Research Statement - Yekaterina Epshteyn http://www.math.utah.edu/~epshteyn/ Fall 2022

1 Introduction

My research interests are in *Computational and Applied Mathematics*. In particular, I work on the development and analysis 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 the mathematical and numerical analysis of the developed models.

2 Materials Microstructures: Modeling, Simulation, Analysis and Experiments

One of the major efforts of my recent and current research work is data-driven mathematical and computational modeling and analysis of polycrystalline materials. This research is interdisciplinary, with the main emphasis being on the development of a predictive theory of microstructure evolution during grain growth (coarsening) in polycrystalline materials (most technologically useful materials are polycrystalline microstructures). Our work has made important contributions to the development of high-resolution structure-preserving/physics-preserving numerical algorithms and simulations for grain growth, to novel and improved modeling of grain growth that informs and guides the design of new critical experiments, to the development of new mathematical analysis techniques, as well as to the analysis and theory development of coarsening in polycrystalline systems, e.g., [9, 8, 12, 7, 6, 30, 29, 11, 31, 28, 27, 50, 52].

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 complex 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 [60]: 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, 40, 55, 56]. This has led to the discovery and notion of the Grain Boundary Character Distribution (GBCD) [2, 1, 40, 55, 56].

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, 40, 55, 56]. 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, [41], [8, 12], [6], [29]. Moreover there is consistency between experimental GBCD's and simulated GBCD's [55].

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 is among the simplest non-random distributions, corresponding to independent trials with respect to the energy). This offers compelling evidence that the GBCD is a material property. Why does such a "simple" distribution emerge from such a complex multiscale and multi-physics 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 [42], 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 α , we derived a new entropy based theory for the evolution of the GBCD.



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 α (x-axis) at times corresponding to 20%, 40%, 60% and 80% removal of the initial boundaries, [6].

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

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

and, see Fig. 1. In Fokker-Planck equation above (2.1), α denotes the misorientation, $\rho(\alpha, t)$ is the GBCD (scaled to be a probability density), $\psi(\alpha)$ is the grain boundary energy density, σ is a diffusion coefficient and ν 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 [55, 47, 51].

In our very recent work, [30, 29], we developed a new model for the evolution of the 2D grainboundary network with finite mobility of the triple junctions (triple junctions are where three grain boundaries meet) and with dynamic lattice misorientations. In [30, 29], using the energetic variational approach, we derived a system of geometric differential equations to describe the motion of such grain boundaries, and we established a local well-posedness result, as well as large time asymptotic behavior for the model. Our results included obtaining explicit energy decay rate for the system in terms of mobility of the triple junction and the misorientation parameter. In addition, similar to our work on GBCD [8, 6], we conducted several numerical experiments for the 2D grain boundary network in order to further understand/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 [29, 11]. In [11, 50], we also presented and discussed relevant experimental results of grain growth in thin films which are consistent with the proposed grain growth model. Furthermore, in [50], for the first time, using experimental data in thin films, it was shown the limitations of assuming the force balance (Herring condition) at the triple junctions in nanocrystalline thin films. This important insight points to other driving forces in the development of the geometry of the grain boundary network and character distribution in thin films and is in agreement with the results of the developed mathematical theory and simulations modeling grain growth with dynamic lattice misorientations and with finite triple junction mobility [30, 29]. Moreover, in [31], using the idea of the Langevin equation approximation (where the interactions among triple junctions and misorientations modeled as a white noise) to model evolution of the network of triple junctions and misorientations (namely, to model the evolution of the planar grain boundary network in polycrystals), we further extended our work in [30, 29] and developed a 2D stochastic model of grain growth (in order to be able to model and analyze critical/disappearance events efficiently during grain growth, e.g., grain disappearance, facet/grain boundary disappearance, facet interchange, splitting of unstable junctions). We derived a Fokker-Planck model for the evolution of the planar grain boundary network. The proposed model considers anisotropic grain boundary energy (which depends on lattice misorientation) and takes into account mobility of the triple junctions, as well as independent dynamics of the misorientations. We established long time asymptotics of the Fokker-Planck solution, namely the joint probability density function of misorientations and triple junctions, and closely related the marginal probability density of misorientations, and hence further extended theory for the GBCD to the 2D grain boundary network. Moreover, for an equilibrium configuration of a boundary network, we derived explicit local algebraic relations, a generalized Herring Condition formula, as well as a formula that connects grain boundary energy density with the geometry of the grain boundaries that share a triple junction. Although the stochastic model in [31], neglects the explicit interactions/correlations among triple junctions and grain boundary misorientations. the considered specific form of the noise, under the fluctuation-dissipation assumption, provides crucial partial information about evolution of a planar grain boundary network, and is consistent with the results of extensive large-scale grain growth simulations. At this point, the derived theory [9, 8, 12, 7, 6, 31] is the only existing mathematical theory for the evolution of the GBCD (a leading metric to characterize texture of the boundary network in polycrystalline materials).

