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Drop dynamics on textured materials

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ABSTRACT

Adding textures at solid surfaces often markedly modifies their wetting properties. More specifically, we discuss how hydrophobic textures and impregnated textures indeed trigger, in different ways, unique dynamical wetting situations - respectively referred to as water-repellent and oleo-planning. After recalling the very low adhesion on such materials, we shall focus on the newly-studied characteristics of the friction they generate.

Other contributors to this talk: Armelle Keiser, Hélène de Maleprade, Timothée Mouterde, Pascal Raux and Christophe Clanet

Nearly-zero contact angle hysteresis on lubricated surfaces

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ABSTRACT

The ability of liquid lubricant on surfaces to reduce *solid-solid* friction has been widely known since antiquity. The idea of using lubricant to reduce *solid-liquid* friction is relatively new: when infused with suitable lubricants, surfaces can exhibit excellent liquid-repellency, with nearly zero contact angle hysteresis. Such surfaces, known in the literature as Slippery Lubricant Infused Porous Surfaces (SLIPS), also show promise in various applications, including in biomedical devices and anti-ice materials. Here, I would show that on such surfaces, the droplet levitates over a thin oil film— akin to how tyres hydroplane on a wet road—with minimal dissipative force and no contact line pinning. The thickness of this intercalated lubricant film follows the Landau-Levich-Derjaguin law. Based on this insight, I will then derive (and experimentally verify) a simple scaling law for the contact angle hysteresis of the levitating droplet. Finally, I will briefly contrast this with droplet dynamics on superhydrophobic surfaces.

Why a droplet can contact smooth surface so rapidly?

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ABSTRACT

When a droplet gently lands on an atomically-smooth substrate, it will most likely contact the underlying surface in about 0.1 second. However, theoretical estimation from fluid mechanics predicts a contact time of 10 to 100 seconds. What causes this large discrepancy and how does nature speed up contact by two orders of magnitude? To probe this fundamental question, we prepare atomically-smooth substrates by either coating a liquid film on glass or using a freshly-cleaved mica surface, and visualize the droplet contact dynamics with 30nm resolution. Interestingly, we discover two distinct speed-up approaches: (1) droplet skidding due to even minute perturbations breaks rotational symmetry and produces early contact at the thinnest gap location, and (2) for the unperturbed situation with rotational symmetry, a previously-unnoticed boundary flow around only 0.1mm/s expedites air drainage by over one order of magnitude. Together these two mechanisms universally explain general contact phenomena on smooth substrates. The fundamental discoveries shed new light on the contact and drainage research [1, 2].

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The threshold dynamics method and applications

Xiao-Ping Wang

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ABSTRACT

In this talk, I will review some recent work on the threshold dynamics method for diffusion generated motion of the interface on solid surface. We also analyze the contact line behavior of the method from asymptotic expansion and the contact line dynamics is also derived. Applications to wetting on solid surface, image segmentation are presented.

Modelling and analysis for contact angle hysteresis on rough surfaces

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ABSTRACT

Wetting on rough surface is common in nature and industry applications. Mathematically, it is a free interface problem proposed in a domain with rough boundary. Due to plenty of local minimizers in the system, there are many interesting phenomena in wetting, like contact angle hysteresis, etc. In this talk, we will show some recent analysis for this problem. We first derive a homogenized equation to describe the macroscopic contact angle on rough surfaces. The equation can reduce to a modified Wenzel (or Cassie) equation on geometrically rough(or chemically patterned) surfaces. It describes the local minimizers in the system and can be used to understand the contact angle hysteresis phenomena. Then, we show some analysis for contact angle hysteresis by using a phase-field model with a relaxed boundary condition. By asymptotic analysis, we derive an ordinary differential equation which can characterize some interesting phenomena for contact angle hysteresis.

