Lin Lin

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Position

Professor, Department of Mathematics, University of California, Berkeley, 2022–present

Associate Professor, Department of Mathematics, University of California, Berkeley, 2018–2022

Challenge Institute of Quantum Computation, University of California, Berkeley, 2020–present

Faculty Scientist, Computational Research Division, and Center for Applied Mathematics for Energy Research Applications (CAMERA), Lawrence Berkeley National Laboratory, 2014–present

Assistant Professor, Department of Mathematics, University of California, Berkeley, 2014–2018

Research Scientist (Career Track), Lawrence Berkeley National Laboratory, 2013–2014

Luis W. Alvarez Postdoctoral Fellow, Lawrence Berkeley National Laboratory, 2011–2013

Education

Ph. D. Applied Mathematics, Princeton University, USA, 2011

Advisors: Professor Weinan E (Mathematics) and Professor Roberto Car (Chemistry)

B.S. Mathematics, Peking University, China, 2007

Awards

Simons Investigator in Mathematics, 2021

ACM Gordon Bell Prize (Team), 2020

Presidential Early Career Awards for Scientists and Engineers (PECASE), 2019

Department of Energy Early Career Award, 2017–2022

National Science Foundation CAREER Award, 2017–2022

SIAM Computational Science and Engineering (CSE) Early Career Prize (inaugural), 2017

Alfred P. Sloan Fellowship, 2015–2017

Luis W. Alvarez Fellowship, Lawrence Berkeley National Laboratory, 2011–2013

Harold W. Dodds Honorific Fellowship, Princeton University, 2010

Ray Grimm Memorial Prize in Computational Physics, Princeton University, 2010

Research Area

Numerical analysis; Quantum many-body problems; Computational quantum chemistry; Computational materials science; Multiscale modeling; Scientific machine learning; Quantum computing; Parallel Computing

Grants

Principal Investigator: Simons Investigator in Mathematics. 2021–2026.

Principal Investigator: Google Quantum Algorithms Grant, 2021-2022, *Efficient quantum algorithms for preparing ground and thermal states on early fault-tolerant computers*

Co-Investigator (Lead PI: Alan MacDonald). Simons Institute. *Moire Materials Magic*, 2021–2026

Co-Investigator (Lead PI: Martin Head-Gordon). SciDAC-5, DOE. 2021–2025. *Large-scale algorithms and software for modeling chemical reactivity in complex systems*

Co-Investigator (Lead PI: Vojtech Vleck). SciDAC-5, DOE. 2021–2025. *Real-time dynamics of driven correlated electrons in quantum materials*

Co-Investigator (Lead PI: James Sethian). DOE. 2020–2023 *Frontiers in computation: new methods for fluids and interfaces, advanced materials, quantum science, and physics-guided machine learning*.

Co-Investigator (Lead PI: Irfan Siddiqi). DOE. 2020–2025. Quantum Information Science Research Center. *Quantum Systems Accelerator*.

Co-Investigator (Lead PI: Dan Stamper-Kurn). NSF. 2020–2025. *Quantum Leap Challenge Institute: Present and Future Quantum Computation*.

Co-Investigator (Lead PI: Andre Walker-Loud). DOE. 2020–2022. *Connecting Quantum Chromodynamics to Nuclear Physics with Adiabatic Quantum Computing*.

Co-Investigator (Lead PI: K. Birgitta Whaley). Google Quantum Algorithms Focused Award ,2020–2021. *Robust control for performing QAOA on a NISQ computer*.

Principle Investigator. Google Quantum Algorithms Focused Award, , 2019-2020. *New discretization method for accelerating quantum simulation*.

Co-Investigator (Lead PI: Wibe de Jong). DOE. Quantum algorithm teams (QAT) 2017–2020. *Quantum Algorithms, Mathematics and Compilation Tools for Chemical Sciences*.

Principle Investigator. Early Career, DOE. 2017–2022. *Green's function methods for multiphysics simulations*.

Principle Investigator. CAREER, NSF. 2017–2022. *Turbo-Charging Hybrid Functional Electronic Structure Calculations via Adaptive Compression Methods*

Co-Investigator (Lead PI: Garnet Chan). MURI, AFOSR. 2017–2022. *Revolutionary Advances in Correlated Electron Materials: From strongly correlated electrons to large scale DFT and quantum embedding*

Co-Investigator (Lead PI: Volker Blum). SI2-SSI, NSF. 2015–2019. *ELSI-Infrastructure for Scalable Electronic Structure Theory.*

Co-Investigator (Lead PI: Martin Head-Gordon). SciDAC-4, DOE. 2017–2021. *Advancing catalysis modeling: from atomistic chemistry to whole system simulation*

Co-Investigator (Lead PI: James Sethian). DOE. 2017–2020. *Frontiers in Computation: New Methods for Fluids, Structures and Interfaces, Advanced Materials, and Stochastics.*

Principal Investigator. LDRD, LBNL. 2014–2017. *Fast numerical methods for Green's function in mesoscale simulation*.

Co-Investigator (Lead PI: John Pask). SciDAC-3, DOE ASCR & BES. 2012–2017. *Discontinuous methods for accurate, massively parallel quantum molecular dynamics: Lithium ion interface dynamics from first principles.*

Co-Investigator (Lead PI: Roberto Car). SciDAC-3, DOE ASCR & BES. 2012–2017. *Advanced Modeling of Ions in Solutions, on Surfaces, and in Biological Environments.*

Co-Investigator (Lead PI: James Sethian). DOE ASCR & BES. 2014–2019, 2019–2024. *CAMERA: Center for Applied Mathematics for Energy Research Applications*.

Principal Investigator. LDRD, LBNL. 2011–2013. *Computational algorithms and mathematical software tools for materials science and chemistry.*

Oberwolfach travel grant, 2011, 2013

Synergistic Activities

Editorial board

Associate editor, SIAM Journal of Scientific Computing (SISC), 2020–

Associate editor, Journal of Computational Physics, 2020–

Associate editor, SIAM Journal on Matrix Analysis and Applications (SIMAX), 2021–

Associate editor, Communications of Mathematical Sciences (CMS), 2021–

Associate editor, Journal of Computational Mathematics (JCM), 2021–

Associate editor, Springer Nature (SN) Partial Differential Equations and Applications, 2019–2021

Referee for

CMAME, CMS, CPC, CPAM, CPL, JAMS, JCP, JCTC, MMS, NM, PNAS, PRB, PRL, PRX, Quantum, SIMA, SIMAX, SINUM, SISC, TOMS, among many others.

