Introduction. In my PhD studies, I have focused on designing and implementing high-performance numerical algorithms for modeling and simulations of problems based on partial differential equations (PDEs) that arise from materials science, biological/biomedical science, etc. Highly accurate and efficient numerical algorithms are crucial for such PDE-based models, especially when the models involve complex geometries (with interfaces, corners or evolving boundaries), and when standard numerical algorithms fail to capture the solutions accurately. In particular, together with my collaborators, I have worked on (i) higher order numerical algorithms for two dimensional elliptic/parabolic interface problems, based on Difference Potentials Method (DPM); and (ii) highly accurate and efficient numerical methods for three dimensional chemotaxis models in irregular domains, using a domain decomposition approach based on DPM.

The DPM was originally proposed by V. S. Ryaben’kii in 1969 for elliptic boundary value problems. Since then, DPM has been extensively developed by Prof. Ryaben’kii, his collaborators and other researchers for applications ranging from wave propagation to crack modeling, to name a few. See [1, 2, 3, 8, 9, 12, 21, 24, 27, 29, 30, 31, 32, 35, 36] among other references.

The main idea behind DPM is to reduce a well-posed boundary value problem in the domain to an equivalent Boundary Equation with Projections (BEP) defined on a thin layer of mesh nodes that straddles the continuous boundary. Broadly speaking, DPM can (i) handle arbitrary complex geometry using, but not limited to, uniform Cartesian meshes; (ii) handle general interface/boundary conditions; (iii) employ fast solvers on uniform meshes; (iv) work without explicit knowledge of Green’s function; and (v) easily be parallelized.

Numerical methods for elliptic interface problems in 2D. Interface problems often arise from real-world computational modeling in biology, material science, fluid dynamics, etc. The PDE-based models, regularity of the solutions, and/or the material properties might differ in different sub-domains. The major challenge here is to design a robust method that can accurately capture such differences across the interface. In addition, the interface might be of irregular shapes. In general, standard numerical methods designed for smooth solutions often fail to produce accurate approximations of solutions near the interface, or might be difficult to extend to higher order accuracy in space.

To handle these challenges, we designed and implemented high-order accurate and efficient DPM-based numerical methods for elliptic interface problems in our work [1]. In particular, the proposed algorithms employed wide stencils for higher order spatial discretization instead of the compact stencil [23], and no continuity was assumed in the interface conditions. Also, comparisons to Immersed Interface Method [18], Mayo’s method [22] and Edge-Based Correction Finite Element Interface method [13] illustrated the high order accuracy of the proposed DPM-based numerical algorithms. Moreover, numerical evidence showed the flexibility of the proposed algorithms – the underlying spatial discretizations, or the non-conforming...
uniform background meshes can be selected independently for each sub-domain, without loss of global accuracy.

Additionally, we applied the proposed algorithms to a biomedical application and computed the induced transmembrane voltage of a circular cell placed in an electric field, a phenomenon known as cell electroporation or electropermeabilization, which can arise in cancer studies. The simulation results obtained using the developed algorithms for interface problems demonstrated high order accuracy in space and agreed with results from [28].

**Numerical methods for parabolic interface problems in 2D.** In [2, 20], we extended the proposed DPM-based numerical methods in [1] to parabolic interface problems. The main idea is to formulate a discrete elliptic interface problem at each time step, and after that extend the idea of DPM. Numerical results illustrated the accuracy of the proposed numerical algorithms are not restricted by the boundary conditions and interface conditions.

Additionally, we extended our work in [2] and considered implicitly-defined interface in the DPM framework for the first time in [20]. Numerical tests showed that the DPM-based method can robustly handle explicit and implicit geometries likewise. We also proposed benchmark parabolic problems for both single and composite domains in [20]. Using these benchmark problems, we compared and contrasted the proposed DPM-based method with an immersed cut finite element method (cut-FEM) [4, 33] and summation-by-parts and simultaneous-approximation-term finite difference (SBP-SAT-FD) method [11, 34]. Numerical evidence showed that the two immersed methods (cut-FEM and DPM) recovered 4th order of convergence as expected, while the conforming method (SBP-SAT-FD) suffered a drop in order of convergence for some test problems. Moreover, we observed that DPM achieved the smallest errors in the comparisons of all three modern numerical methods.

