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RESEARCH INTERESTS

Scientific Computing: Direct solvers and preconditioners for sparse and dense linear systems, low-rank and butterfly compression, randomized matrix and tensor algorithms, high-performance computing, autotuning, Bayesian optimization, scientific machine learning, as well as their applications to fusion simulation, accelerator modeling, seismic modeling, optical computing, quantum chemistry, quantum computing, bio-science, nuclear physics, power grid and inverse problem applications.

Computational Electromagnetics: Fast integral and differential equation solvers for large-scale electromagnetic problems, multi-resolution algorithms for transient scattering, multi-physics and multi-scale modeling, inverse scattering, and high-frequency ansatz.

RESEARCH EXPERIENCE

Career (Tenured) Research Scientist, Lawrence Berkeley National Laboratory, Feb. 2022 - Present

- Develop autotuning and uncertainty quantification techniques for DOE applications
- Develop scalable sparse linear solvers
- Develop efficient solvers for kinetic plasma simulations
- Develop new formulations and solvers for acoustic and electromagnetic problems
- Develop fast linear and multi-linear algorithms for quantum chemistry computation
- Develop randomized algorithms for challenging inverse problems
- Develop domain-aware deep learning algorithms

Career-Track Research Scientist, Lawrence Berkeley National Laboratory, Aug. 2019 - Jan. 2022

- Develop butterfly-based direct solvers for sparse linear systems
- Develop autotuning techniques for exascale applications
- Develop GPU-accelerated exascale sparse linear solvers
- Develop efficient direct solver-based RF cavity modeling tools

Postdoctoral Research Fellow, Lawrence Berkeley National Laboratory, Aug. 2017 - Jul. 2019

- Develop low-rank and butterfly-based hierarchical solvers for highly oscillatory problems.
- Develop scalable triangular solution algorithms for sparse direct solvers.

Postdoctoral Research Fellow, University of Michigan, June 2015 - July 2017

- Develop randomized algorithms for butterfly factorizations and butterfly-based fast direct integral equation solvers for high-frequency Helmholtz problems.

Research Assistant, University of Michigan, Sept. 2010 - May 2015

- Develop provably scalable and wavelet-enhanced plane-wave-time-domain algorithms for integral equation analysis of large-scale transient problems.

TEACHING EXPERIENCE

Lecturer, ACES 2024 Conference, May 2024

- Short course: Direct solvers for sparse and dense systems in electromagnetics and multi-physics simulations.

	<p>Lecturer, IEEE NEMO Conference, June 2023</p> <ul style="list-style-type: none"> • Short course: Rank-structured fast direct solvers for electromagnetics and multiphysics simulations. <p>Lecturer, Exascale Computing Project Annual Meeting, May. 2023</p> <ul style="list-style-type: none"> • Tutorial: SuperLU and STRUMPACK: GPU accelerated sparse factorization solvers • Tutorial: Autotuning ECP Codes Using the GPTune Package <p>Lecturer, Exascale Computing Project Annual Meeting, May. 2022</p> <ul style="list-style-type: none"> • Tutorial: GPU Capable Sparse Direct Solvers • Tutorial: Performance Autotuning of ECP Applications with Gaussian Process-Based and Cloud Database-Enhanced GPTune Package <p>Lecturer, Exascale Computing Project Annual Meeting, Apr. 2021</p> <ul style="list-style-type: none"> • Tutorial: GPTune: Performance Autotuner for ECP Applications <p>Lecturer, Exascale Computing Project Annual Meeting, Feb. 2020</p> <ul style="list-style-type: none"> • Tutorial: STRUMPACK / SuperLU: fast parallel direct linear solvers and preconditioners <p>Lecturer, Super Computing, Nov. 2019</p> <ul style="list-style-type: none"> • Tutorial: fast parallel direct linear solvers and preconditioners <p>Lecturer, IEEE NEMO Conference, May 2019</p> <ul style="list-style-type: none"> • Short course: Scalable direct solvers for electromagnetics and multiphysics simulations. <p>Teaching Assistant, Shanghai Jiao Tong University, Mar. 2009 - June 2009</p> <ul style="list-style-type: none"> • Instruct students in FPGA programming for digital circuit designs.
EDUCATION	<ul style="list-style-type: none"> • Ph.D., Electrical Engineering, University of Michigan, May 2015 Advisor: Eric Michielssen • M.S., Mathematics, University of Michigan, Nov. 2014 • B.S., Electrical Engineering, Shanghai Jiao Tong University, June 2010
HONORS AND AWARDS	<ul style="list-style-type: none"> • DOD SBIR Award (Co-PI), 2023 • LBNL Laboratory Directed Research and Development (LDRD) Award (PI), 2022 • Young Scientists Award, 3rd URSI Atlantic Radio Science Meeting (AT-AP-RASC), 2022 • Sergei A. Schelkunoff Transactions Prize Paper Award, IEEE Antennas and Propagation Society, 2018 • 1st Place in Student Paper Competition, 12th International Workshop on Finite Elements for Microwave Engineering, 2014 • 2nd Place in Student Paper Competition, 28th Annual Review of Progress in Applied Computational Electromagnetics, 2012 • Rackham Travel Grant, University of Michigan, 2012 to 2014 • Outstanding Graduate Award, Shanghai Jiao Tong University, 2010 • Third Prize in National Electronic Contest, China, 2009
SOFTWARE DEVELOPMENT	<ul style="list-style-type: none"> • ButterflyPACK, https://github.com/liuyangzhuan/ButterflyPACK • GPTune, https://github.com/gptune/GPTune • Superlu_DIST, https://github.com/xiaoyeli/superlu_dist • STRUMPACK, https://github.com/pghysels/STRUMPACK
REVIEWER EXPERIENCE	<p>Proposals</p> <ul style="list-style-type: none"> • DOE SBIR/STTR proposals • Dutch Research Council (NWO) proposals

