Final Scientific Report on DOE Project:

Scalable Adaptive Multilevel Solvers for Multiphysics Problems

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1 Summary

In this project, we carried out many studies on adaptive and parallel multi-level methods for numerical modeling for various applications, including Magnetohydrodynamics (MHD) and complex fluids. We have made significant efforts and advances in adaptive multilevel methods of the multiphysics problems.

1.1 Multigrid Methods Discretization of mathematical models described by partial differential equations (PDEs) often leads to linear algebraic equations with sparse matrices of huge dimension. How to solve such algebraic linear systems efficiently is a fundamental question in scientific and engineering computing and numerical PDEs. Multigrid (MG) methods are among the most efficient methods for accomplishing such task, especially in applications governed by elliptic PDEs.

As part of this project we have developed multilevel/multigrid solvers for scalar PDEs as well as coupled systems of PDEs discretized on unstructured grids. We devised a novel multilevel algorithm for Poisson equation discretized on unstructured shape-regular grids using the auxiliary space preconditioning framework [31]. The auxiliary grids and spaces are constructed with the help of a cluster tree. In this work we showed that the multilevel method have nearly-optimal convergence rate and the computational work is of order $\mathcal{O}(N \log N)$ for a problem with N unknowns on a general unstructured grid. We also used such a technique to develop a parallel auxiliary grid algebraic multigrid (AMG) method to leverage the power of graphics processing units (GPUs). Numerical experiments achieved an average relative speedup of over 15 on quasi-uniform grids and 6 on shape-regular grids when compared to the state of the art AMG implementation on CPUs. When compared with AMG implementations in CUSP (a GPU software program developed by NVIDIA), our new algorithm achieved an average speedup of over 4 on quasi-uniform grids and 2 on shape-regular grids. A purely AMG method has also been developed for isotropic graph Laplacian problems on GPUs based on an unsmoothed aggregation framework [22]. In [13], we developed a hybrid preconditioning framework that combines an iterative method and a preconditioner in a complementary fashion. We proved that the combined preconditioner is positive definite and derived sharp estimates on the condition number of the preconditioned system. Numerical results from reservoir simulations showed the efficiency of the solver based on this hybrid preconditioner. In [5], local MG method on adaptive finite element grids obtained via the bisection refinement was developed. We have theoretically shown its robustness as a preconditioner in Krylov iterative method for the symmetric elliptic problems with large jump coefficients in both two and three dimensions. In [16], we developed an efficient multigrid method for finite element discretizations of the Stokes equations on both structured grids and unstructured grids based on a novel distributive Gauss-Seidel smoother and least squares commutator. Our method was shown to be very efficient and outperforms the popular block preconditioned Krylov subspace methods. The multigrid solver we developed for the Stokes equations was the fastest when compared with many of the existing Stokes solvers. Such MG solver is successfully generalized to a first order unwinding MAC discretization Oseen problem in [16]. Defect-correction techniques are applied to further improve the performance. Numerical results are presented to demonstrate the proposed solver is robust to the Reynolds number.

Regarding the theoretical analysis of multilevel solvers, we studied the convergence of two-grid and multigrid methods for linear systems discretized by the conforming linear finite element method for the second-order elliptic equations with anisotropic diffusion [18]. With a specially designed block smoother, we showed that both aligned and non-aligned grids have uniform convergence with respect to the anisotropy ratio and the mesh size in the energy norm. In [12], we provided the first comprehensive convergence analysis of a nonlinear Algebraic MultiLevel Iteration (AMLI)-cycle method for symmetric positive definite problems and showed that the nonlinear AMLI-cycle MG is at least as good and usually better than the n-fold V-cycle MG method in terms of convergence rate and computational cost. In [27], we develop and analyze multilevel methods for the so-called alpha-harmonic extension to localize fractional powers of elliptic operators. We present a multilevel method with line smoothers and obtain a nearly uniform convergence result on anisotropic meshes.

1.2 Adaptive Finite Element Methods Adaptive methods are now widely used in scientific and engineering computation to optimize the relation between accuracy and computational labor (degrees of freedoms). Understanding the convergence, as well as the rate of convergence, of adaptive finite element methods (AFEM) has been an active research topic in recent years. The key behind this technique is to design a good a posteriori error estimator that provides a guidance on how and where grids should be refined.

