RESEARCH STATEMENT

SHIBIN DAI

My research interests lie in nonlinear partial differential equations, applied analysis and numerical analysis. Specifically, I am interested in the modeling, analysis and numerical simulation of the dynamics of nonlinear complex systems. These include

- complex network structures in amphiphilic mixtures with applications to lipid bilayer evolution, biomaterials, and the morphology in polymer electrolyte materials;
- domain coarsening and self similarity in materials science, phase transitions and thin films;
- free boundary problems.

My research is supported by the NSF grant DMS-1411438: *Degenerate diffusion in complex amphiphilic network structures, 2014-2017*. The following is a summary of my research activities.

(i) . In four of my recent papers [12, 13, 14, 15], together with Qiang Du of Columbia University I studied the coarsening dynamics of the Cahn-Hilliard equation with degenerate diffusion mobility, both theoretically and numerically. This equation is a model of the fine structures in composite materials, such as nickel-based super alloys.

(ii) . In two of my recent papers [20, 21], together with Keith Promislow of Michigan State University, I studied the geometric evolution of lipid bilayers and elongated filaments. These are closely related to the functionality of biological membranes and artificial lipid vesicles that are used for drug encapsulation and delivery.

(iii) . In a paper that was recently submitted to *Archive for Rational Mechanics and Analysis* [16], together with Bo Li of UCSD and Jianfeng Lu of Duke University, I studied a phase-field variational model for the solvation of charged molecules with an implicit solvent.

(iv) . In two papers [9, 11] I studied the late stage dynamics of thin liquid films. I concentrated on the nonlinear patterns in thin liquid films caused by the dewetting instabilities.

(v) . I also studied other models on coarsening in materials science. In [18, 19] together with Bob Pego (now at Carnegie Mellon University) I studied a phase-field model and the Lifshitz-Slyozov-Wagner (LSW) mean field model. In [17] with Brabara Niethammer (now at the University of Bonn) and Bob Pego I studied the monopole approximation of the three dimensional Mullins-Sekerka model with kinetic drag. In [10] I studied the area-preserving curvature flow.

(vi) . In addition to the numerical simulations for degenerate Cahn-Hilliard equations [14], my work on numerical analysis also include the study of adaptive finite element methods [6, 7]. These were done with Zhiming Chen of Institute of Computational Mathematics, Chinese Academy of Sciences.

(vii) . In collaboration with Xiang Ma in the Department of Chemistry of Idaho State University, I developed mathematical models for amphiphilic structures and the structures and functionalities of nanoparticles and bio-inspired materials. My ongoing work includes theoretical and numerical studies of these mathematical models. By comparing the mathematical results with experiments, we will obtain a better understanding of the properties of known biomaterials, and shed light on how to design novel biomaterials.

1. The Cahn-Hilliard equation with degenerate diffusion mobility.

---

Updated on March 8, 2017.
For traditional phase transitions, the Cahn-Hilliard energy
\[ \mathcal{E}(u) = \int_{\Omega} \left( \frac{\varepsilon}{2} |\nabla u|^2 + \frac{1}{\varepsilon} W(u) \right) \, dx \]  

is a classical way to model the free energy of binary systems [3, 4]. Here \( u \) is the relative concentration of the two phases, \( W(u) \) is a double-well potential with two equal minima at \( u^\pm \), corresponding to the two phases. The small parameter \( \varepsilon > 0 \) measures the thickness of the transition layer between the two phases. The Cahn-Hilliard equation is the corresponding \( H^{-1} \) gradient flow of \( \mathcal{E}(u) \):
\[ u_t = \nabla \cdot \left( M(u) \nabla \left( -\varepsilon^2 \Delta u + W'(u) \right) \right) \quad \text{in } \Omega \subset \mathbb{R}^n. \]

