RESEARCH STATEMENT

by Lili Ju

I have worked on diverse research projects involving design, analysis, implementation, and applications of algorithms for problems arising from science and engineering. My research efforts have encompassed areas of numerical analysis, mesh optimization, image processing, computational geoscience, mathematical modeling, and parallel computing, with applications ranging from biology (medical imaging), physics (superconducting vortices), materials science (polymers) to environmental science (ocean and ice modeling) and etc. My research projects have been continuously supported by the US National Science Foundation under grant numbers DMS-0609575 (2006-2009) and DMS-0913491 (2009-2012), and the US Department of Energy under grant number DE-FG02-07ER64431 (2007-2011). Together with my collaborators, we have made significant contributions to several topics in computational and applied mathematics as demonstrated by citations shown in the Google Scholar. A detailed description of my research projects and achievements is presented below.

1 Algorithms and Applications of Centroidal Voronoi Tessellations

A comprehensive study of centroidal Voronoi tessellations (CVTs) was first provided in the 1999 review article [12]. While the CVT concept initially was phrased as a model and method for optimal point distributions and spatial tessellations of regions/volumes or within sets of discrete data, the generality and universality of CVTs have also made it widely applicable in many areas of science and engineering [12, 61, 17]. Given an open convex set \( \Omega \subset \mathbb{R}^d \) and a set of points \( \{x_i\}_{i=1}^n \) in \( \Omega \), let \( V_i = \{ x \in \Omega \mid \|x - x_i\| < \|x - x_j\| \text{ for } j = 1, \ldots, k, j \neq i \} \) for \( i = 1, \ldots, k \). The set \( \{V_i\}_{i=1}^k \) is referred to as a Voronoi tessellation (VT) of \( \Omega \) [61], the members of the set \( \{x_i\}_{i=1}^n \) are referred to as generators, and each \( V_i \) is referred to as the Voronoi region corresponding to \( x_i \). It is clear that the Voronoi regions \( \{V_i\}_{i=1}^n \) are polygons in two dimensions and polyhedrons in three dimensions. The dual of a Voronoi tessellation in the graph-theoretical sense is called a Delaunay triangulation (DT) associated with the point set \( \{x_i\}_{i=1}^n \). Given a density function \( \rho(x) \geq 0 \) defined on \( \Omega \), for each Voronoi region \( V_i \), we define the mass center or centroid of \( V_i \) by

\[
x_i^* = \frac{\int_{V_i} x \rho(x) \, dx}{\int_{V_i} \rho(x) \, dx}, \quad \text{for } i = 1, \ldots, k.
\]

We refer a Voronoi tessellation \( \{(x_i, V_i)\}_{i=1}^n \) of \( \Omega \) to as a centroidal Voronoi tessellation [12] if and only if \( x_i = x_i^* \) for \( i = 1, \ldots, k \). The corresponding dual triangulation is then called a centroidal Voronoi Delaunay triangulation (CVDT). A generic Voronoi tessellation usually does not satisfy the CVT property; see Figure 1 (left pair) for an illustration. On the other hand, given a density and the number of generators, the CVT of a domain always exists although it may not be unique. CVTs possess an optimization property that can be used as a basis for an alternate definition. Given a set of points \( \tilde{X} = \{\tilde{x}_i\}_{i=1}^n \) in \( \Omega \) and any tessellation \( \tilde{V} = \{\tilde{V}_i\}_{i=1}^n \) of \( \Omega \), define a clustering energy \( K \) by

\[
K(\tilde{X}, \tilde{V}) = \sum_{i=1}^n \int_{V_i} \rho(x) ||x - \tilde{x}_i||^2 \, dx.
\]

Then it can be shown that \( K \) is minimized only if \( (\tilde{X}, \tilde{V}) \) forms a CVT of \( \Omega \) [12]. Although the energy \( K \) may not be directly identified with the energy of some physical systems, it is often naturally associated with quantities such as quantization error, variance and cost in many applications. Asymptotically as the number of generators gets larger and larger, Gersho’s Conjecture [32] states that the optimal CVT (in the sense of minimizing the energy) forms a regular tessellation consisting of the replication of a single polytope whose shape depends only on the spatial dimension. There are two classic algorithms for constructing CVTs based on minimizing the bove energy: one is the MacQueen’s [58] method that is an elegant random sampling method, the other is the Lloyd’s method [54] which is a deterministic method requiring accurate calculations of Voronoi diagrams.

