Research Summary
(for external reviews only)

1. Three-layer dielectric models for generalized Coulomb potentials

In this direction, my research [2-4] is primarily concerned with the calculation of the generalized Coulomb potential \( \Phi(r, r_s) \) at location \( r \) generated by a charge \( e_s \) located inside or outside a dielectric object with the coordinate \( r_s \), which verifies the Poisson equation

\[
\nabla \cdot \varepsilon(r) \nabla \Phi(r, r_s) = -4\pi e_s \delta(r - r_s). 
\]

(1)

Here, \( \varepsilon(r) \) is the spatially dependent dielectric function. Two representative applications of such a problem are in the fields of quantum dots and biomolecular physics.

The three-dimensional solution of (1), even assuming the spherical geometry and only the radial dependence for \( \varepsilon(r) \), is quite complicated to find. The classical step-like model admits an analytical solution, but it not only is unphysical but also leads to divergent self-polarization at the dielectric interface. On the other hand, distance-dependent dielectric models such as various three-layer dielectric models can overcome the mathematical divergence of the step-like model, but the resulting equation (1) no longer admits analytical solutions and thus has to be solved numerically. In particular, when assuming the radial symmetry, the most widely used numerical approach so far is the one proposed by Bolcatto et al., whose very basic idea is to subdivide the transition layer into multiple layers and then in each one of them approximate the continuous dielectric function by a constant value. It is my belief, however, that this approach has a fundamental limitation: as its numerical nature requires the discretization of a continuous radial dielectric function into a piecewise constant one within the transition layer, new numerical divergence inevitably emerges.

In 2009, Qin et al. proposed a novel “quasi-harmonic” three-layer dielectric model that can admit an analytical solution! Then based on this new discovery and using a procedure analogous to the analysis of a transmission line, in [4] I developed a robust numerical method for solving (1) with essentially any continuous, radially symmetric dielectric function \( \varepsilon(r) \). The idea is still simple: Like in the Bolcatto approach, the spherical domain is subdivided into multiple concentric layers, but unlike in the Bolcatto approach, in each of these layers the dielectric function is now approximated by a quasi-harmonic one. Overall, the approximating dielectric function is still continuous rather than piecewise constant! The resulting numerical method can not only overcome the inherent mathematical divergence in the self-polarization energy which arises for the simplest and most widely used step-like model of the dielectric interface, but also completely eliminate the potential numerical divergence which may occur in the Bolcatto approach. Moreover, numerical experiments have demonstrated the convergence of the robust numerical method as the number of layers used to discretize the spherical computational domain goes to infinity, an important property that the Bolcatto approach appears not necessarily to possess. Later, I further extended the novel quasi-harmonic three-layer dielectric model and the robust numerical method from the spherical geometry to the prolate/oblate spheroidal geometries in [3] and [2], respectively.

Currently, I am applying both the novel quasi-harmonic models and the robust numerical methods in simulations of quantum dots, such as the calculation of the electronic ground state energy of spherical/spheroidal quantum dots with off-centered impurities.
2. Methods of images in hybrid biomolecular solvation models

Computer simulation by molecular dynamics (MD) is nowadays commonplace for investigating properties of bio-macromolecules. Central to this numerical simulation is how to account for electrostatic interactions in the crowded environment of ions, solvents and macromolecules, which are well-known to provide a crucial contribution to the structure, dynamics and function of biomacromolecules. Electrostatic interactions are long-range, and strongly dependent on the solvent and the ions surrounding the macromolecule under study. When modeling biological systems numerically, it has been challenging, however, to account for such solvent environment in a manner that is computationally efficient and physically accurate at the same time. Although bio-molecular simulation methods have advanced dramatically in recent years, a well-known bottleneck of computational efficiency of MD bio-molecular simulations is still the lack of fast and accurate methods to calculate these long-range electrostatic interactions in biological systems.

In this direction, with the so-called hybrid explicit/implicit solvent bio-molecular simulations being my target applications, my research is primarily concerned with fast and accurate calculation of electrostatic interactions between charges inside a spherical dielectric cavity $V_{in}$ immersed in an implicit solvent medium $V_{out}$. Mathematically, the problem can reduce to the solution of the following Poisson and the linearized Poisson-Boltzmann equations:

$$\nabla \cdot (\epsilon_{in} \nabla \Phi_{in}(r)) = -4\pi \rho_{in}(r), \quad r \in V_{in}, \quad (2)$$

$$\nabla^2 \Phi_{out}(r) - \lambda^2 \Phi_{out}(r) = 0, \quad r \in V_{out}, \quad (3)$$

where the charge distribution $\rho_{in}(r) = \sum_i q_i \delta(r - r_i)$ contains all explicit charges from the solute (e.g. a bio-macromolecule) and the solvent molecules inside the cavity $V_{in}$, and $\lambda$ is the inverse Debye screening length ($\lambda = 0$ indicates the pure water solvent outside the cavity.)

