabla\phi) * \zeta \; .$$

The second term in force density

$$(\frac{1}{\epsilon}(\phi^3-\phi)\nabla\phi) * \zeta = \nabla\left((\frac{1}{4\epsilon}(\phi^2-1)^2) * \zeta\right)$$

is a gradient term, thus included in pressure,

$$\begin{cases} u_t = \mu\triangle u - (\epsilon\triangle\phi\nabla\phi) * \zeta + \nabla p \; , \\ \nabla\cdot u = 0 \; , \\ \phi_t + (u * \zeta)\cdot\nabla\phi = 0 \; . \end{cases} \tag{4.2}$$

Moreover, for any polynomial $f = f(x)$,

$$\begin{aligned}\frac{d}{dt}\int_\Omega f(\phi)\,dx &= \int_\Omega f'(\phi)\partial_t\phi\,dx \\ &= -\int_\Omega f'(\phi)\nabla\phi\cdot(u*\zeta)\,dx \\ &= -\int_\Omega \nabla f(\phi)\cdot(u*\zeta)\,dx \\ &= 0\end{aligned}$$

Particularly,

$$\frac{d}{dt}\int_\Omega \frac{1}{4\epsilon}(\phi^2-1)^2\,dx = 0\ .$$

Thus, the energy $E = E[\phi]$ is effectively controlled as long as proper estimates on the Dirichlet integral type energy

$$\frac{\epsilon}{2}\int_\Omega |\nabla\phi|^2\,dx \tag{4.3}$$

can be derived from the model equations.

Before the actual proof, the main analytical result concerning the well-posedness of equation (4.2) is stated here first.

Theorem 4.1 (Well-posedness theorem for a deterministic model)**.** *Let Ω be a unit cell of periodic domain in $\mathbb{R}^N$ with $N \leq 3$. Under the conditions that the kernel $\zeta \in C^2$ and the initial condition $u_0 \in H_d(\Omega)$, $\phi_0 \in H^2(\Omega)$, there exists a unique pair of functions u and ϕ with*

1. *$u \in L^2(0,T;H_d(\Omega))$ and $\partial_t u \in L^2(0,T;H_d^{-1}(\Omega))$,*

2. $\phi \in L^2(0,T;H^2(\Omega))$ *and* $\partial_t\phi \in L^2(0,T;L^2(\Omega))$,

such that (u,ϕ) *is a weak solution to the system (4.2) with the initial condition* $u(0,x) = u_0(x)$ *and* $\phi(0,x) = \phi_0(x)$.

In the above theorem,

1. $H_d(\Omega)$ is the divergence free subspace of $H^1(\Omega)$ with average 0.

2. And $H_d^{-1}(\Omega)$ is the dual space of $H_d(\Omega)$.

To better organize the proof, several formal estimates on the solution are prepared first, then the theorem is proved by applying the Galerkin approximation.

4.1.1 Formal Estimates on Solution

Several formal estimates for the transport equation and the nonlinear force density in the momentum equation are needed. Here $\|\cdot\|_{L^2}$ and $\|\cdot\|_{L^\infty}$ denote norms in the spatial variables.

Lemma 4.1 (Estimate of transport equation)**.** *Let* $u = u(t,x)$ *be a divergence free velocity field, if* ϕ *is defined by*

$$\begin{cases} \phi_t + u \cdot \nabla\phi = 0\ , \\ \phi(0) = \phi_0(x)\ . \end{cases}$$

Then there exists some constant C *such that,*

1. *for any* $t \in (0,T)$,

$$\|\phi_t(t)\|_{L^2} \le \|u(t)\|_{L^\infty} \cdot \|\nabla\phi(t)\|_{L^2}\,,$$

2. *for* $u \in L^1(0,T;W^{1,\infty}(\Omega))$,

$$\|\nabla\phi(t)\|_{L^2}^2 \le \|\nabla\phi_0\|_{L^2}^2 \exp\left(C\int_0^t \|\nabla u(s)\|_{L^\infty}\,ds\right)\,,$$

3. *for* $u \in L^1(0,T;W^{2,\infty}(\Omega))$,

$$\|\triangle\phi(t)\|_{L^2}^2 \le \|\triangle\phi_0\|_{L^2}^2 \exp\left(C\int_0^t \|\triangle u\|_{L^\infty} + \|\nabla u\|_{L^\infty}\,ds\right)\,.$$

Proof. The first result is obvious. Differentiate $\phi_t + u\cdot\nabla\phi = 0$,

$$\nabla\phi_t + u\cdot\nabla(\nabla\phi) = -\nabla u\cdot\nabla\phi.$$

Then multiply $\nabla\phi$ to the above equation and integrating by parts,

$$\begin{aligned}\frac{d}{dt}\left(\frac{1}{2}\|\nabla\phi\|_{L^2}^2\right) &= -\int_\Omega \nabla u\cdot\nabla\phi\cdot\nabla\phi\,dx\\ &\le C\cdot\|\nabla u\|_{L^\infty}\,\|\nabla\phi\|_{L^2}^2.\end{aligned}$$

Similarly,

$$\triangle\phi_t + u\cdot\nabla\triangle\phi = -\triangle u\cdot\nabla\phi - 2\nabla u\cdot(\nabla\,\nabla\phi),$$

which implies

$$\begin{aligned}\frac{d}{dt}\left(\frac{1}{2}\|\triangle\phi\|_{L^2}^2\right) &= -\int_{\Omega_p} \triangle u\cdot\nabla\phi\cdot\triangle\phi + 2\nabla u\cdot\nabla\nabla\phi\,dx\\ &\le C\cdot(\|\triangle u\|_{L^\infty} + \|\nabla u\|_{L^\infty})\|\triangle\phi\|_{L^2}^2.\end{aligned}$$

Then the Gronwall inequality implies the results 2 and 3 of the lemma. □

In the above and thereafter, The notation C is frequently used to denote a generic positive constant as long as there is no ambiguity.