1.1 Theory and construction algorithms for CVT

Extensions of CVTs to surfaces/manifolds in the Euclidean space – In [15] we generalized the CVT concept to surfaces/manifolds by giving a precise definition of constrained centroidal Voronoi
tessellations (CCVTs) and then derived a number of properties for such tessellations including the characterization as minimizers of an “energy”. In particular, we call it a *spherical centroidal Voronoi tessellation* (SCVT) when the underlying surface is the surface of a sphere; see Figure 1 (right pair) for an example. Some probabilistic and deterministic algorithms for construction of CCVTs were also proposed. We implemented the software package “SCVT” using Fortran for generating SCVTs which can be downloaded from my webpage [http://www.math.sc.edu/~ju](http://www.math.sc.edu/~ju).

**Efficient algorithms for computing CVTs** – We proposed in [40] a new probabilistic method for determining CVTs that can be viewed as a generalization or combination of the two classic methods. It is very important to point out that these probabilistic algorithms do not require, at any stage, the construction of Voronoi diagrams nor the determination of the centroids of the Voronoi cells. Moreover, the algorithms are highly amenable to fully scalable parallelization. Based the results from [40], we developed some algorithms for determination of point sets and associated support regions based on the CVT methodology in [14], that can be used for meshless computing methods [2]. The algorithms are probabilistic in nature so that they are totally meshfree. We are currently investigating nonlinear conjugate methods for fast computation of CVTs. It is worth noting that some effective acceleration schemes for computing CVTs such as Newton or quasi-Newton methods and multigrid-based methods were recently proposed in [9, 10, 57].

**Convergence analysis of the Lloyd’s method** – Since Lloyd’s pioneering work many studies have been made on convergence properties of the Lloyd iteration. Local convergence of the algorithm has been proved for the constant density function and strictly *logarithmically concave* density functions (i.e., \((\log \rho)'' < 0\)) in one dimension [12]; especially, the convergence rate is linear for the constant density function. We rigorously proved in [11] the global convergence of the Lloyd’s algorithm in one dimension for any positive and smooth density function based on compactness and non-degeneracy of the Lloyd’s iteration. Furthermore, we gave an explicit lower bound for the distance between generators in this case. However, this result can not be easily extended to higher dimensions since the proof partly depends on the property that the generators in one dimension are well-ordered while this does not hold for the spaces of dimensions higher than two. We made a big progress towards this problem and proved in [30] the weak global convergence of the Lloyd’s algorithm in general dimensions provided that the domain \(\Omega\) is a convex and bounded set and the density function belongs to \(L^1(\Omega)\).

1.2 CVT-based mesh generation and adaptive computation

We have applied the CVT methodology to high-quality mesh generation and adaptive meshing schemes for numerical partial differential equations.

**Mesh generation and optimization** – Mesh generation often forms a crucial part of the numerical solution procedure in many applications, especially PDE-based applications. When CVT/CVDT is applied to the numerical solution of PDEs, some modifications are needed to handle geometric constraints [13, 26]: for example, an obvious one is that some of the CVT generators have to be constrained to lie on the boundary of the domain so that the boundary conditions of the problem can be enforced. We developed in [42, 38] a *conforming centroidal Voronoi Delaunay triangulation* (CfCVDT) for CVT-based mesh generation; in particular, a *lifting* process that allows the boundary generators (vertices) to return to the interior domain is associated with a *projection* process so that the number of boundary generators will be able to automatically change according to the

![Figure 1: Left pair: a Voronoi tessellation of the unit square with 10 generators randomly selected and a 10-point centroidal Voronoi tessellation of the square; Right pair: a Voronoi tessellation of the surface of the unit sphere with 64 generators randomly selected and a 64-point spherical centroidal Voronoi tessellation of the surface. A uniform density function is used for both cases.](image-url)
density function and consequently the dependence of resulting mesh on the initial guess will be weaken. We implemented the software package “MESHGEN” [38] for the CfCVDT generation using C on the base of the popular 2D meshing package “Triangle” [69] and can be downloaded from http://www.math.sc.edu/~ju. Furthermore, our implementation even allows domains with a curved boundary. Figure 2 presents some sample CfCVDT meshes in two dimensions. Quality comparisons of the CfCVDT meshing scheme with some other triangular mesh generators were reported in [59].

Figure 2: [38] Two-dimensional CfCVDT meshes for various domains and density functions.

