1 Introduction

My research interests are in Computational and Applied Mathematics. In particular, I work on the development of accurate and efficient numerical methods for solving partial differential equations (PDEs). My other main research focus is the development of reliable mathematical models based on PDEs with applications to problems in material sciences, biology and fluid dynamics, as well as on mathematical analysis of the developed models.

2 Methods based on Difference Potentials

Highly-accurate numerical methods that can efficiently handle irregular and evolving geometries, as well as interface problems (usually described by mathematical models that have input data and solutions with discontinuities/non-smoothness across the interfaces), are crucial for the resolution of different temporal and spatial scales of physical, biological, biomedical problems, and problems from material sciences (models for composite materials, fluids, chemotaxis models, biofilms), to name a few. The major challenge here is to design a robust method that accurately captures certain properties of the solutions in different domains/subdomains (different regularity of the solutions in the domains, positivity, etc.), while handling the arbitrary geometries of the domains/subdomains. Moreover, any standard numerical method designed for smooth solutions, in general and in any dimension, will fail to produce accurate solutions to interface problems due to discontinuities in the model’s parameters/solutions.

In spite of great advances in the past 40 years in the numerical methods for problems in arbitrary domains and/or interface problems, it is still a challenge to develop efficient numerical algorithms that can deliver high-order accuracy in space, and that can handle general boundary/interface conditions. Therefore, some of my current research is focused on the development and analysis of efficient and high-order accurate numerical methods based on Difference Potentials for the elliptic, parabolic and some nonlinear PDEs in domains with complex geometries and/or with interfaces.

Difference Potentials Method (DPM) can be understood as the discrete version of the method of generalized Calderon’s potentials and Calderon’s boundary equations with projections in the theory of PDEs. DPM introduces computationally simple auxiliary domain. The original domain of the problem is embedded into an auxiliary domain, and the auxiliary domain is discretized using Cartesian grids. After that, the main idea of DPM is to define a Difference Potentials operator, and to reformulate the original discretized PDEs (without imposed boundary conditions yet) as an equivalent discrete generalized Calderon’s boundary equations with projections (BEP). These BEP are supplemented by the given boundary conditions (the resulting BEP are always well-posed, as long as the original problem is well-posed), and solved to obtain the values of the solution at the points near the continuous boundary of the original domain (at the points of the discrete grid boundary which approximates the continuous boundary from the inside and outside of the domain). Using the obtained values of the solution at the discrete grid boundary, the approximation to the solution in the original domain is constructed through the discrete generalized Green’s formula. DPM offers geometric flexibility (without the use of unstructured meshes or “body-fitted” meshes), but does not require explicit knowledge of the fundamental solution, is not limited by the constant coefficient problems, does not involve singular integrals, and can handle general boundary and/or interface conditions [40, 38].
Difference Potentials Method (DPM) for Chemotaxis Models: Chemotaxis refers to mechanisms by which cellular motion occurs in response to an external stimulus, usually a chemical one. Chemotaxis is an important process in many medical and biological applications, such as bacteria/cell aggregation, pattern formation mechanisms, and tumor growth. The mathematical models of chemotaxis are usually described by highly nonlinear time dependent systems of PDEs, which in general can only be solved by numerical methods. Moreover, a common property of many existing chemotaxis systems is their ability to model a concentration phenomenon that mathematically results in rapid growth of solutions in small neighborhoods of concentration points/curves. The solutions may blow up or may exhibit a very singular, spiky behavior. This blow-up represents a mathematical description of a cell concentration phenomenon that occurs in real biological systems. In either case, capturing such solutions numerically is a very challenging problem. Moreover, often, modeling of real biomedical problems has to deal with the complex structure of the computational domains. Therefore, there is a need for accurate, fast, and computationally efficient numerical methods for different chemotaxis models that can handle arbitrary geometries.