In [21], we revealed that the equidistribution principle can be severely violated but asymptoticly optimal error estimates can still be maintained, which led to the following practical statement: linear adaptive finite element approximation of second order elliptic equations in two dimensions will achieve optimal rate of convergence. In [8], a cell conservative flux recovery technique was developed for vertex-centered finite volume methods of second order elliptic equations. The recovery-based and residual-based a posteriori error estimators obtained in this article are apparently the first results on a posteriori error estimators for high order finite volume methods. The recovered flux was found in the broken H(div) elements. In [7], a residual type a posteriori error estimator was presented and analyzed for Weak Galerkin (WG) finite element methods for second order elliptic problems. The error estimator was proved to be efficient and reliable through estimates from below and from above, in terms of an H1-equivalent norm for the exact error. Since WG solution is related to mixed finite element approximation, our a posteriori error estimates are combinations of techniques used for continuous elements and ones used for H(div)-conforming elements. In [17], adaptive mesh refinement and the Borgers algorithm were combined to generate a body-fitted mesh which can resolve the interface with fine geometric details. Standard linear finite element method based on such body-fitted meshes was applied to the elliptic interface problem and proven to be superclose to the linear interpolant of the exact solution. An efficient solver for solving the resulting linear algebraic systems was also developed and shown be robust with respect to both the problem size and the jump of the diffusion coefficients.

Comparing with the uniform refinement of the computational grid, adaptive finite element methods through mesh adaptation are more preferred to locally increase mesh densities in the regions of interest, thus saving the computer resources. The a posteriori error estimator we have developed for several equations will expand the application range of AFEM. The adaptive mesh generator and the corresponding finite element method for the interface problem will have impact on numerical simulation of free surface problem in fluid dynamics and material science, fluid-structure interaction, multiphase material and so on.

1.3 Applications We have also made significant advance in the structure-preserving discretizations for PDEs, and the efficient solution of the resulting systems. We developed an adaptive Eulerian-Lagrangian method in [11] where a new a posteriori error estimate for time dependent problem was proposed and we derived the an a posteriori error bound. In [36], we designed and analyzed some structure-preserving finite element schemes for the MHD system. The main feature of the method is that it naturally preserves the important Gauss's law, namely $\nabla \cdot \mathbf{B} = 0$. For this new finite element method, an energy stability estimate can be naturally established in an analogous way as on the continuous level. Furthermore, well-posedness was rigorously established for both the Picard and Newton linearization of the fully nonlinear systems by using Brezzi's theory for both the continuous and discrete cases. This well-posedness naturally led to robust preconditioners for the linearized systems. In [17, 20], we developed two-grid algorithms to the Maxwell's eigenvalue problem and Cahn-Hillard equation, respectively. We also presented a detailed and rigorous proof for the two-grid algorithm for solving Maxwell's eigenvalue problem. The analysis was technical and highly non-trivial. The two-grid method we have developed for solving the Maxwell's eigenvalue problem will result in significant savings in computational time and resources.

Stokes equations play a central role in the Computational Fluid Dynamics (CFD). In [9], we generalized the classical marker-and-Cell (MAC) scheme on the rectangular grids to the triangular grids and retains all the desirable properties of the MAC scheme: exact divergence-free, solver-friendly, and local conservation of physical quantities. The triangular MAC scheme we have developed and the multigrid solver is expect to have a large impact to the CFD community.

In [38], the minimal speeds (c^*) of the Kolmogorov-Petrovsky-Piskunov (KPP) fronts at small diffusion ($\epsilon \ll 1$) in a class of time-periodic cellular flows with chaotic streamlines is investigated. The variational principal of c^* reduces the computation to that of a principal eigenvalue problem on a periodic domain of a linear advection-diffusion operator with space-time periodic coefficients and small diffusion. To solve the advection dominated time-dependent eigenvalue problem efficiently over large time, a combination of finite element and spectral methods, as well as the associated fast solvers, are utilized to accelerate computation. In contrast to the scaling $c^* = \mathcal{O}(\epsilon^{1/4})$ in steady cellular flows, a new relation $c^* = \mathcal{O}(1)$ as $\epsilon \ll 1$ is revealed in the time-periodic cellular flows due to the presence of chaotic streamlines. Residual propagation speed emerges from the Lagrangian chaos which is quantified as a sub-diffusion process.