Secretary, SIAM SIAM Activity Group on Mathematical Aspects of Materials Science (SIAG/MS), 2021–2022

Co-organizer, IPAM semester program on Mathematical and Computational Challenges in Quantum Computing, September–December, 2023

Co-organizer (with Eric Cances, Maria J. Esteban, Giulia Galli, Alejandro Rodriguez, Alexandre Tkatchenko), IPAM semester program on Advancing Quantum Mechanics with Mathematics and Statistics, March–June, 2022

Co-editor (with Eric Cances, Gero Friesecke and Jianfeng Lu), Springer book series on *Mathematics and Molecular Modeling*, 2017–present

Co-organizer (with James Sethian and Jianfeng Lu). MSRI Summer School on "Mathematical Introduction to Electronic Structure Theory", 2016.

Conference and seminar organization

Co-organizer (with Aram Harrow, Thomas Vidick and Nathan Wiebe) IPAM Workshop on Quantum Numerical Linear Algebra, January, 2022

Co-organizer (with Eric Cances, Maria J. Esteban, Giulia Galli, Alejandro Rodriguez, Alexandre Tkatchenko), IPAM long program on Advancing Quantum Mechanics with Mathematics and Statistics, March–June, 2022

Co-organizer (with Giuseppe Carleo, Yixiao Chen, Jiequn Han, Jianfeng Lu, James Stokes), AIM SQuaRE (virtual), Deep learning and quantum Monte Carlo, June 2021.

Co-organizer (with Roel van Beeumen, Daan Camps and Chao Yang) SIAM Conference on Applied Linear Algebra (SIAM LA21, virtual), May 2021

Co-organizer (with Amartya Banerjee, Felipe Jornada, Refaely-Abramson) 2021 Virtual MRS Spring Meeting (virtual), April 2021

Co-organizer (with Andrew Childs) SIAM Conference on Computational Science & Engineering (SIAM CSE21, virtual), February 2021

Co-organizer (with Jianfeng Lu and Lexing Ying), AIM Workshop, Deep learning and partial differential equations, October 2019

Co-organizer (with Chao Yang), Minisymposium, SIAM Conference on Computational Science & Engineering (SIAM CSE19), Spokane, February 2019

Co-organizer (with Volker Blum, William Huhn, Jianfeng Lu, Alvaro Vazquez-Mayagoitia, Chao Yang): MolSSI Workshop / ELSI Conference, Richmond, August 2018

Co-organizer (with Kaushik Bhattacharya, Kaushik Dayal and Phanish Suryanarayana): Minisymposium, SIAM Conference on Mathematical Aspects of Materials Science (SIAM MS18), Portland, July 2018

Co-organizer (with Anil Damle and Chao Yang): Minisymposium, SIAM Conference on Applied Linear Algebra (SIAM LA18), Hongkong, May 2018

Co-organizer (with Eric Cances, Gero Friesecke and Trygve Helgaker): Oberwolfach Workshop on Mathematical methods in quantum chemistry, March 2018

Co-organizer (with Virginie Ehrlacher, Benjamin Stamm, Chao Yang): Minisymposium, SIAM Conference on Computational Science & Engineering (SIAM CSE17), Atlanta, February 2017

Co-organizer (with Wei Cai, Limin Liu, Jianfeng Lu and ChiYung Yam): International Conference on Algorithms and Applications for Excited State Electronic Structure Theories, CSRC, 2016

Co-organizer (with Gero Friesecke and Jianfeng Lu). Minisymposium, SIAM Conference on Mathematical Aspects of Materials Science (SIAM MS16), Philadelphia, May 2016

Co-organizer (with Jianfeng Lu). Minisymposium, The International Congress on Industrial and Applied Mathematics (ICIAM), Beijing, 2015

Co-organizer (with Eric Polizzi and Chao Yang). Minisymposium, SIAM Conference on Computational Science & Engineering (SIAM CSE15), Utah, March 2015

Co-organizer (with Eric Cances, Gero Friesecke and Chao Yang).Minisymposium, SIAM Conference on Mathematical Aspects of Materials Science (SIAM MS13), Philadelphia, June 2013

Co-organizer (with Chao Yang). Minisymposium, SIAM Conference on Parallel Processing for Scientific Computing (SIAM PP12), Savannah, February 2012

Member of *Society for Industrial and Applied Mathematics* (SIAM)

Thesis Advisor and Postgraduate-Scholar Sponsor (current and past):

Graduate student (UCB): Dong An, Yulong Dong (joint with Birgitta Whaley), Gil Goldshlager, Zhen Huang, Raehyun Kim, Michael Lindsey, Jeffmin Lin, Yu Tong, Ze Xu, Jiahao Yao, Jiasu Wang, Jiefu Zhang, Qinyi Zhu

Postgraduate-Scholar (UCB): Nilin Abrahamsen (Simons postdoctoral scholar, joint with Umesh Vazirani), Anil Damle (NSF postdoctoral scholar), Zhiyan Ding (Morrey Assistant Professor), Di Fang (Morrey Assistant Professor), Fabian Faulstich, Weile Jia, Jin-Peng Liu (Simons postdoctoral scholar, joint with Umesh Vazirani), Subhayan Roy Moulik, Avijit Shee (joint with Martin Head-Gordon and Birgitta Whaley), Kevin Stubbs, Xiaojie Wu, Xin Xing, Leonardo Zepeda-Nunez,

Postgraduate-Scholar (LBNL): Amartya Banerjee (joint with Chao Yang), Wei Hu (joint with Chao Yang), Senwei Liang (joint with Chao Yang), Yuanran Zhu (joint with Chao Yang)

Recent Teaching Activities

Math 54: Linear algebra and its applications, UC Berkeley, Fall 2022

Math 275: Topics in Applied Mathematics: Quantum algorithms for scientific computation, Fall, 2021

Math 228A: Numerical Solutions of Differential Equations, Fall, 2021

Math 54: Linear algebra and its applications, UC Berkeley, Spring 2020

Math 228A: Numerical Solutions of Differential Equations, Fall, 2019

Math 228A: Numerical Solutions of Differential Equations, Fall, 2018

Math 275: Topics in Applied Mathematics: Mathematical Introduction to Electronic structure Theory, Fall, 2018

Math 54: Linear algebra and its applications, UC Berkeley, Fall 2017

Math 228A: Numerical solutions of differential equations, UC Berkeley, Fall 2017

Math 54: Linear algebra and its applications, UC Berkeley, Fall 2016

Math 128B: Mathematical tools for the physical sciences, UC Berkeley, Spring 2016

Math 128A: Mathematical tools for the physical sciences, UC Berkeley, Spring 2016