Several numerical methods have been proposed in the literature for the chemotaxis models but only a few for models in irregular domains (for a more detailed review see for example [16]). In our previous work [24, 21, 23], we developed discontinuous Galerkin method (DG) for the Patlak-Keller-Segel chemotaxis model which was designed to handle rectangular domains. However, in spite of many advantages (see for example [34]), some known drawbacks with the discontinuous Galerkin schemes are their high memory and computational costs, as well as their involved implementation compared to continuous Galerkin finite element, finite volume, or finite difference methods.

Therefore, in our work [16, 15], we develop a novel and efficient upwind-difference potentials method that can handle irregular geometry without the use of unstructured meshes (with the consideration of only Cartesian grids), and that can be employed with fast Poisson solvers. Our method combines the simplicity of positivity-preserving upwind scheme for chemotaxis models on Cartesian meshes [12] with the geometric flexibility and efficiency of the difference potentials method. The extension of the developed methods in [16, 15, 12] to high-order efficient numerical schemes for chemotaxis models in irregular domains will be part of our future research.

DPM for Problems in Composite Domains/Models with Interfaces: In [41, 39, 29, 22], we developed an efficient Algorithms Composition Approach based on DPM for 2D Poisson and 2D heat equations in irregular domains and with curved interfaces (these problems play the role of simplified models for more realistic systems of materials, chemicals, or fluids). The developed methods are second-order accurate in space and first-order in time (for the heat equation). The complexity of the approach reduces to the solutions of simple auxiliary problems on Cartesian grids. Compared to some established finite difference methods for problems in irregular domains and interface problems, our algorithms are not restricted by the type of boundary or interface conditions (as long as the continuous problem is well-posed). The methods are well-suited for parallel computations and can be applied to interface problems, heterogeneous models from biology, material sciences, etc. The work was the first extension of the Difference Potentials approach to elliptic and parabolic interface/composite domains problems, see [41, 39, 29] (2D Poisson problems) and [22] (2D heat equations).

High-Order Accurate DPM for Elliptic and Parabolic Composite Domains/Interface Models: In [4] with J. Albright and K. Steffen (Ph.D students), and in [18] with S. Phippen (REU student), we employed 1D parabolic [4] and 1D elliptic type models [18] as a starting point to develop and numerically test the second-order and the fourth-order accurate in space DPM for
variable coefficient parabolic and elliptic composite domains/interface models. While the method and analysis are simpler for the 1D problems, they illustrate and test the main ideas/properties of high-order accurate DPM. The performance of the proposed second-order and fourth-order DPM, as well as a comparison of the second-order DPM with the second-order Immersed Interface Method (IIM) are illustrated in numerical tests [18, 4]. The work [18, 4] was the first extension of high-order accurate (higher than second-order in space) DPM to interface/composite domains models.

Our ongoing work on high-order (second-order and fourth-order accurate) DPM in [17] is the extension of the work in [18, 41, 39, 29] to 2D variable coefficients elliptic interface problems.

**Current and Future Research:** As the next/future research steps, we plan to further develop and extend the work in [41, 39, 29, 16, 15, 22, 18, 4, 17] to high-order methods for variable coefficient elliptic and parabolic models in 2D and 3D domains with complex geometries and/or with interfaces. We anticipate that the constructed high-order numerical methods will handle general boundary/interface conditions. Moreover, we also plan to apply/adapt the developed efficient and high-order accurate schemes to the solution of Stefan’s type problems, multi-physics problems (such as Stokes-Darcy and Navier-Stokes/Darcy problems), as well as to the solution of biological models (chemotaxis models and blood flow models) in domains with irregular/complex geometry.

3 Materials Microstructures

Another major effort of my recent and ongoing research work is the mathematical and computational modeling and analysis of polycrystalline materials. In particular, together with my collaborators I have been working on the development of a predictive mathematical theory of microstructure evolution and texture development in polycrystalline materials.