2 Research Results

2.1 Penn State Team The team led by the PI at Penn State mainly focuses on adaptive method, fast and parallel multilevel methods for numerical models including magnetohydrodynamics and complex fluids. The results are summarized as follows:

1. In [11], we considered the adaptive Eulerian-Lagrangian method (ELM) for linear convection-diffusion problems and derived a new a posteriori error estimator. Unlike the classical a posteriori error estimation, which might overestimate the temporal error, we estimate the temporal error along with the characteristics and derive a new a posteriori error bound for ELM semi-discretization. With the help of this proposed error bound, we are able to show the optimal convergence rate of ELM for solutions with minimal regularity. Furthermore, by combining this error bound with a standard residual-type estimator for the spatial error, we obtained a posteriori error estimators for a fully discrete scheme. Numerical tests showed that the new temporal error estimator gives a better estimate of the temporal error, and also demonstrates the efficiency and robustness of our adaptive algorithm.

2. In [13], we developed a simple algorithmic framework to solve large-scale linear systems arising from various applications. The framework assumes that two components are present: (1) a norm-convergent iterative method and (2) a preconditioner, which is not necessarily efficient as a stand alone solver. The resulting preconditioner, which we refer to as a combined (hybrid) preconditioner, is more robust and efficient than the iterative method and preconditioner when used in Krylov subspace methods. We proved that the combined preconditioner is positive definite and showed estimates on the condition number of the preconditioned system. As an example, we combined an algebraic multigrid method and an incomplete factorization preconditioner to test the proposed framework on multiphase flow problems in petroleum reservoir simulations. The numerical experiments demonstrated noticeable speed up when we compare the combined method with the standalone algebraic multigrid method or with the incomplete factorization preconditioner.

3. In [18], we derived convergence analysis for two-grid and multigrid methods for linear systems arising from conforming linear finite element discretization of the second-order elliptic equations with anisotropic diffusion. The multigrid algorithm with a line smoother is known to behave well when the discretization grid is aligned with the anisotropic direction;

however, this is not the case with a non-aligned grid. The analysis in this paper was mainly focused on two-level algorithms. For aligned grids, a lower bound was given for the point-wise smoother, and this bound showed a deterioration in the convergence rate. For maximally non-aligned grids (with no edges in the triangulation parallel to the direction of the anisotropy), though, the point-wise smoother results in a robust convergence. With a specially designed block smoother, we showed that for both aligned and non-aligned grids the convergence is uniform with respect to the anisotropy ratio and the mesh size.

4. In [12], we provided a comprehensive convergence analysis of a nonlinear AMLI-cycle multigrid method for symmetric positive definite problems. Based on classical assumptions for approximation and smoothing properties, we showed that the nonlinear AMLI-cycle MG is uniformly convergent. In addition, we provided a comparison analysis in terms of convergence bounds between the nonlinear AMLI-cycle and the n-fold V-cycle MG method and showed that the nonlinear AMLI-cycle is always at least as good as and usually better than the n-fold V-cycle MG method in terms of the bound of the convergence rate as well as numerically.

5. In [15], we developed a new parallel auxiliary grid algebraic multigrid (AMG) method to leverage the power of graphic processing units (GPUs). In the construction of the hierarchical coarse grid, we used a simple and fixed coarsening procedure based on a region quadtree generated from an auxiliary grid. This allows us to explicitly control the sparsity patterns and operator complexities. This feature provides (nearly) optimal load balancing and predictable communication patterns, which makes our new algorithm suitable for parallel computing, especially on GPU clusters. We also designed a parallel smoother using special coloring based on the quadtree to accelerate the convergence rate and improve the parallel performance of this solver. Based on the CUDA toolkit, we implemented our new parallel auxiliary grid AMG method on GPU, and the numerical results of this implementation demonstrate the efficiency of our new method. The results showed an average speedup of over 4 on quasi-uniform grids and 2 on shape-regular grids when compared to the AMG implementation in CUSP (a GPU software program developed by NVIDIA).

6. In [2], we constructed Discontinuous Galerkin approximations of the Stokes problem where the velocity field is H(div)-conforming, which implies that the velocity approximation is divergence-free. We used this property to design a simple and effective preconditioner for the final linear system based on the auxiliary space (or fictitious space) framework. The proposed preconditioner was the solution of several elliptic problems: a vector Laplacian discretized with DG-H(div)-conforming methods, and another elliptic problem discretized with an H1-conforming method. The solution of such systems can then be effectively computed with a classical method,

for instance, the multigrid method. Numerical results were presented to support the theoretical results.

