Snapshots of Jinchao Xu's Research Results on Numerical Methods for PDEs and Deep Learning

STATEMENT OF ACCOMPLISHMENTS

Xu has made many fundamental and impactful contributions to numerical methods, especially the multi-grid (MG) and domain decomposition (DD) methods, for solving partial differential equations (PDEs).

- He is renowned for the Bramble-Pasciak-Xu (BPX) preconditioner [1990] (a basic algorithm for solving elliptic PDEs) and the Hiptmair-Xu (HX) preconditioner [2007] (an effective Maxwell solver featured in a 2008 report by the U.S. Department of Energy as one of the top 10 breakthroughs in computational science in recent years). (see §1.1 and §1.2)
- He developed the framework and theory of the Method of Subspace Corrections [1992] that have been widely used in the literature for design and analysis of iterative methods and later established the Xu-Zikatanov (XZ) identity [2002], giving the optimal theory for these methods. (see §4.1 and §4.2)

Other contributions by him (with collaborators) include:

- the first optimal algorithms and theory based on auxiliary grid etc. [1996] and asymptotically exact a posteriori error estimator [2003], both for PDEs discretized on unstructured grids; (see §1.3)
- the only known canonical construction of finite element family for any order of elliptic PDEs in any spatial dimensions [2013]; (see §3.1)
- the design and analysis of new algorithms for modeling non-Newtonian flows with high Weissengberg numbers [2006]; (see §3.2)
- the first uniform convergence theory [1991] for the multiplicative DD and MG methods with minimal regularity assumptions for the underlying PDE; (see §4.3)
- the development of MgNet which provides a unified frameworks for two different research fields: multigrid methods for solving partial differential equations and convolutional neural networks for machine learning. In particular, MgNet yields a new family of convolutional neural networks that have almost identical algorithmic structure of a geometric multigrid method that is mathematically well-understood. (see §6.1)
- the FASP software-package (http://fasp.sourceforge.net/) providing advanced solvers for coupled PDE systems. (see §7.5)
- the two-grid discretization techniques [1996] which opened new research avenues for solving linear and nonlinear PDEs;

Jinchao Xu's research involve the study of discretization, grid adaptation, iterative methods, applications for partial differential equations and deep learning. Below are some examples.

1 Basic Iterative and Preconditioning Algorithms

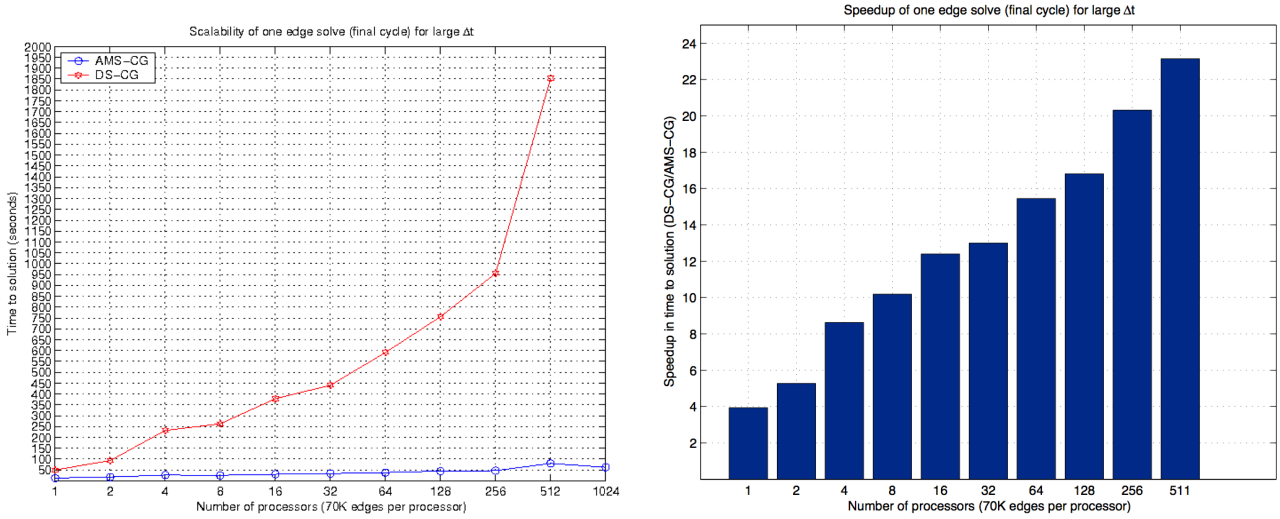
This line of works are concerned with fast iterative methods (mostly based on preconditioned Krylov space methods) for solving discretized partial differential equations.

1.1 BPX preconditioner

Bramble-Pasciak-Xu ([3], 1990) introduced what is now known as the BPX-preconditioner. This method, originally described in Xu's PhD thesis ([29], 1989), is one of the two most powerful multigrid approaches for solving large-scale algebraic systems that arise from the discretization of models in science and engineering described by partial differential equations. The method has been widely used by researchers and practitioners since 1990.

1.2 HX Preconditioner

Xu ([31], 1996) developed the auxiliary space method, a technique that uses a more structured space to construct an efficient subspace correction method for less structured problems. A generalization of this idea when used in concert with the BPX preconditioner led to the optimal preconditioner of Hiptmair-Xu ([14], 2007). The method, now known as HX-preconditioner, is a theoretically optimal and practically easy-to-use iterative method for the so-called H(curl) and H(div) systems that have direct applications to electro-magnetic equations and porous media flows. In this algorithm, for example, a (vector) Maxwell equation in 3 dimensions is transformed into solution of 4 (scalar) Poisson equations. The HX-preconditioner was identified in 2008 by the U.S. Department of Energy as one of the top ten breakthroughs in computational science in recent years. Researchers from Sandia, Los Alamos, and Lawrence Livermore National Labs use this algorithm for modeling fusion with magnetohydrodynamic equations. Moreover, this approach will also be instrumental in developing optimal iterative methods in structural mechanics, electrodynamics, and modeling of complex flows.



