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 materials science, biology and fluid dynamics, as well as on mathematical analysis of the developed models.

2 Materials Microstructures

One of the major efforts of my recent and current research work is data-driven 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 theory of microstructure evolution 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 cells/grains separated by interfaces called grain boundaries, and thus comprise cellular networks, see Fig. 2. The energetics and connectivity of the grain boundary network play a crucial role in determining the properties of a material across multiple scales. Therefore, a grand challenge problem in engineering of polycrystals is the development and implementation of processing technologies to create a microstructure associated with desirable materials properties.

One method of grain structure engineering is via the promotion of grain growth or coarsening from a starting structure, a process that can be viewed as the evolution of a large metastable grain network. 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 [57]: cell growth according to a local evolution law and space filling constraints. In such case, the process may be mathematically described by a set of deterministic local evolution laws for the growth of an individual grain (area of the grain in 2D/volume of the grain in 3D) combined with deterministic and stochastic models to describe grain interactions (e.g., grain deletion, facet interchange).

Traditionally, during grain growth, the focus has been on understanding the 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 experiments and simulations permit harvesting large amounts of information about both the geometric features and crystallography of the boundary network in material microstructures, [2, 1, 39, 52, 53]. This has led to the discovery and notion of the Grain Boundary Character Distribution (GBCD) [2, 1, 39, 52, 53].

The GBCD is an empirical distribution of the relative length (in 2D) or area (in 3D) of interface with a given lattice misorientation (difference in the orientation between two neighboring grains that share the grain boundary) and grain boundary normal. It was discovered that the GBCD can be viewed as a leading statistical descriptor to characterize the texture of the grain boundary network, e.g. [2, 1, 39, 52, 53]. During the growth process, an initially random grain boundary arrangement ultimately reaches a state (described by the GBCD) that is inversely related to the
grain-boundary energy density. In simulation, a stationary GBCD is always observed, [40], [8], [12], [6], [27]. Moreover there is consistency between experimental GBCD's and simulated GBCD's, [52].

Furthermore, it was also observed that in the special situation where the given grain boundary energy density depends only on lattice misorientation, the steady-state GBCD and the energy density are related by a Boltzmann distribution. This offers compelling evidence that the GBCD is a material property. Why does such a simple distribution emerge from such a complex system? To understand this pattern of the cellular network described by the GBCD, in our work [9], [8], [12], [7], [6], and for a perspective on the topic, see also the article by R. V. Kohn [41], using a simplified one-dimensional “coarse-grained” model of grain growth and assuming that the interfacial energy density $\psi = \psi(\alpha)$ depends only on the misorientation of the interface $\alpha$, we derived a new entropy based theory for the evolution of the GBCD.

The developed theory suggests that the evolving GBCD satisfies a Fokker-Planck Equation, an equation whose stationary state is a Boltzmann distribution:

$$\nu \frac{\partial \rho}{\partial t} = \frac{\partial}{\partial \alpha} \left( \sigma \frac{\partial \rho}{\partial \alpha} + \psi' \rho \right) \text{ in } \Omega, \quad 0 < t < \infty, \quad (2.1)$$

and, see Fig. 1. In Fokker-Planck equation above (2.1), $\alpha$ denotes the misorientation, $\rho(\alpha, t)$ is the GBCD (scaled to be a probability density), $\psi(\alpha)$ is the grain boundary energy density, $\sigma$ is a diffusion coefficient and $\nu$ is a positive constant. One of the cornerstones of our analysis in [9], [8], [12], [7], [6] was 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 theory [9], [8], [12], [7], [6] for the 1D simplified coarsening system predicts the results for the GBCD of our 2D large-scale computations, see Fig. 1 (simulations) and is consistent with the experiments [52], [46], [49].

In our recent work, [28], we propose a new model for the evolution of the 2D grain-boundary network with finite mobility of the triple junctions (triple junctions are where three grain boundaries meet) and with dynamic lattice misorientations (possibility of grain rotations). In [28], using the energetic variational approach, we derive a system of geometric differential equations to describe the motion of such grain boundaries, and we establish a local well-posedness result, as well as large time asymptotic behavior for the model. In addition, similar to our work on GBCD [8], we conducted several numerical experiments for the 2D grain boundary network in order to further illustrate the effect of relaxation time scales, e.g. of the curvature of grain boundaries, mobility of triple junctions, and dynamics of misorientations on how the grain boundary system decays energy and coarsens with time [27], [11]. In [11], we also presented and discussed relevant experimental results of grain growth in thin films.