Math 228A: Numerical solutions of differential equations, UC Berkeley, Fall 2015

Math H54: Linear algebra and differential equations, UC Berkeley, Fall 2014

Books

1. L. Lin and J. Lu, A mathematical introduction to electronic structure theory, SIAM, 2019

Peer reviewed publications

1. Z. Ding and L. Lin, Even shorter quantum circuit for phase estimation on early fault-tolerant quantum computers with applications to ground-state energy estimation, PRX Quantum 4, 020331, 2023
2. F. M. Faulstich, K. D. Stubbs, Q. Zhu, T. Soejima, R. Dilip, H. Zhai, R. Kim, M. P. Zaletel, G. Kin-Lic Chan, L. Lin, Interacting models for twisted bilayer graphene: a quantum chemistry approach, Phys. Rev. B 107, 235123 (Editor's suggestion)
3. S. Lee, J. Lee, H. Zhai, Y. Tong, A. M. Dalzell, A. Kumar, P. Helms, J. Gray, Z.-H. Cui, W. Liu, M. Kastoryano, R. Babbush, J. Preskill, D. R. Reichman, E. T. Campbell, E. F. Valeev, L. Lin, G. K.-L. Chan, Evaluating the evidence for exponential quantum advantage in ground-state quantum chemistry, Nature Communications 14, 1952, 2023
4. D. Fang, L. Lin, Y. Tong, Time-marching based quantum solvers for time-dependent linear differential equations, Quantum, 7, 955, 2023
5. Z. Huang, E. Gull, L. Lin, Robust analytic continuation of Green's functions via projection, pole estimation, and semidefinite relaxation, Phys. Rev. B, 107, 075151, 2023
6. J. Lin, G. Goldshlager, L. Lin, Explicitly antisymmetrized neural network layers for variational Monte Carlo simulation, J. Comput. Phys. 474, 111765, 2023
7. Y. Peng, L. Lin, L. Ying, L. Zepeda-Nunez, Efficient long-range convolutions for point clouds, J. Comput. Phys., 473 111692, 2023
8. F. M. Faulstich, X. Wu, L. Lin, Discontinuous Galerkin method with Voronoi partitioning for quantum simulation of chemistry, Res. Math. Sci. 9, 68, 2022
9. J. Wang, Y. Dong, L. Lin, On the energy landscape of symmetric quantum signal processing, Quantum 6, 850, 2022
10. Y. Dong, K. B. Whaley, L. Lin, A Quantum Hamiltonian simulation benchmark, npj Quantum Information, 8, 131, 2022
11. Y. Dong, L. Lin, Y. Tong, Ground state preparation and energy estimation on early fault-tolerant quantum computers via quantum eigenvalue transformation of unitary matrices, PRX Quantum, 3, 040305
12. J. Yao, H. Li, M. Bukov, L. Lin, L. Ying, Monte Carlo tree search based hybrid optimization of variational quantum circuits, Math. Sci. Mach. Learn. (MSML 2022) PMLR 190:49, 2022.
13. E. N. Epperly, L. Lin, Y. Nakatsukasa, A theory of quantum subspace diagonalization, SIAM J. Matrix Anal. Appl., 43, 1263, 2022
14. L. Lin and M. Lindsey, Variational embedding for quantum many-body problems, Commun. Pure Appl. Math. 75, 2033, 2022

15. D. An, L. Lin, M. Lindsey, Towards sharp error analysis of extended Lagrangian molecular dynamics, J. Comput. Phys., 466, 111403, 2022

16. S. Jiao et al, KSSOLV 2.0: An efficient MATLAB toolbox for solving the Kohn-Sham equations with plane-wave basis set, Comput. Phys. Commun., 279, 108424, 2022

17. D. An, D. Fang, L. Lin, Time-dependent Hamiltonian simulation of highly oscillatory dynamics, Quantum 6, 690, 2022

18. J. Han, Y. Li, L. Lin, J. Lu, J. Zhang, L. Zhang, Universal approximation of symmetric and anti-symmetric functions, Commun. Math. Sci. 20, 1397, 2022

19. F. M. Faulstich, R. Kim, Z.-H. Cui, Z. Wen, G. K.-L. Chan, L. Lin, Pure state v-representability of density matrix embedding theory, J. Chem. Theory Comput. 18, 851, 2022

20. X. Xing, L. Lin, Staggered mesh method for correlation energy calculations of solids: Random phase approximation in direct ring coupled cluster doubles and adiabatic connection formalisms, J. Chem. Theory Comput. 18, 763, 2022

21. D. An and L. Lin, Quantum linear system solver based on time-optimal adiabatic quantum computing and quantum approximate optimization algorithm, ACM Trans. Quantum Comput. (TQC), 3 Article 5, 2022

22. L. Lin, Y. Tong, Heisenberg-limited ground state energy estimation for early fault-tolerant quantum computers, PRX Quantum 3, 010318, 2022

23. D. An, D. Fang, L. Lin, Parallel transport dynamics for mixed quantum states with applications to time-dependent density functional theory, J. Comput. Phys. 451, 110850, 2022

24. J. Yao, L. Lin, M. Bukov, Reinforcement learning for many-body ground state preparation based on counter-diabatic driving, Phys. Rev. X 11, 031070, 2021

25. J. Yao, P. Kottering, H. Gundlach, L. Lin, M. Bukov, Noise-robust end-to-end quantum control using deep autoregressive policy networks Math. Sci. Mach. Learn. (MSML 2021) PMLR 2021

26. D. An, L. Lin and Z. Xu, Split representation of adaptively compressed polarizability operator, Res. Math. Sci. 8, 51, 2021

27. H. Ma, L. Wang, L. Wan, J. Li, X. Qin, J. Liu, W. Hu, L. Lin, C. Yang, J. Yang, Realize effective cubic-scaling COHSEX approximation in periodic systems via interpolative separable density fitting with plane-wave basis set, J. Phys. Chem. A, 125, 7545, 2021

28. Y. Tong, D. An, N. Wiebe and L. Lin, Fast inversion, preconditioned quantum linear system solvers, fast Green's-function computation, and fast evaluation of matrix functions, Phys. Rev. A 104, 032422

29. L. Lin and M. Lindsey, Bold Feynman diagrams and the Luttinger-Ward formalism via Gibbs measures: Non-perturbative analysis, Arch. Ration. Mech. Anal. 242, 527, 2021

30. L. Lin and M. Lindsey, Bold Feynman diagrams and the Luttinger-Ward formalism via Gibbs measures: Perturbative approach, Arch. Ration. Mech. Anal. 242, 581, 2021

31. X. Xing, X. Li, L. Lin, Staggered mesh method for correlation energy calculations of solids: Second order Moller-Plesset perturbation theory, J. Chem. Theory Comput. 17, 4733, 2021

32. L. Zepeda-Nunez, Y. Chen, J. Zhang, W. Jia, L. Zhang, L. Lin, Deep Density: circumventing the Kohn-Sham equations via symmetry preserving neural networks, J. Comput. Phys. 443, 110523, 2021