(a) Scalability

(b) Speedup

Figure 1: Scalability and Speedup of HX preconditioner

Compared with algorithms previously used by LLNL, the HX preconditioner:

- Speeds up computational time on 512 processors by a factor of 24.
- Speeds up the magnitude by more than order of 2 on 1,024 processors.

And, the HX preconditioner:

- Takes less than 2 minutes to provide an accurate solution to a Maxwell equation with more than 35 million unknowns on 1,024 processes.
- The scalability of HX preconditioner is verified to 125,000 cores, for the problem with 12 billion DOFs in total.

1.3 Optimal preconditioners for 2nd and 4th order elliptic equations discretized on unstructured grids

With FFT or geometric multigrid methods, it is well-known the discretized system from the finite element approximation of both 2nd and 4th order elliptic boundary value problems discretized on structured grids with N unkowns can be solved within $\mathcal{O}(N \log^m N)$ operations. But a rigorous theoretical extension of such results to unstructured grids is difficult. In Xu ([31], 1996), he developed a multigrid algorithm and a rigorous theory showing its near-optimality of $\mathcal{O}(N \log^m N)$ for unstructured quasi-uniform grids. Recently, Grasedyck, Wang and Xu ([12], 2016) extended this result to more general unstructured which need not to be quasi-uniform.

Recently, Xu with his former postdoc Zhang ([39], 2014) made a nontrivial extension of the above results to 4th order elliptic problems. They proposed the first mathematically provable $\mathcal{O}(N \log N)$ algorithm for linear systems arising from the direct finite element discretization of fourth-order problems on an unstructured grid of an arbitrary domain. This one-grid multilevel method presents a new approach to applying the divide-and-conquer strategy. It shows that some mixed-form discretizations of the fourth-order problems, which of themselves lead to non-desirable — i.e., either non-optimal or nonconvergent approximations of the original solution, can provide optimal preconditioners for direct finite element discretizations. It is rigorously shown that the preconditioners can be reduced to the solution of a fixed number of discrete Poisson equations. This approach will also be instrumental in the development of optimal iterative methods in high-order problems.

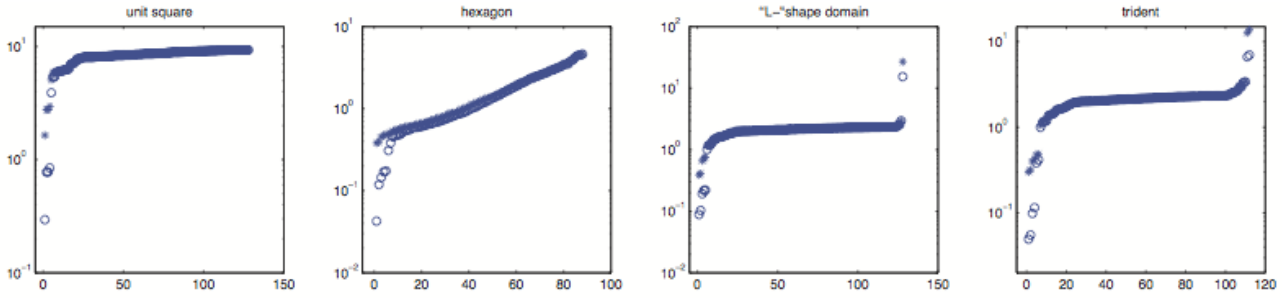


Figure 2: Eigenvalue distribution of a preconditioned system: Only a few bad?? eigenvalues are evident, which is favorable for the PCG method.

2 Algebraic Multigrid Methods

In addition to the GMG and single-grid multilevel method, Algebraic multigrid (AMG) methods were designed in an attempt to start from the algebraic linear system directly.

Recently, Xu and Zikatanov ([37]) provides an overview of AMG methods for solving large-scale systems of equations, such as those from discretizations of partial differential equations. AMG is often understood as the acronym of "algebraic multigrid", but it can also be understood as "abstract multigrid". Indeed, they demonstrate how and why an algebraic multigrid method can be better understood at a more abstract level. They try to develop a unified framework and theory that can be used to derive and analyse different algebraic multigrid methods in a coherent manner. Given a smoother R for a matrix A, such as Gauss–Seidel or Jacobi, they prove that the optimal coarse space of dimension n_c is the span of the eigenvectors corresponding to the first eigenvectors $\bar{R}A$. They also prove that this optimal coarse space can be obtained via a constrained trace-minimization problem for a matrix associated with $\bar{R}A$, and demonstrate that coarse

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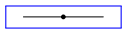
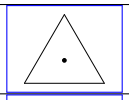
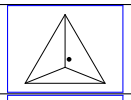
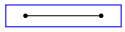
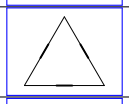
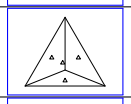
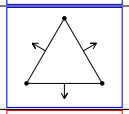
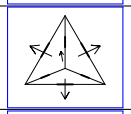
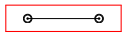
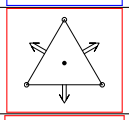
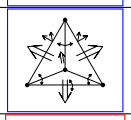
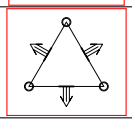
0			
1			
2			
3			
4			

Table 1: Degrees of freedom of MWX elements

spaces of most existing AMG methods can be viewed as approximate solutions of this trace-minimization problem. Furthermore, they provide a general approach to the construction of quasi-optimal coarse spaces, and prove that under appropriate assumptions the resulting two-level AMG method for the underlying linear system converges uniformly with respect to the size of the problem, the coefficient variation and the anisotropy. Their theory applies to most existing multigrid methods, including the standard geometric multigrid method, classical AMG, energy-minimization AMG, unsmoothed and smoothed aggregation AMG and spectral AMGe.