- Israel Science Foundation (ISF) proposals

Conference Proceedings

- PC member for International Parallel and Distributed Processing Symposium (IPDPS) 2023, 2024
- PC member for IEEE Cluster 2021
- PC member for International Conference on Parallel Processing (ICPP) 2021, 2023
- PC member for Supercomputing (SC) 2021, 2022
- IEEE AP-S/URSI Symposium 2021, 2022, 2023
- PC member for SIAM Conference on Parallel Processing for Scientific Computing (PP), 2022, 2023

Journals

- Communications in Computational Physics
- CCF Transactions on High Performance Computing
- CSIAM Transactions on Applied Mathematics
- Journal of Computational Physics
- ACM Transactions on Mathematical Software
- Applied and Computational Harmonic Analysis
- The Journal of the Acoustical Society of America
- SIAM Journal of Scientific Computing
- SIAM Journal on Matrix Analysis and Applications
- Mathematical Reviews of AMS
- IEEE Transaction on Antennas and Propagation
- IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control
- IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems
- IEEE Antennas and Propagation Magazine
- IEEE Transaction on Microwave Theory and Techniques
- IEEE Transactions on Parallel and Distributed Systems
- IEEE Antennas and Wireless Propagation Letters
- IEEE Journal on Multiscale and Multiphysics Computational Techniques
- International Journal of Numerical Modelling: Electronic Networks, Devices and Fields
- Concurrency and Computation: Practice and Experience
- Journal of Applied Computational Electromagnetics Society
- International Journal of Antennas and Propagation
- The Open Electrical and Electronic Engineering Journal
- Journal of Microwaves, Optoelectronics and Electromagnetic Applications
- Mathematics of MDPI

SESSION
ORGANIZER

- Chair for “Fast Algorithms,” IEEE NEMO Conference, May 2024
- Chair for “Fast Algorithms,” ACES 2024 Conference, May 2024
- Publication chair for IEEE NEMO Conference, 2023
- Committee Member for “DOE SciDAC FASTMath Seminar Series”, 2021, 2022
- Chair for “Low-Rank Compression-Based Fast Sparse Direct Solvers,” SIAM Conference on Parallel Processing for Scientific Computing, 2020
- Chair for “Fast and Accurate Integral Methods for Highly Oscillatory Phenomena,” SIAM Conference on Computational Science and Engineering, 2019
- Chair for “Time-Domain Computational Methods for Complex Electromagnetic and Multiphysics Problems,” IEEE International Symposium on Antennas and Propagation and USNC-URSI Radio Science Meeting, 2019
- Chair for “Parallel Sparse Triangular Solve on Emerging Platforms,” SIAM Conference on Applied Linear Algebra, 2018

- Chair for “Acceleration Techniques for Integral Equations,” IEEE International Symposium on Antennas and Propagation and USNC-URSI Radio Science Meeting, 2017.
- Chair for “Time-Domain Numerical Methods,” IEEE International Symposium on Antennas and Propagation and USNC-URSI Radio Science Meeting, 2012
- Judge for the 10th Annual Engineering Graduate Symposium, University of Michigan, 2015
- Steering Committee for “Celebrating Maxwell’s Equations: 150 Years” workshop, 2015.
- Chapter Treasurer for IEEE Southeastern Michigan Section, Chapter IV, 2011-2016.
- Secretary for Technical Activities Committee, IEEE Southeastern Michigan Section, 2015-2016.