Moreover, in our work [12], we further developed and improved a sharp interface structure-preserving algorithm for grain growth simulation in 2D, first proposed in [40]. The 2D sharp interface algorithms [12], [6], [27] are based on a variational principle which assures the discrete dissipation inequality for the total grain boundary energy, and hence ensures the important stability properties of the algorithms. In addition, explicit front-tracking methods, like numerical algorithms in our work [12], [6], [27] make it possible to study effects of different time scales such as those for boundary migration, grain rotations and mobility of the triple junctions on grain growth, as well to handle full system anisotropy accurately.

Figure 1: Average over 10 1D trials with $2^{18}$ initial boundaries (left) and over 10 2D trials with $2 \cdot 10^4$ initial boundaries (right): Comparison of the GBCD (blue) with the Fokker-Planck solution (2.1) (red) as functions of misorientation $\alpha$ (x-axis) at times corresponding to 20%, 40%, 60% and 80% removal of the initial boundaries, [6].
Figure 2: Left figure - experimental microstructure: bright-field transmission electron micrograph of a polycrystalline platinum (Pt) film from an instance of an in-situ experiment [10]. Middle figure - microstructure from simulation: example of a time instance during the simulated evolution of a cellular network. Right figure - a zoom on three grain boundaries that meet at a single triple junction TJ: an arc Γ (represents one of the grain boundary) with normal n, tangent b, and lattice misorientation α, illustrating lattice elements [8, 6, 28, 27].

Current and Future Research: In [29], we are further extending our work in [28, 27] and developing a 2D stochastic model of grain growth with finite mobility of the triple junctions and with dynamic misorientations. Currently, we are working on large time asymptotic analysis of the proposed stochastic model and we expect to use the new stochastic model as a part of the theory development for the evolution of the GBCD of the 2D grain boundary system (this work is motivated by our work in [9, 8, 12, 7, 6]). Future work will include experimental studies to validate the developed mathematical models in [28, 27, 29]. In particular, new in-situ experiments [10] will allow us to capture accurate dynamics of grain growth during experiments, which will be an important part of the validation step of the proposed models. We are also working on developing an efficient sharp interface numerical algorithm and simulation that can deliver accurate approximation of microstructure evolution during coarsening of the polycrystalline system in 3D. The algorithm development is based on the extension of previously developed 2D algorithms and simulations [12, 6, 27]. The 2D and 3D grain growth computational models will be closely integrated with experimental data and will guide modeling, analysis and experiments. Using developed data-driven mathematical and computational models of grain growth, we will study the evolution laws/derive master equations for various statistical metrics of coarsening and look for possible connections between these metrics and their links to materials properties. The ultimate goal of our research is to improve the understanding of grain growth mechanisms and to develop a predictive theory of grain growth (coarsening) in polycrystalline materials.

This work is interdisciplinary, and is currently partially supported by collaborative research NSF grant DMS-1905463/DMS-1905492. It was also previously partially supported by my Simons Foundation grant No. 415673 and by my NSF grant DMS-1112984.

3 Methods based on Difference Potentials

Highly-accurate numerical methods that can efficiently handle irregular and evolving geometries, as well as interface problems are crucial for the resolution of different temporal and spatial scales of physical, biological, biomedical problems, and problems from materials science (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 may fail to produce accurate solutions to interface problems due to possible discontinuities in the model’s parameters/solutions.

In spite of great advances 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 recent and 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 [56, 54]. DPM introduces a computationally simple auxiliary domain. The original domain of the problem is embedded into this simple 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.

**Accurate and efficient Difference Potentials methods for chemotaxis systems in 2D and 3D:** Chemotaxis refers to mechanisms by which cellular motion happens 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 known property of many existing chemotaxis systems is their ability to model a concentration phenomenon that mathematically results in a fast growth of solutions in small regions of concentration points/curves. The solutions may blow up or may exhibit a very singular behavior. This blow-up can be viewed as a mathematical description of a cell concentration phenomenon that occurs in real biological systems. Capturing such singular/“spiky” 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.

In our work [20, 19, 37], we developed novel, efficient and accurate difference potentials based
methods 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. The proposed methods [20, 19, 37] combine the simplicity of the second-order positivity-preserving hybrid finite-volume-finite-difference schemes in space (the hybrid finite-volume-finite-difference schemes in space [20, 19] are modified versions/extensions of the scheme from [14]) with the geometric flexibility and efficiency of the difference potentials method. Moreover, in [37], under suitable conditions, we established the positivity-preserving property of the proposed numerical method in irregular bounded domains in 3D. In addition, to further enhance computational efficiency of the method in 3D, we developed a new accurate non-iterative Difference-Potentials based domain decomposition method that allows mesh adaptivity and easy parallelization of the algorithm in space [37] and see also Fig. 3.