3 New Discretization Methods

Xu has done a lot of works on the construction of finite element discretization for problems ranging from basic model problems to complicated coupled systems of nonlinear partial differential equations. For coupled nonlinear PDEs, Xu aims to design discretization schemes that are "solver-friendly", namely the resulting discretized systems can be easily solved by preconditioned Krylov space method based on BPX and HX preconditioners.

3.1 Morley-Wang-Xu Elements for High-order PDEs in High Dimensions

Xu and his collaborators have recently given the only canonical and universal construction of a class of convergent finite element spaces for any $2m$-th order of elliptic and parabolic equations in any spatial-dimensions $\mathbb{R}^n$. Their results are a generalization of the Morley elements for $m = n = 2$ and they give piecewise polynomials of the lowest-order degree to be used in constructing convergent, stable, and practical finite element discretization methods for higher-order partial differential equations. Wang and Xu ([25], 2013) gives the construction for the case that $1 \leq m \leq n$. Wu (Xu's current postdoc) and Xu ([26], 2017) are now finishing the construction for the more difficult case in which $m = n + 1$. Table 1 depicts the degrees of freedom for the case that $n \leq 3, m \leq n + 1$.

An alternative generalization when $m > n$ is developed by Wu and Xu ([27], 2017) by combining the interior penalty and nonconforming methods. The finite element is the nonconforming element with shape function spaces $\mathcal{P}_m$, which is therefore minimal. The degrees of freedom are carefully designed to preserve the weak-continuity as much as possible. For the case in which $m > n$, the corresponding interior penalty terms are applied to obtain the convergence property.

All other known finite element space families have been constructed for only a given n with $m \leq 2$ and the construction given by Xu and collaborators are the only known constructions that are universal. It has many other interesting theoretical properties. This new family of finite element methods provide practical discretization methods for, say, a 6-th order elliptic equations in 2-dimension (which only has 12 local degrees of freedom) and 3-dimensions (which only requires the use of 3rd order piecewise polynomials).

3.2 New discretization techniques for computational rheology

Xu and Young-Ju Lee (his former Ph.D. student) has developed an algorithm ([22], 2006) and relevant theory that provides a solution to the so-called *High Weissenberg Number Problem* in numerical simulations for complex fluids. Complex fluids, which include shampoos, paints and lubricants in our daily lives, are of universal industrial importance due to their unique mechanical properties, their capacity to solubilize and transport materials and their internal microstructures. On the other hand, the complex physics of such fluids called non-Newtonian fluids presents many challenges for the computational rheologists.

In ([22], 2006), they developed a numerical method that does preserve the positivity of the conformation tensor and theoretically proved and numerically verified that their new method is stable with respect to any size of the Weissenberg number. Their results indeed confirmed the importance of keeping the positivity of conformation tensor on the discrete level and also theoretically explained why. But the positive preserving property of the scheme is only one of the many important components that make their method work. Their method depends on careful use of many sophisticated mathematical and numerical tools and techniques, including a reformulation of the constitutive relation as a generalized Riccati equation in terms of convective derivatives, Eulerian-Lagrangian discretization for both the convective derivatives and material derivatives, special positivity preserving schemes for temporal variable, positivity preserving schemes for spatial variable, proper stable finite element spaces for velocity and pressure and volume preserving schemes for the characteristic feet. The scheme can be applied to most of existing models in a unified framework.

In addition, Lee-Xu-Zhang ([18], 2011) developed numerical methods for non-Newtonian fluids that guarantee the discrete system has a unique solution and there exists an iterative algorithm that converges uniformly with respect to the Weissenberg number and Reynolds number.

One important feature of this new method is that only a linear Stokes-like equation needs to be solved at each time step (in addition to various independent nonlinear ODEs associated with each grid point). The Stokes-like equation can be effectively solved by (either geometric or algebraic) multigrid method. Furthermore, adaptive finite element techniques can be easily applied to enhance the efficiency of the method.

This work was solicited by Professor T. Hughes to publish in a journal that he edits. Hughes is a world leading researcher in computational mechanics and he regards this work highly.

3.3 Structure-preserving Discretization and Efficient Solvers of MHD Problems

Magnetohydrodynamics (MHD) is a coupled system of fluid dynamics and electromagnetism, with many important applications in plasma physics, liquid metal industry, astrophysics and so on. Due to the complication of physics and nonlinear coupling, it is challenging to design numerical schemes which preserve important physical laws. Gauss's law ($\mathrm{div}\boldsymbol{B} = 0$) and the normal continuity of the magnetic field are considered to be crucial, both for the physics and for the success of numerical simulations. On the other hand, how to solve such a large algebraic system remains to be another challenging problem.