In particular, my collaborators and I are interested in developing high-order accurate reaction field-based methods. More specifically, we discovered a systematic procedure in constructing images to represent the reaction field (RF) in a spherical dielectric cavity within either the pure water solvent or an ionic solvent, and developed a series of methods of images for RF approximations, including a method for the pure water solvent [13,16], 2nd-, 4th-, and 6th-order methods for ionic solvents of low concentrations [5,12,14], and 2nd-order methods for ionic solvents of high concentrations [8]. Compared to the direct Kirkwood expansion (KE) solution to the RF, at equivalent accuracy the proposed methods of images are much more efficient computationally, especially when the RF in the whole cavity has to be evaluated. For example, it has been numerically demonstrated that, without combining with any fast algorithm for many-body problems, the methods of images alone could perform at least 20 to 30 times faster than the KE approach in typical high-order accuracy calculations. On the other hand and also most importantly, the proposed methods of images can be combined in a rather straightforward way with existing fast algorithms for many-body problems such as pre-corrected FFT methods or fast multipole methods (FMM), leading to efficient $O(N \log N)$ or even $O(N)$ algorithms for electrostatic calculations. In addition, in the effort to extend the proposed methods of images from the spherical cavity to ellipsoidal cavities (for non-spherical bio-molecular applications), I produced another two publications [7,9].

Currently, to ensure their general applicability, we are testing and calibrating the proposed methods of images with a few simple but biologically important systems, including bulk water [6], ion-solvation and ion-ion interactions. Success of these efforts should have immediate and far-reaching impact on the state-of-the-art capability in bio-molecular simulations.
3. Computational electromagnetics and its applications

In this direction, I had a total of 8 publications, and my primary interest was to develop high-order accurate numerical algorithms for solving Maxwell’s equations in inhomogeneous media.

First in [22], motivated by the immersed interface method (IIM) for solving elliptic equations with discontinuous coefficients, I proposed a globally second-order upwinding embedded boundary method (UEBM) to solve time-domain Maxwell’s equations in media with material interfaces. Then in [18], I developed another globally second-order accurate upwinding boundary condition capturing method for the time-domain Maxwell’s equations by using ghost points instead. Next in [10], through a simple least squares procedure I extended the second-order IIM proposed for two-dimensional acoustic wave equations with piecewise constant coefficients to Maxwell’s equations, and the resulting augmented IIM was found to greatly improve the long-time stability of the time-domain solution. Finally in [18], I presented a fourth-order UEBM for solving Maxwell’s equations with horizontal (or vertical) material interfaces by utilizing the idea of the ghost fluid method to construct finite difference approximation of spatial derivatives at Cartesian grid points near the material interfaces and the idea of the UEBM to evolve solutions at the interfaces. All these finite difference-type methods appear to allow time step sizes independent of the interface locations. However, it should be pointed out that my effort to extend the fourth-order method to solve Maxwell’s equations with arbitrary material interfaces was unsuccessful due to stability issues.

On the application side, I was interested in numerical simulation of optical coupling and light propagation in the so-called Coupled Resonator Optical Waveguide (CROW) structures. Such devices can provide the possibilities of controlling light propagation speed and manipulating light propagation path in a very different way from that in the conventional optical fiber waveguides, and thereby have potential applications in many areas of telecommunication. Theoretically, it is known that in CROW devices, waveguiding is achieved by optical coupling of evanescent whispering gallery modes (WGMs) in individual optical resonators, and the mechanism of such optical coupling can be well understood qualitatively by the tight binding method. However, the formalism is not convenient for real physical CROW structures because, for example, it does not account for different resonator sizes. Moreover, more quantitative study of optical coupling and light propagation in CROW structures may be needed to address various issues such as the sensitivity of the coupling strength and the propagation efficiency to the inter-resonator gap size, etc.

In [20], after formulating the Maxwell equations for coupled microcylinders, I introduced a high-order time-domain discontinuous spectral element method (DSEM) for the study of the optical coupling by evanescent WGMs between two microcylinders, and demonstrated the successful coupling between the microcylinders and also the dependence of such coupling on the separation and size variation of the microcylinders. (This work has received good responses from some good optics people.) Later in [21], I further applied the DSEM to analyze evanescent wave coupling of WGMs in microcylinder CROWs, and demonstrated successful light propagation by WGMs through a chain of coupled cylinder resonators and also obtained some other interesting results. Finally, in [17], I applied the DSEM to specifically study optical coupling and light propagation in coupled microcylinder optical waveguides with slight size disorder. In addition, in [19], I proposed and analyzed an orthogonal non-polynomial nodal basis on triangles for DSEMs for Maxwell’s equations. It is based on the standard tensor product of the Lagrange interpolation polynomials and a “collapsing” mapping between the standard square and the standard triangle.
4. Large-eddy simulations by the SHNSE model

