Research Statement

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1 Introduction

My research interests are focused on numerical methods and analysis for partial differential equations (PDEs), and integro-differntial equations, e.g. the peridynamic (PD) models, using finite element method (FEM) and/or finite volume method (FVM).

The mesh quality can essentially effect the accuracy of finite element schemes, so I have extensively studied the mesh generation algorithm for different model problems. In [8], we proposed an adaptive FEM for Navier-Stokes equations, based on centroid Voronoi tessellation (CVT), which could optimally distribute error and result in high-quality meshes. An adaptive spline FEM was discussed in [14], where the local refinement with spline basis functions was solved by using hierarchical mesh. Other than mesh generation for FEM, I have built an optimal nonstandard control volume for FVM in [10], for solving convection-dominated problems. This kind of control volumes are generated based on local Peclet's number and upwind method, therefore the resulting scheme is both stable and of optimal convergence rate.

My research also covers PDEs on general surfaces, which are useful in various applications. I have studied the numerical approximations for high-order PDEs, e.g. fourth-order equations and Cahn-Hilliard equations, over surfaces, in [3, 4]. I have proposed an adaptive method for elliptic equations on surfaces using FVM in [9], where a robust a posteriori error estimator was proposed and analyzed.

Moreover, I have applied a posteriori error analysis and adaptive algorithms to the PD model in [5, 7], that is a solid mechanics model dealing with cracks and fractures through nonlocal approach and integral equations. Adaptive method is one of the most efficient numerical methods for PD models, because solutions of PD equations allow discontinuities, as a result of which, large errors arise at breakages. It has been seen, in our research, that adaptive method could reduce the computational cost dramatically and lead to optimal convergence.

2 Research Summary

2.1 Numerical Method for PDEs

For the past few years, I have been working on the numerical schemes for PDEs using FEM or FVM, both on theory and implementation. The goal of my research is to design efficient numerical schemes for mathematical and physical models, and several results have been obtained.

2.1.1 Adaptive Methods and Related Research

It is well known that the efficiency and accuracy of FEM can be largely effected by the mesh discretization of the computational domain. Adaptive methods can essentially reduce the computational cost and have been studied by many researchers, with the ultimate goal to build a series of meshes that will eventually equal-distribute the approximation errors. The quality of mesh could be compromised by bad mesh regularity, hanging nodes, and some other factors. My co-researchers and I have introduced several mesh generation algorithms to get high-quality mesh.

In [8], an adaptive method is studied and corresponding numerical simulations are performed on steady Navier-Stokes equations using CVTs, where a density function decides the distribution of 2D triangular grids. We define the density function according to the a posteriori estimator, and therefore the errors will be equally distributed over the mesh in an optimal way while keeping the triangles very well shaped at all levels of refinements as in Figure 1. The generation of adaptive CVT is more convenient and computationally efficient than traditional mesh refinement strategies, and can be easily extended to higher dimensions.

In order to exactly present geometries, more general basis functions such as splines are composed into FEMs. A long term problem of adaptive computations with splines is that the local refinement could not be efficiently carried out, due to a rectangular grid of control points in the parameter space. In [14], we find one solution to this problem. With our algorithm, the rectangular meshes can be locally refined very

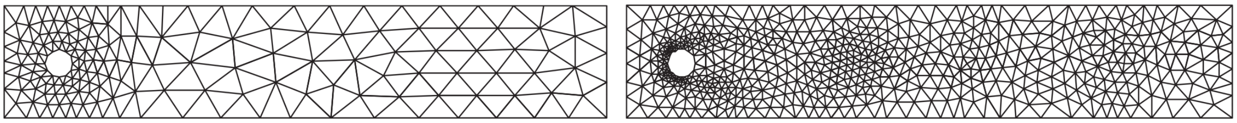

Figure 1: [8] Adaptively refined CVT meshes for steady Navier-Stokes equation where the flow passes a circular cylinder in a channel.

effectively, no efforts are needed to deal with hanging nodes since they are not counted as degrees of freedom. Residual-based error estimator is derived, and is proved to be both efficient and reliable.

Different from FEM, the performance of FVM depends more on the quality of *control volumes* or *covolumes*, since these covolumes have great influence upon the computation of numerical flux. In [10], we study a covolume-upwind FVM on rectangular meshes for solving convection-dominated problems with mixed boundary conditions. It is well-known that for convection-dominated problems, non-physical oscillations may rise on boundary layers. Although standard upwind method can be applied to avoid these oscillations, the convergence rate of upwind method is low. To overcome this issue, we constructed nonstandard covolumes based on local Peclet's numbers and upwind principle. The resulting schemes are both stable and optimally convergent.

2.1.2 PDEs on General Surfaces

Problems related to PDEs on general surfaces have been received growing interests over the past few years, due to a variety of applications such as image processing, geometry, physiology, cell-biology and so on. Therefore I have extensively studied several topics in this area.