33. Y. Dong and L. Lin, Random circuit block-encoded matrix and a proposal of quantum LINPACK benchmark, Phys. Rev. A 103, 062412, 2021

34. D. An, D. Fang, L. Lin, Time-dependent unbounded Hamiltonian simulation with vector norm scaling, Quantum 5, 459, 2021

35. D. An, S. Cheng, T. Head-Gordon, L. Lin and J. Lu, Convergence of stochastic-extended Lagrangian molecular dynamics method for polarizable force field simulation, J. Comput. Phys. 438, 110338 2021

36. L. Lin and X. Wu, Numerical solution of large scale Hartree-Fock-Bogoliubov equations, ESIAM: Math. Model. Numer. Anal. (M2AN), 55, 763, 2021

37. L. Lin and Y. Tong, Low-rank representation of tensor network operators with long-range pairwise interactions, SIAM J. Sci. Comput. 43, A164, 2021

38. Y. Dong, X. Meng, K. B. Whaley, L. Lin, Efficient phase factor evaluation in quantum signal processing, Phys. Rev. A 103, 042419, 2021

39. D. Lu, H. Wang, M. Chen, J. Liu, L. Lin, R. Car, W. E, W. Jia, L. Zhang, 86 PFLOPS Deep Potential Molecular Dynamics simulation of 100 million atoms with ab initio accuracy, Comput. Phys. Commun. 259, 107624, 2021

40. L. Lin and Y. Tong, Optimal quantum eigenstate filtering with application to solving quantum linear systems, Quantum 4, 361, 2020

41. Y. Khoo, L. Lin, M. Lindsey, L. Ying, Semidefinite relaxation of multi-marginal optimal transport for strictly correlated electrons in second quantization, SIAM J. Sci. Comput. 42, B1462, 2020

42. W. Jia, H. Wang, M. Chen, D. Lu, J. Liu, L. Lin, R. Car, W. E, L. Zhang, Pushing the limit of molecular dynamics with ab initio accuracy to 100 million atoms with machine learning, SC'20 Proceedings of the International Conference for High Performance Computing, Article No. 5 (ACM 2020 Gordon Bell Prize)

43. L. Lin and Y. Tong, Optimal quantum eigenstate filtering with application to solving quantum linear systems, Quantum 4, 361, 2020

44. L. Lin and M. Lindsey, Sparsity pattern of the self-energy for classical and quantum impurity problems, Ann. Henri Poincare 21, 2219–2257, 2020

45. S. Tan, I. Leven, D. An, L. Lin and T. Head-Gordon, Stochastic constrained extended system dynamics for solving charge equilibration models, J. Chem. Theory Comput. 16, 5991, 2020

46. K. J. Sung, J. Yao, M. P. Harrigan, N. C. Rubin, Z. Jiang, L. Lin, R. Babbush, J. R. McClean, Using models to improve optimizers for variational quantum algorithms, Quantum Sci. Tech. 5, 044008, 2020

47. X. Wu, M. Lindsey, T. Zhou, Y. Tong and L. Lin, Enhancing robustness and efficiency of density matrix embedding theory via semidefinite programming and local correlation potential fitting, Phys. Rev. B, 102, 085123, 2020 (Editor's Suggestion)

48. J. R. McClean, F. M. Faulstich, Q. Zhu, B. O'Gorman, Y. Qiu, S. R. White, R. Babbush, L. Lin, Discontinuous Galerkin discretization for quantum simulation of chemistry, New J. Phys. 22, 093015, 2020

49. L. Muechler, W. Hu, L. Lin, C. Yang, R. Car, Influence of point defects on the electronic and topological properties of monolayer WTe2, Phys. Rev. B, 102, 041103 (Rapid communication)

50. J. Zhang, L. Zepeda-Nunez, Y. Yao and L. Lin, Learning the mapping $\mathbf{x} \mapsto \sum_{i=1}^{d} x_i^2$: the cost of finding the needle in a haystack, Commun. Appl. Math. Comput. 2020

51. V. Wen-zhe Yu, et al, ELSI–An Open Infrastructure for Electronic Structure Solvers, Comput. Phys. Commun. 256, 107459, 2020

52. F. Henneke, L. Lin, C. Vorwerk, C. Draxl, R. Klein, C. Yang, Fast optical absorption spectra calculations for periodic solid state systems, Comm. Appl. Math. Comput. Sci. 15, 89, 2020

53. D. An and L. Lin, Quantum dynamics with the parallel transport gauge, SIAM Multiscale Model. Simul. 18, 612, 2020

54. A. Garcia, et al, The SIESTA method: recent developments and applications, J. Chem. Phys. 152, 204108, 2020

55. J. Yao, M. Bukov, L. Lin, Policy Gradient based Quantum Approximate Optimization Algorithm, Math. Sci. Mach. Learn. (MSML) 2020

56. Y. Dong, X. Meng, L. Lin, R. Kosut, K. B. Whaley, Robust control optimization for quantum approximate optimization algorithm, 21st IFAC, Berlin 2020

57. C. T. Kelley, J. Bernholc, E. Briggs, S. Hamilton, L. Lin, and C. Yang, Mesh independence of the generalized Davidson algorithm, J. Comput. Phys. 409, 109322, 2020

58. C. Mejuto-Zaera, L. Zepeda-Nunez, M. Lindsey, N. Tubman, K. B. Whaley, L. Lin, Efficient hybridization fitting for dynamical mean-field theory via semi-definite relaxation, Phys. Rev. B, 101, 035143, 2020

59. J. Lee, L. Lin, and M. Head-Gordon, Systematically improvable tensor hypercontraction: interpolative separable density-fitting for molecules applied to exact exchange, second- and third-order Moller-Plesset perturbation theory, J. Chem. Theory Comput. 16, 243, 2020

60. L. Lin and L. Zepeda-Nunez, Projection based embedding theory for solving Kohn-Sham density functional theory, SIAM Multiscale Model. Simul. 17, 1274, 2019

61. W. Jia, L.-W. Wang and L. Lin, Parallel transport time-dependent density functional theory calculations with hybrid functional on Summit, SC '19 Proceedings of the International Conference for High Performance Computing, Article No. 79 2019

62. Y. Fan, L. Lin, L. Ying and L. Zepeda-Nunez, A multiscale neural network based on hierarchical matrices, SIAM Multiscale Model. Simul. 17, 1189, 2019

63. X. Wu, Z.-H. Cui, Y. Tong, M. Lindsey, G. K.-L. Chan and L. Lin, Projected density matrix embedding theory with applications to the two-dimensional Hubbard model, J. Chem. Phys. 151, 064108, 2019