Cellular networks are ubiquitous in nature. They exhibit behavior on many different length and time scales and are usually metastable. Most technologically useful materials are polycrystalline microstructures composed of a myriad of small monocrystalline grains separated by interfaces called grain boundaries, and thus comprise cellular networks. The energetics and connectivity of the grain boundary network plays a crucial role in determining the properties of a material across a wide range of scales. A central problem in materials is to develop technologies capable of producing an arrangement of grains that provides for a desired set of material properties. Traditionally the focus has been on distributions of geometric features, like cell size, and a preferred distribution of grain orientations, termed texture. Attaining these gives the configuration order in a statistical sense. More recent mesoscale experiment and simulation permit harvesting large amounts of information about both geometric features and crystallography of the boundary network in material microstructures, [2, 1, 31, 36, 37]. This has led to the discovery and notion of the Grain Boundary Character Distribution (GBCD) [2, 1, 31, 36, 37].

The GBCD is an empirical distribution of the relative length (in 2D) or area (in 3D) of interface with a given lattice misorientation and grain boundary normal. It is a leading candidate to characterize texture of the boundary network [2, 1, 31, 36, 37]. During the growth process, an initially random grain boundary arrangement reaches a steady state that is strongly correlated to the interfacial energy density. In simulation, a stationary GBCD is always found. Moreover there is consistency between experimental GBCD’s and simulated GBCD’s. The boundary network of a cellular structure is naturally ordered.

In the special situation where given interfacial energy depends only on lattice misorientation, the steady state GBCD and the interfacial energy density are related by a Boltzmann distribution. This is among the simplest non-random distributions, corresponding to independent trials with respect to the density. Such straightforward dependence between the character distribution and
Figure 1: Left figure - example of an instant during the simulated evolution of a cellular network. This is from a small simulation with constant energy density and periodic conditions at the border of the configuration. Right figure - an arc $\Gamma$ with normal $n$, tangent $b$, and lattice misorientation $\alpha$, illustrating lattice elements.

the interfacial energy offers evidence that the GBCD is a material property. Why does such a simple distribution emerge from such a complex system?

The main result of our work in \cite{8, 5, 6, 9, 10, 7} has been the derivation of a new entropy based theory, which suggests that the evolving GBCD satisfies a Fokker-Planck Equation, an equation whose stationary state is a Boltzmann distribution.

Coarsening in polycrystalline systems is a complicated process involving details of material structure, chemistry, arrangement of grains in the configuration, and environment. In this context, we consider just two competing global features, as articulated by C. S. Smith \cite{42}: cell growth according to a local evolution law and space filling constraints. We impose curvature driven growth for the local evolution law, cf. Mullins \cite{33}. Space filling requirements are managed by critical events, rearrangements of the network involving deletion of small contracting cells and facets. The interaction between the evolution law and the constraints is governed primarily by the balance of forces at triple junctions. This balance of forces, often referred to as the Herring Condition \cite{30}, is the natural boundary condition associated with the equations of curvature driven growth. It determines a dissipation relation for the network as a whole. The properties of this system that characterize the GBCD must be identified and appropriately upscaled or ‘coarse-grained’. For a perspective on these issues, see also the article by R. V. Kohn \cite{32}.

Therefore, to understand the evolution of GBCD, we assumed in our work \cite{8, 5, 6, 9, 10, 7}, that the interfacial energy density $\psi = \psi(\alpha)$ depends only on the misorientation of the interface $\alpha$, and employed a 1D simplified critical event model that is driven by the boundary conditions, and reflects the dissipation relation of the grain growth system. This simplified critical event system is more accessible for analysis. It resembles an ensemble of inertia-free spring-mass-dashpots. For this simpler network, we derived in \cite{8, 5, 6, 9, 10, 7} a new entropy-based theory to suggest that the evolving GBCD satisfies a Fokker-Planck Equation. The cornerstone of our analysis is a novel implementation of the iterative scheme for the Fokker-Planck Equation in terms of the system free energy and a Kantorovich-Rubinstein-Wasserstein metric. The developed theory predicts the results for GBCD of our 2-D large scale simulations and is consistent with the experiments.