Lemma 4.2 (Estimate on nonlinear force density)**.** *There exists some constant C,*

$$\|(\triangle\phi\nabla\phi) * \zeta\|_{H^{-1}} \leq C \cdot \|\nabla\phi\|_{L^2}^2 \,.$$

Proof. Note that $\triangle\phi\nabla\phi = \nabla\cdot\tau$, where $\tau = \nabla\phi\otimes\nabla\phi - \frac{1}{2}|\nabla\phi|^2$.

For any test function $\eta \in H_d^1(\Omega)$,

$$\begin{aligned}\left|\int_\Omega (\triangle\phi\nabla\phi) * \zeta \cdot \eta \, dx\right| &= \left|\int_\Omega \nabla\cdot\tau \; \eta_\zeta \, dx\right| \\ &= \left|\int_\Omega \tau\cdot\nabla\eta_\zeta \, dx\right| \\ &\leq \|\nabla\eta_\zeta\|_{L^\infty} \int_\Omega |\tau| \, dx \\ &\leq C\cdot\|\eta\|_{H_d^1}\cdot\|\nabla\phi\|_{L^2}^2 \,.\end{aligned}$$

Then, the conclusion follows. □

4.1.2 Proof of the Well-posedness Theorem

Proof. 1. Let $S_n = span\{\omega_k(x),\, k \leq n\}$, the finite dimensional space spanned by the eigenfunctions of the Stokes operator with periodic boundary condition on the domain Ω. Π_n is the L^2 projection to S_n.

Construct the approximate equation as,

$$\begin{cases} \partial_t u = \mu \triangle u + \Pi_n [(\nabla E[\phi] \cdot \nabla \phi) * \zeta], \\ \partial_t \phi + u_\zeta \cdot \nabla \phi = 0, \\ \nabla \cdot u = 0. \\ u(0,x) = \Pi_n u_0(x), \\ \phi(0,x) = \phi_0(x). \end{cases} \tag{4.4}$$

The velocity field u is naturally restricted in S_n. The divergence-free condition $\nabla \cdot u = 0$ implies $\nabla \cdot (u * \zeta) = 0$ so $u * \zeta$ is also a volume preserving map. Then for the given initial data, ϕ is defined by the transport equation. Moreover, given the regularity on ϕ_0 and using the lemma 4.1, the nonlinear term in the first equation of (4.4) is at least Lipschitz continuous in time. The local solution exists, see [53] for similar discussion. Furthermore,

$$\frac{d}{dt}\left(\frac{1}{2}\|u\|_{L^2}^2 + E[\phi]\right) = -\mu \int_\Omega |\nabla u|^2 dx \,. \tag{4.5}$$

So ,

$$\|u(t)\|_{L^2} \leq \|u(0)\|_{L^2} \,, \quad \forall\, 0 \leq t < \infty \,.$$

It implies the globe existence of $u \in S_n$ and hence the corresponding ϕ.

2. For each S_n, let u_n and ϕ_n be the solution to the system (4.4). By the energy law (4.5), the sequence $\{u_n\}$ is uniformly bounded in $L^\infty(0,T;L^2(\Omega))$ and $L^2(0,T;H^1_d(\Omega))$. Next, by the properties of the kernel ζ,

$$\|\nabla u_n * \zeta\|_{L^\infty} \leq C' \|u_n\|_{L^2} \,.$$

Then, according to Lemma 4.1, there exist some constants C, C' such that

$$\begin{aligned}\|\nabla\phi_n(t)\|_{L^2}^2 &\leq \|\nabla\phi_0\|_{L^2}^2 \exp\left(C\int_0^t \|\nabla(u_n * \zeta)(s)\|_{L^\infty}\, ds\right) \\ &\leq \|\nabla\phi_0\|_{L^2}^2 \exp\left(CC'\int_0^t \|u_n(s)\|_{L^2}\, ds\right).\end{aligned}$$

So, ϕ_n is uniformly bounded in $L^\infty(0,T;H^1(\Omega))$. By repeating a similar argument, ϕ_n is also uniformly bounded in $L^\infty(0,T;H^2(\Omega))$. This in turn implies that $\partial_t\phi_n$ is uniformly bounded in $L^\infty(0,T;L^2(\Omega))$.

Following from Lemma 4.2, $(\triangle\phi\nabla\phi)*\zeta$ is uniformly bounded in $L^\infty(0,T;H_d^{-1}(\Omega))$. So, $\partial_t u_n$ is uniformly bounded in $L^2(0,T;H_d^{-1}(\Omega))$.

Consequently by the Aubin-Lions compactness result, there exists a subsequence $\{(u_{n_k},\phi_{n_k})\}$ and (u,ϕ) such that

- $u_{n_k} \rightharpoonup u$ weakly in $L^2(0,T;H^1(\Omega))$;
- $u_{n_k} \to u$ strongly in $L^2(0,T;L^p(\Omega))$, for $1 \leq p < 6$;
- $\phi_{n_k} \rightharpoonup \phi$ weakly in $L^2(0,T;H^2(\Omega))$;
- $\phi_{n_k} \to \phi$ strongly in $L^2(0,T;W^{1,p}(\Omega))$, for $1 \leq p < 6$.

3. Let $\alpha = \alpha(t) \in C^1([0,T])$, for any test functions $\nu = \nu(x) \in S_n$ and

$\eta = \eta(x) \in L^2(\Omega)$,

$$\int_0^T \alpha < \frac{\partial}{\partial t} u_{n_k} \,,\, \nu > dt = -\int_0^T \alpha < \nabla u_{n_k} \,,\, \nabla \nu > \, dt$$
$$-\epsilon \int_0^T \int_\Omega \alpha \triangle \phi_{n_k} \nabla \phi_{n_k} \, \nu_\zeta \, dx \, dt \;,$$
$$\int_0^T \alpha < \frac{\partial}{\partial t} \phi_{n_k} \,,\, \eta > \, dt = \int_0^T \alpha \int_\Omega (u_{n_k} * \zeta) \, \nabla \phi_{n_k} \, \eta \, dx \, dt \;.$$

Let $n_k \to \infty$, we get

$$\int_\Omega u_t \nu \, dx = -\mu \int_\Omega \nabla u \cdot \nabla \nu dx - \epsilon \int_\Omega (\triangle \phi \nabla \phi) * \zeta \cdot \nu \, dx \;,$$
$$\int_\Omega \phi_t \eta dx + \int_\Omega (u * \zeta) \cdot \nabla \phi \, \eta \, dx = 0 \;.$$

Since $\nu = \nu(x)$ is arbitrarily chosen in S_n, by a density argument, the above equations remain valid for any $\nu \in H_d(\Omega)$, and one can also check that the initial condition is satisfied.

