

# Research Statement Burak Aksoylu

## 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. I am particularly 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. Even in modern day simulations, *solvers* usually take more than half the computation time. Hence, solver technologies, especially equipped with ML adaptive techniques, will surely continue to be a decisive factor for the future of high performance modeling and simulation. My primary areas of interest include biophysics, computer graphics, and geosciences. In particular, the simulation of electrostatics in biomolecules, digital geometry processing in the form of surface parameterization and remeshing, and multiphase flow problems in reservoir and groundwater simulations, respectively.

## 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  $J \sim \log N$  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 in adaptive refinement regimes for achieving optimal storage complexity, but not computational complexity. The wavelet modified (stabilized) hierarchical basis (WHB) method addressed this difficulty. Eventually, optimality of computational complexity under uniform refinement was proved. However, adaptive refinement cases were not studied. I targeted both computational and theoretical optimality for the above methods under adaptive refinement procedures.

In [3], I gave the first optimality proof of the additive variant of the multigrid, Bramble-Pasciak-Xu (BPX) preconditioner, extended to an implementable and realistic 3D local red-green refinement procedure. Red refinement means quadrisection and octasection in 2D and 3D respectively; red-green is red refinement complemented by bisection. The theoretical framework supports arbitrary spatial dimension. This optimality is the fundamental assumption for the HB methods in [4] and lays the foundation of various results in adaptive refinement. In [4], I gave the first optimality result of the additive WHB method with general PDE coefficients in  $L_\infty$  for 3D and 2D local red-green refinement procedures. 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. Nearly optimal estimates can be obtained for the multiplicative version of the WHB method with the help of  $H^1$ -stability of the linear operators employed in the WHB construction.

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 the local red-green refinement procedure. 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 [4].

The methods described above have been implemented using the Finite Element ToolKit (FETk) [7]. 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 [2]. The hierarchical solvers are the core libraries in FETk for adaptive numerical solutions of PDEs.

Parameterization of unstructured surface meshes is of fundamental importance in many applications of *digital geometry processing* such as remeshing and texture mapping. The resulting systems are large and exceedingly ill-conditioned. Hence, they are difficult or impossible to solve without the use of sophisticated ML preconditioning strategies. Since the underlying meshes are very fine to begin with, such ML preconditioners require mesh coarsening to build an appropriate hierarchy. In [5], we examined several mesh simplification strategies for the construction of hierarchies. We introduced two novel hierarchy construction schemes and demonstrated their superior performance when used in conjunction with ML preconditioners. This gave rise to orders of magnitude enhancement in computation time over traditional computer graphics methods.

In [6], I am currently developing solvers to address severe contrasts in geophysical properties for reservoir and groundwater simulations. I combined ML technology with eigenvalue deflation techniques. The constructed *physics based isotropic deflation* technique gives rise to *optimal* preconditioners for multiphase flow in porous media.

### 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, as shown in [2], due to large constants in the complexity statements. I plan to design and implement effective yet reasonably expensive methods.

Theoretically ML methods promise optimal complexity independent of the contrasts in the PDE coefficients. As mentioned above, these methods suffer from large constants in practice. Problems with severe contrasts in the PDE coefficients are ubiquitous in geoscience. Deflation techniques are promising to address the extremal eigenvalues that are associated to these severe contrasts. Within the deflation framework, I plan to analyze strategies to capture and attenuate the effect of extremal eigenvalues. *Physics-based isotropic collapsing* in the ongoing work [6] seems to be quite effective, in which, regions with isotropic geophysical properties are collapsed. This can be interpreted as a semicoarsening process which effectively reduces the 3D problem to a set of 2D problems according to the underlying geological system; and the 2D problems are treated with ML techniques. I also plan to explore the interplay between deflation, isotropic collapsing/coarsening, and ML preconditioning in adaptive regimes.

Mixed and discontinuous Galerkin (DG) FE methods have been extensively used for flow problems due to local mass conservation. However, the preconditioning technology for these methods is not as effective as that for the standard Galerkin methods. In the subdomains of interest, where local mass conservation is imperative, mixed FE and DG can be coupled with Galerkin FE in the complementary subdomain. This will enable the use of the right discretization with the appropriate preconditioner. I plan to pursue such hybrid methods dictated by the underlying discretization.

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 *Poisson-Boltzmann* equation (PBE). The PBE is an elliptic nonlinear partial differential equation which becomes quite challenging to solve especially for realistic biomolecules. There is a 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 [1].

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. Our work in [5] heavily relies on this.

## References

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