In Hu, Ma and Xu ([15], 2017), we proposed a structure-preserving finite element scheme for unstructured mesh on any Lipschitz domain, which achieved all the desired properties mentioned above. Magnetic field $\boldsymbol{B}$ and electric field $\boldsymbol{E}$ are solved at the same time. The energy stability and well-posedness are rigorously proved. For the stationary problems, Hu and Xu proposed a new scheme in ([16], 2015) to achieve the above properties. Magnetic $\boldsymbol{B}$ and electric current $\boldsymbol{j}$ are used as variables, so that there is no restriction on the Reynolds number. They use a new Lagrange multiplier to guarantee the precise divergence-free condition of the magnetic field. Geometric and topological structures of the MHD systems play an important role in the above study.

In order to solve the large algebraic systems, Ma, Hu, Hu and Xu ([24], 2016) designed efficient preconditioners and solvers. The mathematical properties of the MHD systems are fully employed. The proposed preconditioners are robust with various physical and discretization parameters, which are verified by both theory and numerical experiments.

There are some ongoing work. Using the idea developed above, we can design structure-preserving finite element methods for Navier-Stokes-Maxwell systems with displacement current, which is considered as a more difficult problem in the numerical simulations and analysis. We can prove the well-posedness in a stronger norm. For the nonlinear problems, we can prove the existence of solutions and convergence of linearized iterations rigorously.

3.4 Extended Galerkin Methods

Extended Galerkin (XG) method [42], which is a further result of the unified study of continuous and discontinuous Galerkin methods in [40, 41], is a general framework for the derivation and analysis of many different types of finite

element methods (including various discontinuous Galerkin methods). For second order elliptic equation, this framework employs four different discretization variables, $u_h, \boldsymbol{p}_h, \breve{u}_h$ and $\breve{p}_h$, where u_h and $\boldsymbol{p}_h$ are for approximation of u and $\boldsymbol{p} = -\alpha\nabla u$ inside each element, and $\breve{u}_h$ and $\breve{p}_h$ are for approximation of residual of u and $\boldsymbol{p}\cdot\boldsymbol{n}$ on the boundary of each element. The resulting 4-field discretization is proved to satisfy inf-sup conditions that are uniform with respect to all discretization and penalization parameters. As a result, most existing finite element and discontinuous Galerkin methods can be derived and analyzed using this general theory by making appropriate choices of discretization spaces and penalization parameters.

We first propose the XG method for elliptic problem. As we know, there are two major variational formulations for elliptic problem. The first one, namely the primal method, is to impose the continuity of $u \in H^1(\Omega)$. The second one, namely the mixed method, is to impose the continuity of $\boldsymbol{p} \in H(\mathrm{div}, \Omega)$. In correspondence to the two variational formulations, two different conforming finite element methods can be developed. The first one, which approximates $u \in H^1_D(\Omega)$ and known as primal finite element methods (FEMs) contain one unknown, namely u, to solve. The second one, which approximates $\boldsymbol{p} \in H_N(\mathrm{div};\Omega)$ and $u \in L^2(\Omega)$ based on a mixed variational principal, is called the mixed FEMs. These mixed methods solve two variables, namely flux variable $\boldsymbol{p}$ and u, and the condition for the well-posedness of mixed formulations is known as inf-sup or the Ladyzhenskaya-Babuška-Breezi condition.

As a key step in XG method, two additional residual corrections are introduced, which gain the flexibility of boundary finite element spaces for both u and $\boldsymbol{p}\cdot\boldsymbol{n}$. More specifically, XG method is presented in terms of four discretization variables, namely

$$\boldsymbol{p}_h, \quad \breve{p}_h, \quad u_h, \quad \breve{u}_h.$$

Given a triangulation of Ω=$\{\mathrm{K}\}$, the u_h and $\boldsymbol{p}_h$ are discontinuous piecewise polynomial approximations of u and $\boldsymbol{p}$, respectively. The variable $\breve{u}_h$ and $\breve{p}_h$ are introduced for the following approximation on element boundary

$$u \approx \bar{u}_h + \breve{u}_h, \qquad \boldsymbol{p}\cdot\boldsymbol{n}_e \approx \bar{\boldsymbol{p}}_h\cdot\boldsymbol{n}_e + \breve{p}_h, \quad e = K^+ \cap K^-.$$

where $\bar{u}_h$ and $\bar{\boldsymbol{p}}_h$ are numerical traces on the common edge or face. The Nitsche's trick for $\breve{u}_h$ and $\breve{p}_h$ will be used. Hence, XG method develops a concise formulation in terms of four variables $\boldsymbol{p}_h, \breve{p}_h, u_h, \breve{u}_h$, which contain all the possible variables in most of the existing FEMs. Therefore, it has the flexibility to unify most of the existing FEMs:

1. Under proper choices of the discrete spaces, XG recovers the H^1 conforming finite element if we eliminate all the discretization variables except u_h. By eliminating $\breve{p}_h$, XG recovers the hybrid methods in which $\breve{u}_h$ serves as a Lagrange multiplier to force the continuity of $\boldsymbol{p}\cdot\boldsymbol{n}$ across the element boundary. If we further eliminate the Lagrange multiplier, the resulting system needs to solve two variables $\boldsymbol{p}_h$ and u_h, which recovers the $H(\mathrm{div})$ conforming mixed finite element method.

2. The relationship between XG and discontinuous Galerkin methods is twofold. First, by simply taking the trivial spaces for $\breve{u}_h$ and $\breve{p}_h$, XG recovers most of discontinuous Galerkin methods.