The diffusion mobility \( M(u) \) is non-negative and may depend on the phase, and may be degenerate in one or both pure phases \( u^\pm \). When coupled with periodic or Neumann boundary conditions on \( \partial \Omega \), the total mass \( \int_{\Omega} u \, dx \) is preserved and the system dissipates the Cahn-Hilliard free energy \( \mathcal{E}(u) \). The Cahn-Hilliard energy \( \mathcal{E} \) \( \Gamma \)-converges to a multiple of the area of the single layer interface separating the two phases. Hence minimizers of \( \mathcal{E} \) correspond to minimizers of the interface area. Fig. 1.1 shows the morphologies in three different situations: constant mobility, one-sided degenerate mobility, and two-sided degenerate mobility.

\[ \begin{align*}
\text{Fig. 1.1: [14] Comparison of morphological differences caused by different diffusion mobilities. The initial values are the same. Top row: } t = 1; \text{ Bottom row: } t = 20. \quad \text{(left column) } M(u) = 1; \quad \text{(middle column) } M(u) = \frac{1}{2} |u - u^-|; \quad \text{(right column) } M(u) = |(u - u^-)(u^+ - u)|. 
\end{align*} \]

In the Cahn-Hilliard equation, when the mobility \( M(u) \) is degenerate in one or both pure phases, the dynamics is very interesting and counter-intuitive. In collaboration with Qiang Du of Columbia University, I studied the Cahn-Hilliard equation with a diffusion mobility that is degenerate in one or both phases and a double-well potential that is continuously differentiable.
1.1. Highly disparate or one-sided degenerate diffusion mobility. In [12], we considered a two-phase system governed by a Cahn-Hilliard equation with a highly disparate diffusion mobility. It has been observed from recent numerical simulations [30] that the microstructure evolution described by such a system displays a coarsening rate different from that associated with the Cahn-Hilliard equation having either a constant diffusion mobility or a mobility that degenerates in both phases. Using the asymptotic matching method, we derived sharp interface models of the system under consideration to theoretically analyze the interfacial motion with respect to different scales of time $t$. In a very short time regime, the transition layer stabilizes into the well-known hyperbolic tangent single-layer profile. On an intermediate $t = O(1)$ time regime, due to the small mobility in one of the phases, the sharp interface limit is a one-sided Stefan problem, determined by data in the phase with constant nonzero mobility. On a slower $t = O(\varepsilon^{-1})$ time scale, the leading order dynamics is a one-sided Hele-Shaw problem. When this one-sided Hele-Shaw dynamics is equilibrated, the system evolves in $t = O(\varepsilon^{-2})$ time scale according to the combination of a one-sided modified Mullins–Sekerka problem in the phase with nonzero constant mobility and a nonlinear diffusion process that solves a quasi-stationary porous medium equation in the phase with small mobility. Scaling arguments suggest that there should be a crossover in the coarsening rate from $t^{1/3}$ to $t^{1/4}$.

1.2. Two-sided degenerate diffusion mobility. The results in [12] motivated us to re-investigate the Cahn-Hilliard equation with two-sided degenerate mobility, and our findings were reported in [13]. Using asymptotic analysis, we found that for the two-sided degenerate Cahn-Hilliard equation with a smooth double-well potential, the interface motion is determined by a quasi-stationary porous medium diffusion processes in both bulk phases, together with a surface diffusion process along the interface itself. In addition, in off-critical systems where one phase—the minor phase—occurs only a small fraction of the system and consists of many disjoint components, it is the quasi-stationary porous medium diffusion process that provides communications between the disjoint components and accounts for the occurrence of coarsening.

1.3. Numerical simulations. In [14], we studied computationally coarsening rates for the Cahn-Hilliard equation with a smooth double-well potential, and with phase-dependent diffusion mobilities. The latter makes accurate numerical simulations challenging. Our numerical simulations confirm earlier theoretical predictions on the coarsening dynamics based on asymptotic analysis. We demonstrated that the numerical solutions are consistent with the physical Gibbs-Thomson effect, even if the mobility is degenerate in one or both phases. For the two-sided degenerate mobility, we reported computational results showing that the coarsening rate is on the order of $l \sim c t^{1/4}$, independent of the volume fraction of each phase. For the one-sided degenerate mobility, that is non-degenerate in the positive phase but degenerate in the negative phase, we showed that the coarsening rate depends on the volume fraction of the positive phase. For large positive volume fractions, the coarsening rate is $l \sim c t^{1/3}$ and for small positive volume fractions, the coarsening rate becomes $l \sim c t^{1/4}$.