64. X. Yang, X. Wan, L. Lin and H. Lei, A general framework of enhancing sparsity of generalized polynomial chaos expansions, Int. J Uncertain. Quan. 9, 221, 2019

65. J. Hu, B. Jiang, L. Lin, Z. Wen and Y. Yuan, Structured quasi-Newton methods for optimization with orthogonality constraints, SIAM J. Sci. Comput. 41, 2239, 2019

66. L. Lin, J. Lu and L. Ying, Numerical methods for Kohn-Sham density functional theory, Acta Numer. 2019

67. W. Jia and L. Lin, Fast real-time time-dependent hybrid functional calculations with the parallel transport gauge and the adaptively compressed exchange formulation, Comput. Phys. Commun. 240, 21, 2019

68. L. Lin, Numerical methods for Hartree-Fock-like equations (in Chinese), Math. Numer. Sinica, 41, 113, 2019

69. W. Hu, Y. Huang, X. Qin, L. Lin, E. Kan, X. Li, C. Yang, J. Yang, Room-temperature magnetism and tunable energy gaps in edge-passivated zigzag graphene quantum dots, npj 2D Mater. Appl. 3, 17, 2019

70. Y. Fan, J. Feliu-Faba, L. Lin, L. Ying and L. Zepeda-Nunez, A multiscale neural network based on hierarchical nested bases, Res. Math. Sci. 6, 21, 2019

71. L. Lin and M. Lindsey, Convergence of adaptive compression methods for Hartree-Fock-like equations, Commun. Pure Appl. Math. 72, 451, 2019

72. Y. Li and L. Lin, Globally constructed adaptive local basis set for spectral projectors of second order differential operators, SIAM Multiscale Model. Simul., 17, 92, 2019

73. A. Damle, A. Levitt and L. Lin, Variational formulation for Wannier functions with entangled band structure, SIAM Multiscale Model. Simul., 17, 167, 2019

74. W. Jia, D. An, L.-W. Wang and L. Lin, Fast real-time time-dependent density functional theory calculations with the parallel transport gauge, J. Chem. Theory Comput. 14, 5645, 2018

75. A. Damle and L. Lin, Disentanglement via entanglement: A unified method for Wannier localization, SIAM Multiscale Model. Simul., 16, 1392, 2018

76. W. Hu, M. Shao, A. Cepelloti, F. H. Jornada, L. Lin, K. Thicke, C. Yang and S. Louie, Accelerating Optical Absorption Spectra and Exciton Energy Computation for Nanosystems via Interpolative Separable Density Fitting, ICCS, 604, 2018

77. A. S. Banerjee, L. Lin, P. Suryanarayana, C. Yang, J. E. Pask, Two-level Chebyshev filter based complementary subspace method for pushing the envelope of large-scale electronic structure calculations, J. Chem. Theory Comput. 14, 2930, 2018

78. X. Li, L. Lin, J. Lu, PEXSI-Σ: A Green's function embedding method for Kohn-Sham density functional theory, Ann. Math. Sci. Appl. 3, 411, 2018

79. L. Lin and M. Lindsey, Variational structure of Luttinger-Ward formalism and bold diagrammatic expansion for Euclidean lattice field theory, Proc. Natl. Acad. Sci. 115, 2282, 2018

80. M. Shao, F. da Jornada, L. Lin, C. Yang, J. Deslippe and S. G. Louie, A structure preserving Lanczos algorithm for computing the optical absorption spectrum, SIAM J. Matrix Anal. 39, 683, 2018

81. K. Dong, W. Hu and L. Lin, Interpolative separable density fitting through centroidal Voronoi tessellation with applications to hybrid functional electronic structure calculations, J. Chem. Theory Comput. 14, 1311, 2018

82. M. Jacquelin, L. Lin and C. Yang, PSelInv – A distributed memory parallel algorithm for selected inversion: the non-symmetric case, Parallel Comput. 74, 84, 2018

83. M. Jacquelin, L. Lin, W. Jia, Y. Zhao and C. Yang, A left-looking selected inversion algorithm and task parallelism on shared memory systems, HPC Asia, 54, 2018

84. V. Wen-zhe Yu, F. Corsetti, A. Garcia, W. Huhn, M. Jacquelin, W. Jia, B. Lange, L. Lin, J. Lu, W. Mi, A. Seifitokaldani, A. Vazquez-Mayagoitia, C. Yang, H. Yang and V. Blum, ELSI: A Unified Software Interface for Kohn-Sham Electronic Structure Solvers, Comput. Phys. Commun. 222, 267, 2018

85. W. Hu, L. Lin, R. Zhang, C. Yang and J. Yang, Highly efficient photocatalytic water splitting over edge-modified phosphorene nanoribbons, J. Amer. Chem. Soc. 139, 15429, 2017

86. W. Hu, L. Lin and C. Yang, Interpolative separable density fitting decomposition for accelerating hybrid density functional calculations with applications to defects in silicon, J. Chem. Theory Comput. 13, 5420, 2017

87. W. Hu, L. Lin and C. Yang, Projected Commutator DIIS Method for Accelerating Hybrid Functional Electronic Structure Calculations, J. Chem. Theory Comput. 13, 5458, 2017

88. W. Jia and L. Lin, Robust Determination of the Chemical Potential in the Pole Expansion and Selected Inversion Method for Solving Kohn-Sham density functional theory, J. Chem. Phys. 147, 144107, 2017

89. A. Damle, L. Lin and L. Ying, Accelerating selected columns of the density matrix computations via approximate column selection, SIAM J. Sci. Comput. 39, 1178, 2017

90. L. Lin and B. Stamm, A posteriori error estimates for discontinuous Galerkin methods using non-polynomial basis functions. Part II: Eigenvalue problems, Math. Model. Numer. Anal. (M2AN), 51, 1733, 2017

91. L. Lin, Randomized estimation of spectral densities of large matrices made accurate, Numer. Math. 136, 183, 2017

92. L. Lin, Localized spectrum slicing, Math. Comp. 86, 2345, 2017

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101. L. Lin, Y. Saad and C. Yang, Approximating spectral densities of large matrices, SIAM Rev. 58, 34, 2016

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111. W. Hu, L. Lin and C. Yang, Edge reconstruction in armchair phosphorene nanoribbons revealed by discontinuous Galerkin density functional theory, Phys. Chem. Chem. Phys. 17, 31397, 2015

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115. W. Hu, L. Lin, C. Yang and J. Yang, Electronic structure of large-scale graphene nanoflakes, J. Chem. Phys. 141, 214704, 2014

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117. H. M. Aktulga, L. Lin, C. Haine, E. Ng and C. Yang, Parallel eigenvalue calculation based on multiple shift-invert Lanczos and contour integral based spectral projection method, Parallel Comput. 40, 195, 2014