Isotropic adaptive schemes – Essential ingredients of adaptive methods are a posteriori error estimates and mesh refinement (or possible coarsening) schemes. An interesting relation between the density function $\rho$ and the local mesh sizes possessed by the CVT is $h_i/h_j \approx (\rho(x_j)/\rho(x_i))^{1/(d+2)}$ where $h_i$ denotes the diameter of the Voronoi region $V_i$ corresponding to $x_i$ (It is still a conjecture in dimensions higher than two but has been numerically verified by many experiments). This property makes adaptive methods based on CfCVDT meshing scheme for numerical solution of PDEs have many advantages over most of existing adaptive methods. The main idea is to refine the old mesh and then optimize it by CVT/CVDT algorithms according to some local a posteriori error estimators. A major advantage of this approach is that we can explicitly determine a density function based on some posteriori error estimator and the CVT mesh size relation to generate the new mesh so that the errors of the new approximate solution will be equally distributed over the element in an optimal way. In particular, the density functions and resulting meshes could be different if different type of error estimators are used for the same problem (for example, $H^1$-type vs. $L^2$-type estimators). Another advantage of CfCVDT-based adaptive methods is that the resulting CfCVDT mesh always has good quality (isotropic) while most adaptive method often degenerates the mesh quality along the refinements. We developed some algorithms and reported numerical results of this method for second-order elliptic PDEs in [42, 48] and the Navier-Stokes equations in [44]. Some examples are presented in Figure 3.

Figure 3: [48] Adaptively refined CfCVDT meshes (left three) and the approximate solution (right) for a convection-dominated problem with a discontinuous solution (having a jump).

Anisotropic adaptive schemes – For convection-dominated problems, one often encounters the difficulty that the overall accuracy of the numerical approximation is deteriorated by local singularities such as interior and boundary layers or sharp shock-like fronts. It is thus interesting to connect the density function to a posteriori error estimates and anisotropic metrics for determining point distributions with special properties such as high aspect ratio spacings that would be useful for resolving boundary layers. We developed such an adaptive anisotropic meshing scheme for solving two-dimensional steady convection-dominated problems in [60]; in particular, the meshes are generated by the ACVDT algorithm [27] in combination with metric tensor information at each level of refinement. Numerical results showed that the adaptive ACVT approach results in substantial improvements compared to using regular isotropic CVT meshes; see Figure 4 for an illustration.
1.3 CVT-based image segmentation

**Basic CVT segmentation** – In the image processing context and in its simplest form, the CVT-based methodology reduces to the well-known $k$-means clustering technique based on similarity. By viewing the latter within the CVT context, very useful generalizations can be easily made; we exploited several such generalizations in [18] and proposed CVT-based algorithms for image compression and segmentation applications. However, the classic CVT model lacks the regularity term, thus often produces too many details during segmentation and fails to accurately detect the target objects in heavily noisy images.

**Segmentation by edge-weighted CVT** – In [71] we developed a model called edge-weighted centroidal Voronoi tessellation (EWCVT) for image segmentation; in particular, the EWCVT model beautifully combines the global color/intensity information and the physical information by adding a regularity term in the original CVT model, and can handle very sophisticated situations; see Figure 5 for an example of EWCVT-based segmentation. We note that the EWCVT model sometimes has difficulties in segmenting images with background inhomogeneity. More recently, the local variation and edge-weighted centroidal Voronoi tessellation LVEWCVT model proposed in [72] improves the EWCVT model by replacing the classic clustering energy term by the local variation energy. It now can easily handle images with background inhomogeneity. Figure 6 shows segmentation results of an inhomogeneous image of a blood vessel into two clusters by the EWCVT method and the LVEWCVT method. We also proposed in [3] a multichannel edge-weighted centroidal Voronoi tessellation (MCEWCVT) method for automatic segmentations of 3D superalloy volumes in the non-interactive fashion. Overall, image segmentation algorithms based on CVT methodologies are essentially clustering algorithms like the $k$-means method, so they are computationally much less expensive than the PDE-based variational models, especially when the number of clusters is large.
2 Ocean and Ice Sheet Modeling and Simulations