1.4. Weak solutions. In [15], we studied the well-posedness of Cahn-Hilliard equations with a smooth double-well potential $W(u)$ and a two-sided degenerate mobility $M(u) = |(u - u^-)(u^+ - u)|^m$, where $m > 0$ is the degree of degeneracy. Due to the degeneracy of $M(u)$ in the two pure phases $u^{\pm}$, it has been conceived that if the initial value of $u$ is inside $[u^-, u^+]$, then the solution $u$ remains confined in $[u^-, u^+]$ for all time [5, 31]. Indeed it was proved in [23] (and in [32] for the 1D case) that there exists such a $u$, confined in $[u^-, u^+]$ for all time, as a solution for the Cahn-Hilliard equation in a weak sense. Apparently the weak solution studied in [23] is not consistent with the physical Gibbs-Thomson effect, which says the concentration of “pure” phases can only
be achieved when the interface has zero mean curvature. The concentration of a phase inside small particles of high mean curvature is higher than that of the corresponding pure phase, due to excessive surface tension. This means, mathematically that if a model accommodates the Gibbs-Thomson effect, then the relative concentration \( u \) may not remain inside \([u^-, u^+]\), as long as the interface separating the two phases has nonzero mean curvature. In [15], we proved the existence of a solution, in a weak sense and different from the weak solution in [23], that is consistent with the Gibbs-Thomson effect.

2. The Functionalized Cahn-Hilliard energy.

The Functionalized Cahn-Hilliard (FCH) energy [24, 25] is a model for the free energy in amphiphilic mixtures. For a binary mixture consisting of water and an amphiphilic lipid phase, take \( u \) as the dimensionless rescaled concentration of the lipid phase. The assumption is that the network structure can be described as selective critical points, but not the minimizers, of the Cahn-Hilliard free energy (1), with a double well potential \( W \) which has two unequal minima at \( u^\pm \). The selection mechanism describes the physics of the specific system under consideration. For complex structures in amphiphilic mixtures, the FCH energy is chosen as [20, 21, 24, 25]

\[
F(u) = \int_{\Omega} \left\{ \frac{1}{2} \left( -\varepsilon \Delta u + \frac{1}{\varepsilon} W'(u) \right)^2 - \varepsilon \left( \frac{\eta_1}{2} |\nabla u|^2 + \frac{\eta_2}{\varepsilon} W(u) \right) \right\} \, dx. \tag{3}
\]

The negative terms parameterized by \( \eta_1 \) and \( \eta_2 \) are, respectively, surface tension induced by hydrophilic interaction and the mixture entropy. So when \( \eta_1 > 0 \), the minimizers of \( F \) are critical points of \( \mathcal{E} \) with maximal surface area, hence complex network structures are induced. The precise ingredients of the network structure is selected by the entropy term. Notably single layer structures, even if they are minimizers of the Cahn-Hilliard energy, become unstable under the FCH energy. In the FCH energy, \( W \) is a tilted double well and it is this feature that guarantees the existence of stable, strongly incompressible bilayer, filamentous pore, and micelle structures, see Fig. 2.1.

![Fig. 2.1: Stable structures generated by minimizing the FCH energy with identical random initial data, but different parameter values: (a) bilayer; (b) pore network; (c) micelles [25].](image)

The functionalized Cahn-Hilliard equation is a gradient flow

\[
u_t = \nabla \cdot \left\{ M(u) \nabla \left( \left( -\varepsilon \Delta + \frac{1}{\varepsilon} W''(u) - \varepsilon \eta_1 \right) \left( -\varepsilon \Delta u + \frac{1}{\varepsilon} W'(u) \right) + (\eta_1 - \eta_2) W'(u) \right) \right\}. \tag{4}
\]
Under periodic or no-flux boundary conditions, equation (4) preserves the volume fraction of the lipid phase while decreasing the FCH energy via a local flux relation.