7. In [31], we developed a multigrid method on unstructured shape-regular grids. For a general shape-regular unstructured grid with N elements, we presented a construction of an auxiliary coarse grid hierarchy on which a geometric multigrid method can be applied together with a smoothing on the original grid by using the auxiliary space preconditioning technique. Such a construction is realized by a cluster tree which can be obtained in $\mathcal{O}(N \log N)$ operations. This tree structure in turn is used for the definition of the grid hierarchy from coarse to fine. For the constructed grid hierarchy we prove that the convergence rate of the multigrid preconditioned CG for an elliptic PDE is $1 - \mathcal{O}(1/\log N)$. Numerical experiments confirmed the theoretical bounds and show that the total complexity is in $\mathcal{O}(N \log N)$.

8. In [37], we discussed the linear element methods for interface boundary value problems of the diffusion equation and the incompressible Stokes equation. The schemes were proved to be of optimal accuracy, provided the underlying grid is interface-fitted and maximal-angle-bounded. We also presented an optimal multigrid method solver of the generated linear system.

9. In [26], we developed a unified framework using energetic variational approaches for generalized complex fluids, including viscoelastic materials, free interface motion in mixtures of fluids and magnetohydrodynamics. The paradigm revealed the competition and couplings between different parts of the energy and dissipation functionals. It also focused on the coupling between the kinematic transport of the internal variables and the induced stress in the momentum equations.

10. In [14] we derived a three-term recurrence relation for computing the polynomial of best approximation in the uniform norm to $1/x$ on a finite interval with positive endpoints. In terms of applications, we considered two-level methods for scalar elliptic partial differential equations (PDE), where the relaxation on the fine grid uses the aforementioned polynomial of best approximation. Based on a new smoothing property of the matrix polynomial, combined with a proper choice of the coarse space, allowed us to show that the convergence rate of the resulting two-level method was uniform with respect to the mesh parameters, the coarsening ratio, and the variations in the PDE coefficient.

11. In [1], we considered the approximation of incoming solutions to Maxwell's equations with dissipative boundary conditions whose energy decays exponentially with time. Such solutions are called asymptotically disappearing (ADS), and they play an important role in inverse back-scattering problems. For the exterior of a sphere, such solutions have been constructed analytically in earlier works by specifying appropriate initial conditions.

However, for more general domains of practical interest (such as Lipschitz polyhedra), the existence of such solutions is not evident. We considered a finite-element approximation of Maxwell's equations in the exterior of a polyhedron, whose boundary approximates the sphere. We used structure preserving discretization with Nédélec–Raviart–Thomas elements were used with a Crank-Nicholson scheme to approximate the electric and magnetic fields. We show numerically that the finite-element approximations of the ADS also decay exponentially with time.

12. In [22], we designed and implemented a parallel algebraic multigrid method for isotropic graph Laplacian problems on multicore Graphical Processing Units (GPUs). The proposed AMG method is based on the unsmoothed aggregation framework. The coarse space construction is based on a parallel maximal independent set algorithm in forming aggregates and the resulting coarse-level hierarchy is then used in a K-cycle iteration solve phase with an ℓ^1-Jacobi smoother. Numerical tests of a parallel implementation of the method for graphics processors were presented to demonstrate its effectiveness.

13. In [23], we introduced the concept of a visible point of a convex set relative to a given point and we prove a number of basic properties of such visible point sets. In particular, we showed that this concept is useful in the study of best approximation from polyhedral sets, and it also has potential applications in robotics.

14. In [24], we constructed a two-grid method for mimetic finite difference approximation of scalar elliptic partial differential equation. We proved the uniform convergence of the method using graph analogues of the Poincaré/Cheeger inequalities. The method has application in solving systems coming from discretizations based on partitioning of the domain with arbitrary polygons/polyhedra such as Virtual Element Methods (VEM) or mimetic Finite Difference methods.