Moreover, our work [12, 6, 29] has also contributed to further development and improvement of a sharp interface structure-preserving/physics-preserving algorithm for grain growth simulation in 2D, first proposed in [41]. The 2D sharp interface algorithms [12, 6, 29] 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, numerical algorithm in [29] (extension of the algorithms from [12, 6]) makes it possible to study effects of different relaxation time scales such as those for boundary migration, grain rotations and mobility of the triple junctions on grain growth, and to handle full system anisotropy accurately (note, to the best of our knowledge, such important studies of the effect of different relaxation time scales on microstructure evolution are not possible with existing level-set based/phase-field based algorithms for grain growth simulations).

Current and Future Research: As a part of our current/future research, we are extending further our work in [31, 52]. Our goal is to incorporate more accurate grain growth mechanisms in the model, in particular, to identify and explicitly model interactions among triple junctions and lattice misorientations in the grain boundary network.

Moreover, future work will include new experimental studies to more closely validate the developed models in [30, 29, 31, 52]. 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 inter-



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, 30, 29].

face numerical algorithm and simulation that can deliver accurate approximation of microstructure evolution during coarsening of the polycrystalline systems in 3D. The algorithm development is based on the extension of previously developed 2D algorithms and simulations [12, 6, 29]. 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 among 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 grants DMS-2118172/DMS-2118206/DMS-2118181/DMS-2118197 and 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 Fast Numerical 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 [59, 57]. 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, for example, 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 nonlinear time dependent systems of PDEs (often, system of nonlinear convection-diffusion equations), which in general can only be solved by numerical methods. Moreover, a known property of many existing chemotaxis models is their ability to model a concentration phenomenon that mathematically results in a rapid growth of solutions in small regions of concentration points/curves.



Figure 3: Isosurface plots of the cell density ρ (left) and the chemoattractant concentration c (right). Example of the earlier time (t = 0.04) of the test in 3D where cells first move to the north pole of the sphere and is expected to aggregate (solution is expected to blow-up) at the north pole at a later time. Illustration of the Difference Potentials based domain decomposition algorithm [38].

The solutions may blow up or may exhibit a 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 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, 38], 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, 38] combine the simplicity of the secondorder positivity-preserving hybrid finite-volume finite-difference schemes in space (the hybrid finitevolume 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 [38], 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 [38] 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 and adaptivity (e.g., [53]), these methods can be computationally expensive. Hence, in [15], we developed simpler and more efficient high-order positivity-preserving hybrid finite-volume finitedifference methods for chemotaxis and related 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 [58, 24, 34, 4, 32, 3, 5], high-order accurate and fast numerical methods have been developed for elliptic and parabolic interface model problems, the methods in [58, 24, 32, 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. Additionally, in [48], 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 [39], 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 [39], 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 [39] 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, 34, 4, 32, 3, 5, 38] was partially supported by my NSF grant DMS-1112984 and the work in [5, 48, 39] was partially supported by Simons Foundation grant No. 415673. The work in [48] was also partially supported by the Swedish Foundation for International Cooperation in Research and Higher Education Grant No. STINT-IB2016-6512 and the work [39] was also partially supported by my current NSF grant DMS-1905463.