One key feature of the FCH energy $F(u)$ is that although $\eta_1, \eta_2 > 0$, it is well-defined for any fixed $\varepsilon > 0$. The small parameter $\varepsilon > 0$ measures the thickness of lipid bilayers, or the radius of filamentous pores, or the radius of micelles. A single bilayer, pore, or micelle structure consists of a very small amount of lipid. We summarize some of its known properties.

**Properties of $F(u)$:**

(i) Let $\Omega$ be a bounded domain with smooth boundary. For any fixed positive parameters $\varepsilon, \eta_1, \eta_2$, $F(u)$ is bounded from below for all $u \in H^2(\Omega)$. That is, there exists a constant $C > 0$ depending on $\Omega, \varepsilon, \eta_1, \eta_2$ such that

$$\inf_{u \in H^2(\Omega)} F(u) > -C.$$ 

Consequently $F$ has a minimizer over various classes of admissible set of functions. In addition, $F$ has other critical points corresponding to various new structures.

(ii) The FCH equation (4) admits solutions corresponding to bilayers, filamentous pores, and micelles. The bilayer solution $u_b$ corresponds to when the lipid phase occupies $O(\varepsilon)$ fraction of the system; the pore solution $u_p$ corresponds to when the lipid phase occupies $O(\varepsilon^2)$ fraction of the system. In addition, bilayer and pore structures may co-exist [20, 21].

2.1. Geometric evolution of bilayers, pores, and their competition. The FCH equation supports amphiphilic structures including bilayers, filamentous pores, and micelles. In collaboration with Keith Promislow of Michigan State University, I studied the geometric evolution laws of bilayer [20] and filamentous pores [21]. For smooth bilayers, the evolution follows an area-preserving Willmore flow. For filamentous pores, the evolution follows a Willmoresque flow that preserves the total length of the filaments. We extended these results to a sharp-interface reduction for the competitive evolution of disjoint collections of bilayer interfaces and closed-loop pores. In particular, for a mixture of spherical bilayers and circular, closed pores we explicitly identified two regimes: one in which spherical bilayers extinguish and the circular pores arrive at a common radius, and a complimentary regime in which spherical bilayers of differing radii stably coexist with common-radius, closed-loop, circular pores.

3. Phase-field model for molecular solvation.

In the variational implicit-solvent model [22], the molecular solvation free energy consists of the surface energy, the solute excluded volume, the solute-solvent van der Waals dispersion energy, and the electrostatic free energy. Let $\Omega \subset \mathbb{R}^3$ be the region occupied by the solute-solvent mixture, and $\{x_1, \ldots, x_N\} \subset \Omega_m$ be the charged solute atoms. For any possible configuration, let $\Omega_m$ be the region occupied by the solute, and $\Gamma := \partial \Omega_m$ be the interface between the solute and solvent regions. The total free energy is written as

$$G[\Gamma] := P_0 \text{Vol}(\Omega_m) + \gamma_0 \text{Area}(\Gamma) + \rho_0 \sum_{i=1}^{N} \int_{\Omega \cap \Omega_m} U(||x - x_i||) \, dx$$

$$+ \int_{\Omega_m} \left( -\frac{\varepsilon_m}{2} |\nabla \psi_T|^2 + \rho \psi_T \right) \, dx + \int_{\Omega \setminus \Omega_m} \left( -\frac{\varepsilon_w}{2} |\nabla \psi_T|^2 + \rho \psi_T - B(\psi_T) \right) \, dx.$$  

(5)

Here $P_0, \gamma_0, \rho_0$ are positive constants, $U(\cdot)$ is the van der Waals attraction-repulsion potential, $\varepsilon_m$ is the solute permittivity, $\varepsilon_w$ is the solvent permittivity, $\rho$ is the charge density, $B(\cdot)$ is a convex potential, and $\psi_T$ solves the Poisson-Boltzmann equation in $\Omega_m$ and $\Omega \setminus \Omega_m$, respectively,
with a proper boundary condition on the interface $\Gamma$. The optimal configurations of the interface $\Gamma$ correspond to minimizers of $G$. Given any initial configuration $\Gamma_0$, the gradient flow of $G$ corresponds to the geometric evolution equation $V_n = -\delta T G[\Gamma]$, in which the normal velocity is determined by the shape variation of $G$.