15. In [36], we designed and analyzed structure-preserving finite element schemes for the MHD system. The main feature of the method is that it naturally preserves the important Gauss law, namely $\nabla \cdot \mathbf{B} = 0$. In contrast to most existing approaches that eliminate the electrical field variable and give a direct discretization of the magnetic field, our new approach discretizes the electric field by Nédélec type edge elements, and the magnetic field by Raviart-Thomas type face elements. As a result, the divergence-free condition for the magnetic field holds exactly on the discrete level. For this new finite element method, an energy stability estimate can be naturally established in an analogous way as in the continuous case. Furthermore, well-posedness was rigorously established in the paper for both the Picard and Newton linearization of the fully nonlinear systems by using the Brezzi theory for both the continuous and discrete cases. This well-posedness naturally led to robust (and optimal) preconditioners for the linearized systems.

16. In [37], we discussed linear finite element methods for interface boundary value problems of the diffusion equation and the incompressible Stokes equation. The schemes were proved to be of optimal accuracy, provided the underlying grid is interface-fitted and the maximal-angle of mesh is bounded.

17. In [29], we developed a novel domain decomposition method and a scalable implementation of the method using the semistructured geometric multigrid solver, PFMG, available in Hypre for solving the time dependent and nonlinear magnetic Thomas-Fermi model used in studying surface temperature inhomogeneities of neutron stars. The method we developed may be seen as a prototype for the general class of problems involving nonlinear charge screening of periodic, quasi-low-dimensionality structures, e.g. liquid crystals. Physically, our findings include low density elastic instabilities for both bcc and fcc lattices, reminiscent of the situation in some light actinides, and phonon thermal conductivity three orders of magnitude larger than that derived from the plasma model. The former result suggested there is a symmetry-lowering transition to a tetragonal or orthorhombic lattice. The latter indicated transport anisotropy may be greatly reduced within 10 meters of the surface, giving the effect of a "heat-spreader cladding" which may significantly increase the size of polar hot spots and alter pulse profiles.

2.2 UCSD team The team at UCSD mainly works on the *hp* adaptive method, theory for finite element exterior calculus, and adaptivity for nonlinear problems. The results are summarized as follows:

1. In [3], we show that interpolation error and best approximation error or finite element error behave in a similar fashion. The three estimates taken together show that interpolation error is both efficient and reliable as an a posteriori error estimate, provided that interpolation error can be estimated from the finite element approximation u_h. Procedures for doing this were developed by Bank, Xu, and Zheng in [40]. This has immediate application to adaptive finite element methods.

2. In [25], new a priori and a posteriori error estimates and discrete pointwise estimates for critical and subcritical nonlinear problems with no angle conditions on the underlying mesh were established. In [34, 35] we developed an adaptive finite element method (AFEM) convergence theory for a class of goal-oriented adaptive algorithms (GOAFEM). Following Mommer and Stevenson (2009) for symmetric problems, in [34] we establish GOAFEM contraction for nonsymmetric problems. Our approach uses newer contraction frameworks. In [35], we prove convergence of GOAFEM for semilinear problems. We first establish quasi-error contraction of primal problem, then establish contraction of combined primal-dual quasi-error, giving convergence with respect to the quantity of interest. Sequence of numerical experiments presented in both papers; behavior of implementations follow predictions of the theory.

3. We study finite element exterior calculus (FEEC); our interest has been to develop adaptive FEEC methods with a corresponding convergence theory. AFEM convergence theory for mixed methods (the target of FEEC) is not complete; the main difficulty is lack of error (quasi-)orthogonality. In earlier work of Chen, Holst, and Xu (2006), we established convergence and optimality of AFEM for mixed Poisson on simply connected domains in two dimensions. Our argument was based on a quasi-orthogonality result that exploits error orthogonal to divergence free subspace, with non-divergence-free part bounded by data oscillation via discrete stability. In another related development, Demlow and Hirani (2012) developed an FEEC a posteriori indicator with provably good properties. In [32,33], we use the FEEC framework to develop AFEM convergence and complexity results for Hodge-Laplace problem (k=n) on domains of arbitrary topology and spatial dimension. Our supporting results hold for general B-Hodge-Laplace problem ($k \neq n$).

4. In [30], the theory of finite element exterior calculus was extended to non-linear problems and evolution problems and to problems on hypersurfaces arising in geometric analysis and general relativity.