4 Structure-Preserving Numerical Methods for Nonlinear Hyperbolic Balance Laws and Related Models: 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" system of deterministic shallow water equations, known as the Saint-Venant system, is a nonlinear hyperbolic system of conservation/balance laws. The Saint-Venant model can admit non-smooth solutions that may have shocks, rarefaction waves, and if the bottom topography is discontinuous, contact discontinuities. In the latter case, the solution may not be unique, which makes the development of accurate and efficient algorithms 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.

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 on the so called "lake at rest" steady-state solutions. The well-balanced property will diminish the appearance of unphysical waves (the so-called "numerical storm"), which are usually present when computing quasi steady-states. 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.

The central Nessyahu-Tadmor schemes, their generalization into higher resolution 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 [49, 44, 45, 43]. 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 nonlinear 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.

Our work has made important contributions to the development of efficient structure-preserving numerical methods for shallow water models [13, 46, 16, 33, 17]. In [13, 46] we developed a robust second-order well-balanced positivity preserving central-upwind finite-volume scheme for computing the solutions of the Saint-Venant system and related models on triangular grids. The scheme in [46] is a further improvement of the scheme from [13]. In [46] we developed a special wellbalanced positivity-preserving 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, 46] are well-suited for models with discontinuous bottom topography and irregular channel widths. In [33], 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 [33] is an extension of the scheme from [46]. 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 [33].



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].

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 finite-volume 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: The hyperbolicity-preserving framework that we developed in [16, 17] can be used with other solvers for hyperbolic balance laws and can be adapted to related models. Our goal is to extend work in [13, 46, 16, 33, 17] to the design of adaptive high-order structure-preserving methods (including energy-stable methods) for nonlinear hyperbolic balance laws with uncertainty and related models (e.g., design of a high-order central-upwind finite-volume and DG methods will be studied as a part of high-order accurate deterministic solvers for such models).

This work is currently partially supported by the NSF grant DMS-2207207.

5 Ph.D. Research and Selected Previous Research Projects

Besides the current/recent research mentioned above, in the past I was also involved in several other projects: for example, 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, 35, 22, 36], where we designed and analyzed hp DG finite element methods for such problems in porous media. 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 [37, 54], 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 [61], we investigated a microscale property of

sea ice, namely, the effect that microbiology has on the effective fluid permeability of Arctic sea ice.

References

- B.L. Adams, D. Kinderlehrer, I. Livshits, D. Mason, W.W. Mullins, G.S. Rohrer, A.D. Rollett, D. Saylor, S Ta'asan, and C. Wu. Extracting grain boundary energy from triple junction measurement. *Interface Science*, 7:321–338, 1999.
- [2] BL Adams, D Kinderlehrer, WW Mullins, AD Rollett, and S Ta'asan. Extracting the relative grain boundary free energy and mobility functions from the geometry of microstructures. *Scripta Materiala*, 38(4):531–536, Jan 13 1998.
- [3] Jason Albright, Yekaterina Epshteyn, Michael Medvinsky, and Qing Xia. High-order numerical schemes based on difference potentials for 2D elliptic problems with material interfaces. Appl. Numer. Math., 111:64–91, 2017.
- [4] Jason Albright, Yekaterina Epshteyn, and Kyle R. Steffen. High-order accurate difference potentials methods for parabolic problems. Appl. Numer. Math., 93:87–106, 2015.
- [5] Jason Albright, Yekaterina Epshteyn, and Qing Xia. High-order accurate methods based on difference potentials for 2D parabolic interface models. *Commun. Math. Sci.*, 15(4):985–1019, 2017.
- [6] Patrick Bardsley, Katayun Barmak, Eva Eggeling, Yekaterina Epshteyn, David Kinderlehrer, and Shlomo Ta'asan. Towards a gradient flow for microstructure. Atti Accad. Naz. Lincei Rend. Lincei Mat. Appl., 28(4):777–805, 2017.
- [7] K. Barmak, E. Eggeling, M. Emelianenko, Y. Epshteyn, D. Kinderlehrer, R.Sharp, and S.Ta'asan. Predictive theory for the grain boundary character distribution. In *Proc. Re*crystallization and Grain Growth IV, 2012.
- [8] K. Barmak, E. Eggeling, M. Emelianenko, Y. Epshteyn, D. Kinderlehrer, R. Sharp, and S. Ta'asan. Critical events, entropy, and the grain boundary character distribution. *Phys. Rev. B*, 83:134117, Apr 2011.
- [9] K. Barmak, E. Eggeling, M. Emelianenko, Y. Epshteyn, D. Kinderlehrer, and S. Ta'asan. Geometric growth and character development in large metastable networks. *Rend. Mat. Appl.* (7), 29(1):65–81, 2009.
- [10] Katayun Barmak. Experimental data, K. Barmak's Laboratory, Columbia University. 2022.
- [11] Katayun Barmak, Anastasia Dunca, Yekaterina Epshteyn, Chun Liu, and Masashi Mizuno. Grain Growth and the Effect of Different Time Scales, pages 33–58. Springer International Publishing, Cham, 2022.
- [12] Katayun Barmak, Eva Eggeling, Maria Emelianenko, Yekaterina Epshteyn, David Kinderlehrer, Richard Sharp, and Shlomo Ta'asan. An entropy based theory of the grain boundary character distribution. *Discrete Contin. Dyn. Syst.*, 30(2):427–454, 2011.