4. For uniqueness, assume that there exist two solutions (u_1, ϕ_1) and (u_2, ϕ_2) with the same initial condition. Let $\tilde{u} = u_1 - u_2$, $\tilde{\phi} = \phi_1 - \phi_2$. Then $\tilde{u}$, $\tilde{\phi}$ satisfy the equation

$$\begin{cases} \tilde{u}_t = \mu \nabla \tilde{u} + \nabla \tilde{p} - \epsilon [(\triangle \tilde{\phi} \nabla \phi_1)_\zeta + (\triangle \phi_2 \nabla \tilde{\phi})_\zeta] \;, \\ \tilde{\phi}_t + \tilde{u}_\zeta \nabla \phi_1 + (u_2 * \zeta) \nabla \tilde{\phi} = 0 \;. \end{cases} \tag{4.6}$$

Multiply $\tilde{u}$ to the first equation in (4.6)and $-\epsilon \triangle \tilde{\phi}$ to the second equation, then integrate over the whole domain,

$$\frac{d}{dt} \left(\frac{1}{2} \|\tilde{u}\|_{L^2}^2 + \frac{\epsilon}{2} \|\nabla \tilde{\phi}\|_{L^2}^2 \right) \;\leq\; -\mu \|\nabla \tilde{u}\|_{L^2}^2 - \epsilon \int_\Omega \triangle \phi_2 \nabla \tilde{\phi} \tilde{u}_\zeta \, dx$$
$$+\epsilon \int_\Omega \nabla \tilde{\phi} \triangle \tilde{\phi} (u_2 * \zeta) \, dx$$

There exists constant C such that,

$$\begin{aligned}\left|\int_\Omega \triangle\phi_2 \nabla\tilde{\phi}\tilde{u}_\zeta \, dx\right| &\leq \frac{1}{2}\|\nabla\tilde{\phi}\|_{L^2}^2 + \frac{1}{2}\|\triangle\phi_2\|_{L^2}^2\|\tilde{u}_\zeta\|_{L^\infty}^2 \\ &\leq \frac{1}{2}\|\nabla\tilde{\phi}\|_{L^2}^2 + \frac{C}{2}\|\triangle\phi_2\|_{L^2}^2\|\tilde{u}\|_{L^2}^2 \,.\end{aligned}$$

$$\begin{aligned}\left|\int_\Omega \nabla\tilde{\phi}\triangle\tilde{\phi}\,(u_2 * \zeta)\, dx\right| &= \left|\int_\Omega \nabla\cdot\tilde{\tau}\,(u_2 * \zeta)\, dx\right| \\ &\leq \|\nabla(u_2 * \zeta)\|_{L^\infty}\cdot\|\tilde{\tau}\|_{L^2}^2 \\ &\leq C\cdot\|u_2\|_{L^2}\cdot\|\nabla\tilde{\phi}\|_{L^2}^2 \,,\end{aligned}$$

where $\tilde{\tau} = \nabla\tilde{\phi}\otimes\nabla\tilde{\phi} - \frac{1}{2}|\nabla\tilde{\phi}|^2$.

Recall that u_1 and u_2 are uniformly bounded in $L^\infty(0,T;L^2(\Omega))$ and ϕ_1 and ϕ_2 are uniformly bounded in $L^\infty(0,T;H^2(\Omega))$. Then there exists some constant C', such that

$$\frac{d}{dt}\left(\frac{1}{2}\|\nabla\tilde{u}\|_{L^2}^2 + \frac{\epsilon}{2}\|\tilde{\phi}\|_{L^2}^2\right) \leq C'\cdot\left(\frac{1}{2}\|\tilde{u}\|_{L^2}^2 + \frac{\epsilon}{2}\|\nabla\tilde{\phi}\|_{L^2}^2\right) \,.$$

So the Gronwall inequality implies that if the two solutions share the same initial data, then the two solutions remain identical afterwards.

□

Remark 4.1. Through a boot-strapping argument, if the initial conditions are smooth, the solutions discussed in the theorems are actually smooth classical solutions to the coupled systems. □

Remark 4.2. As mentioned, a relatively simple form of the phase field energy corresponding to surface tension is chosen to illustrate the idea of proof but the techniques work for other forms of the phase field or level set energies as well. The main ingredients are: first, the dissipative energy law (4.5) holds independent of the choice of energy. The energy law provides uniform bounds of $\|u(t)\|_{L^2}^2$ in time. Secondly, by differentiating the transport equation of ϕ in space, the evolution equations of the spatial derivatives of ϕ are derived. And such derivatives are bounded by initial data and the fluid velocity field (Lemma 4.1). For different energy, there is different nonlinearity in $\nabla E[\phi]\nabla\phi$. As long as ζ is smooth enough, it is always possible to differentiate the transport equation as needed in order to obtain the bounds on the high order spacial derivatives of ϕ. Finally, all those bounds provide compactness, then pass to the limit to get the existence of solution. $\square$

Remark 4.3. The well-posedness result given here for the deterministic case is new as many other existence results in the literature on the coupled phase field Navier Stokes equations have been proved in the cases where extra dampings were applied to the transport equation, for instance the analysis of PFNS equation in Chapter 2, which would lead to stronger control on the nonlinear force density term. $\square$

4.2 Analysis of SIIM

As discussed in previous chapter, the stochastic implicit interface model (SIIM) derived in Proposition 3.4 could be rewritten in a more abstract form,

$$\begin{cases} u_t = \mu\triangle u + \nabla p + (\nabla E[\phi]\nabla\phi) * \zeta + \sigma Q^{\frac{1}{2}}\dfrac{dW}{dt}, \\ \nabla\cdot u = 0, \\ \phi_t + (u*\zeta)\nabla\phi = 0, \end{cases} \tag{4.7}$$

where μ is the viscosity and σ is a small constant.

