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Two-grid methods for semilinear elliptic interface problems by immersed finite element methods

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ABSTRACT

In this talk, two efficient two-grid algorithms are proposed and analyzed for semi-linear interface problems with discontinuous diffusion coefficients in two dimension. Because of the advantages of simple structure of Cartesian grids and the finite element formulation, we use immersed finite element discretization. To linearize the finite element method equations, two-grid algorithms based on some Newton iteration approach and residual-correction technique are applied. It is shown that the coarse space can be extremely coarse, and yet one can still achieve asymptotically optimal approximations as good as solving the original nonlinear problem on the fine mesh. As a result, solving such a large class of nonlinear equation will not be much more difficult than solving one linearized equation.

Thermodynamic-consistent multiple-relaxation-time lattice Boltzmann equation model for nonideal fluids with Peng-Robinson equation of state

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ABSTRACT

In this work, a multiple-relaxation-time (MRT) lattice Boltzmann (LB) equation model with Beam-Warming (B-W) scheme is proposed to simulate multiphase fluid system with Peng-Robinson (P-R) equation of state (EOS). The mathematical model of the multi-phase fluid flow is derived based on the NVT-based framework, where the Helmholtz free energy of P-R fluid is introduced. The nonideal force in multi-phase flow is directly computed from the free energy so that a more compact formulation of hydrodynamic equations, which is termed as potential form, can be obtained. The MRT-LB model is developed based on the potential form of hydrodynamic equations, which can eliminates the parasitic currents effectively. In addition, to capture the tiny nonconvex perturbation from the linear trend of P-R model precisely, the B-W scheme is utilized in the present MRT-LB model, which leads to an adjustable Courant-Friedrichs-Lewy (CFL) number and the second order accuracy can be naturally achieved by this scheme without any other requirement and numerical boundary conditions. In the numerical experiments, a realistic hydrocarbon component, such as isobutane, in three dimensional space is simulated by the proposed MRT-LB model. Numerical results show that the magnitude of parasitic currents can be significantly reduced by the present MRT-LB model. In addition, our numerical predictions of surface tension agree well with the experimental data, which verify the effectiveness of the proposed MRT-LB model.

Equation-of-State Based Diffuse Interface Modeling of Multi-Component Two-Phase Flow with Partial Miscibility

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ABSTRACT

Petroleum reservoir engineers spent great efforts studying the flow of fluid mixture involving two or multiple phases, where oil, gas and water are often produced and transported together. Darcy's law based field-scale simulation has conventionally and routinely used for this purpose, but this approach requires a number of poorly known parameters including absolute permeability, relative permeability and capillary pressure. In recent decades, advancement of digital rock technology allows pore-scale simulation of single-phase and two-phase flows, which can be used to predict absolute permeability, relative permeability, capillary pressure and many others. However, very little work has been done for the pore-scale simulation of two-phase systems with **partial miscibility**. In this work, we consider two-phase flow with partial miscibility at a pore scale. Specifically, we study the modeling and simulation of possibly compressible, partially miscible, fully compositional two-phase hydrocarbon systems using a diffuse interface model together with Peng-Robinson Equation of State (EOS). This research has an eventual goal of applying to realistic modeling of petroleum and other reservoir fluids in pores or pore networks within geological formation. Our model is based on the coupling of the Navier-Stokes equation for flow and a Cahn-Hilliard-like equation with Peng-Robinson chemical potentials for phase behaviors of hydrocarbon fluids, and the entire modeling approach is self-consistent and complies with the principles of non-equilibrium thermodynamics including the second law of thermodynamics and the Onsager reciprocity principle. To solve the continuum model expressed as a coupled nonlinear partial differential equation (PDE) system, we propose an efficient numerical solution strategy, focusing on discrete energy stability, local mass conservation and numerical accuracy. We compare our computational results with laboratory experimental data reported in the literature, which have good agreement. This report is partially based on joint work with Xiaolin Fan (KAUST), Jisheng Kou (Hubei Eng. U.), Yiteng Li (KAUST), Zhonghua Qiao (HK PolyU), and Tao Zhang (KAUST).

Asymptotic analysis and numerical method for singularly perturbed eigenvalue problems

Zhongyi Huang

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ABSTRACT

In this talk, we study the asymptotic analysis and numerical method for singularly perturbed eigenvalue problems (SPEP) which arise in fluid mechanics and quantum mechanics. We first make a close asymptotic analysis on the SPEP, and prove the main theorems about the asymptotic behavior of the eigenvalues and eigenfunctions. Then we introduce a new tailored finite point method (TFPM) for numerical solutions of SPEP with higher accuracy. Our numerical examples verify our theory and show the feasibility and efficiency of our method.