- [13] Steve Bryson, Yekaterina Epshteyn, Alexander Kurganov, and Guergana Petrova. Wellbalanced positivity preserving central-upwind scheme on triangular grids for the Saint-Venant system. ESAIM Math. Model. Numer. Anal., 45(3):423–446, 2011.
- [14] A. Chertock and A. Kurganov. A positivity preserving central-upwind scheme for chemotaxis and haptotaxis models. *Numer. Math.*, 111:169–205, 2008.
- [15] Alina Chertock, Yekaterina Epshteyn, Hengrui Hu, and Alexander Kurganov. High-order positivity-preserving hybrid finite-volume-finite-difference methods for chemotaxis systems. Adv. Comput. Math., 44(1):327–350, 2018.
- [16] Dihan Dai, Yekaterina Epshteyn, and Akil Narayan. Hyperbolicity-preserving and wellbalanced stochastic galerkin method for shallow water equations. SIAM Journal on Scientific Computing, 43(2):A929–A952, 2021.
- [17] Dihan Dai, Yekaterina Epshteyn, and Akil Narayan. Hyperbolicity-preserving and wellbalanced stochastic galerkin method for two-dimensional shallow water equations. *Journal* of Computational Physics, 452:110901, 2022.
- [18] A. Dunca and Y. Epshteyn. On the Stolz-Adams deconvolution model for the large-eddy simulation of turbulent flows. SIAM J. Math. Anal., 37(6):1890–1902 (electronic), 2006.
- [19] Y. Epshteyn. Upwind-difference potentials method for chemotaxis models. 2012. in the proceedings of "European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2012)".
- [20] Y. Epshteyn. Upwind-difference potentials method for Patlak-Keller-Segel chemotaxis model. Journal of Scientific Computing, 53(3):689 – 713, 2012.
- [21] Y. Epshteyn and B. Rivière. On the solution of incompressible two-phase flow by a p-version discontinuous Galerkin method. Comm. Numer. Methods Engrg., 22:741–751, 2006.
- [22] Y. Epshteyn and B. Rivière. Fully implicit discontinuous finite element methods for two-phase flow. Applied Numerical Mathematics, 57:383–401, 2007.
- [23] Yekaterina Epshteyn. Discontinuous Galerkin methods for the chemotaxis and haptotaxis models. J. Comput. Appl. Math., 224(1):168–181, 2009.
- [24] Yekaterina Epshteyn. Algorithms composition approach based on difference potentials method for parabolic problems. *Commun. Math. Sci.*, 12(4):723–755, 2014.
- [25] Yekaterina Epshteyn and Ahmet Izmirlioglu. Fully discrete analysis of a discontinuous finite element method for the Keller-Segel chemotaxis model. J. Sci. Comput., 40(1-3):211–256, 2009.
- [26] Yekaterina Epshteyn and Alexander Kurganov. New interior penalty discontinuous Galerkin methods for the Keller-Segel chemotaxis model. SIAM J. Numer. Anal., 47(1):386–408, 2008/09.
- [27] Yekaterina Epshteyn, Chang Liu, Chun Liu, and Masashi Mizuno. Nonlinear inhomogeneous Fokker-Planck models: Energetic-variational structures and long-time behavior. Analysis and Applications, 20(06):1295–1356, 2022.