If the domain is the unit cell of periodic domain, then let $e_k(x) = e^{i2\pi kx}$. Collect all the constants such as Boltzmann constant K_b, temperature T into σ, then

$$Q^{\frac{1}{2}}\frac{dW}{dt} = \sum_k |k|\frac{d\beta_k}{dt}\cdot e_k(x) \ ,$$

and $\{\beta_k\}$ are the standard complex Wiener processes. The subsequent discussion will focus on this special case.

Denote the semigroup generated by $\mu\triangle$ operator by $S(t)$. Let P be the L^2 projection to the divergence free space. Formally the first equation in (4.7) is rewritten as an integral equation,

$$u(t) = S(t)u_0 + \int_0^t S(t-s)P(\nabla E[\phi]\nabla\phi)_\zeta ds + \sigma\int_0^t S(t-s)PQ^{\frac{1}{2}}dW(s) \ .$$

Let

$$G(t) \triangleq \int_0^t S(t-s)PQ^{\frac{1}{2}}dW(s),$$

and $v(t) = u(t) - \sigma G(t)$. Then,

$$v(t) = S(t)u_0 + \int_0^t S(t-s)P((\nabla E[\phi]\nabla\phi) * \zeta)ds \ ,$$

and

$$v(0) = u(0) \ .$$

That is,

$$\begin{cases} v_t = \mu\triangle v + \nabla p + (\nabla E[\phi]\nabla\phi)_\zeta \ , \\ \nabla \cdot v = 0 \ , \\ \phi_t + (v_\zeta + \sigma G_\zeta)\nabla\phi = 0 \ , \end{cases} \tag{4.8}$$

together with initial condition,

$$\begin{cases} v(0) = u_0(x) \ , \\ \phi(0) = \phi_0(x) \ , \end{cases} \tag{4.9}$$

and periodic boundary condition. The actual analysis is on equation (4.8). The solution to (4.8) is interpreted as a solution to (4.7).

Remark 4.4. $G(t)$ has infinite variance. In fact,

$$\begin{aligned} G(t) &= \int_0^t S(t-s)P\,Q^{\frac{1}{2}}\,dW(s) \\ &= \sum_k \left(P_k \int_0^t e^{-4\pi^2\mu|k|^2(t-s)}|k|\,d\beta_k(s) \right) \cdot e_k(x) \end{aligned}$$

where $P_k = I - \frac{k\otimes k}{|k|^2}$ as used before. So,

$$\begin{aligned}
\mathbb{E}\|G(t)\|_{L^2}^2 &= \sum_k \mathbb{E}\left\| P_k \int_0^t e^{-4\pi^2\mu|k|^2(t-s)}|k|\,d\beta_k(s)\right\|^2 \\
&= \sum_k tr(P_k)\left(\int_0^t e^{-8\pi^2\mu|k|^2(t-s)}|k|^2\,ds\right) \\
&= C\cdot\left(\sum_k\left(1-e^{-8\pi^2\mu|k|^2 t}\right)\right) \\
&= \infty
\end{aligned}$$

However after the mollification, $\mathbb{E}\|G_\zeta(t)\|_{L^2}^2 \le C\cdot\|\zeta\|_{L^2}^2$, thus G_ζ is well defined. $\square$

4.2.1 Some Technical Estimates

First, the following energy law holds

$$\frac{d}{dt}\left(\frac{1}{2}\|v\|_{L^2}^2 + E[\phi]\right) = -\mu\|\nabla v\|_{L^2}^2 - \sigma\int_\Omega \nabla E[\phi]\nabla\phi\, G_\zeta(t)\,dx. \qquad (4.10)$$

In the later discussion, several estimates on G_ζ is required. So a lemma is prepared here first.

Lemma 4.3. *1. If $\zeta\in C^m$, then the Ornstein-Uhlenbeck process $\nabla^\alpha G_\zeta(t)\in C(0,T;L^2(\Omega))$ almost surely for $|\alpha|\le m$, and there exist a constant C such that*

$$\mathbb{E}\|G_\zeta\|_{H^m}^2 \le C\cdot\|\zeta\|_{H^m}^2\ .$$

2. If in addition,

$$\zeta = \zeta_1 * \zeta_2 \in C^{m+1}\,, \quad \textit{for} \quad \zeta_1\in C^m, \zeta_2\in C^1\,, \qquad (4.11)$$

then there exists a constant C that depends on ζ_2, when $|\alpha| \le m$.

$$\|\nabla^\alpha G_\zeta(t)\|_{L^\infty} \le C \cdot \|\nabla^\alpha G_{\zeta_1}\|_{L^2} .$$

Proof. The continuity of the process is the direct consequence of Theorem 1 and its corollary in [38].

$$\begin{aligned}\mathbb{E}\|\nabla^\alpha G_\zeta(t)\|_{L^2}^2 &\le C \cdot \sum_k tr(P_k) \left(\int_0^t e^{-8\pi^2\mu|k|^2(t-s)} |k|^2 \, ds \right) \hat{\zeta}_k^2 \cdot |k|^{2|\alpha|} \\ &\le C\|\nabla^\alpha \zeta\|_{L^2}^2 .\end{aligned}$$

And

$$\begin{aligned}\|\nabla^\alpha G_\zeta(t)\|_{L^\infty} &= \|\nabla^\alpha G_{\zeta_1} * \zeta_2\|_{L^\infty} \\ &\le C\|\nabla^\alpha G_{\zeta_1}\|_{L^2} .\end{aligned}$$

□

4.2.2 Well-posedness of SIIM

Again the analysis focuses on the special case where $E = E[\phi]$ as in (4.1). Similar to the discussion of the deterministic model, the existence of the solution is proved for almost all realization of noise.