2.3 UCI team The focus of the UCI group is the Laplacian preconditioner , centrodial Voronoi tessellation, and design of solver-friendly discretizations for Stokes and Navier-Stokes equations based on the finite element exterior calculus framework. The results are summarized as follows:

1. In [10], a new and effective graph Laplacian preconditioner and a two-grid method were proposed to speed up the computation of Centrodial Voronoi Tessellation (CVT), i.e., Voronoi tessellations in which the generators are the centroids for each Voronoi region. Numerical tests show that the preconditioned optimization method converges fast and has nearly linear complexity. CVTs have many applications to computer graphics, image processing, data compression, mesh generation, and optimal quantization. Consequently, our fast methods will be useful in these areas.

2. In [16], a distributive Gauss-Seidel relaxation based on the least squares commutator is devised for the saddle-point systems arising from the discretized Stokes equations. Based on that, an efficient multigrid method is developed for finite element discretizations of the Stokes equations on both structured grids and unstructured grids. On rectangular grids, an auxiliary space multigrid method using one multigrid cycle for the Marker and Cell scheme as auxiliary space correction and least squares commutator distributive Gauss-Seidel relaxation as a smoother is shown to be very efficient and outperforms the popular block preconditioned Krylov subspace methods.

3. In [6], an efficient multigrid solvers for the Oseen problems discretized by Marker and Cell (MAC) scheme on staggered grid is developed in this pa-

per. Least squares commutator distributive Gauss-Seidel (LSC-DGS) relaxation is generalized and developed for Oseen problems and overweighting and defect-correction techniques are applied to further improve the performance. Some numerical results are presented to demonstrate the efficiency and robustness of the proposed solver.

4. In [17], adaptive mesh refinement and the Börgers algorithm were combined to generate a body-fitted mesh that can resolve the interface with fine geometric details. The standard linear finite element method based on such body-fitted meshes was applied to the elliptic interface problem and proven to be superclose to the linear interpolant of the exact solution. An efficient solver for solving the resulting linear algebraic systems was also developed and shown to be robust with respect to both the problem size and the jump of the diffusion coefficients.

5. In [5], a local multigrid methods on adaptive grids was used as a preconditioner and shown to be robust for symmetric elliptic problems with possibly large jump coefficients in both two and three dimensions.

6. In [19,20], we applied two-grid algorithms to the Maxwell eigenvalue problem and Cahn-Hillard equation, respectively. We also presented a detailed and rigorous proof for the two-grid algorithm for solving Maxwell eigenvalue problem. The analysis was technical and highly non-trivial.

7. In [21], we revealed that the equidistribution principle can be severely violated but asymptoticly optimal error estimates can still be maintained and we are led to conclude the following practical statement: linear adaptive finite element approximation of second order elliptic equations in two dimensions will achieve optimal rate of convergence.

8. In [8], a cell conservative flux recovery technique was developed for vertex-centered finite volume methods of second order elliptic equations. The recovery-based and residual-based a posteriori error estimators obtained in this article was apparently the first results on a posteriori error estimators for high order finite volume methods. The recovered flux was found in the broken $H(\mathrm{div})$ elements.

9. In [7], a residual type a posteriori error estimator was presented and analyzed for Weak Galerkin (WG) finite element methods for second order elliptic problems. The error estimator was proved to be efficient and reliable through two estimates, one from below and the other from above, in terms of an H1-equivalent norm for the exact error. Since WG solution was more close to mixed finite element approximation, our a posteriori error estimates was a combination of that for conforming element and that for $H(\mathrm{div})$ elements.

10. In [4], a Fortin operator is constructed to verify the discrete inf-sup condition for $P_0^2 - P^1$ Taylor-Hood element and its variant $P_0^2 - (P^1 + P_0)$

in two dimensions. The constructed Fortin operator for $P_0^2 - P^1$ element is uniformly bounded in both H^1 and L^2 norm for general shape regular triangulations.

11. In [9], we generalize the classical MAC scheme on rectangular grids to triangular grids and retains all the desirable properties of the MAC scheme: exact divergence-free, solver-friendly, and local conservation of physical quantities. We address the error estimate of the element pair RT_0-P_0, which is known to be suboptimal, and render the error estimate optimal by the symmetry of the grids and by the superconvergence result of Lagrange interpolant. By enlarging RT_0 such that it becomes a modified BDM-type element, we develop a new discretization $\mathrm{BDM}_1^{\mathrm{b}}$-$\mathrm{P}_0$ and prove that the proposed discretization achieves the optimal convergence rate for both velocity and pressure on general quasi-uniform unstructured grids, and one and half order convergence rate for the vorticity and a recovered pressure. We demonstrate the validity of theories developed here by numerical experiments.