In addition, our previous work also included the development of discontinuous Galerkin (DG) method for the Patlak-Keller-Segel chemotaxis model [26, 23, 25] on rectangular domains. However, in spite of many attractive features of DG methods, including their high-order accuracy (e.g., [50]), these methods can be computationally expensive. Hence, in [15], we developed simpler and more efficient high-order positivity-preserving hybrid finite-volume-finite-difference methods for chemotaxis models on rectangular domains.

**High-order accurate Difference Potentials based algorithms for elliptic and parabolic composite domains/interface models in 2D and for models with dynamic boundary conditions and bulk-surface problems in 3D:** In [55, 24, 32, 4, 30, 3, 5], high-order accurate and fast numerical methods have been developed for elliptic and parabolic interface model problems, the methods in [55, 24, 30, 3, 5] are designed for models in 2D domains with irregular geometry. The designed algorithms use structured meshes, allow easy parallelization and adaptivity in space. In addition, in [47], we considered a set of benchmark problems for linear parabolic problems on single and composite domains in 2D, and compared with respect to accuracy and efficiency of the developed Difference Potentials-based methods with Cut Finite Element method (Cut-FEM), and with summation-by-parts SAT Finite Difference Method (SBP-SAT-FD). In recent work [38], we considered parabolic models with dynamic boundary conditions and parabolic bulk-surface problems in 3D. Such PDEs based models describe phenomena that happen both on the surface and in the bulk/domain. These problems may appear in many important applications, ranging from cell dynamics in biology, to grain growth models in polycrystalline materials. In [38], using Difference Potentials method, we designed robust numerical algorithms for the approximation of such models. The developed algorithms efficiently and accurately handle the coupling of the models in the bulk and on the surface, approximate 3D irregular geometry in the bulk by the use of only Cartesian meshes, employ Fast Poisson Solvers, and utilize spectral approximation on the surface. Numerical tests illustrate the efficiency and high accuracy of the developed numerical algorithms.

**Current and Future Research:** Currently, we are extending ideas developed in [38] to be a part of numerical algorithm for 3D grain growth simulations (see Section 2). Moreover, in the future we also plan to apply/adapt the developed efficient and high-order accurate algorithms to the solution of multi-physics problems, as well as to the solution of biological/biomedical models defined in domains with irregular/complex geometry.

*The work in [20, 19, 24, 32, 4, 30, 3, 5, 37] was partially supported by my NSF grant DMS-1112984 and the work in [5, 47, 38] was partially supported by Simons Foundation grant No. 415673. The work in [47] was also partially supported by the Swedish Foundation for International Cooperation in Research and Higher Education Grant No. STINT-IB2016-6512 and the work [38] was also partially supported by my current NSF grant DMS-1905463.*
4 Structure-Preserving Numerical Methods for Shallow Water Models

Recently, shallow water models and closely related geophysical applications have also become one of my active research interests. Together with my collaborators I am working on the development of efficient structure-preserving numerical methods for shallow water equations in domains with irregular geometry and for shallow water systems with uncertainty, and related models. 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 development of accurate and efficient numerical methods for the computation of the solutions to shallow water models is an important and challenging active area of research. The “classical” example of shallow water models is the Saint-Venant system. The Saint-Venant system is a hyperbolic system of conservation/balance laws. 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 for example, [13] for more details). In addition, the accuracy and prediction capabilities of shallow water models depend strongly on the presence of various uncertainties that naturally arise in measuring or empirically approximating, e.g., the bottom topography data, or initial and boundary conditions. Hence, it is also essential to consider a stochastic version of the shallow water equations.

Figure 4: Example of stochastic version of small perturbation of a stationary steady-state solution test with uncertain bottom topography. Disk-glyph over mean contours of water surface (the radii of the disks indicate the magnitude of the standard deviation). Mesh is 200 × 200 [17].

An accurate numerical method for deterministic or stochastic Saint-Venant system or for shallow water models in general should satisfy at least two major properties that are crucial for its stability: i) the method should be well-balanced, i.e., should exactly balance the numerical flux and source terms. The well-balanced property will diminish the appearance of unphysical waves, the so-called “numerical storm”. In general, standard numerical methods for conservation laws will fail to preserve the subtle balance between the fluxes and the source terms, and thus will result in unstable approximation; ii) the method should be positivity preserving, that is, the water height should be nonnegative at all times. The positivity preserving property ensures a robust performance of the method on dry (water depth is zero) or almost dry (water depth is near zero) states. The system will lose hyperbolicity and hence, the scheme for Saint-Venant system will fail, if the numerical water height will become negative. The additional challenge for stochastic shallow water models is that, for example, stochastic Galerkin formulation of such models may fail to preserve hyperbolicity of the original system.