Theorem 4.2 (Well-Posedness of Pathwise Solution)**.** *Under the conditions made as before on the initial conditions, the form of the noise, and the additional assumption (4.11) with $m = 2$ on the kernel ζ, for almost every* *realization of noise, there exists a weak solution on time interval* $(0, T)$ *to the system (4.8).*

Proof. 1. Here a sketched proof is provided, because it is similar to the deterministic case. Let

$$W_n \triangleq span\{e_k = e_k(x) : \ |k| \leq n\}$$

be the finite dimensional space spanned by the Fourier modes.

Apply Galerkin approximation and restrict v in the divergence free subspace of W_n, an approximate equation of v is obtained,

$$\partial_t v = \mu \triangle v + P\Lambda_n(-\epsilon \triangle \phi \nabla \phi)_\zeta \ ,$$

where Λ_n is the L^2 projection to W_n and P is the L^2 projection to the divergence-free space. (Note that P commutes with Λ_n).

ϕ is transported via

$$\phi_t + (v_\zeta + \sigma \Lambda_n G_\zeta)\nabla\phi = 0 \ .$$

The energy law says,

$$\frac{1}{2}\frac{d}{dt}\left(\|v\|_{L^2} + \epsilon\|\nabla\phi\|_{L^2}^2\right) = -\mu\|\nabla v\|_{L^2}^2 + \sigma\int_\Omega(\epsilon\triangle\phi\nabla\phi)\cdot P\Lambda_n G_\zeta(t)\,dx. \tag{4.12}$$

Obtaining a priori bounds via energy law is the key to show the existence of solutions. Similar to the proof of the deterministic case, write

$$\triangle\phi\nabla\phi = \nabla\cdot\tau \ ,$$

where $\tau = \nabla\phi\otimes\nabla\phi - \frac{1}{2}|\nabla\phi|^2$. Then,

$$\begin{aligned}
\left|\int_\Omega \triangle\phi\nabla\phi\cdot\Lambda_n G_\zeta dx\right| &= \left|\int_\Omega (\nabla\cdot\tau)\cdot\Lambda_n G_\zeta \, dx\right| \\
&= \left|\int_\Omega \tau\cdot\nabla\Lambda_n G_\zeta \, dx\right| \\
&\leq \|\nabla\Lambda_n G_\zeta\|_{L^\infty}\int_\Omega |\tau| \, dx \\
&\leq C_1\cdot\|\nabla\Lambda_n G_{\zeta_1}\|_{L^2}\|\nabla\phi\|_{L^2}^2 \\
&\leq C_2\cdot\|\nabla G_{\zeta_1}\|_{L^2}\cdot\|\nabla\phi\|_{L^2}^2 \qquad (4.13)
\end{aligned}$$

where C_1, C_2 are two constants.

By Lemma 4.3, $\nabla G_{\zeta_1}\in C(0,T;L^2(\Omega))$ almost surely. There exists a constant C dependent on the realization of the noise, ζ and T, but independent of the W_n, such that

$$\frac{d}{dt}\left(\frac{1}{2}\|v\|_{L^2}^2 + \frac{\epsilon}{2}\|\nabla\phi\|_{L^2}^2\right) \leq -\mu\|\nabla v\|_{L^2}^2 + \sigma\epsilon C\|\nabla\phi\|_{L^2}^2.$$

In each finite dimensional space W_n, an approximate solution v_n and corresponding ϕ_n exist. Then Gronwall inequality implies that there exist some other constant C independent of W_n (but dependent on the realization of noise) such that

$$\frac{1}{2}\|v_n(t)\|_{L^2}^2 + \frac{\epsilon}{2}\|\nabla\phi_n(t)\|_{L^2}^2 \leq e^{Ct}\left(\frac{1}{2}\|v_0\|_{L^2}^2 + \frac{\epsilon}{2}\|\nabla\phi_0\|_{L^2}^2\right)$$

if $0 < t < T$.

Then immediately,

- v_n is uniformly bounded in $L^\infty(0,T;L^2\Omega)$.
- ϕ_n is uniformly bounded in $L^\infty(0,T;H^1(\Omega))$.

By Lemma 4.1,

$$\|\nabla\phi_n(t)\|_{L^2}^2 \leq \|\nabla\phi_0\|_{L^2}^2 \exp\left(C\int_0^t \|\nabla u_n * \zeta(s)\|_{L^\infty} + \sigma\|\nabla\Lambda_n G_\zeta(s)\|_{L^\infty} ds\right).$$

$$\begin{aligned}\|\nabla\Lambda_n G_\zeta(t)\|_{L^\infty} &\leq C\|\nabla\Lambda_n G_{\zeta_1}(t)\|_{L^2}\\ &\leq C\cdot\|\nabla G_{\zeta_1}\|_{L^2}.\end{aligned}$$

Therefore,

- $\nabla\phi_n$ is uniformly bounded in $L^\infty(0,T;L^2(\Omega))$.
- Similarly, $\triangle\phi_n$ is uniformly bounded in $L^\infty(0,T;L^2(\Omega))$.
- u_n is uniformly bounded in $L^2(0,T;H_d^1(\Omega))$.

Using the same argument as in the deterministic case,

- $\partial_t u_n$ is uniformly bounded in $L^2(0,T;H_d^{-1}(\Omega))$.
- $\partial_t\phi_n$ is uniformly bounded in $L^\infty(0,T;L^2(\Omega))$.

The a priori bounds lead to compactness. And passing to the limit recovers the solution. The detail is omitted here.