- [28] Yekaterina Epshteyn, Chang Liu, Chun Liu, and Masashi Mizuno. Local well-posedness of a nonlinear Fokker-Planck model. *Nonlinearity*, revised version submitted, 2022.
- [29] Yekaterina Epshteyn, Chun Liu, and Masashi Mizuno. Large time asymptotic behavior of grain boundaries motion with dynamic lattice misorientations and with triple junctions drag. *Communications in Mathematical Sciences*, 19(5):1403–1428, 2021.
- [30] Yekaterina Epshteyn, Chun Liu, and Masashi Mizuno. Motion of grain boundaries with dynamic lattice misorientations and with triple junctions drag. SIAM Journal on Mathematical Analysis, 53(3):3072–3097, 2021.
- [31] Yekaterina Epshteyn, Chun Liu, and Masashi Mizuno. A stochastic model of grain boundary dynamics: a Fokker-Planck perspective. 2022. In Press, Mathematical Models and Methods in Applied Sciences.
- [32] Yekaterina Epshteyn and Michael Medvinsky. On the solution of the elliptic interface problems by difference potentials method. In Spectral and high order methods for partial differential equations—ICOSAHOM 2014, volume 106 of Lect. Notes Comput. Sci. Eng., pages 197–205. Springer, Cham, 2015.
- [33] Yekaterina Epshteyn and Thuong Nguyen. Adaptive central-upwind scheme on triangular grids for the Saint-Venant system. *Communication in Mathematical Sciences*, 2022. to appear.
- [34] Yekaterina Epshteyn and Spencer Phippen. High-order difference potentials methods for 1D elliptic type models. *Appl. Numer. Math.*, 93:69–86, 2015.
- [35] Yekaterina Epshteyn and Béatrice Rivière. Estimation of penalty parameters for symmetric interior penalty Galerkin methods. J. Comput. Appl. Math., 206(2):843–872, 2007.
- [36] Yekaterina Epshteyn and Beatrice Rivière. Analysis of hp discontinuous Galerkin methods for incompressible two-phase flow. J. Comput. Appl. Math., 225(2):487–509, 2009.
- [37] Yekaterina Epshteyn, Beatrice Rivière, David Swigon, and Yoram Vodovotz. A simple mathematical model of lipopolysaccharide signaling through toll-like receptor 4 results in complex insights on preconditioning. *Journal of Critical Care*, 22(4), 2007.
- [38] Yekaterina Epshteyn and Qing Xia. Efficient numerical algorithms based on difference potentials for chemotaxis systems in 3D. J. Sci. Comput., 80(1):26–59, 2019.
- [39] Yekaterina Epshteyn and Qing Xia. Difference potentials method for models with dynamic boundary conditions and bulk-surface problems. Adv. Comput. Math., 46(5):Paper No. 67, 39, 2020.
- [40] D Kinderlehrer, I Livshits, GS Rohrer, S Ta'asan, and P Yu. Mesoscale simulation of the evolution of the grain boundary character distribution. *Recrystallization and grain growth, pts* 1 and 2, 467-470(Part 1-2):1063–1068, 2004.
- [41] David Kinderlehrer, Irene Livshits, and Shlomo Ta'asan. A variational approach to modeling and simulation of grain growth. SIAM J. Sci. Comp., 28(5):1694–1715, 2006.
- [42] Robert V. Kohn. Irreversibility and the statistics of grain boundaries. *Physics*, 4:33, Apr 2011.
- [43] A. Kurganov, S. Noelle, and G. Petrova. Semi-discrete central-upwind schemes for hyperbolic conservation laws and Hamilton-Jacobi equations. SIAM J. Sci. Comput., 23:707–740, 2001.