Thus far, finite difference scheme was employed as the underlying spatial discretization in our work [1, 2, 20], but the discretization in space can also be finite volume [8, 10] or finite element [35, 36] in the DPM framework. Moreover, even though the proposed algorithms in [1, 2, 20] were for interface of circular/elliptic shapes inside a rectangular domain, the resulting algorithms for interface problems can be applied to arbitrary geometries and interfaces. Indeed, we extended the algorithms for 2D interface problems in [1, 2, 20] to the domain decomposition approach for 3D chemotaxis models in [10].

**Numerical methods for chemotaxis models in 3D.** Chemotaxis refers to mechanisms by which cellular motion occurs in response to an external, chemical stimulus. It plays a crucial role in the evolution of many living organisms. Experimental studies revealed that certain species undergo collective motion driven by attraction to or repulsion from other species (medicine, food, tumor angiogenic factor), despite having no means of self-organization.

In [10], we developed efficient numerical algorithms for the classical “parabolic–parabolic” Patlak–Keller–Segel (PKS) chemotaxis model [15, 16, 26] in a spherical domain. However, the proposed method is not restricted to a spherical domain and will be applied to models in 3D domains with arbitrary geometries as a part of future work. Mathematically, this PKS model is described by a system of two nonlinear PDEs: a convection-diffusion equation (1) for the cell density coupled with a reaction-diffusion equation for the
The chemoattractant concentration (2):

$$\rho_t = \Delta \rho - \nabla \cdot (\chi \rho \nabla c), \quad (x, t) \in \Omega \times \mathbb{R}^+, \quad (1)$$

$$c_t = \Delta c - c + \rho, \quad (x, t) \in \Omega \times \mathbb{R}^+, \quad (2)$$

where $\rho(x, t)$–the cell density and $c(x, t)$–the chemoattractant concentration are subject to homogeneous Neumann boundary condition and non-negative initial conditions, and $\chi$ is the chemotactic sensitivity constant. We used the classical PKS model as an important validation for the development and analysis of the numerical tools for different chemotaxis models. The developed algorithms can be extended in a straightforward way to other chemotaxis systems, or even haptotaxis systems for modeling tumor growth.

Chemotaxis models are highly nonlinear due to the density-dependent cross-diffusion term, which models the chemotactic behavior. Hence, any realistic chemotaxis model is analytically intractable. Therefore, development of accurate and efficient numerical methods is crucial for the modeling and analysis of chemotaxis systems. Furthermore, a common property of many chemotaxis models is their ability to describe a concentration phenomenon that mathematically results in quick growth of solutions in small regions of concentration points or curves. The quick growth of solutions may lead to a blowup phenomenon, which introduces singularities in the solutions. The blowup phenomenon is a mathematical description of rapid unbounded aggregation of organisms at an accumulation point in a real biological system. It is numerically challenging to capture such spiky behaviors. Additionally, we wished to design a structure-preserving method that preserves the positivity of the density $\rho$ and concentration $c$ in a 3D irregular domain.

To address these challenges, we first proposed positivity-preserving upwind DPM in a single domain in 3D, following work in [7, 8]. The method is based on a hybrid finite-difference-finite-volume scheme as the underlying discretization in space, combined with the idea of Difference Potentials for the highly accurate and efficient approximation of solutions in 3D irregular domains. The positivity of solutions $\rho$ and $c$ in the 3D irregular domain was shown both theoretically and numerically. Additionally, to improve the efficiency of the algorithms, we employed Fast Poisson Solver on uniform Cartesian meshes that uses FFTW3 library with openMP enabled. The Fast Poisson Solver makes the DPM-based algorithms for 3D simulations suitable not only for high performance computing clusters, but also for personal laptops.