Freezing impacts

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ABSTRACT

We investigate the dynamics of water drop impacts on solid substrate at very low temperature, that is below the freezing temperature. The coupling between rapid surface deformation and the solidification leads to the formation of surprising patterns. We will show, using a model solving the heat transfers in a simple geometry that these patterns are controlled by the competition between the thermal layer and the free surface dynamics. Finally, the formation of cracks within the frozen structure will be discussed.

Modeling and Simulation of Moving Contact Lines in Fluids

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ABSTRACT

It is well-known that the no-slip boundary condition leads to an infinite rate of energy dissipation when combined with hydrodynamic equations. To overcome this difficulty, we derive a slip model based on molecular dynamics simulations and thermodynamic principles. We illustrate how this model can be used to analyse the behaviour of the apparent contact angle, hysteresis and other important physical problems for the moving contact line. We also discuss the distinguished limits of the slip model as the slip length tends to zero.

Macroscopic Equations of Motion for Grain Boundaries

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ABSTRACT

Grain boundaries (GBs) are interfaces between crystallites of the same crystal structure (i.e., grains) within a polycrystalline materials. It is now well established that the microscopic mechanism by which GBs (codimension 1 objects) move is through the motion of line defects (codimension 2 objects) that lie within the GB plane. Disconnections are characterized by both a step height h and Burgers vector $\mathbf{b}$ which are defined in terms of the relative orientation of the two grains meeting at the GB. In this presentation, I will introduce disconnections, explain how their motion gives rise to GB migration, shear across grain boundaries, grain boundary sliding,... Then, I will discuss continuum description of GB dynamics that are based upon disconnection motion. Finally, I will discuss why the constraints that 3-dimensional grains fill space within polycrystals have profound effects on GB dynamics and microstructural evolution in polycrystals. The latter discussion focuses on mechanical constrain that the triple junctions (codimension 2 defects along which three GBs meet) and mechanical constraint.

Energy and Dynamics of Grain Boundaries Based on Underlying Mircrostructure

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ABSTRACT

Grain boundaries are the interfaces of grains with different orientations in polycrystalline materials. Energetic and dynamic properties of grain boundaries play essential roles in the mechanical and plastic behaviors of the materials. These properties of grain boundaries strongly depend on their microscopic structures. We present continuum models for the energy and dynamics of grain boundaries based on the continuum distribution of the line defects (dislocations or disconnections) on them. The long-range elastic interaction between the line defects is included in the continuum models to maintain stable microstructure on grain boundaries during the evolution. The continuum models is able to describe both normal motion and tangential translation of the grain boundaries due to both coupling and sliding effects that were observed in atomistic simulations and experiments.

Mound Formation during Epitaxial Growth studied by Kinetic Monte Carlo and Island Dynamics Simulations

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ABSTRACT

In this talk we will discuss the formation of mounds during epitaxial growth studied by kinetic Monte Carlo (KMC) simulations as well as Island Dynamics simulations that employ the level set method. In the presence of a step edge barrier (that induces an uphill current) mounds form during epitaxial growth. The slopes of these mounds are stabilized by a downward transport mechanism. We study two different downward transport mechanisms, referred to as downhill funneling and transient mobility. Our results show that the scaling exponents that are associated with mound formation depend continuously on the model parameters.

The role of grain boundary and interface diffusion in solid state dewetting of thin metal films deposited on ceramic substrates

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ABSTRACT

We studied the solid state dewetting of thin Au [1], Ni [2] and Fe [3] films, and Au-Fe bilayers [4] deposited on sapphire substrates. Both Au and Fe films were nanocrystalline, while the Ni and Au-Fe films exhibited a strong heteroepitaxy to the substrate. The single crystalline particles formed at the late stages of dewetting exhibited stable faceted shapes that were far from those predicted by equilibrium considerations. We discussed high stability of faceted particles in terms of slow mass transport along the singular atomically flat facets. In the case of heteroepitaxial Ni films and Au-Fe bilayers, the formation of faceted pinholes to the substrate is accompanied by the nucleation and growth of twin boundaries parallel to the substrate. These boundaries allow nucleating of defects at the side facets of the pinhole, thus enabling its growth.