2. To prove the uniqueness of solution, assume that there exist two solutions (v_1, ϕ_1), (v_2, ϕ_2), which have the same initial data. Let $\tilde{v} = v_1 - v_2$, and $\tilde{\phi} = \phi_1 - \phi_2$. Then $\tilde{v}$ and $\tilde{\phi}$ satisfy the following equation,

$$\begin{cases} \tilde{v}_t = \mu\triangle\tilde{v} + \nabla\tilde{p} - \epsilon[(\triangle\tilde{\phi}\nabla\phi_1)_\zeta + (\triangle\phi_2\nabla\tilde{\phi})_\zeta] \,, \\ \tilde{\phi}_t + \tilde{v}_\zeta\nabla\phi_1 + ((v_2 * \zeta) + \sigma G_\zeta)\nabla\tilde{\phi} = 0 \,. \end{cases} \tag{4.14}$$

The same as the deterministic case, multiply $\tilde{v}$ to the first equation in (4.14), and $-\epsilon\triangle\tilde{\phi}$ to the second equation.

$$\begin{aligned} \frac{d}{dt}\left(\frac{1}{2}\|\tilde{v}\|_{L^2}^2 + \frac{\epsilon}{2}\|\nabla\tilde{\phi}\|_{L^2}^2\right) \;\; \leq \;\; & -\mu\|\nabla\tilde{v}\|_{L^2}^2 - \epsilon\int_\Omega \triangle\phi_2\nabla\tilde{\phi}\tilde{v}_\zeta\, dx \\ & +\epsilon\int_\Omega \nabla\tilde{\phi}\triangle\tilde{\phi}(u_2 * \zeta + \sigma G_\zeta)\, dx \,. \end{aligned}$$

Recall that $\nabla G_{\zeta_1} \in C(0, T; L^2)$. Using the same argument as in the deterministic case, the uniqueness of the pathwise solution is proved.

□

4.2.3 Uniform Bound in Large Probability

In the above proof, a Gronwall inequality is used to control the energy for a particular path, however, no uniform bound on a family of paths is provided. The following theorem asserts indeed for large probability energy stays uniformly bounded for any finite time.

Theorem 4.3. *Under the conditions made as before on the initial conditions, the form of the noise, and the additional assumption (4.11) with*

$m = 2$ on the kernel ζ, there exist two constants C' and C'' such that for σ small,

$$\mathbb{P}\left(\frac{1}{2}\|v(t)\|_{L^2}^2 + \frac{\epsilon}{2}\|\nabla\phi(t)\|_{L^2}^2 \le (\frac{1}{2}\|u_0\|_{L^2}^2 + \frac{\epsilon}{2}\|\nabla\phi_0\|_{L^2}^2)e^{C't}\right) \ge 1 - \sigma^2 \cdot C'' .$$

Proof. Let v_n and ϕ_n be the approximate solution, as in Theorem 4.2. Following from the estimates (4.12) and (4.13),

$$\frac{d}{dt}\left(\frac{1}{2}\|v_n\|_{L^2} + \frac{\epsilon}{2}\|\nabla\phi_n\|_{L^2}^2\right) \le -\mu\|\nabla v_n\|_{L^2}^2 + \sigma\epsilon\, C \cdot \|\nabla G_{\zeta_1}\|_{L^2}\|\nabla\phi_n\|_{L^2}^2 .$$

∇G_{ζ_1} is a martingale. By martingale inequality, for fixed constant $C_0 > 0$,

$$\mathbb{P}(\sup_{0<t<T} \|\sigma\nabla G_{\zeta_1}\|_{L^2} \ge C_0) \le \frac{\sigma^2}{C_0^2} \sup_{0<t<T} \mathbb{E}(\|\nabla G_{\zeta_1}(t)\|_{L^2}^2)$$

By Lemma 4.3

$$\sup_{0<t<T} \mathbb{E}(\|\nabla G_{\zeta_1}(t)\|_{L^2}^2) \le C_1 \cdot \|\nabla\zeta_1\|_{L^2}^2 .$$

Therefore,

$$\mathbb{P}\left(\sup_{0<t<T} \sigma\|\nabla G_{\zeta_1}(t)\|_{L^2}\|\nabla\phi_n(t)\|_{L^2}^2 \le C_0\,\|\nabla\phi_n\|_{L^2}^2\right) > 1 - \frac{\sigma^2}{C_0^2}C_1 \cdot \|\nabla\zeta_1\|_{L^2} .$$

Under the assumption $\sup_{0<t<T}\|\sigma\nabla G_{\zeta_1}(t)\|_{L^2} < C_0$,

$$\frac{d}{dt}\left(\frac{1}{2}\|v_n\|_{L^2} + \frac{\epsilon}{2}\|\nabla\phi_n\|_{L^2}^2\right) \le -\mu\|\nabla v_n\|_{L^2}^2 + \epsilon\, C\, C_0\|\nabla\phi_n\|_{L^2}.$$

Then Gronwall inequality implies that there exist two constants C' and C'', which are independent of W_n, such that

$$\mathbb{P}\left(\frac{1}{2}\|v_n(t)\|_{L^2}^2 + \frac{\epsilon}{2}\|\nabla\phi_n(t)\|_{L^2}^2 \le (\frac{1}{2}\|u_0\|_{L^2}^2 + \frac{\epsilon}{2}\|\nabla\phi_0\|_{L^2}^2)e^{C't}\right) \ge 1 - \sigma^2 C'' .$$

It is easy to check that v_n converges in $C([0,T];L^2(\Omega))$, and ϕ_n converges in $C([0,T];H^1(\Omega))$. By passing to the limit, the result is obtained. $\square$

Remark 4.5. In the proof, C' and C'' are implicitly connected by the choice C_0 but independent of the time interval $(0,T)$. Bigger C' is, then a smaller C'' has to be chosen, and vice versa. $\square$

4.2.4 Analysis of SIIM with Elastic Bending Energy

The proof to the theorem presented earlier is based on a relatively simple phase field energy (for an interface under constant interfacial tension). Indeed, the technique can extend it to other types of energies, including those involving higher order derivatives or stronger nonlinearities.

In the analysis of phase field Navier Stokes vesicle-fluid interaction model in Chapter 2, the elastic bending energy (1.1) is considered. Recall the phase field approximation with spontaneous curvature $c_0 = 0$ is

$$E_b[\phi] = \frac{\kappa}{2\epsilon}\int_\Omega \left(\epsilon\triangle\phi + \frac{1}{\epsilon}\phi(1-\phi^2)\right)^2 dx\ , \qquad (4.15)$$

It can be shown that the discussion in previous section is also applicable to this energy.