3. XG can be compared with most hybridized discontinuous Galerkin methods if $\breve{p}_h$ is eliminated.

4. XG can be compared with most weak Galerkin methods if $\breve{u}_h$ is eliminated.

In addition, two types of uniform inf-sup conditions for XG method can be established and the relationship between H^1 conforming method, mixed method and XG method can be seen.

Finally, we consider the XG method for elasticity method which contains the conforming mixed method, nonconforming mixed method, hybrid mixed method method as special cases and further some new methods are proposed there.

3.5 Analysis of the numerical schemes for phase field models and modeling of the multiphase problems

In recent years, the Allen-Cahn and Cahn-Hilliard equations have gained great popularity in a variety of moving interface problems in the materials science and fluid dynamics through a phase field approach. Partially implicit (or partially explicit) schemes, such as the convex splitting schemes (CSS in short), are among the most popular numerical schemes used in phase-field modeling. Using both theoretical analysis and numerical experiments, Xu, Li, and Wu ([36], 2016) demonstrate that all existing partially implicit schemes for phase-filed simulations may lack convergence accuracy.

As the main example, they first show that some well-known CSS can be interpreted as some fully implicit schemes (FIS in short) in disguise. For the Allen-Cahn model, we prove that the standard CSS is exactly the same as the standard FIS but with a (much) smaller time step size and as a result, it would provide an approximation to the original solution of the Allen-Cahn model at a delayed time (although the magnitude of the delay is reduced when the time step size is reduced). Such time delay is also observed for other partially implicit schemes when time step size is not sufficient small. For the Cahn-Hilliard model, we prove that the standard CSS is exactly the same as the standard FIS for a different model that is a (nontrivial) perturbation of the original Cahn-Hilliard model.

Motivated by the equivalence between CSS and FIS, they also propose a modification of a typical FIS for the Allen-Cahn model so that the maximum principle will be valid on the discrete level and we further rigorously prove that, the linearization of such a modified FIS can be uniformly preconditioned by a Poisson-like operator.

For the multiphase modeling and discretizations, the mathematical properties and numerical discretizations of multiphase models that simulate the phase separation of an N-component mixture are studied by Wu and Xu ([28], 2017). For the general choice of phase variables, the unisolvent property of the coefficient matrix involved in the N-phase models based on the pairwise surface tensions is established. Moreover, the symmetric positive-definite property of the coefficient matrix on an $(N-1)$-dimensional hyperplane — which is of fundamental importance to the well-posedness of the models — can be proved equivalent to some elegant physical condition for pairwise surface tensions. The N-phase Allen-Cahn and N-phase Cahn-Hilliard equations can then be derived from the free-energy functional. Finite element discretizations for N-phase models can be obtained as a natural extension of the existing discretizations for the two-phase model.

4 Theories

Most of the pure theoretical works done by Xu involve the abstract framework and convergence analysis of various iterative methods including multigrid and domain decomposition methods. Examples of theoretical works are also given on some very basic questions in numerical analysis.

4.1 Framework of the method of subspace correction

In Xu ([30], 1992), a general theoretical framework on iterative methods based on space decompositions and subspace correction is proposed. In this work, many standard linear iterative methods such as multigrid and domain decomposition methods are cast and analyzed in a unified framework. This framework changed the understanding of iterative methods and, together with subsequent research on subspace correction methods, it is considered a milestone in the development of multilevel iterative methods. In particular, [30] is a highly cited paper. This is a highly impactful and highly cited paper (which had 1267 citations according to scholar.google.com as of May 16, 2017).

4.2 XZ identity

Xu-Zikatanov ([33], 2002), published in the Journal of American Mathematical Society (JAMS) made substantial progress in regard to the theory of the subspace correction method and obtained the sharpest possible estimate for the convergence of the subspace correction method. Most of the existing estimates (which have been studied in hundreds of papers) can be easily derived from this identity.

Consider the linear system $Au = f$. Let operator B be defined by the Successive Subspace Correction (SSC) method. Then, the following X-Z identity holds when each subspace problem is solved exactly:

$$\|I - BA\|_A^2 = 1 - \frac{1}{1 + c_0},$$

where

$$c_0 = \sup_{\|v\|_A=1} \inf_{\sum v_i = v} \sum_{i=0}^{J} \|P_i \sum_{j>i} v_j\|_{A_i}^2.$$

Here are some more related works:

- Lee, Wu, Xu and Zikatanov ([19], 2006; [21], 2008) extended the identity to symmetric positive semi-definite system

- Lee, Wu, Xu and Zikatanov ([20], 2007) applied the identity to find a very simple and practical condition that gives uniform convergence for nearly singular systems.

4.3 Optimal theories for iterative methods such as multigrid and domain decomposition methods

In the last three decades, Xu has been a world leading analyst on the theoretical foundation for various iterative methods. He is well-known for various fundamental theoretical results that he has obtained with co-workers for multigrid and domain decomposition methods. In the early stage of his career, in joint of his collaborators, he wrote several fundamental papers on the convergence analysis of multigrid and domain decomposition methods. Here are three examples: In Bramble, Pasciak and Xu ([4], 1991), they provided a convergence theoretical framework for analyzing multigrid algorithms with non-embedded spaces or non-inherited quadratic forms which has a wide range applications (with 267 citations as shown in Google Scholar July 2016). In Bramble, Pasciak, Wang and Xu ([5], 1991), this paper is the first analysis of the uniform convergence of multiplicative overlapping domain decomposition method. Another paper by Bramble, Pasciak, Wang and Xu ([6], 1991) is a new multigrid convergence theory without using elliptic regularity.