118. L. Lin, J. Lu and S. Shao, Analysis of the time reversible Born-Oppenheimer molecular dynamics, Entropy 16, 110-137 (Special issue on Molecular Dynamics), 2014

119. L. Lin and C. Yang, Elliptic preconditioner for accelerating the self consistent field iteration in Kohn-Sham density functional theory, SIAM J. Sci. Comput. 35, S277-S298 (Copper Mountain special issue), 2013

120. L. Lin, M. Chen, C. Yang and L. He, Accelerating atomic orbital-based electronic structure calculation via pole expansion and elected inversion, J. Phys. Condens. Matter 25, 295501, 2013

121. L. Lin, S. Shao and W. E, Efficient iterative method for solving the Dirac-Kohn-Sham density functional theory, J. Comput. Phys 245, 205, 2013

122. C. Mendl and L. Lin, Kantorovich dual solution for strictly correlated electrons in atoms and molecules, Phys. Rev. B 87, 125106, 2013

123. L. Lin, L. Ying, Element orbitals for Kohn-Sham density functional theory, Phys. Rev. B 85, 235144, 2012

124. L. Lin, J. Lu, L. Ying and W. E, Optimized local basis function for Kohn-Sham density functional theory, J. Comput. Phys 231, 4515, 2012

125. D. Flammini, A. Pietropaolo, R. Senesi, C. Andreani, F. McBride, A. Hodgson, M. Adams, L. Lin, and R. Car, Spherical momentum distribution of the protons in hexagonal ice from modeling of inelastic neutron scattering data, J. Chem. Phys. 136, 024504, 2012

126. L. Lin, J. Lu, L. Ying and W. E, Adaptive local basis set for Kohn-Sham density functional theory in a discontinuous Galerkin framework I: Total energy calculation, J. Comput. Phys. 231, 2140, 2012

127. L. Lin, J.A. Morrone and R. Car Correlated tunneling in hydrogen bonds, J. Stat. Phys. 145, 365, 2011

128. L. Lin, J.A. Morrone, R. Car and M. Parrinello, Momentum distribution, vibrational dynamics and the potential of the mean force in ice, Phys. Rev. B 83, 220302(R), 2011.

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131. L. Lin, J. Lu and L. Ying, Fast construction of hierarchical matrix representation from matrix-vector multiplication, J. Comput. Physics, 230, 4071, 2011

132. L. Lin, J.A. Morrone, R. Car and M. Parrinello, Displaced path integral formulation for the momentum distribution of quantum particles, Phys. Rev. Lett. 105, 110602, 2010

133. L. Lin, J. Lu, L. Ying and W. E, Pole-based approximation of the Fermi-Dirac function, Chin. Ann. Math. 30B, 729, 2009

134. 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, 755, 2009

135. J.A. Morrone, L. Lin and R. Car, Tunneling and delocalization effects in hydrogen bonded systems: A study in position and momentum space, J. Chem. Phys. 130, 204511, 2009

136. L. Lin, J. Lu, R. Car and W. E, Multipole representation of the Fermi operator with application to the electronic structure analysis of metallic systems, Phys. Rev. B 79, 115133, 2009

Conference Presentations

1. Modern Applied and Computational Analysis, ICERM, June 2023
2. New Mathematics for the Exascale: Applications to Materials Science, IPAM, March, 2023
3. APS March Meeting, Las Vegas, March, 2023

4. Sanibel Conference on Theoretical Chemistry, St Augustine, February, 2023
5. Joint Mathematics Meeting, Minisymposium on Prospects of eigenvalue problems, Boston, January, 2023
6. CCQ 5th year anniversary conference, New York, December, 2022
7. SIAM SIAM Conference on Mathematics of Data Science (MDS22), Minisymposium on Algorithms of Deep Learning for PDEs in Scientific Computing (virtual), San Diego, September, 2022
8. Conference on Computational Physics (virtual), UT Austin, August, 2022
9. Computational Mathematics for Quantum Technologies (virtual), Bath, August, 2022
10. Workshop on Moire systems, IPAM, May 2022
11. Wannier Summer School (virtual), Trieste, May 2022
12. Workshop on Large-Scale Certified Numerical Methods in Quantum Mechanics, IPAM, May 2022
13. Workshop on Multiscale Approaches in Quantum Mechanics, IPAM, March 2022
14. MolSSI HPC Workshop (virtual), December, 2021
15. Quantum Wave in Computing Reunion (virtual), Simons Institute, July 2021
16. Telluride Workshop on New Frontiers in Electron Correlation (virtual), June 2021
17. Minisymposium on Quantum Numerical Linear Algebra, SIAM Conference on Applied Linear Algebra (SIAM LA21, virtual) May, 2021
18. Useful Quantum Computation For Quantum Chemistry (virtual), February 2021
19. Workshop on Mathematical and Computational Materials Science (virtual), University of Chicago, February 2021
20. Plenary talk, New York Scientific Data Summit (virtual), October 2020
21. Society of Engineering Science (SES) 2020 (virtual), October 2020
22. Google Quantum Symposium, July 2020
23. The Third Conference on Scientific and Engineering Computing for Young Chinese Mathematicians, Beijing, August 2019
24. Diagrammatic Monte Carlo workshop, Flatiron Institute, July 2019
25. Mathematical and Numerical Analysis of Electronic Structure Models, Suzhou, June 2019
26. Workshop on Machine Learning Techniques in Scientific Computing, Wuhan, June 2019
27. Workshop on Scientific Computing Across Scales: Quantum Systems in Cold-matter Physics and Chemistry, Fields Institute, April, 2019
28. Minisymposium on Recent Advances in Modeling and Numerical Analysis for Electronic Structure Calculations, SIAM Conference on Computational Science and Engineering (CSE19), Spokane, February, 2019
29. Workshop on Optimal Transport Methods in Density Functional Theory, Banff, January 2019
30. Minisymposium on Recent Advances in DFT and TDDFT: Theory and Simulations, ACS National Meeting, Boston, August 2018
31. Workshop and Summer School Parallel Computing in Molecular Sciences, Berkeley, August 2018
32. Solid Math 2018, Montreal, August 2018
33. Minisymposium on Electronic Structure of Materials, SIAM Conference on Mathematical Aspects of Materials Science (SIAM MS18), Portland, July 2018