Further, in consideration of the locality of the solutions $\rho$, we proposed a domain decomposition approach based on DPM. The main idea is to introduce an artificial interface that separates two subdomains: one contains relatively large values of the solution and the other does not. Then we treated the domain decomposition problem in a manner similar to interface problems we had considered in 2D [2, 20]. Both convergence studies and long-time simulations based on DPM showed that the domain decomposition approach gives almost identical accuracy as the single domain approach. In contrast...
to the single domain approach, we recovered similar accuracy of solutions and obtained 4×–8× speedup for some simulations in the domain decomposition approach, by introducing mesh adaptivity and reducing the number of degrees of freedom. Note that the DPM-based domain decomposition approach is compatible with Fast Poisson Solvers.

**Current and Future Work.** Currently, I have three ongoing projects: (i) higher order numerical methods for free boundary problems with Y. Epshteyn and K. R. Steffen; (ii) statistical analysis of the effectiveness of FDA approved drugs for breast cancer using patient-derived xenograft models, with Y. Epshteyn and researchers from Huntsman Cancer Institute at the University of Utah; and (iii) highly accurate and efficient algorithms for PDEs with dynamic boundary conditions with Y. Epshteyn. In particular, my focus is on algorithms for dynamic boundary condition. Let me briefly discuss some ideas below related to project (iii).

**Dynamic Boundary Condition.** The dynamic boundary condition indicates that the boundary condition is prescribed by a PDE, which is also known as bulk-surface coupling of PDEs. Such coupling may occur in many applications. For instance, in the modeling of fluorescence loss in photobleaching, a signaling molecule (G-protein Rac) cycles between the cytoplasm (bulk) and cell membrane (surface) [25]. Or, the Cahn-Hillard equation with dynamic boundary conditions [19] might arise in the modeling of phase separation processes of binary mixtures of fluid. However, there have been only a few numerical methods proposed for such coupling (see [6, 5, 14, 17]).

From our experience in designing numerical algorithms based on DPM [1, 2, 10, 20], we noted that DPM-based approach is naturally fit for PDEs with dynamic boundary conditions in complex geometries, based on the following observations: (i) DPM can handle irregular boundary or interface using uniform meshes, with great flexibility, efficiency and no loss of accuracy in domains with complex geometry; (ii) DPM reduces the PDE in the bulk to an equivalent BEP defined on a thin layer of mesh nodes near the boundary, which reduces the dimension of the problem; (iii) the dynamic boundary condition essentially prescribes the dependence of higher order normal derivatives at the boundary on Cauchy data; and (iv) Cauchy data and higher order normal derivatives are incorporated into the BEP via the extension operator.

As the first step, I plan to work on efficient and highly accurate DPM-based numerical methods for problems in the form of:

\[
\begin{align*}
    u_t - \Delta u &= f, \quad (x,t) \in \Omega \times \mathbb{R}^+, \\
    \mu u_t + \alpha u + \beta u_n &= \kappa \Delta_I u, \quad (x,t) \in \Gamma \times \mathbb{R}^+, \\
    u(x,0) &= u_0(x), \quad x \in \Omega.
\end{align*}
\]

Here \( \Gamma \) is the surface of the bulk \( \Omega \), \( n \) is the outward normal and \( \Delta_I \) is the Laplace-Beltrami operator that models surface diffusion on \( \Gamma \). As future work, I plan to extend the algorithms for dynamic boundary condition to more applications, such as Cahn-Hillard equation with dynamic boundary condition or bulk-interface problem in composite domains that arises from modeling fluids in porous media (see [6, 19]).

**Future Work.** As a postdoctoral research fellow and beyond, I hope to extend the proposed numerical methods based on DPM further for numerical modeling and simulations of complex phenomena in arbitrary geometries from more areas. Moreover, my long term goal is to develop practical tools that can handle PDE-based models in complex geometry numerically with high order accuracy and that can be readily used by researchers in other disciplines of science and engineering. For instance, I am interested in developing an adaptive mesh refinement (AMR) library/package based on the Difference Potentials ideas and the domain decomposition approach. The novelty of the proposed AMR is that we can use uniform meshes and employ Fast Poisson Solvers to handle each sub-domain efficiently and parallelly. Additionally, the original problem can be reformulated into equivalent, coupled BEPs at mesh nodes near the boundary/interface and the BEPs
can be solved with less computational cost, in comparison to using AMR based on block mesh refinement, quadtree/octree, or unstructured meshes.

References