One of our interests is fourth-order PDEs defined on general surfaces, which may find its application in chemical coating, cell membrane deformation and computer graphics, in fact, the variation of curvature dependent interfacial energies leads naturally to fourth-order or higher equations on surfaces. Based on these motivations, we have studied a FVM for the numerical solution of a model fourth order PDE defined on a smooth surface in [3]. The discretization is done via a surface mesh consisting of piecewise planar triangles and its dual surface polygonal tessellation. We have provided an error estimate for the approximate solution under the H^1 norm on general regular meshes. In particular, a superconvergent scheme is proposed to compute gradients more accurately when the underlying mesh is constructed by CVT meshes.

Various experimental studies have shown that phase separations could occur on static or dynamic surfaces, such as phase separation on lipid bilayer membranes and crystal growth on curved surfaces. Thus in [4], we extend our research to the phase separation on general surfaces by solving the nonlinear Cahn-Hilliard equation using FEM. 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. Numerical examples are also provided to substantiate the theoretical results, one of which is shown in Figure 2.

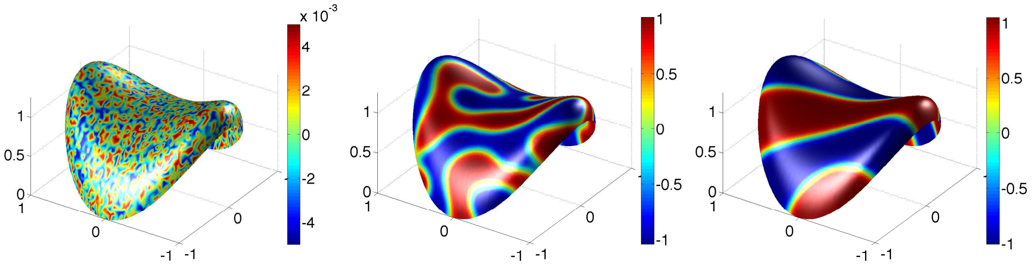

Figure 2: [4] Phase separation on a surface.

Adaptive computation over surfaces is another topic worth studying. In [9], we propose a residual-based a posteriori error estimator for finite volume approximations of elliptic equations on general surfaces. The crucial part is to define a reliable and efficient estimator, and it is not similar as that in planar case where the estimator is just composed of interior and boundary residual. For PDEs on surfaces, one has to consider the difference between the discretized ‘surface’ and the original surface, as well as the difference of data defined on the two domains. Moreover, the refining algorithm require a lifting process onto the original surface. The estimator and refining strategy introduced in this paper work fine on either closed or open surfaces, see Figure 3 for adaptive refinement for equation over a torus, whose solution has large gradient around $(-1, 0, 0)$.

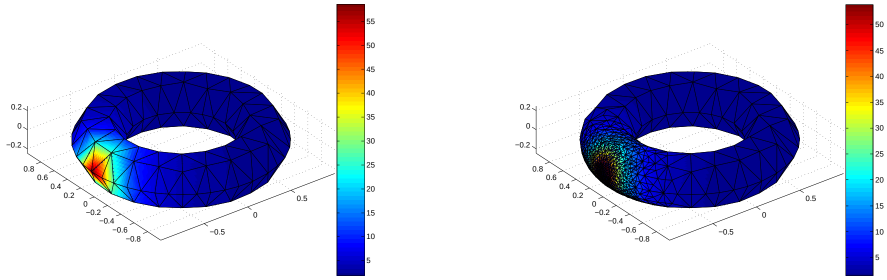

Figure 3: [9] Adaptive refinement for equation over a torus.

2.2 Numerical Method for PD Models

Besides PDEs, I also have interests in the numerical approximation for PD models. PD models are introduced by considering the interaction of material points, which consist of the material, within finite distance [12, 13]. As in Figure 4, let $\mathbf{x}$ and $\mathbf{x}'$ denote initial positions of two material points in the reference configuration Ω, $\mathbf{u}(\mathbf{x})$ and $\mathbf{u}(\mathbf{x}')$ be the displacements of the points with respect to the reference positions. Denote $\mathbf{f}(\mathbf{u}(\mathbf{x}', t) - \mathbf{u}(\mathbf{x}, t), \mathbf{x}' - \mathbf{x})$ the pairwise force function for *bond* $\mathbf{x}' - \mathbf{x}$ and relative displacement $\mathbf{u}(\mathbf{x}', t) - \mathbf{u}(\mathbf{x}, t)$. PD model (bond-based) of solid mechanics then follows from the Newton’s second law

$$\mathbf{u}_{tt}(\mathbf{x}, t) = \int_{B_\delta(\mathbf{x})} \mathbf{f}(\mathbf{u}(\mathbf{x}', t) - \mathbf{u}(\mathbf{x}, t), \mathbf{x}' - \mathbf{x})\, d\mathbf{x}' + b(\mathbf{x}, t), \tag{1}$$

where b is the external force density, $B_\delta(\mathbf{x}) = \{\mathbf{x}' \in \Omega : |\mathbf{x}' - \mathbf{x}| < \delta\}$ denotes the interaction range of $\mathbf{x}$, with *horizon* $\delta > 0$. This nonlocal model is closely connected with classical differential equations in the sense that PD equations reduce to PDEs as $\delta \to 0$.