4.4 Removal of "1"

Xu-Zikatanov ([34], 2003) made a key observation on abstract error estimates for Galerkin approximations based on Babuska-Brezzi conditions. In all the earlier papers and textbooks, the following error estimate is often presented:

$$\|u-u_h\|_U \leq (1+C)\inf_{w_h}\|u-w_h\|_U.$$

Here u_h is a general Galerkin approximation of u which can often be written as $u_h = P_h u$ for some idempotent operator P_h and $C = \|P_h\|$. By observing the identity that $\|P\| = \|I-P\|$ for any nontrivial idempotent operator P. Xu-Zikatanov ([34], 2003) removed the constant "1" from the above estimate to get the following sharp estimate:

$$\|u-u_h\|_U \leq C\inf_{w_h}\|u-w_h\|_U.$$

Given the fundamental nature of these estimates in numerical analysis, this simple improvement is mathematically pleasing.

4.5 Lower Bounds of the Discretization Error for Piecewise Polynomials

Lin, Xie and Xu ([23], 2014) proved the sharp lower-bound error estimate of the approximation error by piecewise polynomials function spaces. Precisely, the following lower error bounds are valid for finite element (consisting of piecewise polynomials of a degree less than r) approximation to $2m$-th order elliptic boundary value problems:

$$\|u-u_h\|_{j,p,h} \geq Ch^{r-j}, \qquad 0 \leq j \leq r, \qquad \forall u \in W^{r+\delta,p}(\Omega),$$

where the positive constant C is independent of the mesh size h. This result is further extended to various situations including general shape regular grids and many different types of finite element spaces. This appears to be a very fundamental question in approximation theory in general and in particular it has been used especially in the analysis lower-bound eigenvalue approximations in the literature.

5 Adaptivity: a new class of error estimators for adaptive finite element methods

A finite element discretization based on more or less uniform grids, even though it is stable, robust and can be applied with fast algebraic solvers such as multigrid, may still not be efficient enough for solution that change much more rapidly in some parts of the region than the other. One practical approach, known as adaptive finite element method, is to use grids that are locally adapted according to the behavior of the solution, namely more grid points will be placed in the region where the solution changes more rapidly. The problem is that the solution is unknown in advance and a good adaptive procedure requires a computable and reliable error estimator. It has been a very active

research subject in recent years to develop a posterior error estimates (that are mostly problem-dependent) for such a purpose.

One major limitation of the existing adaptive finite element methods is that the underlying a posterior error estimators are often problem-dependent. In a recent work, Bank and Xu ([1, 2], 2003) developed a new class of error estimates that are problem-independent and can be applied to various different problems (such as the aforementioned complex fluids models) with no or very little modification. They also showed that the estimators are asymptotically exact for a variety of applications. While there are many other problem-independent error estimators that have been used in practice, the Bank-Xu method seems to be the only one that has a solid mathematical foundation and yet is practically efficient for various applications. This new error estimator has replaced the more traditional error estimators that have been used for about two decades in Randy Bank's popular PLTMG code and it gives outstanding performances for many applications.

Other works on adaptivity

Here are some other works that Xu has done on adaptivity:

- [1, 2] (2003) and [17] (2008) obtained superconvergence for linear and quadratic elements respectively on mildly structured grids, and some theoretical justification for the Zienkiewicz-Zhu error estimator ([32], 2004).
- Chen, Sun and Xu ([8], 2007) have developed anisotropic refinement and mesh optimization techniques based on minimizing the interpolation error in L^p norm. Chen and Xu ([11], 2004) further defined and studied optimal triangulations using the interpolation error as a quality of the triangulation and got some properties of the optimal triangulations and sufficient conditions for a triangulation to be near optimal. The anisotropic refinement and mesh optimization techniques are successfully applied to convection dominated problem by Chen, Sun and Xu ([7], 2005). Chen and Xu ([9], 2005; [10], 2008) gave a theoretical justification of the algorithm for a 1-d convection dominated problem and obtain optimality of the streamline diffusion finite element method.

6 Deep Learning

6.1 MgNet: A Unified Framework of Multigrid and Convolutional Neural Network

Recently, Xu and his collaborator proposed an abstract and unified mathematical framework, known as MgNet, that simultaneously recovers some convolutional neural networks (CNN) for image classification and multigrid methods for solving discretized partial differential equations. Different from the viewpoint of approximation and dynamic systems, MgNet is based on close connections that they have observed and uncovered between the CNN and MG methodologies. For example, pooling operation and feature extraction in CNN correspond directly to restriction operation and iterative smoothers in MG, respectively. As the solution space is often the dual of the data space in PDEs, the analogous concept of feature space and data space (which are dual to each other) is introduced in MgNet. By investigating the iterative schemes for dual variables, they established the connections between different ResNet type CNN architectures and smoothers in MG. With such connections and new concept in the unified model, the function of various convolution operations and pooling used in CNN can be better understood.

The MgNet framework opens a new door to the mathematical understanding, analysis and improvements of deep learning models. The very preliminary results presented in ([13], 2019) have demonstrated the great potential of MgNet from both theoretical and practical viewpoints. Obviously many aspects of MgNet should be further explored and expect to be much improved. In fact, only very few techniques from multigrid method have been tried and many more in-depth techniques from multigrid require further study for deep neural networks, especially CNN. In particular, it is believed that the MgNet framework will lead to improved CNN that only has a small fraction of the number of weights that are required by the current CNN. On the other hand, the techniques in CNN can also be used to develop new generation of multigrid and especially algebraic multigrid methods ([37], 2017) for solving partial differential equations.