For convenience, Let $f_\epsilon(\phi) = \frac{1}{\epsilon^2}(\phi - \phi^3)$, $H_\epsilon(\phi) = \triangle\phi + f_\epsilon(\phi)$. For the elastic bending energy defined by (4.15), the force density term is given by

$$\nabla E_b[\phi]\nabla\phi = \kappa\epsilon\left(\triangle^2\phi + \triangle f_\epsilon(\phi) + H_\epsilon(\phi)\cdot f'_\epsilon(\phi)\right)\cdot\nabla\phi\ .$$

First rewrite the force density in terms of stress tensor, i.e. $-\nabla E_b[\phi]\nabla\phi = \kappa\epsilon\nabla\cdot\tau$, where

$$\tau = 2H_\epsilon(\phi)\nabla^2\phi - \nabla(H_\epsilon(\phi)\nabla\phi) - \frac{1}{2}H_\epsilon(\phi)^2\cdot I.$$

Then the estimates start with the last term in (4.10).

$$\left|\int_\Omega \nabla E_b[\phi]\nabla\phi\, G_\zeta(t)\, dx\right| = \kappa\epsilon\left|\int_\Omega \tau\,\nabla G_\zeta(t)\, dx\right| \,,$$

in which

$$\begin{aligned}
&\left|\int_\Omega \tau\,\nabla G_\zeta(t)\, dx\right| \\
&\quad\leq\; 2\left|\int_\Omega H_\epsilon(\phi)\nabla^2\phi\,\nabla G_\zeta(t)\, dx\right| + \left|\int_\Omega H_\epsilon(\phi)\nabla\phi\,\triangle G_\zeta(t)\, dx\right| \\
&\qquad + \left|\frac{1}{2}\nabla H_\epsilon(\phi)^2\, G_\zeta(t)\, dx\right| \\
&\quad=\; 2\,J_1 + J_2 + J_3\;.
\end{aligned}$$

J_1, J_2 and J_3 are estimated respectively.

$$\begin{aligned}
J_1 &\leq \left|\int_\Omega \triangle\phi\nabla^2\phi\,\nabla G_\zeta(t)\, dx\right| + \left|\int_\Omega f_\epsilon(\phi)\nabla^2\phi\,\nabla G_\zeta(t)\, dx\right| \\
&\leq C_1\cdot\|\nabla G_\zeta(t)\|_{L^\infty}(\|\triangle\phi\|_{L^2}^2 + \|f_\epsilon(\phi)\|_{L^2}^2).
\end{aligned}$$

Since $\partial_t f(\phi) + ((u_\zeta + G_\zeta)\cdot\nabla)f(\phi) = 0$, $|f(\phi(t)| \leq |f(\phi_0)|$. Therefore,

$$\begin{aligned}
J_1 &\leq C_1'\cdot\|\nabla G_\zeta\|_{L^\infty}(E_b[\phi(t)] + 1) \\
&\leq C_2'\cdot\|\nabla G_{\zeta_1}\|_{L^2}(E_b[\phi(t)] + 1)\;.
\end{aligned}$$

Similarly,

$$\begin{aligned} J_2 &\leq C_2 \|\triangle G_\zeta\|_{L^\infty} \cdot (E_b[\phi] + 1) \\ &\leq C_2' \|\triangle G_{\zeta_1}\|_{L^2} \cdot (E_b[\phi] + 1) \ . \end{aligned}$$

G_ζ is divergence free, so

$$J_3 = 0 \ .$$

Put the pieces together,

$$\frac{d}{dt}\left(\frac{1}{2}\|v\|_{L^2}^2 + E_b[\phi]\right) = -\mu\|\nabla v\|_{L^2}^2 + \sigma\epsilon\kappa C\|\triangle G_{\zeta_1}\|_{L^2} \cdot (E_b[\phi] + 1)$$

for some constant C. This then gives the Gronwall type inequality so that for some generic constant C, we have

$$\frac{d}{dt}\left(\frac{1}{2}\|v\|_{L^2}^2 + E_b[\phi] + 1\right) \leq -\mu\|\nabla v\|_{L^2}^2 + C\sigma\|\triangle G_{\zeta_1}\|_{L^2}^2 \cdot \left(\frac{1}{2}\|v\|_{L^2}^2 + E_b[\phi] + 1\right) \ .$$

Assume that ζ is sufficiently regular. By the continuity of $\triangle G_\zeta(t)$, its each realization on time interval $(0\,T)$ is bounded. So the solution is bounded, the existence theorem can be further proved. Moreover, $\triangle G_\zeta$ is martingale. Martingale inequality implies for large probability $\sigma\|\triangle G_\zeta(t)\|_{L^2}^2$ is bounded. Therefore, for large probability the solution remains bounded for any finite time.

To conclude the analysis of SIIM, the discussion above is summed up as the following theorem.

Theorem 4.4. *Under the conditions as before on the initial conditions, the form of the noise, and the additional assumption (4.11) with* $m = 3$ *on the kernel* ζ*, for the energy given by the phase field elastic bending energy (4.15), there exists a unique weak solution to the deterministic model (3.17). And for any time interval* $(0, T)$*, the stochastic model (4.8-4.9) has a unique weak solution almost surely. Moreover, there exist two constants* C', C''*, such that*

$$\mathbb{P}\left(\frac{1}{2}\|v(t)\|_{L^2}^2 + E_b[\phi(t)] + 1 \leq (\frac{1}{2}\|u_0\|_{L^2}^2 + E_b[\phi_0] + 1)e^{C't}\right) \geq 1 - \sigma^2 \cdot C'' .$$

Chapter 5

Summary and Future Plan

5.1 A Summary of Thesis Work

This thesis research has concentrated on modeling fluid elastic surface (or interface) interaction. The representation of elastic surface (or interface) is implicit interface formulations. While the phase field method is the primary implicit interface formulation considered, most of the discussion on modeling and analysis also works for level set framework.