We propose that the slow pace of surface diffusion in thin textured films brings to the forefront other types of short-circuit diffusion, such as grain boundary diffusion and metal self-diffusion along the metal-ceramic interface. We illustrated the importance of these short-circuit diffusion paths in the framework of new quantitative models of solid state dewetting. For example, the observed shape of thermal grain boundary grooves in Ni thin films on sapphire deviated substantially from Mullins' classical solution, and showed an apparent negative mass balance. We proposed a model which explains this by considering Ni self-diffusion along the Ni-sapphire interface accompanied by the homogeneous thickening of the film [2]. Further examples in which the metal self-diffusion along the metal-ceramic interface plays an important role are the capillary-driven growth of Fe [5] and Au [6] nanowires from the respective thin films deposited on sapphire and silica. Finally, we discuss the atomistic origins of fast metal self-diffusion along the metal-ceramic interfaces.

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Equilibria for Thin Grain Systems: Surface Diffusion and Grain Migration

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ABSTRACT

Consideration of the motion of a thin system of, say, metallic grains whose exterior surface is exposed to an ambient vapor or vacuum can lead to quite complicated models, involving a large variety of physical effects. To gain intuition, we focus on a particularly simple but relatively classical model in which the exterior surface is taken to evolve by motion by surface diffusion and the grain boundaries, which separate between neighboring grains, are taken to evolve by mean curvature motion. Even with this simplistic context, the dynamics can be quite complicated. To emphasis the wealth of possible behaviors, we consider a number of special 3D geometries and demonstrate a severe lack of uniqueness even within the class of possible steady state solutions. Recent results reflect joint work with V. Derkach and J. McCuan.

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Modeling and Simulation for Solid-State Dewetting Problems

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ABSTRACT

In this talk, I present sharp interface models with anisotropic surface energy and a phase field model for simulating solid-state dewetting and the morphological evolution of patterned islands on a substrate in two and three dimensions. We show how to derive the sharp interface model via thermovariation dynamics, i.e. variation of the interfacial energy via an open curve with two triple points moving along a fixed substrate. The sharp interface model tracks the moving interface explicitly and it is very easy to be handled in two dimensions via arc-length parametrization. The phase field model is governed by the Cahn-Hilliard equation with isotropic surface tension and variable scalar mobility and it easily deals with the complex boundary conditions and/or complicated geometry arising in the solid-state dewetting problem. Since the phase field model does not explicitly track the moving surface, it naturally captures the topological changes that occur during film/island morphology evolution. Efficient and accurate numerical methods for both sharp interface models and phase field models are proposed. They are applied to study numerically different setups of solid-state dewetting including short and long island films, pinch-off, hole dynamics, semi-infinite film, etc. Our results agree with experimental results very well.

This talk is based on joint works with Wei Jiang, David J. Srolovitz, Carl V. Thompson, Yan Wang and Quan Zhao.

Reciprocal theorem: From local equations to symmetry over the whole system

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ABSTRACT

Onsager's reciprocal symmetry is typically used to derive local constitutive equations through a variational approach. We consider a non-equilibrium system close to the global equilibrium state. We show that the reciprocal symmetry for local constitutive equations can be extended to a new symmetry over the whole system. This symmetry is manifested in the kinetic coefficients connecting the forces and fluxes defined at the system boundary. Our results generalize the Lorentz theorem for Stokes flows. A phase field model, a micropolar fluid, and heat transport will be used to demonstrate the generalized theorem.

This work is supported by Hong Kong Research Grants Council.