12. In [27], we develop and analyze multilevel methods for nonuniformly elliptic operators whose ellipticity holds in a weighted Sobolev space with an A2–Muckenhoupt weight. Using the so-called Xu-Zikatanov (XZ) identity, we derive a nearly uniform convergence result, under the assumption that the underlying mesh is quasi-uniform. We also consider the so-called alpha-harmonic extension to localize fractional powers of elliptic operators. Motivated by the scheme proposed in [R.H. Nochetto, E. Otarola, and A.J. Salgado. A PDE approach to fractional diffusion in general domains: a priori error analysis. arXiv:1302.0698, 2013] we present a multilevel method with line smoothers and obtain a nearly uniform convergence result on anisotropic meshes. Numerical experiments reveal a competitive performance of our method.

13. In [28], we derive a computable a posteriori error estimator for the α-harmonic extension problem, which localizes the fractional powers of elliptic operators supplemented with Dirichlet boundary conditions. Our a posteriori error estimator relies on the solution of small discrete problems on anisotropic cylindrical stars. It exhibits built-in flux equilibration and is equivalent to the energy error up to data oscillation, under suitable assumptions. We design a simple adaptive algorithm and present numerical experiments which reveal a competitive performance.

14. In [38], the minimal speeds (c^*) of the Kolmogorov-Petrovsky-Piskunov (KPP) fronts at small diffusion ($\epsilon \ll 1$) in a class of time-periodic cellular flows with chaotic streamlines is investigated. The variational principal of c^* reduces the computation to that of a principal eigenvalue problem on a periodic domain of a linear advection-diffusion operator with space-time periodic coefficients and small diffusion. To solve the advection dominated time-dependent eigenvalue problem efficiently over large time, a combination of finite element and spectral methods, as well as the associated fast

solvers, are utilized to accelerate computation. In contrast to the scaling $c^* = \mathcal{O}(\epsilon^{1/4})$ in steady cellular flows, a new relation $c^* = \mathcal{O}(1)$ as $\epsilon \ll 1$ is revealed in the time-periodic cellular flows due to the presence of chaotic streamlines. Residual propagation speed emerges from the Lagrangian chaos which is quantified as a sub-diffusion process.

3 Achievements of Goals and Objectives

The primary goal of this project is to extend the applicability of AFEM and MG methods to various particular problems for which these methods are difficult to apply, including viscoelastic fluids and magnetohydrodynamics(MHD). We plan to pursue an integrated approach, combining mathematical modeling, numerical discretization using AFEM, and optimal solvers based on MG methods. Specially, we aim to:

1. *Derive improved mathematical models and numerical discretizations for viscoelastic fluids and resistive MHD;*

   To achieve this goal, we have derived improved mathematical models and numerical discretizaitons for viscoelastic fluids and resistive MHD. For example, in [26], we developed a unified framework using energetic variational approaches for generalized complex fluids, including viscoelastic materials, free interface motion in mixtures of fluids and magnetohydrodynamics; in [36], we designed and analyzed of some structure-preserving finite element schemes for the MHD system. The main feature of the method is that it naturally preserves the important Gauss law, namely $\nabla \cdot \mathbf{B} = 0$.

2. *Develop (nearly) optimal and practical AFEM for multiphysics systems;*

   To achieve this goal, we have developed several new a posteriori error estimators and extended the applicability of AFEM to various problems. Below is of a list of results achieved in this direction.

   - In [11], we considered the adaptive Eulerian-Lagrangian method (ELM) for linear convection-diffusion problems and derived a new a posteriori error estimator. We showed the optimal convergence rate of ELM for solutions with minimal regularity.
   - In [25], new a priori and a posteriori error estimates and discrete pointwise estimates for critical and subcritical nonlinear problems with no angle conditions on the underlying mesh were established and the convergence theory for goal-oriented adaptive methods for both linear and nonlinear problems was developed in [34, 35].
   - In [32, 33], we use the FEEC framework to develop AFEM convergence and complexity results for Hodge-Laplace problem (k=n) on domains of arbitrary topology and spatial dimension. Our supporting results hold for general B-Hodge-Laplace problem ($k \neq n$).

