Final Report

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1 Center description and goals

For many problems in computational science and engineering, the so-called forward problemsolution of the underlying mathematical model to yield output quantities of interest, given input parametersis difficult enough for frontier complex models, which are often characterized by coupled multiphysics and possibly stochastic behavior over a wide range of length and time scales. However, we face the need to move beyond the forward problem, to address what is often the ultimate goal of computational science and engineering (CS&E): decision making. This requires us to tackle a spectrum of mathematical problems that subsume, and are thus even more difficult than, the forward problem. First, given experimental data, we wish to estimate unknown parameters characterizing a model of a natural or engineered system by solving an inverse problem. Second, we seek the optimal configuration of the system (or experiments) by solving an optimal design problem. Third, the optimal operation of the system must be determined by solving an optimal control problem. And fourth, we must quantify uncertainties as they propagate through all of the preceding problems, from data to model inference to prediction and finally to optimal design and control.

Optimal mathematical methods and algorithms for such end-to-end, data-to-decisions modeling and simulation of complex problemsrequiring integrated solution of forward, inverse, optimization, and UQ problems for large, multiphysics, multiscale modelsentails challenges of the highest order, while also presenting great opportunities for applied mathematics research. Unfortunately, research on forward, inverse, optimization, and UQ problems has all-too-often progressed in isolation. This has led to mathematical methods that perform well when considering the forward simulation in isolation, but are prohibitive or suboptimal or unstable when combined with other methods within the framework of inversion, optimization, or UQ. The reverse is also true: general-purpose methods developed within the inversion, optimization, and UQ fields often become prohibitive when applied to complex CS&E problems since they do not exploit their structure.

DiaMonD is a multi-institutional DOE MMICC effort that aims to address the challenges of end-to-end, data-to-decisions modeling and simulation for complex CS&E problems in a unified, systematic, and integrated fashion. Institutions involved are Colorado State, Florida State, Los Alamos, MIT, Oak Ridge, Stanford, and UT-Austin. The goals of DiaMonD are (1) to develop advanced mathematical methods and analysis for multimodel, multiphysics, multiscale model problems driven by frontier DOE applications, including those in subsurface energy and environmental flows, materials for energy storage and conversion, and ice sheet dynamics; (2) to create theory and algorithms for integrated inversion, optimization, and uncertainty quantification for these complex problems; and (3) to disseminate the philosophy of an integrated end-to-end, data-to-decisions approach to modeling and simulation of complex problems to the broader applied math and computational science communities through workshops and other outreach.

2 Accomplishments

At Stanford University, we have been focusing on the following projects.

2.1 1. Data-sparse factorization for operators of linear and nonlinear PDEs

In this topic, we construct data-sparse factorizations for linear and nonlinear PDEs. These factorizations give rise to efficient algorithms and preconditioners for the solutions of these PDE problems.

Elliptic problems. For elliptic PDEs, we have developed the *hierarchical interpolative factorization*, which is the first to achieve linear complexity (with respect to the unknowns) for general 2D/3D elliptic problems in both differential and integral formulations. The main idea is to build data-sparse representation of these operators via exploiting the low-rank properties of the Green's function and introducing novel interlacing hierarchical decompositions.

- Yingzhou Li and Lexing Ying. Distributed-memory hierarchical interpolative factorization. Research in Mathematical Sciences 4 (2017).
- Victor Minden, Kenneth Ho, Anil Damle, and Lexing Ying. A recursive skeletonization factorization based on strong admissibility. SIAM Multiscale Modeling and Simulation 15-2 (2017).
- K. Ho and L. Ying. Hierarchical interpolative factorization for elliptic operators: differential equations. Communications in Pure and Applied Mathematics 69-8 (2016).
- K. Ho and L. Ying. Hierarchical interpolative factorization for elliptic operators: integral equations. Communications in Pure and Applied Mathematics 69-7 (2016).

High frequency time-harmonic wave equations. For the high-frequency time-harmonic wave equations, the problems are much harder due to the oscillatory nature of the solution. We have designed many fast algorithms for rapid solution of these equations. For the PDE formulations of these operators, we have developed the sweeping preconditioner, which is the first to achieve near-linear complexity for general non-resonant problems. The main idea of the sweeping preconditioner is to guide the factorization process using the geometric nature of the wave propagation and then compress the factorization using tools such as perfectly matched layers (PMLs).

