Research Statement

1 Overview

As the complexity of problems increases in all practical fields of science and engineering, "ad hoc" methods are reaching their limits. Thus, "provably good" methods have gained an unprecedented weight in scientific computing. My research concentrates on the design, analysis, and implementation of *provably good* numerical methods. In particular, I am interested in approximation theory and numerical solutions to partial differential equations (PDE) using the finite element method coupled with multilevel (ML) adaptive techniques. *Adaptivity* is the most critical feature in my research. My primary areas of interest are in biophysics and computer graphics: simulation of electrostatics in biomolecules, namely numerically solving the *Poisson-Boltzmann* equation (PBE), and surface processing in the form of parameterization and remeshing.

2 Research Accomplishments

Traditional ML preconditioning analysis revolves around uniform refinement. Conventional ML methods (e.g., multigrid) have been proven to be optimal ($O(N)$ where N is the number of degrees of freedom) by exploiting the geometric increase in the size of the problem. In adaptive refinement this geometric increase is hard or simply impossible to attain. The multigrid method suffers from both suboptimal computational and storage complexity, $O(JN)$, where J is the number of levels of refinement. As the refinement depth is increased, it is this suboptimality that prevents conventional ML methods from being a viable tool in realistic applications. The hierarchical basis (HB) methods are superior to multigrid methods in adaptive refinement regimes where they promise optimal computational and storage complexity. My research includes theoretical treatment and implementation of the HB methods under adaptive refinement procedures.

In [2], I extended the optimality of an additive variant of multigrid, Bramble-Pasciak-Xu (BPX) preconditioner, to 3D red-green, 3D/2D red refinements. Red refinement means quadrasection and octasection in 2D and 3D respectively; red-green is red refinement complemented by bisection. The theoretical framework supports arbitrary spatial dimension only the geometrical relations must be re-established. This optimality is the fundamental assumption for the HB methods in [3] and lays the foundation of various results in adaptive refinement.

The HB methods were the remedy to multigrid for achieving optimal storage complexity, not computational complexity. The wavelet stabilizations to HB methods by Vassilevski and Wang, known as the wavelet modified hierarchical basis (WHB) method, addressed this difficulty by proving the optimality of computational complexity under uniform refinement. The adaptive refinement cases were not studied.

In [3], I gave the first optimality result of the additive WHB method with a general PDE coefficient in L_∞ for all the five local refinement procedures under consideration: 3D/2D red-green, 3D/2D red, and an other version of 2D red refinement. In addition, as in the BPX case, the theoretical framework of the additive method supported extensions of these classes of refinement procedures to higher spatial dimensions greater than 3, provided that the necessary geometrical abstractions are in place. With continuously differentiable PDE coefficients, optimality of the multiplicative WHB method was given for 3D/2D red refinement. Without such coefficients, a nearly optimal estimate can be obtained with the help of H^1-stability of the linear operators employed in the WHB method.

An interesting consequence of the optimality of the BPX preconditioner was a proof of the H^1-stability of L_2-projection restricted to finite element spaces under the same class of local red-green and red refinement algorithms. This question has been under intensive study due to its relationship to ML preconditioning. The existing theoretical results involve *a posteriori* verification of somewhat complicated mesh conditions after refinement has taken place. If such mesh conditions are not satisfied, one has to redefine the mesh. My stability result appears to be the first *a priori* H^1-stability result for the L_2-projection.

The methods described above have been implemented using the Finite Element ToolKit (FEtk) [4]. FEtk contains *a posteriori* error estimation, mesh refinement algorithms, and iterative solution methods. All of the preconditioners mentioned have been implemented as ANSI-C class library extensions to FEtk. A collection of our numerical results has been published in [1]. The hierarchical solvers are the core libraries in FEtk for adaptive numerical solution of PDEs.

3 Future Research

I am interested in multiresolution approximation theory techniques. In particular, practical applications of such techniques to the discretization of the PDEs so that ML hierarchical solvers can effectively be exploited. Wavelet modifications to hierarchical basis have been somewhat successful in discretizing PDEs. Although such methods are provably optimal, the computation is rather expensive due to large constants in the complexity statements. I plan to design and implement effective yet reasonably expensive methods.

The finite element machinery is notoriously expensive to construct. Completing a package takes many years of code development. The finite element theory can accommodate adaptive techniques, but implementation can be quite problematic. I was attracted to adaptive finite difference schemes because of their convenience and simplicity. As an alternative to finite element and successive refinement techniques, I plan to examine the theoretical treatment of adaptive finite difference schemes together with moving mesh methods.

The biochemistry community is intensely interested in the complicated range of interactions between enzymes and their substrates. My graduate work contained applications to *diffusion-influenced bimolecular reactions*. Simulation of such reactions are often approximated with continuum mechanics, leading to the PBE. The PBE is an elliptic nonlinear partial differential equation which becomes quite challenging to solve especially for realistic biomolecules. There is substantial amount of research dedicated to numerically solving the PBE. However a comprehensive theoretical treatment of the PBE is still missing, and I plan to address this issue. There is also ongoing work with a number of colleagues to efficiently solve the PBE.

Although ML methods' superior performance is known in computing circles, the deployment of the code into the existing software is far from being complete. I am going to extend the existing application program interfaces (API) in order to support hierarchical solvers in a wide collection of applications. The standardization of such API is critical to interdisciplinary collaborations.

References

[1] B. Aksoylu, S. Bond, and M. Holst, *An odyssey into local refinement and multilevel preconditioning III: Implementation and numerical experiments*, in Proceedings of the 7th Copper Mountain Conference on Iterative Methods, H. van der Vorst, ed., Copper Mountain, CO, 2002, SIAM J. Sci. Comput. Copper Mountain special issue, accepted.

[2] B. Aksoylu and M. Holst, *An odyssey into local refinement and multilevel preconditioning I: Optimality of the BPX preconditioner*, SIAM J. Numer. Anal., (2002). in review.

[3] ——, *An odyssey into local refinement and multilevel preconditioning II: Stabilizing hierarchical basis methods*, SIAM J. Numer. Anal., (2002). in review.

[4] M. Holst, *Adaptive numerical treatment of elliptic systems on manifolds*, Advances in Computational Mathematics, 15 (2001), pp. 139–191.