Time domain modeling and computation for waves in some complex mediums

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ABSTRACT

In this talk, we first introduce several models describing waves in some complex mediums, including waves in incompressible liquid medium, electromagnetic waves in compressible and incompressible fluids, electromagnetic waves in metals, elastic waves in porous medium. We design and analyze discontinuous or continuous Galerkin schemes for numerical solutions of these models, and numerical results will be presented to illustrate the accuracy and efficiency of the proposed scheme.

A new numerical method for the study of liquid-vapor transition

Wenqi Yao

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ABSTRACT

The hydrodynamical fluctuation included diffuse interface model is an effective model to describe noise induced phase transition in liquid-vapor isothermal system. This system is obviously non-gradient by using macroscopic density and velocity as the system coordinates, and the phase transition between metastable states of the system could be studied via Minimum Action Method. By introducing smoothed particle hydrodynamics, the original macroscopic equations could be interpolated with those smoothed particles, and the Minimum Energy Path in the N smoothed particle Langevin system is theoretically obtained. A new numerical method for searching of Minimum Action Path in the interpolated system is proposed, which is efficient as the String Method and robust as the Minimum Action Method. Two typical numerical examples on liquid-vapor transition are subsequently studied to verify the feasibility of the new numerical method, one of which is a isolate system without external force exerted, while the other is in a external force field which is generated by a delicately designed potential to introduce shear flow in the system.

Story on the Ericksen-Leslie system of liquid crystal with and without the penalty function

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ABSTRACT

Here we will talk about the story the Ericksen-Leslie system of liquid crystal with and without the penalty function. What is the advantage and disadvantage of the model with and without the penalty function, including the different numerical approach and phenomena. We present the development and interaction of the defects. These results are partly consistent with the observation from the experiments. Thus this scheme illustrates, to some extent, the kinematic effects of the defects.

Maximum principle preserving exponential time differencing schemes for the nonlocal Allen-Cahn equation

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ABSTRACT

The nonlocal Allen-Cahn (NAC) equation is a generalization of the classic Allen-Cahn equation by replacing the Laplacian with a parameterized nonlocal diffusion operator, and satisfies the maximum principle as its local counterpart. In this talk, we develop and analyze first and second order exponential time differencing (ETD) schemes for solving the NAC equation, which unconditionally preserve the discrete maximum principle. The fully discrete numerical schemes are obtained by applying the stabilized ETD approximations for time integration with the quadrature-based finite difference discretization in space. We derive their respective optimal maximum-norm error estimates and further show that the proposed schemes are asymptotic compatible, i.e., the approximate solutions always converge to the classic Allen-Cahn solution when the horizon, the spatial mesh size and the time step size goes to zero. We also prove that the schemes are energy stable in the discrete sense. Various experiments are performed to verify these theoretical results and to investigate numerically the relationship between the discontinuities and the nonlocal parameters.

A Boundary Integral Equation Method for the Laplace Equation with Dynamic Boundary Conditions

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ABSTRACT

We present a numerical algorithm for the accurate and efficient solution of the Laplace equation with dynamic boundary conditions on complex geometry, which represents a primitive model for the moving contact lines, electro-wetting, and more general interactions of fluids with solid boundaries. We reformulate the partial differential equation to a time-dependent boundary integral equation using layer potentials where the unknowns are only defined on the boundary of the domain, and study the stability of the numerical discretization and its efficient solution. In particular, we show how existing state-of-the-art techniques for near-singular and singular integrals can significantly change the high frequency spectrum of the integral operators, which will cause numerical instability and unphysical solutions in the dynamic simulations. We present techniques to avoid the instability, and justify our analysis and demonstrate the accuracy and efficiency of the algorithm through several numerical experiments.

Solid-state dewetting on curved substrates

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ABSTRACT

Employing a thermodynamic variational method, we propose a sharp interface model combined with a relaxed contact angle boundary condition for simulating solid-state dewetting of thin films on rigid curved substrates. In this model, film/vapor interfacial anisotropy is easily included, and the movement of the contact line can be explicitly described by the relaxed boundary condition. We implement the model by a semi-implicit parametric finite element method to study the equilibrium configuration of small islands and the pinch-off of large islands. We also apply the model to simulate the migration of tiny particle and the templated solid-state dewetting on inverted pyramidal pits. The simulation results capture many of the complexities associated with solid-state dewetting experiments.