- Fei Liu and Lexing Ying, Sparsifying preconditioner for the time-harmonic Maxwells equations. Journal of Computational Physics 376 (2019).
- Fei Liu and Lexing Ying. Sparsify and sweep: an efficient preconditioner for the Lippmann-Schwinger equation. SIAM Journal on Scientific Computing 40-2 (2018).
- Fei Liu and Lexing Ying. Localized sparsifying preconditioner for periodic indefinite systems. Communications in Mathematical Sciences 15-4 (2017).
- F. Liu and L. Ying. Additive sweeping preconditioner for the Helmholtz equation. SIAM Multiscale Modeling and Simulation 14-2 (2016).
- F. Liu and L. Ying. Recursive sweeping preconditioner for the 3D Helmholtz equation. SIAM Journal on Scientific Computing 38-2 (2016).
- J. Poulson, B. Engquist, S. Li and L. Ying. A parallel sweeping preconditioner for heterogeneous 3D Helmholtz equations. SIAM Journal on Scientific Computing 35 (2013)
- B. Engquist and L. Ying. Sweeping preconditioner for the Helmholtz equation: Moving perfectly matched layers. SIAM Multiscale Modeling and Simulation 9 (2011)
- B. Engquist and L. Ying. Sweeping preconditioner for the Helmholtz equation: Hierarchical matrix representation. Communications in Pure and Applied Mathematics 64 (2011)

In many situations, one prefers to work with the integral equation formulation in order to achieve better accuracy or reduce the number of unknowns. We have also developed a list of efficient preconditioners for various settings, each of which is significantly faster and more effective than existing methods. The main idea is to build data-sparse approximations and inverses using the ray geometry of high frequency wave propagation or the underlying PDE structure.

- L. Ying. Directional preconditioner for high frequency obstacle scattering. SIAM Multiscale Modeling and Simulation 13-3 (2015).
- L. Ying. Sparsifying preconditioner for the Lippmann-Schwinger equation. SIAM Multiscale Modeling and Simulation 13-2 (2015).
- L. Ying. Sparsifying preconditioner for pseudospectral approximations of indefinite systems on periodic structures. SIAM Multiscale Modeling and Simulation 13-2 (2015).

Fourier integral operators. Building on top of our previous work, we have developed a few novel compression techniques for Fourier integral operators with applications in high-frequency wave propagation. These new techniques put the into a more algebraic framework. As a result, it is now possible to carry out a rather complete calculus for the FIOs.

- Victor Minden and Lexing Ying. A simple solver for the fractional Laplacian in multiple dimensions. Submitted.
- Yingzhou Li, Haizhao Yang, and Lexing Ying. Multidimensional butterfly factorization. To appear in Applied and Computational Harmonic Analysis 44-3 (2018).
- Y. Li, H. Yang, E. Martin, K. Ho, and L. Ying. Butterfly factorization. SIAM Multiscale Modeling and Simulation 13-2 (2015).
- Y. Li, H. Yang, and L. Ying. A multiscale butterfly algorithm for multidimensional Fourier integral operators. SIAM Multiscale Modeling and Simulation 13-2 (2015).

Fast algorithm for kinetic equations. We have also developed efficient and accurate algorithms for simulating the kinetic equations. The main challenge is to gain computational efficiency while still maintaining part of mass, energy, and momentum conservation.

- Yuwei Fan, Jing An, and Lexing Ying. Fast algorithms for integral formulations of steady-state radiative transfer equation. Journal of Computational Physics, 380 (2019).
- Zhenning Cai, Yuwei Fan, and Lexing Ying. An entropic Fourier method for the Boltzmann equation. SIAM J. Sci. Comput. 40(5) (2018).

2.2 Algorithm and sparse representation for electronic structure analysis

In the past several years, we have been actively working on developing efficient and accurate algorithms for electronic structure calculation.

Pole expansion and selected inversion. Kohn-Sham density functional theory (KSDFT) is the most widely used electronic structure theory for molecules and condensed matter systems. In recent years, we have developed a new framework for solving KSDFT called the pole expansion and selected inversion (PEXSI) method. The PEXSI method solves KSDFT without solving any eigenvalue and eigenvector, and directly evaluates physical quantities including electron density, energy, atomic force, and density of states. The overall algorithm scales as at most quadratically for all materials including insulators, semiconductors and the difficult metallic systems.

- L. Lin, J. Lu, L. Ying, R. Car and W. E, Fast algorithm for extracting the diagonal of the inverse matrix with application to the electronic structure analysis of metallic systems, Commun. Math. Sci. 7 (2009).
- L. Lin, J. Lu, L. Ying, and W. E. Pole-based approximation of the Fermi-Dirac function. Chinese Annals of Mathematics - Series B 30 (2009).
- L. Lin, C. Yang, J. Lu, L. Ying, and W. E. A fast parallel algorithm for selected inversion of structured sparse matrices with application to 2D electronic structure calculations. SIAM Journal on Scientific Computing 33 (2011).

- L. Lin, C. Yang, J. Meza, J. Lu, L. Ying, and W. E. SelInv–an algorithm for selected inversion of a sparse symmetric matrix. ACM Trans. Math. Software 37 (2011).