7 Practical Applications

In recent years, Xu has spent significant portion of his time in applying advanced numerical techniques to very practical problems.

7.1 Reservoir Simulation

Reservoir simulation is the art of combining physics, mathematics, reservoir engineering, and computer programming to develop a tool for predicting hydrocarbon reservoir performance via various operating strategies. It is an important decision-making tool. For example, engineers use it to obtain information pertaining to the processes that take place in oil reservoirs. Such information enables an analysis of the various recovery strategies in order to effect optimal oil recovery. The crucial part of reservoir simulations is to solve large-scale discretized PDEs (highly coupled, nonsymmetric, and indefinite) over and over again. However, this is also the most time-consuming process of any modern petroleum reservoir simulator (more than 75%). The complexity of the geometry and of the physical model, heterogeneity, and size of reservoir model are continuing to grow, which makes these linear systems more difficult to solve using standard direct or iterative solvers.

The FASP Method for Reservoir Simulations The FASP method takes full advantage of the underlying physical and analytic properties of the mathematical model.

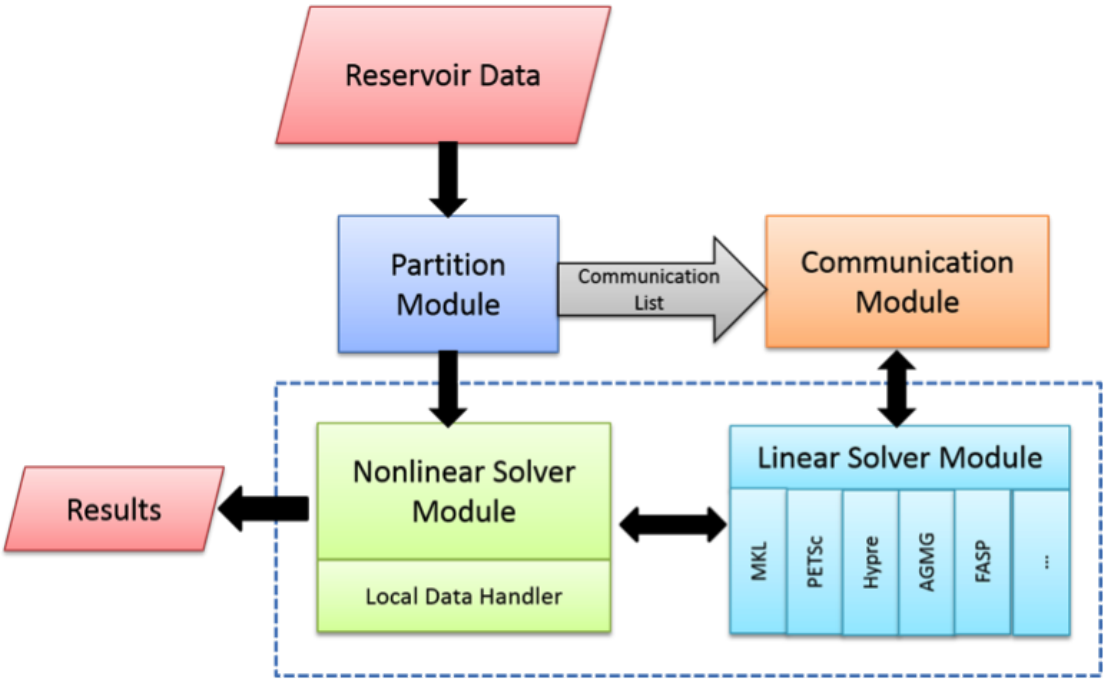


Figure 3: FASP structure

- Transforms the complicated Jacobian system into three simpler auxiliary problems: an elliptic problem for the pressure variables, a hyperbolic problem for the saturation variables, and a purely algebraic problem for the well bottom-hole pressure variables.
- Thus, it can be used to design efficient and robust smoothers or preconditioners for each auxiliary problem.
- It then couples the auxiliary problems and applies the preconditioned Krylov subspace methods.

7.2 Fluid Structure Interaction

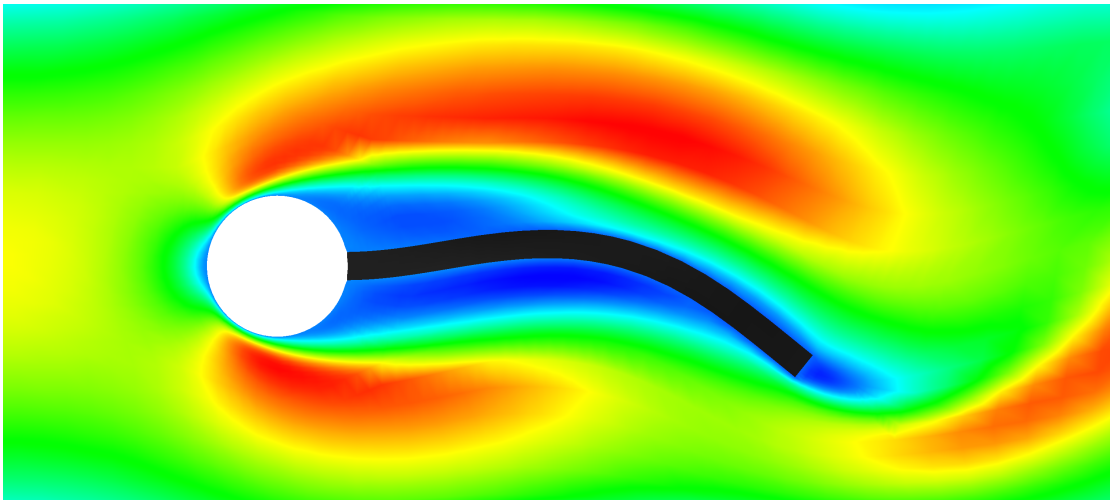
Fluid-structure interaction (FSI) aims at understanding the interaction between moving structure and fluid and how their interaction affects the interface between them. FSI has a wide range of applications in many areas including hemodynamics and wind/hydro turbines simulation. FSI problems are computationally challenging. The computational domain of FSI consists of fluid and structure subdomains. The position of the interface between fluid domain and structure domain is time dependent. Therefore, the shape of the fluid domain is one of the unknowns, increasing the nonlinearity of the FSI problems.