34. Minisymposium on Numerical Methods for Ground and Excited State Electronic Structure Calculations, SIAM Conference on Applied Linear Algebra (SIAM LA18), Hong Kong, May 2018
35. MaX Conference on the Materials Design Ecosystem at the Exascale: High-Performance and High-Throughput Computing, Trieste, January 2018
36. Minisymposium on Numerical Linear Algebra, Joint Mathematics Meeting, San Diego, January 2018
37. Minisymposium on Extending Accuracy & Scales with Emerging Computing Architectures & Algorithms, ACS National Meeting, Washington DC, August 2017
38. Workshop on Density-Functional Theory and Beyond: Accuracy, Efficiency, and Reproducibility in Computational Materials Science, Berlin, August, 2017
39. Workshop on Density Functional Theory and Beyond, Warwick, July 2017
40. Workshop on Electronic Structure Theory (ES17), Princeton, June 2017
41. Workshop on New Frontiers in Electron Correlation, Telluride, June 2017
42. Minisymposium on Optimization and Quantum Chemistry, SIAM Conference on Optimization, Vancouver, May 2017
43. Workshop on Emerging Topics in Optics, IMA, Minneapolis, April 2017
44. Computational Physics at the Petascale and Beyond (invited talk), APS March Meeting, New Orleans, March, 2017
45. Minisymposium on electronic structure theory for excited states, SIAM Conference on Computational Science and Engineering, Atlanta, February, 2017
46. IPAM: Collective Variables in Quantum Mechanics, Los Angeles, November 2016
47. Mean-field modeling and multiscale methods for complex physical and biological systems, Santa Barbara, October 2016
48. EMN Meeting on Computation and Theory, Las Vegas, October 2016
49. USACM "Recent Advances in Computational Methods for Nanoscale Phenomena", Ann Arbor, August 2016
50. International Conference on Algorithms and Applications for Excited State Electronic Structure Theories, CSRC, Beijing, August 2016
51. Mathematical and Numerical Analysis of Electronic Structure Models, Roscoff, July 2016
52. Workshop on Optimization and Eigenvalue Computation, BICMR, Beijing, June 2016
53. 2nd Computational and Theoretical Chemistry Research PI Meeting, Washington D.C., May 2016
54. Workshop on Mathematical and Computational Methods in Quantum Chemistry, Yale, May 2016
55. SIAM Conference on Mathematical Aspects of Materials Science (SIAM MS16), Philadelphia, May 2016
56. Workshop on Workshop on Computational Quantum Systems, Shanghai, December 2015
57. Minisymposium on New Numerical Linear Algebra Methods Meet New Challenges of Physics, SIAM Applied Linear Algebra Meeting (SIAM LA15), Atlanta, October, 2015
58. Upscaling Electronic Structure: Reduced-Scaling and Multi-Scale Methods (invited talk), Psi-k 2015, San Sebastian, September 2015
59. Minisymposium on Electronic structure theory for large scale systems, 250th ACS National Meeting, Boston, August 2015
60. Minisymposium on Mathematics and Algorithms in Quantum Chemistry; Computational Methods of PDE-based Eigenvalue Problems and Applications in Nanostructure Simulations, ICIAM 2015, Beijing, August 2015

61. Workshop on Multiscale Modeling and Analysis in Materials Science, Shanghai, August 2015
62. Minisymposium on Recent Progress in Multi-scale Modeling at the Intersection of Ab-initio Methods, Mechanics and Mathematics, 13th U.S. National Congress on Computational Mechanics (USNCCM13), July 2015
63. Minisymposium on Recent developments of mathematical aspects of computational chemistry, 26th Biennial Numerical Analysis Conference, Glasgow, June 2015
64. Workshop on Dimension Reduction: Mathematical Methods and Applications, Penn State University, March 2015
65. Workshop on Numerical Methods for Quantum Chemistry, Tromso, 2015
66. Workshop on Fundamental Aspects of DFT, Oslo, 2015
67. Workshop on New and Future Directions in Atomistic Simulation and Modeling, Seattle, 2014
68. Minisymposium on Mathematical Theory and Computational Techniques for Multiscale Materials Modeling, 7th International Conference on Multiscale Materials Modeling, Berkeley, 2014
69. Workshop on Mathematical and Numerical Analysis of Electronic Structure Models, Berlin, April 2014
70. Workshop on Mathematical and Numerical Methods for Complex Quantum Systems, Chicago, March 2014
71. Session on High Performance Computing in Density Functional Theory, APS March Meeting, Portland, March 2014
72. Minisymposium on Density Functional Theory: Large-scale Algorithms and O(N) Methods, SIAM Conference on Parallel Processing for Scientific Computing (SIAM PP14), Portland, February 2014
73. Workshop on Numerical Solution of PDE Eigenvalue Problems, Oberwolfach, November 2013
74. Minisymposium on Electronic structure, and minisymposium on Computational methods for nano scale materials and devices, SIAM Conference on Mathematical Aspects of Materials Science (SIAM MS13), Philadelphia, June 2013
75. Workshop on quantum systems: a mathematical journey from few to many particles, University of Maryland, College Park, May 2013
76. Session on Recent developments in density functional theory, APS March Meeting, Baltimore, March 2013
77. Minisymposium on Recent advances in preconditioning techniques, SIAM Conference on Computational Science and Engineering, Boston, February, 2013
78. Bay Area Scientific Computing Day, SLAC, December, 2012
79. 2012 Young Researchers Workshop: Kinetic Description of Multiscale Phenomena, University of Wisconsin-Madison, October, 2012
80. Materials defects: Mathematics, Computation, and Engineering Workshop I: Quantum and Atomistic Modeling of Materials Defects, IPAM, October 2012
81. Minisymposium on Structured matrices and scientific computing, SIAM Conference on Applied Linear Algebra (SIAM LA12), Valencia, June 2012
82. Workshop on Mathematical and Numerical Analysis of Electronic Structure Models, Beijing, June 2012
83. Workshop on Computational Problems in Material Sciences, Beijing, June 2012
84. Session on Nonlinear solution methods, 12th Copper Mountain Conference on Iterative Methods, Copper, March 2012
85. Session on Electronic structure: calculations, APS March Meeting, Boston, March 2012
86. Workshop on Structure & Dynamics of Water & Aqueous Solutions, Seattle, February 2012

87. Minisymposium on Large-scale parallel first principles calculation for quantum many-particle systems, SIAM Conference on Parallel Processing for Scientific Computing (SIAM PP12), Savannah, February 2012
88. Workshop on Structure & Dynamics of Water & Aqueous Solutions, Seattle, February 2012
89. Thematic Minisymposia: Quantum modeling in molecular simulation, International Council for Industrial and Applied Mathematics (ICIAM 2011), Vancouver, July 2011
90. Workshop on Mathematical Methods in Quantum Chemistry, Oberwolfach, June 2011
91. Session on Numerical PDE, International Conference on Interdisciplinary Applied Mathematics and Computational Mathematics (ICIACM 2011), Hangzhou, June 2011
92. Workshop on Electronic Structure Analysis and Computation, Shanghai, June 2011
93. Session on Condensed phase dynamics and structure, APS March Meeting, Dallas, March 2011
94. Workshop on Density Functional Theory: Fundamentals and Applications in Condensed Matter Physics, Banff, January 2011
95. Workshop on Structure & Dynamics of Water & Aqueous Solutions,Princeton, December 2010
96. Workshop on High Energy Neutrons for Science and Society, Rome, October 2010
97. Minisymposium on Electronic structure, SIAM Conference on Mathematical Aspects of Materials Science (SIAM MS10), Philadelphia, May 2010
98. Minisymposium on Large-scale parallel computing for scientific modeling and simulation, SIAM Conference on Parallel Processing for Scientific Computing (SIAM PP10), Seattle, February 2010
99. Session on Theoretical chemistry, APS March Meeting, Portland, March 2010