Small deformations of biomembranes

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ABSTRACT

In this talk, we introduce a mathematical model for small deformations induced by external forces of closed surfaces that are minimisers of Helfrich-type energies. Our model is suitable for the study of deformations of cell membranes induced by the cytoskeleton. We describe the deformation of the surface as a graph over the undeformed surface. A new Lagrangian and the associated Euler-Lagrange equations for the height function of the graph are derived. This is the natural generalisation of the well-known linearisation in the Monge gauge for initially flat surfaces. We discuss energy perturbations of point constraints and point forces acting on the surface. We establish existence and uniqueness results for weak solutions on spheres and on Clifford tori. Algorithms for the computation of numerical solutions in the general setting are provided. We present numerical examples. This is based on joint work, [1, 2, 3].

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Interface dynamics of model systems: from local properties to boundary conditions

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ABSTRACT

Despite its wide interest in many applications, modeling accurately two-phase (fluid-fluid and fluid-solid) interface dynamics still remains quite challenging. This is even more complex when three-phase (fluid-fluid-solid) interface dynamics is dealt with. The difficulties are mostly due to the multi-scale (in time and space) nature of these systems [1]. In addition to experiments, one possible way to improve our understanding is to use nano-scale molecular simulations in which the interface dynamics behavior emerges without any *a priori* [2].

Thus, during the presentation, we will illustrate how molecular dynamics simulations of idealized configurations can shed light on the small scales phenomena occurring at interfaces. In particular, we will focus on:

- viscosity at fluid-solid interfaces [3]
- slip at fluid-fluid interfaces [4]
- nanodroplet dynamics on a perfect surface [5]
- contact line boundary conditions when all scales are resolved [6]

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Large Scale Direct Dynamic Contact Line Simulations And The Forced Dewetting Transition

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ABSTRACT

We investigate the contact line dynamics using an adaptive direct solver of the Navier–Stokes equations. The discretization of the surface tension is based on a Volume-of-Fluid method that includes a modification of the capillary force near the contact line to impose a specified contact angle [1]. This numerical contact angle condition can be thought of as a regularization of the Navier–Stokes equation by a partial (Navier) slip model, yielding an implicitly dynamic contact angle model that involves a numerical slip length. We carry out our study in the context of forced dewetting transition, also known as the transition to Landau–Levich–Derjaguin film, and provide a framework that yields a dynamic contact angle measurable at scales larger than the grid size, which depends logarithmically on the distance to the contact line. A distinguished feature of the proposed numerical model is the consideration of large contact angles ($\geq 90^\circ$) and arbitrary viscosity ratios, in contrast to available asymptotic models. By means of large scale direct numerical simulation, we verify that the Cox-Voinov theory, combined with lubrication theory, provides a unique relationship between the dynamic contact angle, the grid size near the contact line and the critical Ca for the forced dewetting transition [2].

This work was done in collaboration with Stéphane Zaleski from Sorbonne Universites, UPMC Univ Paris 06, France.

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Simulations of Particle Structuring Driven by Electric Fields

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ABSTRACT

Recent experiments show intriguing surface patterns when a uniform electric field is applied to a droplet covered with colloidal particles. Depending on the particle properties and the electric field intensity, particles organize into an equatorial belt, pole-to-pole chains, or dynamic vortices. Here we present simulations of the collective particle dynamics, which account for electrohydrodynamic and dielectrophoresis of particles. In order to better understand the collective particle dynamics, we will also discuss the solution of a model problem of a dielectric particle on a planar interface in an applied electric field. Analytical and numerical results will be presented including the derivation of the interaction force between two particles.

Solid-state dewetting: modeling and numerics

Wei Jiang

Wuhan University, China

ABSTRACT

In this talk, I will talk about our work about modeling solid-state dewetting problems. Taking the 2D case for example, I will explain the main idea behind these approaches; some extensions to the 3D case will be also presented. If time permits, I will talk about our recent work about using Onsager's variational principle to derive reduced models with applications to solid-state dewetting.