Simulator	ECL100	tNavigator	HiSim
CPU Time (hours)	**120**	**50**	**0.63**

Figure 4: SPE 10 benchmark and result

Monolithic Solver for FSI Numerical solutions of FSI are roughly classified into partitioned approaches and monolithic approaches. Partitioned approaches employ single-physics solvers to solve the fluid and structure problems separately and then couple them by the interface conditions. Monolithic approaches solve the fluid and structure problems simultaneously. Monolithic approaches are considered more stable, although it is accompanied with larger linear systems and higher computational cost. In ([35], 2015), Xu and Yang (his former Ph.D. student) developed a well-posed numerical methods for fluid–structure interaction and designed several robust preconditioners for discretized systems.

- Lagrangian coordinate is used for structure equations, and Eulerian coordinate for fluid equations. They use ALE method to update the fluid mesh.
- They discretize the coupled fluid and structure equations in a single linear system.
- In order to solve it efficiently, they develop block preconditioners for this problem, which proves to be robust with respect to varying parameters and problems sizes.



Number of iterations for preconditioned MINRES for different time step sizes

	$k = 0.01$				$k = 0.001$				$k = 0.0001$			
preconditioner	**M1**	**M2**	**M3**	SC	**M1**	**M2**	**M3**	SC	**M1**	**M2**	**M3**	SC
mesh 1	9	6	11	37	9	6	11	25	8	7	11	23
mesh 2	9	6	11	59	9	7	11	28	7	7	11	23
mesh 3	9	6	11	132	8	7	11	48	9	5	12	29

Figure 5: Turek benchmark and result

Hydroelectric Generator Hydroelectric generator simulation involves the moving fluid domain, which is due to the rotation and deformation of the blade of the generator. Therefore, efficient monolithic solver for the couple system is

difficult to construct. In order to simulation fluid coupled with rotating structures, like hydroturbine in hydroelectric , Yang, Sun, Wang, Xu and Zhang ([38], 2016) develop a new ALE method to update the fluid mesh so that it can handle arbitrary rotation.

Artificial Heart Artificial heart is a kind of effective treatment for heart failure, which is the finial battlefield of cardiovascular disease. The artificial heart significantly changes the hemodynamics of the aorta. The main difficulty of artificial heart simulation is the complex interaction between blood, aorta and artificial heart.

7.3 Energy Storage

Lithium Ion Battery Lithiumion batteries are rechargeable, and they are characterized by lithium ions that move from the negative electrode to the positive electrode during discharge and then back again during charging.

Newton-Krylov-Multigrid Schemes for Lithium Ion Battery Simulation

- Finite volume method
- Newton's method for the Butler-Volmer equation, and the whole nonlinear system
- Krylov subspace method (GMRes) with block Gauss-Seidel preconditioner
- Multigrid method for solving the Poisson-like problems in the preconditioner

7.4 Fuel Cells

A fuel cell is a device that converts a fuel's chemical energy from a fuel into electricity through a chemical reaction with oxygen or another oxidizing agent. Hydrogen is the most commonly used fuel for this purpose, but hydrocarbons such as natural gas and alcohols like methanol are sometimes used.

Robust Methods for Fuel Cells

- Newton's method for the nonlinear system
- Kirchhoff transformation
- Finite element-upwind finite volume method
- Nonoverlapping Schwarz domain decomposition method
- Overlapping domain decomposition method with non-matching grids Newton-Krylov-based solvers

7.5 Software development: FASP

Over the last few decades, researchers have expended significant effort on developing efficient iterative methods for solving discretized partial differential equations (PDEs). Though these efforts have yielded many mathematically optimal solvers such as the multigrid method, the unfortunate reality is that multigrid methods have not been much used in practical applications. This marked gap between theory and practice is mainly due to the fragility of traditional multigrid (MG) methodology and the complexity of its implementation. In the last few years, Xu and his group aim to develop techniques and the corresponding software that will narrow this gap, specifically by developing mathematically optimal solvers that are robust and easy to use in practice.

We believe that there is no one-size-for-all solution method for discrete linear systemsfrom different applications. And, efficient iterative solvers can be constructed by taking the properties of PDEs and discretizations into account. In this project, we plan to construct a pool of discrete problems arising from partial differential equations (PDEs) or PDE systems and efficient linear solvers for these problems. We mainly utilize the methodology of Auxiliary Space Preconditioning (ASP) to construct efficient linear solvers. Due to this reason, this software package is called Fast Auxiliary Space Preconditioning or FASP for short.

FASP contains the kernel part and several applications (ranging from fluid dynamics to reservoir simulation). The kernel part is open-source and licensed under GNU Lesser General Public License or LGPL version 3.0 or later. Some of the applications contain contributions from and owned partially by other parties.

For details, see http://fasp.sourceforge.net

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