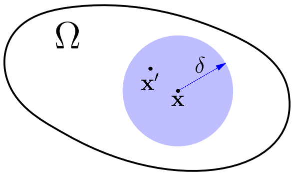

Figure 4: Bond-based peridynamic model.

Recently, the PD model is receiving more and more attentions, the effectiveness of PD models has been demonstrated in a number of applications, e.g. fracture and failure of composites, fracture of polycrystals, nanofiber networks and so on, where numerical simulations of singular behavior such as crack growth or damage are involved. Numerical methods for PD models have been extensively studied by mathematicians while the PD adaptive FEM is still lacking. Since PD models are capable of describing material cracks and fractures without knowing the positions of breakage, adaptive computations are even more demanding than PDEs. Notice that there have been some efforts made (see [1, 2]), however no systematic nonlocal a posteriori error analysis has been established within our knowledge, and our research is aiming to fill in such a gap.

In [5], a posteriori error analysis for steady-state PD models is studied, a residual-based estimator was introduced to recover the exact error. Although we adopt the similar framework as in the classical a posteriori analysis for PDEs, the nonlocal a posteriori error analysis is quite different. Unlike the PDE case, there is no jump terms on interior edges due to the lack of derivative. Considering the connection between PD equations and PDEs, we have also established the relationship between nonlocal estimator and its local counterpart by showing that the nonlocal error estimator actually reduces to the local error estimator, as $\delta \to 0$, element-wisely.

Later, a convergent adaptive finite element algorithm for PD models is introduced in [7], we basically prove the error-reduction of adaptive refinement. Although similar conclusion has been proved for PDEs, it is essentially different methodology for PD models. Since PD models are proposed to deal with discontinuous solutions, therefore uniform refinement usually would not lead to optimal convergence rate. Various numerical experiments have been performed to show that the optimal convergence rate can be achieved by adaptive refinements, no matter the solution is continuous or not. One of the computational result is shown in Figure 5, optimal rate is achieved under adaptive refinement (right), while the accuracy of uniform refinement is not as good (left).

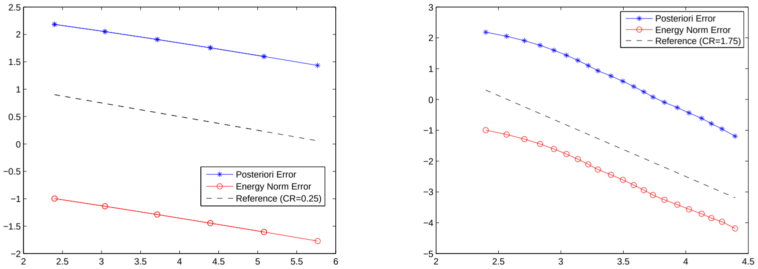

Figure 5: [7] Uniform and adaptive refinement for a PD model with discontinuous solution.

Other than the above topics, my research also covers the numerical methods for SDEs. Since SDEs are often driven by a high-dimensional Brownian motion and coupled with other types of stochastic problems, efficient and accurate solvers for high-dimensional SDEs are urgently needed. The operator splitting scheme is one of the most popular ways to deal with multi-dimensional problems of PDEs, and we apply the similar idea to SDEs. We propose a splitting method, which is suitable to deal with high-dimensional case, for SDEs in [15], and show that the convergence rate is the same as the traditional Euler-Maruyama method.

3 Future Research Plan

For the next few years, I will extend my current work, and meanwhile try to investigate some new research areas.

CVT has great advantages in adaptive mesh generating, such as good quality, the easiness of implementation, and flexibility of application. While the application of CVT for time-evolving problem has not been well developed, with the main problem being the lack of efficient interpolation algorithm between meshes. One of my research plans is to work on this project.

Spline is useful in describing the geometry of surfaces or thin films, therefore can be applied in areas like biological cell formation and computer graphics. We plan to apply our spline adaptive algorithm in [14] onto general surfaces, as well as evolving surfaces. Moreover, we are working to design a coarsening-refining algorithm with spline basis functions, which is more flexible and efficient than the existing one.

For future research on numerical approximations for PD models, my plan includes:

- Analyses: To continue the nonlocal a posteriori error analysis and convergent adaptive methods for PD models. Several results have been obtained on this topic for now, while a complete systematic framework is yet to be established. Besides residual-based estimator, there are other types of estimator, e.g. adjoint-based and recover-based estimators, are worthy of study. Moreover, discontinuous galerkin method is another topic within our interests.
- Applications: Various numerical schemes and meshes will be investigated for different PD models. We plan to study the effect of quality of 2D triangular meshes on the condition number of the linear system,

when using FEMs to implement PD models. Multigrid schemes will be introduced to PD computations. Meshless adaptive methods for PD models, and numerical schemes for nonlocal advection problems are to be considered. Application of PD models for adaptive multiscale material modeling will also be studied.

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