Recently Bo Li of UCSD and his collaborators developed a phase-field variational implicit-solvent model for the solvation of biomolecules. The model involves a phase-field $\phi$ defined on $\Omega$ and a double-well potential $W(\phi)$ with two equal minima at $\phi = 0$ and $\phi = 1$ satisfying $\int_0^1 \sqrt{2W(s)}ds = 1$. The regions $\{\phi \approx 0\}$ and $\{\phi \approx 1\}$ correspond respectively to the water region and the molecule region. Let $\xi$ be a small parameter describing the thickness of the transition layer between the water and the molecule regions. The main idea is to utilize the well-known fact that the Cahn-Hilliard functional $\int_\Omega \left( \frac{\xi}{2} |\nabla \phi|^2 + \frac{1}{\xi} W(\phi) \right) dx$ approximates the surface energy $\text{Area}(\Gamma)$. We can translate all other terms of the molecular-solvation free energy in terms of $\phi$. Consequently the phase-field free energy is written as

$$G_\xi(\phi) := P_0 \int_\Omega \phi^2 dx + \gamma_0 \int_\Omega \left( \frac{\xi}{2} |\nabla \phi|^2 + \frac{1}{\xi} W(\phi) \right) dx + \rho_0 \sum_{i=1}^N \int_\Omega (\phi - 1)^2 U(|x - x_i|) dx \right. \left. + \int_\Omega \left( -\frac{\varepsilon(\phi)}{2} |\nabla \psi_\phi|^2 + \rho \psi_\phi - (\phi - 1)^2 B(\psi_\phi) \right) dx. \quad (6)$$

Here $\varepsilon(\phi)$ is a continuous function describing the permittivity. $\varepsilon(\phi)$ agrees with the solute permittivity $\varepsilon_m$ for $\phi = 1$ and the solvent permittivity $\varepsilon_w$ for $\phi = 0$. $\psi_\phi$ is the solution of the Poisson-Boltzmann equation. The optimal configurations correspond to minimizers of $G_\xi$. For any given initial configuration $\phi_0$, we can study the gradient flow $\phi_t = -\delta_{\phi} G_\xi(\phi)$, whose equilibrium states correspond to critical points of $G_\xi$. Formally when $\xi \to 0$, the phase field $\phi$ converges to a characteristic function $\chi_A$. The functional $G_\xi(\phi)$ then formally converges to $G[\partial A]$.

**3.1. Convergence of free energy and boundary force.** In collaboration with Bo Li of UCSD and Jianfeng Lu of Duke University, I studied the relation between the phase-field variational implicit-solvent model and the sharp-interface variational implicit-solvent model [16]. We proved the continuity of the electrostatics—its potential, free energy, and dielectric boundary force—with respect to perturbations of the dielectric boundary. We also proved the $\Gamma$-convergence of the phase-field free-energy functionals $G_\xi$ to their sharp-interface limit $G$, and the equivalence of the convergence of total free energies to that of all individual parts of free energy. We finally proved the convergence of phase-field forces to their sharp-interface limit. Such forces are defined as the negative first variations of the free-energy functional; and arise from stress tenors. More precisely we proved that for sequences $\xi_k$ and $\phi_k$, if $\xi_k \to 0$, $\phi_k \to \chi_A$ in $L^1(\Omega)$, and $G_{\xi_k}(\phi_k) \to G[\partial A]$, then $-\delta_{\phi} G_{\xi_k}(\phi) \nabla \phi \rightharpoonup \delta \Gamma G[\partial A] n$ in a weak sense. Here $n$ is the outer normal of $\partial A$. In particular, we obtained the force convergence for the Cahn-Hilliard functionals with minimal assumptions.