BOOK
CHAPTERS

- [1] **Y. Liu**, and E. Michielssen “Parallel fast time-domain integral-equation methods for transient electromagnetic analysis,” in *Parallel algorithms in computational science and engineering*. Birkhauser, 2020.

REFEREED
JOURNAL
PUBLICATIONS

- [1] W. Boukaram, Y. Hong, **Y. Liu**, T. Shi, and X. S. Li, “Batched sparse direct solver design and evaluation in SuperLU DIST,” *Int. Journal of High Performance Computing Applications*, 2024. (submitted)
- [2] Z. Wang, A. Aldossary, T. Shi, **Y. Liu**, X. S. Li, and M. Head-Gordon, “Local second-order Møller–Plesset theory with a single threshold using orthogonal virtual orbitals: theory, implementation, and assessment,” *J. Chem. Theory Comput.*, 2023. doi:10.1021/acs.jctc.3c00744.
- [3] **Y. Liu**, T. Luo, A. Rani, H. Luo, and X. Li, “Detecting resonance of radio-frequency cavities using fast direct integral equation solvers and augmented Bayesian optimization,” *IEEE J. Multiscale Multiphysics Comput. Tech.*, 2023. doi:10.1109/JMMCT.2023.3311322.
- [4] L. Claus, P. Ghysels, **Y. Liu**, T. Nhan, R. Thirumalaisamy, A. P. S. Bhalla, and X. Li, “Sparse approximate multifrontal factorization with composite compression methods,” *ACM Trans. Math. Softw.*, 2023. doi:10.1145/3611662.
- [5] X. Li, **Y. Liu**, P. Lin, and P. Sao, “Newly released capabilities in distributed-memory SuperLU sparse direct solver,” *ACM Trans. Math. Softw.*, 2023. doi:10.1145/3577197.
- [6] H. Luo, Y. Cho, J. W. Demmel, X. S. Li, and **Y. Liu**, “Hybrid models for mixed variables in Bayesian optimization,” *Journal of Machine Learning Research*, (arXiv:2206.01409).
- [7] W. Sheng, A. C. Yucel, **Y. Liu**, H. Guo, and E. Michielssen, “A domain decomposition based surface integral equation simulator for characterizing EM wave propagation in mine environments,” *IEEE Trans. Antennas Propag.*, 2023. doi:10.1109/TAP.2023.3256579.
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- [11] H. Luo, J. W. Demmel, Y. Cho, X. S. Li, and **Y. Liu**, “Non-smooth Bayesian optimization

in tuning problems,” *Journal of Machine Learning Research*, (arXiv:2111.01730).

- [12] **Y. Liu**, P. Ghysels, L. Claus, and X. Sherry Li, “Sparse approximate multifrontal factorization with butterfly compression for high frequency wave equations,” *SIAM J. Sci. Comput.*, 2021. doi:[10.1137/20M1349667](https://doi.org/10.1137/20M1349667).
- [13] **Y. Liu**, Xin Xing, H. Guo, E. Michielssen, P. Ghysels, and X. Sherry Li “Butterfly factorization via randomized matrix-vector multiplications,” *SIAM J. Sci. Comput.*, 2021. doi:[10.1137/20M1315853](https://doi.org/10.1137/20M1315853).
- [14] **Y. Liu**, W. Sid-Lakhdar, E. Rebrova, P. Ghysels, and X. Sherry Li, “A parallel hierarchical blocked adaptive cross approximation algorithm,” *Int. Journal of High Performance Computing Applications* 2020. doi:[10.1177/1094342020918305](https://doi.org/10.1177/1094342020918305)
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tion strategies for sparse triangular solver on CPU and GPU clusters," in *The International Conference for High Performance Computing, Networking, Storage, and Analysis*, 2023. doi:[10.1145/3581784.3607092](https://doi.org/10.1145/3581784.3607092)

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- [3] Y. Cho, J. W. Demmel, J. King, X. S. Li, **Y. Liu**, and H. Luo, "Harnessing the crowd for autotuning high-performance computing applications," in *IEEE International Parallel and Distributed Processing Symposium*, 2023. doi:[10.1109/IPDPS54959.2023.00069](https://doi.org/10.1109/IPDPS54959.2023.00069)
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- [5] X. Zhu, **Y. Liu**, P. Ghysels, D. Bindel, and X. S. Li, "GPTuneBand: multi-task and multi-fidelity Bayesian optimization for autotuning exascale applications," in *SIAM PP*, 2022. doi:[10.1137/1.9781611977141.1](https://doi.org/10.1137/1.9781611977141.1)
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- [9] G. Chavez, E. Rebrova, **Y. Liu**, P. Ghysels and X. S. Li "Scalable and memory-efficient kernel ridge regression," in *34th IEEE International Parallel and Distributed Processing Symposium*, 2020. doi:[10.1109/IPDPS47924.2020.00102](https://doi.org/10.1109/IPDPS47924.2020.00102)
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ference, 2024.