- In [21], we revealed that the equidistribution principle can be severely violated but asymptoticly optimal error estimates can still be maintained.
- In [8], a cell conservative flux recovery technique was developed for vertex-centered finite volume methods of second order elliptic equations. The recovery-based and residual-based a posteriori error estimators obtained was apparently the first results on a posteriori error estimators for high order finite volume methods.
- In [7], a residual type a posteriori error estimator was presented and analyzed for Weak Galerkin (WG) finite element methods for second order elliptic problems. The error estimator was proved to be efficient and reliable through two estimates, one from below and the other from above, in terms of an H1-equivalent norm for the exact error.
- In [28], we derive a computable a posteriori error estimator for the α-harmonic extension problem, which localizes the fractional powers of elliptic operators supplemented with Dirichlet boundary conditions. Our a posteriori error estimator relies on the solution of small discrete problems on anisotropic cylindrical stars.

3. *Develop a class of proven optimal MG methods for their solution;* To achieve this goal, we have developed multilevel solvers for solving discretized PDEs, especially on unstructured grids.

   - In [31], we designed a multilevel method for solving the Poisson equation, discretized on unstructured shape-regular grids based on the auxiliary space preconditioning framework. We showed the overall multilevel method has nearly-optimal convergence rate of $1 - \mathcal{O}(1/\log N)$ where N is the number of degrees of freedom.
   - In [22], a purely algebraic MG method has also been developed for isotropic graph Laplacian problems on GPUs based on an unsmoothed aggregation framework.
   - In [13], we developed a hybrid preconditioning framework that combines an iterative method and a preconditioner in a complementary fashion. We proved that the combined preconditioner is positive definite and derived sharp estimates on the condition number of the preconditioned system
   - In [18], we conducted convergence analysis for two-grid and multigrid methods for linear systems arising from conforming linear finite element discretizations of the second-order elliptic equations with anisotropic diffusion. With a specially designed block smoother, we showed that both aligned and non-aligned grids have uniform convergence with respect to the anisotropy ratio and the mesh size in the energy norm.
   - In [12], we provided the first comprehensive convergence analysis of a nonlinear AMLI-cycle multigrid method for symmetric positive

definite problems and showed that the nonlinear AMLI-cycle is at least as good and usually better than the n-fold V-cycle MG method in terms of the bound of the convergence rate.

- In [5], a local multigrid methods on adaptive grids was used as a preconditioner and shown to be robust for symmetric elliptic problems with possibly large jump coefficients in both two and three dimensions.
- In [16], a distributive Gauss-Seidel relaxation based on the least squares commutator is devised for the saddle-point systems arising from the discretized Stokes equations. Based on that, an efficient multigrid method is developed for finite element discretizations of the Stokes equations on both structured grids and unstructured grids.
- In [6], an efficient multigrid solvers for the Oseen problems discretized by Marker and Cell (MAC) scheme on staggered grid is developed in this paper. Least squares commutator distributive Gauss-Seidel (LSC-DGS) relaxation is generalized and developed for Oseen problems and overweighting and defect-correction techniques are applied to further improve the performance.
- In [27], we develop and analyze multilevel methods for the so-called alpha-harmonic extension to localize fractional powers of elliptic operators. We present a multilevel method with line smoothers and obtain a nearly uniform convergence result on anisotropic meshes. Numerical experiments reveal a competitive performance of our method.

4. *develop and implement integrated AFEM-MG methods (iAFEM-MG) for use in DOE application's codes.*

   To achieve this goal, we have integrated the study between adaptive method and multigrid methods. For example, most of the multilevel solvers we developed during the project period were designed for the unstructured grid, which can be directly applied to adaptive grid obtained by different refinement strategies. For example, MG method based on auxiliary space preconditioning framework developed in [15, 31]; AMG method developed in [22]; and local MG method for the bisection adaptive grid [5]. On the other hand, we also developed solver-friendly adaptive finite element methods which leads to linear systems that can be efficiently solved by existing robust solvers. The main tool we used is the ELM method, which has been used for linear convection dominated problem [11]. Moreover, as reported in [39], PLTMG software package 11.0 features two solvers for hp adaptive finite element systems, a sparse block ILU preconditioner based on the multigraph method and a two-level (in p) hierarchical preconditioner. Both of them achieved effective performance empirically.

Overall, we have made significant efforts and advances in adaptive multilevel methods of multiphysics problems. Furthermore, we have successfully extended the applicability of AFEM and MG methods to various practical problems including complex fluids, MHD, and reservoir simulation.

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