Multi-resolution shallow water simulations – We used nonuniform SCVT/SCVDT grids for ocean and ice modeling in [68]; see Figure 7 (left) a SCVDT grid of the North Atlantic where the fourth power of the kinetic energy was used as a proxy to define the density function in the SCVT/SCVDT construction. It suffices to note that SCVT/SCVDT grids take very good advantage of whatever proxy one chooses. The density function as well as the need to resolve boundaries motivate the variations in the grid size. Numerical examples reported in [68, 45, 67] based on the nonlinear shallow-water equations elucidate both the potential benefits of this variable-resolution method and the challenges ahead; see Figure 7 (right) that shows the parallel simulation result of a standard shallow-water test case (test case 5 of [70] for which a flow in geostrophic balance is confronted with a large-scale orographic feature at the start of the simulation) on a nonuniform SCVT mesh using Voronoi-based finite volume discretization. This example clearly illustrates both the potential benefits of this SCVT based multi-resolution method and the challenges ahead.

Parallel FEM ice-sheet modeling – In [74], we presented a prototype 3D thermo-mechanical coupled Stokes ice-sheet model to explore ice-sheet changes under realistic conditions. Finite element approximations with linear elements for all components of the ice sheet (velocity, pressure, temperature, and thickness) on prismatic meshes and parallel algorithms based on domain decomposition were employed to solve the respective sub-models using Message Passing Interface (MPI). To ensure stability for this finite element discretization of the Stokes system, a penalty term was additionally added into the system. In this model the boundary conditions of the Stokes system were simplified to only the no-slip condition at the ice-bedrock boundary and zero velocity lateral boundary condition. We observed that the Picard nonlinear solver is linearly convergent with a contraction constant $\frac{n-1}{n}$, where $n$ denotes the exponent in the Glen’s flow law (thus $2/3$ for the ice sheet case $n = 3$). Based on the observational data of current bedrock topography and ice thickness for Greenland at 5km-resolution, we conducted some preliminary simulation results for the Greenland ice sheet with simplified initial and boundary conditions. Figure 8 presents some simulation results for the top surface velocity field and the current annual change in thickness of the Greenland ice sheet.

Figure 7: [68] Left pair: the original digital image of the kinetic energy in the North Atlantic and the corresponding SCVDT mesh; Right pair: A nonuniform SCVT mesh (decomposed for parallel simulation) and the kinetic energy field at day 10 of the simulation based on this mesh.

Figure 8: [74] Log plot of the distribution of the simulated surface velocity (left pair) and current annual change in thickness (right pair) of the Greenland ice sheet using the Stokes model. For better visualization, we set the upper limit of the values displayed in the left two plots (see the figure legends); these limits correspond to surface speeds of 176.83 and 999 ma$^{-1}$, respectively. The right two plots also have limits as given in the figure legends.
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Table 1: [56] Results of the strong scalability tests using our parallel FEM solver. Mesh size: $80 \times 80 \times 20$, number of tetrahedral elements: 768,000, number of DOF: 3,296,724.

In [56], we greatly improved this method through a new parallel finite element implementation on tetrahedral meshes of the nonlinear Stokes model. Discretizations are based on a high-order accurate scheme using the Taylor-Hood element pair (quadratic elements for velocity and linear elements for pressure) that is stable without any need for penalization. Both no-slip and sliding boundary conditions at the ice-bedrock boundary were studied. In particular, we proposed an efficient and effective approach for handling of the Rayleigh friction boundary condition. In addition, effective solvers using preconditioning techniques for the resulting saddle-point system such as Algebraic Multigrid (AMD) were discussed and implemented. The parallel libraries HYPRE and PETSC were used in our implementation. Through established ice-sheet benchmark experiments, we demonstrated that our finite element nonlinear Stokes model performs at least as well as other published and established Stokes models [65] in the field. The parallel solver was also shown to be efficient, robust, and scalable. Table 1 provides an example of the strong scalability of our Stokes solver.

3 Numerical Methods for PDEs on Surfaces

Finite volume and finite element methods have been widely used in scientific and engineering applications, my work in this area mostly focuses on problems defined on surfaces.

Approximations of convection-diffusion equations – In [16] we developed a Voronoi-based finite volume scheme for discretization of convection-diffusion problems on the sphere based on spherical Voronoi tessellations. For the model problem, the Voronoi-based finite volume scheme was shown to produce first-order accurate approximations with respect to a mesh-dependent discrete first-derivative norm, and in particular, the $L^2$ error of the approximation is of quadratic order when the underlying Voronoi mesh is given by a spherical centroidal Voronoi tessellation (SCVT) [22]. Superconvergence of the approximate solutions on SCVT meshes were also numerically demonstrated.