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- [3] **Y. Liu**, M. Kielstra, T. Shi, H. Luo, and J. Qian, “Fast Iterative Solvers in Tensor Butterfly Format”, in *18th Copper Mountain Conference on Iterative Methods*, 2024.
- [4] **Y. Liu**, “Butterfly Algorithms: from Matrix to Tensor”, in *SIAM Conference on Parallel Processing for Scientific Computing*, 2024.
- [5] **Y. Liu**, “Efficient Matrix, Tensor, Machine Learning Algorithms for Computational Science and Engineering Applications”, in *Purdue University Seminar*, 2024.
- [6] **Y. Liu**, “Babich Ansatz: a Geometrical-Optics-Like Ansatz for Green’s Function of Wave Equations with Variable Coefficients”, in *DOE FASTMath Seminar*, 2023.
- [7] **Y. Liu**, “Progress on Faster Butterfly Construction Based on Randomized Matrix-Vector Multiplication”, in *SIAM CSE*, 2023.
- [8] **Y. Liu**, “Fast Direct Solvers for Electromagnetic, Optics, Acoustic, and Elastic Applications”, in *Physics-2022*.
- [9] **Y. Liu**, “Butterfly Compressed Babich Integrator for Solving Helmholtz Equations in Inhomogeneous Media”, in *BIRS-CMO Workshop on Outstanding Challenges in Computational Methods for Integral Equations*, 2022.
- [10] **Y. Liu**, “Fast Direct Integral and Differential Equation Solvers for Electromagnetic Applications at All Frequency Ranges”, in *Howard University Seminar*, 2021.
- [11] **Y. Liu**, “Fast Direct Integral and Differential Equation Solvers for Electromagnetic, Acoustic, and Elastic Applications at All Frequency Ranges”, in *Michigan MICDE Seminar*, 2021.
- [12] **Y. Liu**, “Fast Direct Integral and Differential Equation Solvers for Electromagnetic, Acoustic, and Elastic Applications at All Frequency Ranges”, in *Flatiron Seminar*, 2021.
- [13] **Y. Liu**, “Autotuning HPC and ML Applications Using GPTune ”, in *Google Research Seminar*, 2021.
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- [16] **Y. Liu**, T. Luo, and S. Tan, “A Fast Direct IE Solver for Characterization of Accelerator Cavities with Waveguide Ports”, in *ICCEM*, 2020.
- [17] **Y. Liu**, P. Ghysels, L. Claus, and X. S. Li, “Butterfly-based Multifrontal Preconditioner for Wave Equations”, in *HPC China*, 2020.
- [18] **Y. Liu**, X. Zhu, W. S-Lakhdar, X. S. Li, O. Marques, and J. Demmel, “Multitask Learning and Multi-Armed Bandit-Based Bayesian Optimization for HPC Applications”, in *NYSDS*, 2020.
- [19] **Y. Liu**, P. Ghysels, and X. S. Li, “Parallel butterfly-based Sherman–Morrison–Woodbury inversion,” in *SIAM Conference on Parallel Processing for Scientific Computing*, 2020.
- [20] P. Ghysels, **Y. Liu**, and X. S. Li, “Incorporating hierarchical matrix compression and butterfly factorizations in a multifrontal LU solver,” in *SIAM Conference on Parallel Processing for Scientific Computing*, 2020.

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- [22] **Y. Liu**, “Fast Algebras on Optimized Butterfly Structures,” in *SIAM Conference on Computational Science and Engineering*, 2019.
- [23] **Y. Liu**, “A blocked adaptive cross approximation algorithm and its hierarchical generalization,” in *Copper Mountain Conference On Multigrid Methods*, 2019.
- [24] **Y. Liu**, M. Jacquelin, and X. S. Li, “Enhancing scalability of parallel sparse triangular solve in SuperLU,” in *SIAM Conference on Applied Linear Algebra*, 2018.
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time domain volume integral equation solver,” in *Proc. IEEE Int. Symp. AP-S/URSI*, 2013.

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