- [44] Alexander Kurganov and Eitan Tadmor. New high-resolution central schemes for nonlinear conservation laws and convection-diffusion equations. J. Comput. Phys., 160(1):241–282, 2000.
- [45] Alexander Kurganov and Eitan Tadmor. New high-resolution semi-discrete central schemes for Hamilton-Jacobi equations. J. Comput. Phys., 160(2):720–742, 2000.
- [46] Xin Liu, Jason Albright, Yekaterina Epshteyn, and Alexander Kurganov. Well-balanced positivity preserving central-upwind scheme with a novel wet/dry reconstruction on triangular grids for the Saint-Venant system. *Journal of Computational Physics*, 374:213 – 236, 2018.
- [47] Xuan Liu, Noel T. Nuhfer, Andrew P. Warren, Kevin R. Coffey, Gregory S. Rohrer, and Katayun Barmak. Grain size dependence of the twin length fraction in nanocrystalline Cu thin films via transmission electron microscopy based orientation mapping. J. Mater. Res., 30:528–537, 2015.
- [48] Gustav Ludvigsson, Kyle R. Steffen, Simon Sticko, Siyang Wang, Qing Xia, Yekaterina Epshteyn, and Gunilla Kreiss. High-order numerical methods for 2D parabolic problems in single and composite domains. J. Sci. Comput., 76(2):812–847, 2018.
- [49] Haim Nessyahu and Eitan Tadmor. Nonoscillatory central differencing for hyperbolic conservation laws. J. Comput. Phys., 87(2):408–463, 1990.
- [50] Matthew J. Patrick, Gregory S. Rohrer, Ooraphan Chirayutthanasak, Sutatch Ratanaphan, Eric R. Homer, Gus W. Hart, Yekaterina Epshteyn, and Katayun Barmak. Relative grain boundary energies from triple junction geometry: Limitations to assuming the Herring condition in nanocrystalline thin films. Acta Materialia, 242:118476, 2023.
- [51] Sutach Ratanaphan, Theerayut Boonkird, Rajchawit Sarochawikasit, Hossein Beladi, Katayun Barmak, and Gregory S. Rohrer. Atomistic simulations of grain boundary energies in tungsten. *Materials Lett.*, 186:116–118, 2017.
- [52] J. Rickman, K. Barmak, Y. Epshteyn, and C. Liu. Point process microstructural model of metallic thin films with implications for coarsening. 2022, submitted.
- [53] Béatrice Rivière. Discontinuous Galerkin methods for solving elliptic and parabolic equations, volume 35 of Frontiers in Applied Mathematics. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2008. Theory and implementation.
- [54] Beatrice Rivière, Yekaterina Epshteyn, David Swigon, and Yoram Vodovotz. A simple mathematical model of signaling resulting from the binding of lipopolysaccharide with Toll-like receptor 4 demonstrates inherent preconditioning behavior. *Math. Biosci.*, 217(1):19–26, 2009.
- [55] Gregory S. Rohrer. Influence of Interface Anisotropy on Grain Growth and Coarsening. Annu. Rev. Mater. Res., 35:99–126, 2005.
- [56] Anthony D. Rollett, S.-B. Lee, R. Campman, and G. S. Rohrer. Three-dimensional characterization of microstructure by electron back-scatter diffraction. *Annual Review of Materials Research*, 37:627–658, 2007.
- [57] V. S. Ryaben'kii. Difference potentials analogous to Cauchy integrals. Uspekhi Mat. Nauk, 67(3(405)):147–172, 2012.

- [58] V. S. Ryaben'kiĭ, V. I. Turchaninov, and E. Yu. Èpshteĭn. An algorithm composition scheme for problems in composite domains based on the method of difference potentials. *Zh. Vychisl. Mat. Mat. Fiz.*, 46(10):1853–1870, 2006.
- [59] Viktor S. Ryaben'kii. Method of difference potentials and its applications, volume 30 of Springer Series in Computational Mathematics. Springer-Verlag, Berlin, 2002. Translated from the 2001 Russian original by Nikolai K. Kulman.
- [60] Cyril Smith. Grain Shapes and Other Metllurgical Applications of Topology. American Society of Metals, pages 65–113, 1952.
- [61] Kyle R. Steffen, Yekaterina Epshteyn, Jingyi Zhu, Megan J. Bowler, Jody W. Deming, and Kenneth M. Golden. Network modeling of fluid transport through sea ice with entrained exopolymeric substances. *Multiscale Model. Simul.*, 16(1):106–124, 2018.