Approximations of the Ginzburg-Landau model – In [21] we proposed a novel finite volume discretization scheme for approximations of the reduced Ginzburg-Landau phenomenological model for superconducting hollow spheres based on SCVT [21] and used to study the behavior of the quantized vortices [20] on a spherical geometry. The scheme utilizes the properties of the SCVT and the discrete gauge invariance automatically is satisfied to accurately compute the various solution branches, vortex nucleation patterns and vortex dynamics on the sphere. For example, the vortex motion (splitting and annihilation near the equator) shown in the Figure 9 from are features unique to our simulations on the spherical surface and have never been reported in the literature.

Figure 9: [20] The nucleation and the splitting of vortex pairs near equator.
Approximations of fourth-order equations – Examples of physical flows modeled by fourth-order PDEs include ice formation, fluids on lungs, brain warping, and designing special curves on surfaces. In [33], by representing a surface in $\mathbb{R}^d$ as the level set of a smooth function, a discretization of these high order PDEs was proposed by using only finite differences on a standard Cartesian mesh. We developed accurate finite volume schemes that may satisfy discrete conservation law for some physical variables in [23]. In [24], we considered the phase separation on general surfaces by solving the nonlinear Cahn-Hilliard equation using a finite element method. A fully discrete approximation scheme is introduced, and we establish a priori estimates for the discrete solution that does not rely on any knowledge of the exact solution beyond the initial time. This in turn leads to convergence and optimal error estimates of the discretization scheme.

Covolume-upwind finite volume approximations – In [49] we studied covolume-upwind finite volume methods on rectangular meshes for solving linear elliptic partial differential equations with mixed boundary conditions. To avoid non-physical numerical oscillations for convection-dominated problems, nonstandard control volumes (covolumes) are generated based on local Peclet’s numbers and the upwind principle for finite volume approximations. Two types of discretization schemes with mass lumping are developed with use of bilinear or biquadratic basis functions as the trial space respectively. Various examples were also carried out to numerically demonstrate stability and optimal convergence of the proposed methods.

4 Geometric and Image Processing of Surfaces/Curves

Cortical surface flattening – Surface representations of the human cortex have become an important tool for brain imaging data analysis in recent years as they could facilitate the visualization and analysis of functional activation data by preserving important geometrical and topological relationships, and they can be parameterized using two dimensional coordinate systems and be very useful for anatomically-driven inter-subject registration. While some elegant flattening schemes minimizing the metric/areal distortion were proposed, three approaches for discrete conformal flattening which preserves the angles were also suggested in [37, 1, 36]. We applied in [47] the so-called least squares conformal mapping (LSCM) approach [53] to flatten a patch of the cortical surface on planar regions and generalized it to produce spherical conformal maps of the entire cortex while minimizing metric distortion within the class of conformal maps. Our method, which preserves angular information and controls metric distortion to some extent, involves the solution of a linear system and a nonlinear minimization problem with three parameters. Some performance comparisons of our method with other techniques was also reported in [43], see Figure 10 for an illustration.

Figure 10: [43] From left to right: a left cerebral hemispheral cortex (in radiological orientation) and spherical maps produced by FreeSurfer, CirclePack and LSCM, respectively.

Open-surface shape correspondence – Shape correspondence [8], which aims at accurately identifying corresponding landmarks from the given population of shape instances, is a major challenge in constructing a statistical shape model, such as the popular Point Distribution Model (PDM) [6]. We developed a new 3D shape correspondence method in [7]. The proposed method bears two important properties. First, while available methods are primarily focused on closed-surface shape correspondence, the proposed method aims to address open-surface shape correspondence, where each shape instance is an open surface with a closed boundary. Second, the proposed method explicitly enforces the topology consistency of the identified landmarks in a way that they constitute consistent and accurate triangulated meshes for the input shape instances. Thus the correspondence of the identified landmarks more accurately reflects the correspondence of the underlying continuous shape instances.
Curve smoothing – In [79] we proposed a variational phase field model for curve smoothing, in which a weight function is associated with the similarity measure term in the model so that important geometric features could be well preserved. Finite element approximation of the proposed model is given for its numerical implementation. Since the model has a linear weak variational form, the discretized system could be solved efficiently by many existing solution techniques. An effective algorithm is also developed, for the purpose of feature preservation, to automatically determine the weight from the given data.