Together with my collaborators, I contributed to the development of efficient structure-preserving central-upwind finite volume methods for shallow water models [13, 45, 16, 31, 17]. The central Nessyahu-Tadmor schemes, their generalization into higher resolution Kurganov-Tadmor central schemes and semidiscrete central-upwind schemes are a family of efficient and accurate Godunov-type Riemann problem-free projection-evolution finite volume schemes for hyperbolic systems, originally developed in [48, 43, 44, 42]. The main advantages of these schemes are high resolution, computational efficiency and their simplicity. For example, the central-upwind schemes do not
involve Riemann solvers or characteristic decompositions, which makes them a very appealing tool for general multidimensional systems of conservation laws and related problems. At the same time, certain upwinding information is incorporated into the semi-discrete central-upwind schemes, since they respect the directions of wave propagation by estimating the one-sided local speeds.

In [13, 45] we developed a robust second-order well-balanced positivity preserving central-upwind scheme for computing the solutions of the Saint-Venant system and related models on triangular grids. The scheme in [45] is a further improvement of the scheme from [13]. In [45] we developed a special reconstruction on unstructured triangular grids of the water surface that ensures accurate treatment of wet and dry interfaces (waves arriving or leaving the shore) which is combined with algorithmic draining time step procedure on unstructured triangular grids. Such an algorithm to handle dry/wet interfaces makes it possible to avoid CFL-type-restrictive time-step on partially flooded regions and allows significant improvement of the computational efficiency of the method. Moreover, the developed schemes [13, 45] are well-suited for models with discontinuous bottom topography and irregular channel widths. In [31], we designed a robust adaptive well-balanced and positivity-preserving central-upwind scheme on unstructured triangular grids for the Saint-Venant system and related models. The numerical method in [31] is an extension of the scheme from [45]. As a part of the adaptive central-upwind algorithm, we derived a local a posteriori error estimator for the efficient mesh refinement strategy. We conducted several challenging numerical tests for shallow water equations and demonstrated that the new adaptive central-upwind scheme maintains important stability properties (i.e., well-balanced and positivity-preserving properties) and delivers high-accuracy at a reduced computational cost [31]. In our very recent work [16], we developed a novel hyperbolicity-preserving stochastic Galerkin formulation for the random Saint-Venant system in 1D physical space. In [16] we carefully tailored polynomial chaos expansion truncation operators for the nonlinear non-polynomial term in the shallow water system using only the conserved variables. Moreover, in an arbitrary finite stochastic dimension we established a sufficient condition to guarantee hyperbolicity of the stochastic Galerkin system through a finite number of conditions at stochastic quadrature points. Further, we developed a well-balanced central-upwind scheme for the stochastic shallow water model and derived the associated hyperbolicity-preserving CFL-type condition. The performance of the new method was illustrated on a number of challenging numerical tests. In [17], we extended the developed method [16] to stochastic shallow water models in 2D physical space, Fig. 4. Note, although the developed framework in [16, 17] can be combined with different choices of solvers for hyperbolic problems, the Riemann-solver-free nature of the central-upwind schemes allowed us to design an efficient deterministic solver as a part of the numerical discretization of the random shallow water models.

Current and Future Research: Currently, we are extending adaptive algorithm [31] to variable density shallow water equations. In addition, hyperbolicity-preserving framework that we developed in [16, 17] can be used with other solvers for balance laws. We will look into the design of adaptive high-order structure-preserving methods for random shallow water models (e.g., design of a high-order central-upwind and DG methods will be studied as a part of high-order accurate deterministic solvers for such models). We also plan to extend the developed methods [13, 45, 16, 31, 17] to different shallow water and related models which are used in scientific and engineering applications.

Besides the current/recent research mentioned above, in the past I was also involved in several other projects: my Ph.D. research under the guidance of Prof. Béatrice Rivière focused on the numerical simulation and analysis of different models of incompressible two-phase flow in porous media [21, 22, 35, 34] - we developed an implicit fully coupled hp-version of DG methods for these models. In [33], we studied one of the primal DG methods, symmetric interior penalty Galerkin
method (SIPG) applied to elliptic PDEs. In [33], we obtained lower bounds on the penalty parameters above which SIPG will produce stable and convergent numerical solutions. The other direction of my past research was [18] where we developed the mathematical analysis of the Stolz-Adams approximate deconvolution model for Large Eddy Simulation (LES) of turbulent flows. In addition, in [36, 51], we developed a simplified mathematical model of signaling (this was a collaborative work with the University of Pittsburgh Medical School (UPMC)). Finally, in a recent work [58], we investigated a microscale property of sea ice, namely, the effect that microbiology has on the effective fluid permeability of Arctic sea ice.

References