Modeling and simulation of moving contact line problem for two-phase complex fluids flow

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ABSTRACT

We introduce the sharp interface models for moving contact lines with polymeric fluids. A continuous model with the boundary conditions is derived for the dynamics of two immiscible fluids with moving contact lines based on thermodynamic principles. An immersed boundary method is developed to solve the resulting free boundary problem. We also discuss the model reduction of the slip model to the no-slip limit by the technique of asymptotic analysis. The work is based on the paper [1, 2] and manuscript [3].

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A new and robust approach to construct energy stable schemes for gradient flows

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ABSTRACT

We propose a new technique, the scalar auxiliary variable (SAV) approach, to deal with nonlinear terms in a large class of gradient flows. The technique is not restricted to specific forms of the nonlinear part of the free energy, it leads to linear and unconditionally energy stable second-order (or higher-order with weak stability conditions) schemes which only require solving decoupled linear equations with constant coefficients. Hence, these schemes are extremely efficient as well as accurate.

We apply the SAV approach to deal with several challenging applications which can not be easily handled by existing approaches, and present convincing numerical results to show that the new schemes are not only much more efficient and easy to implement, but also can better capture the physical properties in these models.

We shall also present a convergence and error analysis under mild assumptions on the nonlinear free energy.

Structure-Preserving Numerical Approximations to Thermodynamically Consistent Dissipative Models

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ABSTRACT

Thermodynamically consistent theories for matter systems are the ones derived systematically following the non-equilibrium thermodynamic protocols and conservation laws. They satisfy the fundamental laws of thermodynamics (1st and 2nd law). For matter systems involving irreversible processes, the second law of thermodynamics dictates that entropy produced in the thermodynamic process must increase, which in many cases implies well-posedness of the underlying mathematical equations. When one numerically approximate the thermodynamically consistent models, consisting of partial differential equations, the physical properties that should be retained in the approximate discrete models include the conservation laws and the second law of thermodynamics. I will present a general approach to design numerical algorithms so that the conservation laws as well as the second law of thermodynamics are preserved at the discrete level. This is known as the structure-preserving numerical approximation. Applications of the numerical treatment of thermodynamically consistent crystal growth model will be discussed as an example.

Numerical simulations for Newtonian vesicles suspended in viscoelastic fluid

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ABSTRACT

In this talk, an immersed boundary method is introduced to simulate the dynamics of Newtonian vesicle in viscoelastic Oldroyd-B fluid under shear flow. The viscoelasticity effect of extra stress is well incorporated into the immersed boundary formulation using the indicator function. Our numerical methodology is first validated in comparison with theoretical results in purely Newtonian fluid, and then a series of numerical experiments is conducted to study the effects of different dimensionless parameters on the vesicle motions. Although the tank-treading (TT) motion of Newtonian vesicle in Oldroyd-B fluid under shear flow can be observed just like in Newtonian fluid, it is surprising to find that the stationary inclination angle can be negative without the transition to tumbling (TB) motion. Moreover, the inertia effect plays a significant role that is able to turn the vesicle back to positive inclination angle through TT-TB-TT transition as the Reynolds number increases.

A systematic approach for fluid & porous media coupling, multi-particles & multi-scale problems

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ABSTRACT

Simulations of fluid and porous media couplings, multi-particles & multi-scale problems are important and challenging because of different governing equations, muilti-scales and multi-connected domain, and complicated interface conditions such as BJ and BJS relations. Most of numerical methods in the literature are based on direct approaches that leads large system of equations, often coupled and ill-conditioned, with lower order accuracy near the interface or boundary.

In this talk, I will first introduce a few examples of these problems, then I explain a systematical approach based on the augmented strategies by introducing one or several intermediate augmented variables along the interface. The augmented variables enable us to have dimension by dimension discretization, improve the stability and CFL constraints, and utilize fast solvers.