5 Numerical Solution of Stochastic Differential Equations

Stochastic differential equations (SDEs) are used in many fields, such as stock market, financial mathematics, stochastic controls, dynamic system, biological science, chemical reactive kinetics and hydrology, and so on. Thus, it is of importance to develop numerical solution for solving SDEs.

Stochastic differential equations – Consider the following (forward) SDEs

\[ \begin{cases} \frac{dy(t)}{dt} = f(y(t))dt + g(y(t))dW(t), & t \in [0, T], \\ y(0) = y_0, \end{cases} \]

where \( T > 0 \) is the terminal time, \( y(t) : [0, T] \times \Omega \to \mathbb{R}^m \), \( f(y) : \mathbb{R}^m \to \mathbb{R}^m \), \( g(y) : \mathbb{R}^m \to \mathbb{R}^{m \times d} \), and \( W(t) = (W_1(t), \ldots, W_d(t))^* \) is a standard \( d \)-dimensional Brownian motion defined on a complete, filtered probability space \((\Omega, \mathcal{F}, P, \{\mathcal{F}_t\}_{0 \leq t \leq T})\). SDEs are often driven by a high-dimensional Brownian motion and coupled with other type stochastic problems [29], thus efficient and accurate solvers for high-dimensional SDEs are urgently needed. In [77] we proposed a splitting scheme for numerical solutions of the SDEs, and showed that the resulted approximate solution converges to the analytic solution of the SDEs with the same convergence rate as the popular Euler-Maruyama method. Furthermore, this scheme allows us to use the latest information inside each iteration in the E-M method so that better approximate solutions could be obtained than standard approach especially when \( d \) is large.

Backward stochastic differential equations – A backward stochastic differential equation (BSDE) for \((y(t), z(t))\) is often given by

\[ \begin{cases} -dy(t) = f(t, y(t), z(t))dt - z(t)dW(t), & t \in [0, T), \\ y(T) = y_T, \end{cases} \]

where \( f(t, y(t), z(t)) \) is an adapted stochastic process with respect to \( \{\mathcal{F}_t\} (0 \leq t \leq T) \) for each \((y(t), z(t))\). Existence and uniqueness of solution of the nonlinear backward stochastic differential equation were originally proved by Pardoux and Peng in [64] in 1990. Since then BSDEs and their solutions have been extensively studied by many researchers. Many important properties of BSDEs and their applications in finance were studied in [62, 29]. In [78] we developed a stable multi-step scheme on the time-space grids for numerically solving BSDEs. In this scheme, the integrands, which are conditional mathematical expectations derived from the original equations, are approximated by the Lagrange interpolating polynomial with values of the integrands at multi-time levels. In particular, they are then numerically evaluated using the Gauss-Hermite quadrature rule and linear interpolation in the spacial grids. In [76], we studied error estimates of the Crank-Nicolson scheme proposed by [75] for solving BSDEs and prove that this scheme is of second-order convergence in solving both \( y_t \) and \( z_t \) without any extra constraint on \( f \).

6 Other Works

Numerical methods for peridynamics

Peridynamics (PD) models were first introduced by Silling in 2000 and has become an attractive emerging tool for the multi-scale material simulations involving crack growth or damage. It is an integral-type nonlocal continuum theory which provides a more general set-up than the classical PDE based elasticity theories for physical problems with discontinuities; on the other hand it can also be viewed as a continuum version of molecular dynamics. In [25], we presented some results on a posteriori error analysis of finite element methods for solving linear bond-based nonlocal diffusion and PD models. In particular, we aimed to propose a general abstract frame work for a posteriori error analysis of the PD problems. A posteriori error estimators were consequently prompted, and the
connection between non-local a posteriori error estimation and classical local estimation is studied. 
The analysis is done with equations for which the operator- induced norm is equivalent to $L^2$ norm, 
due to our choice of kernel function. As shown in [28] and many other references, for different kernel 
functions, we may have equivalence with fractional Sobolev space $H^s (0 < s < 1)$ and this sort of 
situation is still under our investigation.