Using phase field or level set method has several advantages. For instance, if explicitly tracking the interface by a mesh, one might need to worry mesh entangling. Implicit interface formulations do not suffer from such problems. Indeed, it has been showed the phase field method has the ability to handle topological change in physically meaningful way [16].

Given an implicit interface formulation either in phase field or level set framework, one can define a corresponding elastic energy functional. The fluid implicit interface interaction equations could be derived via the least action principle. The least action principle provides a consistent and problem-independent way to derive the exact stress to be added to the conventional Navier-Stokes equation due to the deformation effect of the interface. The stress is expressed in terms of the energy functional and also depends on the transport equation of the phase field (or level set) function.

Thermal fluctuation may involve in fluid elastic surface (or interface) interactions. To further account for fluctuation effects, a noise term has been incorporated to the fluid implicit interface interaction equation. The resulting equation is a system of stochastic PDEs. To capture the fluctuation in a physically meaningful way, the stochastic implicit interface model (SIIM) is proposed. SIIM is based on the stochastic immersed boundary method. It starts with considering a near equilibrium dynamics, through computing the correlation structure of the linearized dynamics and imposing Boltzmann distribution at equilibrium, the proper form of noise to be included in macroscopic field equations is obtained. The heuristic analysis shows it is reasonable to expect the equilibrium distribution of SIIM is consistent with Boltzmann distribution. At the end of Chapter 3, SIIM with a quasi-steady flow is considered, which reduced the stochastic hydrodynamic equation to a Langvine type equation of phase field (or level set) function with multiplicative noise. It has been showed if such equation is interpreted in Stratonovich sense, Boltzmann distribution is also the equilibrium distribution.

The mathematical analysis in this thesis consists of two parts. In Chapter 2, the well-posedness of the phase field Navier-Stokes vesicle-fluid interaction model (PFNS) has been established through a modified Galerkin method. The artificial damping term in the transport equation of phase field function provides extra dissipation of the system, which in turn leads to control over high order spacial derivatives of phase field function. Such a priori estimates are important to obtain compactness results in the proof of existence of weak solutions. Even for conventional Naiver-Stokes equation, the issue of uniqueness of solution is still open. However, with an additional assumption on the regularity of the fluid velocity field, the uniqueness can be established.

The second part of analysis is on the well-posedness of SIIM. Both deterministic and stochastic models are considered. Unlike the PFNS equation, no damping term is introduced to the transport equation of the implicit interface. Instead, a mollification of the fluid velocity field is considered. In the analysis, Galerkin approximation has been used again. The key is also to derive proper a priori estimates on the solutions, particularly on their spacial, time derivatives. In the end the existence and uniqueness of pathwise solutions has been established. And a uniform bound on solutions in probability has been provided.

5.2 Open Questions and Future Plan

This thesis has addressed the modeling and analysis issues arising from the studies of fluid-interface interaction. Both deterministic and stochastic models are considered. And rigorous theory concerning the well-posedness has been developed for both models. However, there remain some open questions that haven't been addressed in this thesis and may be put to further work.

5.2.1 Sharp Interface Limit of Fluid Implicit Interface Interaction Model

In PFNS equation and SIIM, the interface is modeled by a phase field function, which is associated with a small positive parameter ϵ characterizing the width of the interface (or phase transition layer). All the analysis presented in this thesis regards ϵ as a fixed small number, thus cannot be used to study the sharp interface limit as $\epsilon \to 0$.

However, such sharp interface limit has attracted much interest and been extensively studied for Allen-Cahn and Cahn-Hilliard dynamics [2, 19, 34]. This poses an interesting challenge to study the sharp interface limit in coupled hydrodynamic equations.

5.2.2 Consistence of SIIM in Infinite Dimensional Space with Boltzmann Distribution at Equilibrium

As discussed in Section 3.5, to verify the consistence of SIIM with Boltzmann distribution at equilibrium, a truncated finite dimensional system is considered. In finite dimensional space, the probability distribution induced by the truncated system satisfies the corresponding Fokker-Planck equation. So it is straightforward to verify Boltzmann distribution as an equilibrium distribution for the truncated system. Same situation occurs for SIIM considered with a quasi-steady flow in Section 3.6. The rigorous analysis has not been fully carried out for the original infinite dimensional system. Moreover, in Section 3.5, the convergence of the probability measure induced by SIIM to the invariant measure corresponding to Boltzmann distribution is briefly discussed, but has not been established. Those subjects deserve further exploration in the future.

5.2.3 Large Deviation Property of SIIM

The derivation of SIIM is through the linearized dynamics around a steady state of the deterministic hydrodynamic equation. However the noise derived for SIIM is completely determined by the dissipative character of the dynamics, and independent of the choice of the energy functional and the steady state (although the fluid velocity must be at rest). Therefore, it is possible to consider an energy functional with multiple minimizers, which won't affect the form of noise in SIIM.

The randomly perturbed gradient flow system with a double-well potential energy has been extensively studied [31]. Double-well potential energy functional has two energy minimizers, which corresponds to the two most likely (stable) status of the system. When the random perturbation vanishes, the system converges to the deterministic gradient flow. When the random perturbation is small, the solutions wanders around the minimizers most of the time. But in rare event, there is transition from one energy minimizer to another. It has been known the most probable transition path connecting the two energy minimizer passes through the saddle point of the energy functional, which corresponds the lowest energy barrier. The studies of the transition path in rare events and finding the saddle point have many very important applications, for example, in materials science [56]. So it will be very interesting work to study the similar large deviation property of stochastic hydrodynamic equations of SIIM that has multiple energy minimizers.

5.2.4 Numerical Algorithms and Simulations

Finally, the effectiveness of SIIM hasn't been tested in extensive simulations. Indeed designing effective numerical scheme for stochastic partial differential equations is another big research area, and poses many challenges. Moreover, many stochastic models have been established to simulate hydrodynamics, for instance, dissipative particle dynamics [37] and Stokesian dynamics [9]. Then it is interesting to compare SIIM with those existing models and test its feasibility. Such work could be considered in the future.

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