Some numerical examples will be shown to demonstrate the efficiency of the augmented strategies, particularly of the ADI methods for parabolic PDES with multi-inclusions; and Navier-Stokes and Darcy's couplings. The proposed new method has also been utilized to simulate different flow/porous media setting with complicated interfaces which leads to some interesting simulations results such as effect of corners, orientation effect etc.

An efficient adaptive rescaling scheme for computing moving interface problems

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[b] *Shanghai Jiao Tong University, China*
[c] *University of California at Irvine, USA*

ABSTRACT

In this talk, I will present an adaptive rescaling scheme for computing long-time dynamics of expanding interfaces. The main idea is to rescale the temporal and spatial variables so that the interfaces evolve logarithmically fast at early growth stage and exponentially fast at later times. The new scales guarantee the conservation of the area/volume enclosed by the interface. Numerical examples will be presented.
This is joint work with Meng Zhao, Shuwang Li and John Lowengrub.

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Error estimates for a energy stable scheme to a Cahn-Hilliard phase-field model for two-phase in-compressible flows

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ABSTRACT

We carry out a rigorous error analysis for a finite element discretization of the linear, weakly coupled energy stable scheme for a Cahn-Hilliard phase-field model of two-phase incompressible flows with matching density.

Modelling multicomponent fluid flows with the lattice Boltzmann method

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ABSTRACT

I will present a free energy lattice Boltzmann approach to simulate multicomponent fluid flows [1, 2]. The method is flexible, as it allows different number of fluid components to be implemented easily. I will also show how high density ratios between the liquid and gas components can be realised [3]. Focusing on binary and ternary fluid systems, I will then discuss several applications of the method. First, I will present our numerical study on contact line dynamics, where we reconcile two scaling laws that have been proposed in the literature for the slip length associated with a moving contact line in diffuse interface models [4]. Second, I will discuss the dynamics of drops moving across liquid infused surfaces [5]. These are liquid repellent surfaces made by infusing a lubricant into porous or rough solid surfaces. Third, I will present collision dynamics between two immiscible drops [3]. We are able to capture bouncing, adhesive and insertive regimes, in agreement with experimental observations.

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Dislocation network structures in 2D bilayer system

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ABSTRACT

We develop a multiscale continuum model to describe the interlayer defects in bilayer materials. The model incorporates both the anisotropy elasticity of each mono-layer in bilayer materials and the first-principle calculation informed interaction between two layers, i.e., the nonlinear atomistic potential energy between two layers. The equilibrium structures are obtained from the numerical simulations of the force balance differential equations. We apply this approach to determine the structure and energetics of twisted bilayer material. In tBLG, two distinct, modified Moiré structures are observed. We also investigated the dislocation structure in heterogeneous bilayer material such as G/BN. Our model agrees well with the atomistic results. An analytical description is developed based on the obtained structural features.

Asymptotic analysis of phase-field and sharp-interface models for surface diffusion

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ABSTRACT

We study the evolution of solid surfaces and pattern formation by surface diffusion. Phase field models with degenerate mobilities are frequently used to model such phenomena, and are validated by investigating their sharp interface limits. We demonstrate by a careful asymptotic analysis involving the matching of exponential terms that a certain combination of degenerate mobility and a double well potential leads to a combination of both surface and non-linear bulk diffusion to leading order. We also discuss implications for the case with an anisotropic free energy, and analyse the "finger" instability that occurs in solid dewetting.

References

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An immersed finite volume element method for interface problems and its applications

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ABSTRACT

An immersed finite volume element method is developed to solve 2D elliptic interface problems with a variable coefficient that has a finite jump across an interface. The numerical method consists of an immersed finite element method in the physical space and a sparse grid collocation method based on the Smolyak construction in the probability space is proposed for solving elliptic PDEs with both random input and interfaces . At last, a immersed finite element method based on the variational discretization concept is applied to the optimal control problems of elliptic PDEs with interfaces. Numerical experiments demonstrate the convergence rates of the proposed method and confirm the theoretical results.