**4. Late stage dynamics of thin liquid films.**

The dewetting instabilities of a thin liquid film coating a solid substrate cause rupture and complicated morphological changes in the early stage and ultimately the formation of complex nonlinear patterns in the late stage, see Fig. 4.1. The patterns are essentially fluid droplets connected by an ultra thin residual film. The evolution of the droplets exhibits a coarsening phenomena where we observe the decrease of the total number of droplets and an increase in the average droplet size and the average distance between droplets. The thin film has a mixture of dimensions in that the underlying substrate is 2 dimensional while the liquid film is genuinely 3 dimensional. What’s more, the liquid droplets may have high mobility and collisions can be important.
Asymptotic analysis indicates that the liquid droplets are approximately paraboloids. However, little is known about the distribution of droplet sizes. Part of the reason is, it is a challenging problem to retrieve the statistical information from the continuum PDE model for thin films. To facilitate the study of the statistics of liquid droplets, I concentrated on mean field approaches to the late stage dynamics of thin films.

4.1. 1D mean field model. In [9] I studied a mean field model proposed by Gratton and Witelski [26] for the case when the underlying substrate was one dimensional. Estimates on the number and size of droplets were obtained. Also it was found that this mean field model is equivalent to the classical 2 dimensional LSW mean field model for phase transitions after a nonlinear rescaling of time.

4.2. 2D mean field model. In [11] I formally derived a mean field model for the case when the underlying substrate was 2 dimensional. Let \( f(R, t) \) be the distribution density of the radii \( R \) of the bases of droplets. \( f \) satisfies a transport equation

\[
\frac{\partial}{\partial t} f(t, R) + \frac{\partial}{\partial R} \left( -\frac{1}{R^2} \ln \phi^{-1} \left( \frac{1}{R} - P_* \right) f(t, R) \right) = 0.
\]

Here

\[
\phi = \frac{\int_0^\infty R^2 f(t, R) \, dR}{\mathcal{L}^2}, \quad P_* = \frac{\int_0^\infty R^{-1} f(t, R) \, dR}{\int_0^\infty f(t, R) \, dR}.
\]

\( \mathcal{L} \) is the system size. The minimum requirement on \( f(t, R) \) is \( \int_0^\infty R^2 f(t, R) \, dR < \mathcal{L}^2 \) since the droplets can not occupy all the substrate. In addition, the conservation of total volume of droplets translates into \( \int_0^\infty R^2 f(t, R) \, dR = \text{const} \). The coarsening dynamics was then studied by considering a “structural” time scale, which captures part of the statistical information of the size distribution of droplets. I then obtained estimates that in a sense improved the results of Otto, Rump and Slepčev [28]. Note that this mean field model is now not equivalent to the classical LSW models.

The above mentioned mean field models for thin films are valid when collisions of droplets are negligible. When collisions are not negligible, we have to include extra nonlocal terms in those models. This results in a combination of LSW models and Smoluchowski coagulation models. I would like to rigorously study the derivation of such models, their wellposedness and specifically their possible self-similar solutions.

5. Other models on coarsening in materials science.

In addition to my study of the Cahn-Hilliard equation with one and two sided degenerated mobility [12, 13, 14, 15], I also studied several other phase transition models corresponding to different microscopic mechanisms of coarsening.
5.1. Phase-field and the Lifshitz-Slyozov-Wagner (LSW) model. With R. L. Pego, I studied the phase-field model [19] and the classical Lifshitz-Slyozov-Wagner (LSW) mean-field models [18]. Heuristic arguments suggest that, if self-similarity were true, in both models the typical length scale \( l \) such as the characteristic particle radius will grow as a temporal power law \( l \sim ct^{1/3} \), with \( c \) a universal constant independent of any system parameters. We rigorously prove that in these models, the energy density \( \bar{E}(t) \) can not dissipate faster than a negative temporal power law \( ct^{-1/3} \), in the average sense

\[
\int_0^T \bar{E}(t)^2 \, dt \geq C \int_0^T t^{-2/3} \, dt \quad \text{for } T \text{ big enough.} \tag{9}
\]

Since the total energy is proportional to the area of the interface separating the two phases, the energy density \( \bar{E} \) is proportional to the inverse of length. Equation (9) gives an upper bound on the coarsening rate that is consistent with \( l \sim ct^{-1/3} \) if we choose \( l = \bar{E}^{-1} \). Specifically we note that the constant \( C \) in (9) is independent of any system parameters.

