Research Statement (Brief Version) - Yekaterina Epshteyn

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1   Introduction

My research interests are in *Numerical Analysis, Computational and Applied Mathematics*, in particular in the development of reliable and efficient models and numerical methods for partial differential equations (PDEs).

- Some of my recent and ongoing work is to understand and to discover a predictive theory for microstructure evolution. Most technologically useful materials are polycrystalline microstructures composed of a myriad of small monocrystalline grains separated by grain boundaries. 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 science is to develop technologies capable of producing an arrangement of grains—a texture—that provides for a desired set of material properties.
In the collaborative work [2] which involves Departments of Mathematical Sciences and Material Sciences at Carnegie Mellon University we have proposed a theory which accounts for the kinetics of network evolution. In [2], we have introduced the grain boundary character distribution, the GBCD, a basic texture measure, and established an entropy based theory for it which suggests that GBCD satisfies Fokker-Planck type kinetics. For this, a simplified critical event model is introduced and studied.
Current and Future Goals: In [1], our aim is to use accurate large scale simulation to develop multiscale theory of complex evolving networks, exploit dissipation/entropy method for simplified models, and to establish kinetics of Grain Boundary Character distribution (GBCD) evolution.

- The other direction of my research deals with numerical simulation and analysis of different chemotaxis models. *Chemotaxis* is the active orientation of cells and organisms along chemical gradients. Some of the chemotaxis related examples in biomedical sciences are: bacterial infection - invades the body and may be attacked by movement of cells (neutrophil - white blood cells) towards the source as a result of the chemotaxis; development of cancer - very much related to the ability of cancerous cells to move, and thus spread faster than healthy cells. 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. Furthermore, it is known that the solutions of chemotaxis models may blow up or may exhibit very singular spiky behavior. Capturing such solutions numerically is a very challenging problem. In our work [10,8,7] we have introduced and studied a new numerical scheme based on interior penalty high-order discontinuous Galerkin finite element methods (DG) for the Keller-Segel chemotaxis model. We have proved theoretically and confirmed

numerically the stability and high-order of accuracy of the proposed numerical methods. Recently, in [4] we have also proposed Hybrid Central-Upwind-Difference Potentials Scheme to simulate and analyze the newly derived model for the bacterial (Aerobic bacteria) swimming and oxygen transport near contact lines. The proposed method is the positivity preserving and can handle complex geometry. The mathematical model under consideration, which describes the dynamics related to the Boycott effect in sedimentation consists of the coupled partial differential equations describing oxygen diffusion and consumption, chemotaxis and viscous fluid dynamics.

As one of our future directions, we are planning to extend the proposed DG methods for the Keller-Segel chemotaxis system [10,8] to this model and to compare the performance of the Hybrid Central-Upwind-Difference Potentials Method and the DG methods.

Future Goals: One of our goals also is to provide the software based on the developed numerical methods for the chemotaxis models which will be useful to the researchers working on mathematical biology.

- In [5], we are interested in 1D Keller-Segel chemotaxis system $\rho_t = (\sigma \rho_x - \chi c_x \rho)_x, \alpha c_t = c_{xx} - \epsilon c + \rho, \rho_x = 0, c_x = 0$ on $\partial \Omega$. In [5], we introduce a hybrid variational scheme: Given prior states ρ^*, c^* determine ρ, c such that $\frac{1}{2\tau} d(\rho, \rho^*)^2 + \frac{1}{2\tau} \int_\Omega |c - c^*|^2 dx + \int_\Omega F(\rho, c) dx = \min$ subject to $\rho \in L^1(\Omega), \rho \geqq 0, \int_\Omega \rho dx = 1$ $c \in H^1(\Omega)$ where $F(\rho, c) = \sigma \rho \log \rho + \frac{\chi}{2}(c_x^2 + \epsilon c^2) - \chi c \rho$ is the free energy of the system and $d(\rho, \rho^\star)$ is the Wasserstein distance for a pair of non-negative functions $\rho, \rho^\star \in L^1(\Omega)$ with the same mass.

  The hybrid variational approach allows the interpretation of the Keller-Segel system as a generalized gradient flow, and allows for the definition of a robust numerical scheme. Our goal is to provide a new way to prove the existence of the global in time solution.

- A different project that I have been involved with is the development of the robust numerical method for Saint-Venant system of the shallow water equations. This system is widely used in many scientific and engineering applications related to modeling of water flows in rivers, lakes, and coastal areas. The development of robust and accurate numerical methods for the computation of its solutions is an important and challenging problem. In [3], we have introduced and tested on several examples a new simple well-balanced positivity preserving second-order central-upwind scheme for the Saint-Venant system of shallow water equations on triangular grids.

  Future Goals: Extension of the proposed method/ideas to the numerical modeling of the tsunami waves

- In [18] we have began recently investigating the application of optimal-transportation type metrics in understanding large image data sets. As a part of this project, we are developing fast numerical algorithm to compute Wasserstein metric.

Besides the above research I was also involved in the past in the following projects: My Ph.D. research focused on the numerical simulation and analysis of different models of incompressible two-phase flow, namely the flow of a wetting phase (such as water) and a non-wetting phase (such as dense non-aqueous phase liquids), in a porous medium with possibly heterogeneous characteristics. In particular, we introduced and studied numerically and theoretically *implicit, fully coupled hp-version of discontinuous Galerkin (DG) schemes for solving incompressible two-phase flow problem in porous media* ([11,12,14,13]). We also studied one of the primal DG methods, Symmetric Interior Penalty Galerkin Method (SIPG) applied to elliptic

(PDEs) and we obtained *lower bounds on the penalty parameters above which SIPG will produce stable and convergent numerical solutions.*

During my Ph.D I was also involved in the following projects: Difference Potentials Method with application to *the development of algorithms composition and decomposition* ([16,17]); Fluid Dynamics-Large Eddy Simulations (LES), *where we developed mathematical analysis of the fundamental LES model* ([6]); Miscible Displacement Problem, *where we proposed and derived the theoretical error estimates for high order fully discrete discontinuous Galerkin methods*; Optical tomography inverse problems, *where we compared DG and continuous finite element (CFEM) for one dimensional inverse problem applied to breast cancer detection* ([9]); Mathematical modeling of biological processes, *where we developed mathematical model of signaling* [15,19]- collaborative work with University of Pittsburgh Medical School (UPMC).

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