The Navier-Stokes equations (NSE) represent the standard model for studying turbulent incompressible flows. Standout difficulties encountered in direct numerical simulation of the NSE include high-frequency Gibbs oscillation and the requirement of large numbers of degrees of freedom for accurate simulation. In response, large-eddy simulations have been developed, but with their own problems in their numerical implementation. Recently, the so-called spectrally hyperviscous Navier-Stokes equations (SHNSE) was proposed as an outgrowth of the spectral vanishing viscosity method and theoretically investigated by my collaborator Dr. Joel Avrin. As the result, he has demonstrated that the SHNSE model has many unique and robust theoretical properties including convergence of Galerkin approximations with significant improvements in the convergence for high wavenumbers, all suggesting that the SHNSE model has the potential to be a highly robust and accurate platform for studying and modeling three-dimensional turbulences. The three-dimensional SHNSE are

\[
\begin{align*}
\mathbf{u}_t + \nu A \mathbf{u} + \mu A \phi \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla p &= \mathbf{g}, \\
\nabla \cdot \mathbf{u} &= 0.
\end{align*}
\]

where \( A = \Delta \), and \( \mu A \phi \mathbf{u} \) is the so-called spectrally hyperviscous term (The meaning of other notations follows the NSE). For example, one simple choice of \( \mu A \phi \mathbf{u} \) is to let \( \mu A \phi \mathbf{u} = \mu Q(k) A^2 \mathbf{u} \) where \( Q(k) = 1 \) as \( k \geq M \) and \( Q(k) = 0 \) as \( k < M \) with \( M \) being a prescribed cut-off wave number.

In this direction, as a computational mathematician, I am interested in numerically investigating the utility of the SHNSE model in providing a viable computational model for three-dimensional fluid turbulence, in particular, at high Reynolds numbers. In [1], the SHNSE model has been successfully implemented (by a Ph.D. student who is going to join the Mohseni group soon in the Department of Aerospace Engineering Sciences at University of Colorado at Boulder and whom I co-advised with Dr. Avrin) for a periodic box by using pseudo-spectral methods, and applied to simulations of benchmark isotropic homogeneous decaying turbulences, yielding very promising results including excellent agreement with the Kolmogorov energy law for Reynolds numbers as high as \( 10^7 \) (but still with manageable computational cost). Through extensive numerical experiments, we have not only validated some of the nice theoretical properties of the SHNSE, but also obtained two empirical formulas regarding optimal parameter choices in \( M \) and \( \mu \). For example, the preliminary numerical results suggest that the optimal value of \( \mu \) is independent of \( \nu \), depending instead on a small fixed parameter times the square root of the initial total energy. In sum, numerical results obtained so far did indicate that the SHNSE model has strong potential to be a robust platform for modeling three-dimensional turbulence.

Next, we intend to further investigate SHNSE’s capabilities in handling complex geometries and general boundary conditions by modeling the benchmark wall-bounded turbulent channel flow or even the more challenging flow over the “Ahmed body” car model, where the Reynolds number could be as high as \( \text{Re}=768,000 \). And of course, many issues have to be addressed in this endeavour.
5. Immersed interface method for 3D interface problems

This was my dissertation work under the direction of Drs. Zhilin Li and Kazufumi Ito from North Carolina State University. Basically, my goal was to develop finite difference methods with the Cartesian grid for the following three-dimensional elliptic interface problem

\[ \nabla \cdot (\beta \nabla u(x, y, z)) + \lambda u(x, y, z) = f(x, y, z), \quad (x, y, z) \in \Omega - \Gamma, \]

with some given boundary condition on \( \partial \Omega \). Here, \( \Omega \) represents a domain in \( \mathbb{R}^3 \) and \( \Gamma \) is an arbitrary piecewise smooth surface in \( \Omega \). The interface \( \Gamma \) divides \( \Omega \) into two sub-domains \( \Omega^+ \) and \( \Omega^- \). The coefficients \( \beta, \lambda \), and the source term \( f \) may be discontinuous across the interface \( \Gamma \).

In [23], I extended the second-order immersed interface method (IIM) for elliptic equations with discontinuous coefficients and/or singular source terms from two dimensions to three dimensions. More specifically, I developed two second-order accurate elliptic solvers using Cartesian grids for the above three-dimensional elliptic interface problem. One method was designed for general interface problems with variable and discontinuous coefficient. The scheme preserves the discrete maximum principle using constrained optimization techniques, and an algebraic multigrid solver is applied to solve the discrete system. On the other hand, the second method was designed for interface problems with piecewise constant coefficient. The method is based on the fast immersed interface method and a fast three-dimensional Poisson solver. The second method was further modified to solve Helmholtz/Poisson equations on irregular domains. An application of the method to an inverse interface problem of shape identification was also presented. In this application, the level set method was applied to find the unknown surface iteratively.

6. Early work

Between 1991 and 1996, I worked on parallel computing for finite element structural analysis. I published one book and 11 peer-reviewed papers, but all were written in Chinese. The book is in the Computational Methods Series published by the Science Press, Beijing, China.