5.2. Mullins-Sekerka model with kinetic drag. With B. Niethammer and R. L. Pego, I studied a more subtle problem, namely the crossover of coarsening rates for the monopole approximation of the three dimensional Mullins-Sekerka model with kinetic drag [17]. The model that we start from is formulated as follows for a two-phase mixture in a domain \( \Omega \subset \mathbb{R}^n \). Let \( G_t \subset \Omega \) denote the region occupied by one of the phases at time \( t \), and let \( \Gamma_t = \partial G_t \) denote the interface separating the two phases. The system in nondimensional form is then:

\[
\begin{align*}
\Delta u &= 0 \quad \text{in } \Omega \setminus \Gamma_t, \tag{10} \\
u &= \kappa + \beta v \quad \text{on } \Gamma_t, \tag{11} \\
v &= [n \cdot \nabla u] \quad \text{on } \Gamma_t. \tag{12}
\end{align*}
\]

Here \( u \) is a normalized chemical potential or concentration difference, \( n \) is the outward unit normal to the interface \( \Gamma_t \), \( v \) is the normal velocity of the interface \( \Gamma_t \), \( \kappa \) is the mean curvature of \( \Gamma_t \) (taken to be positive when \( G_t \) is convex), and \( \beta > 0 \) is a constant kinetic drag coefficient. The jump of the normal derivative of \( u \) across \( \Gamma_t \) is \( [n \cdot \nabla u] = n \cdot \nabla u^+ - n \cdot \nabla u^- \), where \( u^+, u^- \) are the limits of \( u \) on \( \Gamma_t \) coming along \( n \) from the outside and inside, respectively. One should also apply an appropriate boundary condition on \( \partial \Omega \), for example the no-flux condition

\[
n \cdot \nabla u = 0 \quad \text{on } \partial \Omega.
\]

For this model, the total volume of \( G_t \) is conserved in time.

The kinetic drag coefficient \( \beta \) introduces an extra length scale. As a result, in the early stage when particle sizes are smaller than \( \beta \), \( l \sim c_1(t/\beta)^{1/2} \). In the late stage when particles are much bigger than \( \beta \), the influence of \( \beta \) disappears and \( l \sim c_2 t^{1/3} \). The monopole approximation is the geometrically constrained case when droplets are spherical, which is a reasonable approximation according to [1, 2]. The wellposedness of the monopole model is also proved as a result of the careful study of the gradient flow structure.

5.3. Area-preserving curvature flow. When the interaction on the interface dominates the coarsening process, the dynamics is described by the mean curvature flow, with the restriction that the volume (or area in 2D) of each phase is preserved, respectively. Let \( \Gamma \) be the interface that is a collection of disjoint closed hypersurfaces, \( \kappa \) be the mean curvature, positive when \( \Gamma \) is convex, and \( V \) be the outer normal velocity. The volume-preserving mean curvature flow is written as

\[
V = -\kappa + \frac{1}{|\Gamma|} \int_{\Gamma} \kappa \, ds.
\]
In this case, simple observation indicates that the shapes of the interface have profound influence on the coarsening rate. In [10], I studied the effect of the droplet shapes by considering the area-preserving curvature flow for the case when droplets are disjoint and convex.


Numerical analysis is another area I am interested in. Together with Prof. Zhiming Chen, I worked on the numerical simulation of PDEs using adaptive finite element methods. One is about the simulation of a dynamical Ginzburg-Landau model in superconductivity [6] and another is about the efficiency of adaptive finite element methods for elliptic problems with discontinuous coefficients [7]. Adaptive methods are efficient when dealing with problems with singularities or when both large and small scales are involved. As exhibited in my study of the degenerate Cahn-Hilliard equation [12, 13, 14, 15], it has been a common practice to combine numerical analysis and scientific computing with theoretical analysis to study complex problems in applied mathematics. This is also my approach to the study of complex network structures in amphiphilic mixtures.