Current and Future Research: Currently, we are investigating the Large Deviation approach to further develop the derived mathematical theory for GBCD in \cite{8, 5, 6, 9, 10, 7}. Among other important questions that we study is the development of a theory for GBCD when the interfacial energy density $\psi = \psi(\theta, \alpha)$ depends on both the normal orientation (normal angle) $\theta$, and the misorientation of the interface $\alpha$ (in reality no material has an interfacial energy density which depends only on misorientation. However this simplified assumption is a very effective starting model to study the role of anisotropy).
4 Numerical Schemes based on Hybrid Variational Principle for Chemotaxis Models and Closely Related Problems

An additional direction of my research involves the design of numerical schemes based on the hybrid-variational approach to the Patlak-Keller-Segel chemotaxis model, and closely related systems in one-dimension (as the starting point). In [13], we consider the solution to Patlak-Keller-Segel model in terms of an implicit scheme, or generalized gradient flow, for a natural free energy. The considered hybrid variational method is based on a finite-difference-type scheme for the concentration, and Monge-Kantorovich-Wasserstein method for the density. This hybrid variational method defines a very robust numerical scheme that satisfies both positivity for the density and concentration, mass conservation property for the density, and inherits the energy minimizing properties of the original problem. We anticipate that the designed numerical schemes could provide a very attractive alternative to “conventional methods”.

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5 Numerical Methods for Shallow Water Models

Recently, shallow water models and closely related geophysical applications have also become one of my research interests. Together with my collaborators I am working on the development of efficient and accurate numerical methods for the Saint-Venant system of shallow water equations, and related models in domains with complex geometry. These models arise in a wide variety of applications ranging from coastal and hydraulic engineering, to modeling many atmospheric and oceanographic phenomena including hurricanes/typhoons and tsunamis.

The Saint-Venant system is a hyperbolic system of balance laws. The development of the accurate and efficient numerical methods for the computation of the solutions to shallow water models is a very important and challenging active area of research. One of the difficulties encountered is the fact that the Saint-Venant system of shallow water equations admits non smooth solutions: shocks, rarefaction waves and, when the bottom topography function is discontinuous, contact discontinuities. In the latter case, the solution may not be unique, which makes the design of robust numerical methods more challenging even in the one-dimensional case (see [11] for more details).

To design a good numerical method for the Saint-Venant system, one has to preserve a delicate balance between the flux and the source terms (in other words, the scheme must be well-balanced) to prevent the appearance of the so-called “numerical storm” - when artificial numerical waves have a larger magnitude than the actual water waves to be captured. It is also crucial to design a scheme that can handle dry/almost dry areas without producing negative water depth, that is, the scheme must be positivity preserving. Furthermore, many real world engineering applications have to deal with models in domains with complex geometry, and the design of the accurate numerical scheme becomes even more difficult task in this case.

In [11, 3] we developed a second-order well-balanced positivity preserving central-upwind scheme for computing the solutions of the Saint-Venant system on triangular grids (work [3] is an improved scheme from [11] with a more accurate reconstruction of “dry”/”almost dry states” (waves arriving or leaving the shore)). Moreover, the developed scheme [11, 3] is well-suited for models with discontinuous bottom topography and irregular channel widths.

**Future Research:** As a future extension of the developed numerical method for shallow water
models [11, 3], we plan to design a local mesh refinement strategy (local $h$-refinement) to improve the efficiency and the resolution of the scheme on domains with complex geometry, as well as extend the developed method to other shallow water models, for example, the Ripa system of shallow water equations with horizontal temperature gradients and shallow water systems with Coriolis forces.

Besides the current research mentioned above, previously I was also involved in several other projects: my Ph.D. research under the guidance of Prof. Béatrice Rivièere focused on the numerical simulation and analysis of different models of incompressible two-phase flow in porous media [19, 20, 27, 26] - we developed an implicit fully coupled hp-version of discontinuous Galerkin methods (DG) for these models. In [25], we studied one of the primal DG methods, symmetric interior penalty Galerkin method (SIPG) applied to elliptic PDEs. In this work, [25], we obtained lower bounds on the penalty parameters above which SIPG will produce stable and convergent numerical solutions.

In [14], we developed the mathematical analysis of the Stolz-Adams approximate deconvolution model for Large Eddy Simulations (LES).

In [28, 35], we developed a mathematical model of signaling (this was a collaborative work with University of Pittsburgh Medical School (UPMC)).

References