Localized or data-sparse representations. More recently, we have developed a number of algorithms for computing localized or data-sparse representations of the electron orbitals and interaction integrals of KSDFT. These new sparse representations immediately give rise to new efficient computational methods in computational quantum chemistry. The main idea is to combine the physical nature of the quantum systems (such as the spectral gap of the insulator systems) with the recently developed randomized algorithms in numerical linear algebra.

- Anil Damle, Lin Lin, and Lexing Ying. Computing localized representations of the kohn-sham subspace via randomization and refinement. SIAM Journal on Scientific Computing 39-6 (2017).
- Lin Lin, Ze Xu, and Lexing Ying. Adaptively compressed polarizability operator for accelerating large scale ab initio phonon calculations. SIAM Multiscale Modeling and Simulation 15-1 (2017).
- A. Damle, L. Lin, and L. Ying. SCDM-k: Localized orbitals for solids via selected columns of the density matrix. Journal of Computational Physics 334 (2017).
- J. Lu and L. Ying. Compression of the electron repulsion integral tensor in tensor hypercontraction format with cubic scaling cost. Journal of Computational Physics 302-1 (2015).
- J. Lu and L. Ying, Fast algorithm for periodic density fitting for Bloch waves. Annals of Mathematical Sciences and Applications 1-2 (2016).
- A. Damle, L. Lin, and L. Ying. Compressed representation of Kohn-Sham orbitals via selected columns of the density matrix (SCDM). J. Chem. Theory Comput. 11 (2015).

2.3 Representation of high dimensional functions and distributions

In the past two years, we have started to explore several new directions.

Tensor networks. Tensor network is a novel representation for high-dimensional functions and probability distributions when the degrees of freedoms (DOFs) have certain geometric structure (for example in a typical Ising model, only nearby spins interact with each other). In many applications from statistical and quantum mechanics, tensor networks are able to represent key objects such as ground state wave functions and partition functions accurately and effective. One of the key computational problem in tensor network is how to compute the value of the tensor network (i.e., contract the network) without resorting to exponential computational cost. Recently, we have developed a novel algorithm for this task where the key contribution is a novel way of removing short-range correlation without modifying the geometry structure of the tensor network. This allows one to extend the algorithm relatively easily to higher dimension and, for the first time, results efficient computation for 3D and 4D tensor networks.

- Yuehaw Khoo, Jianfeng Lu, and Lexing Ying. Efficient construction of tensor ring representations from sampling. Submitted.
- L. Ying. Tensor network skeletonization. SIAM Journal of Multiscale Modeling and Simulation 15-4 (2017).

Machine learning and neural networks. Recently, we started to explore new problems and opportunities at the interface of machine learning and PDEs. we will give two examples. In this first example, we have applied the techniques developed in the SCDM work to develop a new algorithm for spectral clustering. This method is based on a column-pivoted QR factorization and may be directly used for cluster assignment or to provide an initial guess for k-means. This algorithm is simple to implement, direct, and requires no initial guess. Furthermore, it scales linearly in the number of nodes of the graph and a randomized variant provides significant computational gains.

- Jing An, Jianfeng Lu, and Lexing Ying, Stochastic modified equations for the asynchronous stochastic gradient descent. To appear in Information and Inference.
- A. Damle, V. Minden, and L. Ying. Simple, direct and efficient multi-way spectral clustering. Information and Inference 8-1 (2019).
- Victor Minden, Anil Damle, Kenneth Ho, and Lexing Ying. Fast spatial Gaussian process maximum likelihood estimation via skeletonization factorizations. SIAM Journal of Multiscale Modeling and Simulation 15-4 (2017).

In the second example, we explored the possibility of solving challenging partial differential equations using neural networks. This is particularly relevant when a certain type of PDEs need to be solved repetitively with different parameters and computing each solution takes significant amount of cost. In the following paper, we successfully trained artificial neural method to solve a problem in numerical homogenization and a nonlinear elliptic eigenvalue problem.

- Yuwei Fan, Lin Lin, Lexing Ying, and Leonardo Zepeda-Nunez, A multiscale neural network based on hierarchical matrices. Submitted.
- Yuwei Fan, Jordi Feliu-Faba, Lin Lin, Lexing Ying, and Leonardo Zepeda-Nunez. A multiscale neural network based on hierarchical nested bases. Research in the Mathematical Sciences, 2019, Vol. 6
- Yuwei Fan, Cindy Orozco Bohorquez, and Lexing Ying. BCR-Net: a neural network based on the nonstandard wavelet form. Journal of Computational Physics, 384 (2019).
- Yuehaw Khoo, Jianfeng Lu, and Lexing Ying. Solving for high dimensional committor functions using artificial neural networks. Research in the Mathematical Sciences 6 (1), 2019.
- Y. Khoo, J. Lu, and L. Ying. Solving parametric PDE problems with artificial neural networks. Submitted.