7. Ongoing and future research topics.

7.1. Complex structures as geometrically constrained local minimizers. The first and most fundamental problem is variational properties of the functionalized Cahn-Hilliard energy. Although for any fixed $\varepsilon > 0$, $F(u)$ is bounded from below for all $u \in H^2(\Omega)$ [29], its lower bound is negative and depends on $\varepsilon$. Specifically the lower bound approaches negative infinity as $\varepsilon \to 0^+$. This feature makes it very challenging to directly apply standard variation techniques such as Gamma convergence. However, this feature is also complemented by the fact that for a bilayer of area in the order of $O(1)$, and a pore of length in the order of $O(1)$, the solute phase occupies only a small fraction of the whole system, in the order of $O(\varepsilon)$ and $O(\varepsilon^2)$, respectively. This observation motivated us to consider the bilayer and pore structures as local minimizers of the FCH energy under energy and geometric constraints. In addition to bilayer and pore structures, some defect structures are also observed and are stable under energy and geometric constraints. Such structures include free edges, end caps and triple junctions. Some results are being organized in the manuscript [8].

7.2. FCH equation with degenerate mobility. In biological or artificial systems, it is known that bilayer vesicles can co-exist, even if they are of various sizes and shapes. Also lipid bilayers are essentially impermeable, in the sense that solvent can not freely go through a lipid membrane. To revise our FCH model to accommodate such features, we modify the FCH equation to include a phase-dependent diffusion mobility. Based on our knowledge about the degenerate Cahn-Hilliard equations [12, 13, 14, 15], a FCH equation with one or two sided degenerate mobility becomes more realistic and captures more features of bilayer vesicles. In addition, it is natural to choose a double-barrier potential rather than a smooth double-well potential.

7.3. Fusion of bilayers through hemifusion: structures and energy barriers. The opening and fusion of bilayers (vesicles) are critical for biological processes like drug delivery or protein transportation and for the formation of networks in amphiphilic mixtures. Because of the bilayer structure, there is an intrinsic resistance for two bilayers to merge. This can be quantified as an energy barrier. Even if two relaxed bilayers are close to each other, they may not merge. Either extra tensions of bilayers, or change of ion densities or electric field around the bilayers, are needed to induce the fusion of vesicles. It is natural to use FCH to handle the topological changes in such processes, and it is capable of handling complex dynamics in large scales when multiple vesicles of various shapes and sizes exist at the same time. This goes well beyond the scope of molecular dynamics or mesoscopic simulations. We expect our analytic techniques in [20] and [21]
to be generalized, although highly nontrivial, to extract information such as energy barriers that need to overcome for vesicle fusion to happen. Since the free energy of bilayer membranes are modeled by the FCH energy, these problems can also be summarized as optimization problems of the FCH energy under various geometric constraints.

7.4. Structures and functionalities of biomaterials. Nanocrystals have wide applications in biological imaging and drug delivery. In vivo applications require these nanoparticles to disperse well in the aqueous media, and to avoid coagulation. The common practice is to encapsulate them in artificial bilayer vesicles called liposomes, or in amphiphilic polymeric micelles. I will study the complex amphiphilic structures and the functionality of nanoparticles/proteins and other bio-inspired materials. I have created mathematical models for the encapsulation of nanoparticles in bilayer liposomes and polymeric micelles, the coating of biomaterials by amphiphilic copolymers, and the change of morphology caused by proteins. My approach is in the framework of the functionalized Cahn-Hilliard (FCH) energy, coupled with proper strong and weak anchoring conditions. Through collaboration with an experimentalist, Xiang Ma in the Department of Chemistry of Idaho State University, this program will advance the understanding of the properties of existing biomaterials and inspire the design of new biomaterials and drug delivery systems such as those based on virus-like particles.

REFERENCES