Sharp interface models for solid-state dewetting and their applications

Quan Zhao

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ABSTRACT

Solid-state dewetting is a ubiquitous physical phenomenon occurring in the solid-solid-vapor system. The solid thin film on the substrate is typically unstable and exhibits complex morphological evolutions, including hole formation, edge retraction, rim pinch-off and so on. In this thesis, we develop mathematical models and efficient numerical schemes for simulating the solid-state dewetting, and the problem is approached in both 2D and 3D via the Cahn-Hoffman $\boldsymbol{\xi}$-vector formulation. The sharp interface models are rigorously derived based on the thermodynamic variation, which includes the surface diffusion flow and moving contact line. The governing equations for the model belong to fourth order geometric partial differential equations with proper boundary conditions such that the total volume is conserved and total surface energy is dissipative. Besides, a semi-implicit parametric finite element method is proposed for solving the models efficiently. Numerical examples are presented to show consistent morphological evolutions observed in physical experiments.

Efficient Methods for Homogenization of Random Heterogeneous Materials

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ABSTRACT

Predicting homogeneous coefficients of random heterogeneous materials involves solving auxiliary problems in volume element. The accuracy of homogeneous coefficients depends not only on the size of volume element, but also on the boundary condition. Dirichlet and Neumann boundary conditions give upper and lower bounds of real homogeneous coefficients respectively. But when the contrast ratio of high and low coefficients is large, these upper and lower bounds will be too broad to predict the homogeneous coefficients. We propose a new boundary condition constructed by combining Dirichlet and Neumann boundary conditions —— Robin boundary condition. As the volume element size goes to infinity, t he c onvergence o f t he a pproximate h omogeneous coefficients under Robin boundary condition is shown. Numerical examples demonstrate that the results lie in that of Dirichlet and Neumann boundary conditions. And by choosing proper parameter, Robin boundary condition does better than Dirichlet-Neumann mixed boundary condition and it may be an optimal boundary condition.

Liquid droplets on soft elastic substrates

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ABSTRACT

A liquid droplet can deform the elastic solid substrate due to the capillary forces. Recent experiments and atomistic simulations considering liquid on soft elastic substrates demonstrate many interesting phenomenon such as the geometry near the contact line, the deformation shape of the elastic solid, and the spreading dynamics. We consider a two-dimensional system of a liquid droplet on a semi-infinite incompressible elastic substrate. A mathematical modelling is established to find the equilibrium shapes of the liquid droplet and elastic substrate. Evolution equations are derived by the variational calculus of the total energy of the system. Based on this model, we also study the dynamics of the contact line in this system for different initial droplet configurations. Numerical simulations and their comparisons to experimental results will be presented.

Discretization and Modelling of the Non-cutoff Boltzmann Collision Operator Using Hermite Spectral method

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ABSTRACT

Based on the Hermite expansion of the distribution function, we introduce a Galerkin spectral method for the spatially homogeneous Boltzmann equation with the non-cutoff inverse-power-law models. A practical algorithm is proposed to evaluate the coefficients in the spectral method with high accuracy, and these coefficients are also used to construct new computationally affordable collision models. Numerical experiments show that our method captures the low-order moments very efficiently. It is probably the first time that a non-cutoff collision operator is simulated numerically. These new collision models are applied to the simulation of Couette flows and the numerical results match the results from Monte-Carlo method very well.

References

[1] Wang Y. and Cai Z., *Approximation of the Boltzmann Collision Operator Based on Hermite Spectral Method*, submitted, arXiv: 1803.11191.

A generalized MBO diffusion generated method for constrained harmonic maps

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ABSTRACT

A variety of tasks in inverse problems and data analysis can be formulated as the variational problem of minimizing the Dirichlet energy of a function that takes values in a certain submanifold and possibly satisfies additional constraints. These additional constraints may be used to enforce fidelity to data or other structural constraints arising in the particular problem considered. I'll present a generalization of the Merriman-Bence-Osher (MBO) method for minimizing such a functional. I'll give examples of how this method can be used for finding Dirichlet partitions and constructing smooth orthogonal matrix valued functions. For the second problem, I'll prove the stability of the method by introducing an appropriate Lyapunov function, generalizing a result of Esedoglu and Otto to matrix-valued functions. I'll also state a convergence result for the method. This is joint work with Braxton Osting.

References

[1] Dong Wang and Braxton Osting, *A diffusion generated method for computing Dirichlet partitions*, submitted 2018.

[2] Braxton Osting and Dong Wang, *A generalized MBO diffusion generated motion for orthogonal matrix-valued fields*, submitted 2017.