**Study of heterogeneous nematic polymers**

In [4], we examined the linear viscoelastic response of heterogeneous nematic polymers to small 
amplitude oscillatory shear flow, paying special attention to the macroscopic influence of strong 
plate anchoring conditions. To predict the dynamic moduli, we modeled the system with Stokes 
hydrodynamic equations with viscous and nematic stresses coupled with orientational dynamics 
driven by the flow, an excluded volume potential, and an elasticity potential. First, we showed that 
for special cases of normal and tangential anchoring, we recover explicitly solvable Leslie-Ericksen-
Frank behavior. In this case we observed significant differences between the moduli for normal and 
tangential anchoring. Then, we turned to a numerical study of oblique anchoring conditions, which 
are more complicated due to the appearance of order parameter gradients at leading order. When 
the anchoring angle is near 45 degrees, we observed significantly different scaling behavior in the 
storage modulus for high frequencies compared to the behavior for normal or tangential anchoring. 
In [5] we extended previous work on the linear viscoelastic moduli of heterogeneous nematic polymers 
in small amplitude oscillatory shear, focusing on the role of the orientational anchoring conditions 
at the plates. When tangential or normal anchoring conditions are applied, the Doi-Marrucci-Greco 
tensor model effectively reduces to the Leslie-Ericksen model, leading to the prediction that director 
distortions dominate the dynamic moduli with negligible contributions from the order parameters. 
We examined oblique anchoring angles which are experimentally feasible and naturally arise in the 
presence of curved boundaries. We used a combination of analysis and numerical simulation on the 
generalized tensor-flow system for arbitrary anchoring conditions to show that any oblique anchoring 
condition induces a nontrivial order parameter contribution to the dynamic moduli, which vanishes 
only in the limit of tangential or normal anchoring. These results provide insight into the relative 
importance of the distortional versus bulk nematic elastic stress in determining the viscoelastic 
moduli, predicting that anchoring conditions tune the relative contributions.

**Numerical methods for the boundary controllability for the wave equation**

The exact boundary controllability problem for the wave equation is defined as follows: Given a 
bounded domain $\Omega \subset \mathbb{R}^d$ with boundary $\Gamma$, the wave equation

$$u_{tt} - \Delta u = f \quad \text{for } x \in \Omega \text{ and } t \in (0, T]$$

and initial conditions

$$u(x, 0) = v_0(x) \quad \text{and} \quad u_t(x, 0) = v_1(x) \quad \text{for } x \in \Omega,$$

(5) determine a boundary control $g = \alpha \frac{\partial u}{\partial n} + \beta u$ such that the terminal conditions

$$u(x, T) = w_0(x) \quad \text{and} \quad u_t(x, T) = w_1(x) \quad \text{for } x \in \Omega$$

(7)

are satisfied. It is known that the control $g$ exists that drives the solution of (5)–(6) to the terminal 
condition (7) so long as $T$ is sufficiently large [51]. We changed the original control problem, after 
discretization, into a quadratic optimization problem with linear constraints. The uniqueness of the 
discrete finite difference solutions obtained in this manner is demonstrated and efficient implement-
ation strategies for the method are also discussed. It is shown that for smooth, minimum $L^2$-norm 
Dirichlet controls, the method results in convergent approximations without the need to introduce 
regularization. Furthermore, for the generic case of non-smooth Dirichlet controls, convergence with 
respect to $L^2$ norms is also numerically demonstrated. One of the strengths of the method is the flex-
ibility it allows for treating other controls and other minimization criteria; such generalizations are 
discussed. In particular, minimum $H^1$-norm Dirichlet controllability problem is approximated and 
solved, as are minimum regularized $L^2$-norm Dirichlet controllability problems with small penalty 
constants. We are also dealing with implementation issues such as efficiency, good linear system 
solvers, and pre-conditioners which need to be addressed for the large-scale optimization systems we 
have to deal with in multiple dimensions; see our work in [34, 41, 35] for details.
Parallel and high-performance computing

I did some research on parallel CFD problems when I was back in the Institute of Computational Mathematics of Chinese Academy of Sciences. We dealt with the parallel implementation on distributed memory systems of a pressure-correction projection scheme (i.e., the Crank-Nickolson modified Temam scheme II) for the unsteady, incompressible Navier-Stokes equations [50]. Various techniques such as pipelining and canon cyclic algorithms were used to ensure the good parallel performance and scalability of the algorithm. The algorithm for the 2D case was implemented using an MPI environment and numerical tests have been carried out on various computers, including the home made Dawn–1000 MPP system and workstation clusters. For one and a half years early in my residence at Iowa State University, I was a member of the high-performance computing research group in ISU Computing Center. My research in this period concentrated on the performance and function evaluation of OpenMP and MPI, including MPI2.0 one-sided communication subroutines, on several supercomputer systems, see [52].

References