Seminar Talks

1. Ordway distinguished lecture, University of Minnesota, April, 2023
2. Math Colloquium, UC Berkeley, March, 2023
3. Math Colloquium, Stanford University, February 2023
4. Applied Math Colloquium, Columbia University, February, 2023
5. PACM Colloquium, Princeton University, February, February, 2023
6. Munich-Berkeley Winter school on quantum information, LBNL, January, 2023
7. Courant Institute, December, 2022
8. Alvarez seminar (virtual), LBNL, September, 2022
9. Psi Quantum seminar (virtual), July, 2022
10. Quantum seminar (virtual), National University of Singapore, July, 2022
11. IBM Quantum seminar (virtual), July, 2022
12. Mathematics Colloquium (virtual), University of South Carolina, February, 2022
13. CAMS Colloquium (virtual), University of Southern California, October 2021
14. Applied Math Seminar (virtual), UC Santa Cruz, May 2021
15. Oden Institute Seminar (virtual), UT Austin, May 2021
16. Distinguished Lecture Series of Computational Science (virtual), ETH Zurich, March 2021

17. Data science seminar, Purdue University (virtual), March 2021
18. School of Mathematical Sciences Colloquium (virtual), Peking University, March 2021
19. Widely Applied Math (WAM) Seminar (virtual), Harvard, March 2021
20. NEXUS Seminar (virtual), UC Irvine, February, 2021
21. MIT Computational Science and Engineering Distinguished Seminar Series (virtual), October 2020 Google Theory seminar (virtual), September 2020
22. Quantum seminar (virtual), Simons Institute, May 2020
23. INS Colloquium (virtual), Shanghai Jiaotong University, April, 2020
24. Applied and Computational Mathematics Seminar, UW Madison, December 2019
25. Computational and Applied Mathematics Colloquium, Cornell University, April 2019
26. Flatiron Seminar, Flatiron Institute, April 2019
27. Department of Scientific Computing Colloquium, Florida State University, April 2019
28. Department of Statistics Seminar, University of Chicago, April 2019
29. Applied Mathematics Seminar, Department of Mathematics, UC Berkeley, February, 2019
30. Applied Mathematics Seminar, Courant Institute, February, 2019
31. PACM Colloquium, Princeton University, February 2019
32. Computational and Applied Mathematics Colloquium, University of Chicago, November 2018
33. Applied Mathematics Seminar, Peking University, June 2018
34. Applied Mathematics Seminar, Department of Mathematics, Hong Kong University of Science and Technology, May 2018
35. Applied Mathematics Seminar, Department of Mathematics, City University of Hong Kong, May 2018
36. Applied Mathematics Seminar, Department of Mathematics, Southern Methodist University, April 2018
37. Theoretical Physics Seminar, Los Alamos National Laboratory, April 2018
38. Theoretical Chemistry Seminar, Department of Chemistry, UC Berkeley, February 2018
39. Applied Mathematics Seminar, Department of Mathematics, UC Irvine, April 2017
40. Applied Mathematics Seminar, Department of Mathematics, UC Berkeley, September, 2016
41. Center for Computational and Applied Mathematics seminar, Purdue University, December 2015
42. School of Mathematical Sciences, Peking University, Beijing, July 2015
43. Algorithms Division, Beijing Computational Science Research Center, Beijing, July 2015
44. Computer Network Information Center, Chinese Academy of Sciences, Beijing, July 2015
45. Software Center for High Performance Numerical Simulation, Chinese Academy of Engineering Physics, Beijing, July 2015
46. PACM Colloquium, Princeton, April, 2015
47. Math/CS Seminar, Emory University, April, 2015
48. Condensed matter theory seminar, UC Berkeley, December, 2014
49. Scientific Computing and Matrix Computations Seminar, UC Berkeley, October, 2014

50. Colloquium, Applied Physics and Applied Mathematics, Columbia University, March 2014
51. Colloquium, Department of Computational and Applied Mathematics (CAAM), Rice University, February, 2014
52. CSCAMM Seminar, University of Maryland at College Park, February, 2014
53. Colloquium, Department of Mathematics, University of Toronto, February, 2014
54. Colloquium, Department of Mathematics, University of Southern California, January, 2014
55. Department of Mathematics, UC Berkeley, January, 2014
56. Colloquium, Department of Mathematics, UNC Chapel Hill, January, 2014
57. Department of Mathematics, Stanford University, January, 2014
58. PDE-Numerical Analysis Seminar, Department of Mathematics, University of Maryland at College Park, December, 2013
59. Applied Mathematics Seminar, Department of Mathematics, UC Santa Barbara, December, 2013
60. Department of Mathematics, National University of Singapore, December, 2013
61. Colloquium, Department of Mathematics, University of Wisconsin at Madison, November, 2013
62. Computational Math Seminar, University of Colorado at Bolder, November, 2013
63. Institute of Mathematics Seminar, Peking University, July 2013
64. Laboratoire Jacques-Louis Lions Seminar, UPMC, June 2013
65. Applied Mathematics Seminar, UC Irvine, April 2013
66. Applied Mathematics Seminar, Stanford University, April 2013
67. Seminar in Quantum Simulations Group, Lawrence Livermore National Laboratory, March 2013
68. Applied Mathematics and Analysis Seminar, Duke University, February, 2013
69. Scientific and Statistical Computing Seminar, University of Chicago, January, 2013
70. NWChem Seminar, Pacific Northwest National Laboratory, October 2012
71. Computer Science Summer Student Program Talk, Lawrence Berkeley National Laboratory, July 2012
72. The State Key Laboratory of Scientific and Engineering Computing (LSEC), Chinese Academy of Sciences, July 2012
73. School of Mathematics and Statistics, Wuhan University, July 2012
74. Statistical Mechanics Seminar, UC Berkeley, March 2012
75. Linear Scaling Theory Seminar, Lawrence Livermore National Lab, March, 2012
76. Scientific Computing and Matrix Computations Seminar, UC Berkeley, March, 2012
77. Applied Mathematics Seminar, Courant Institute, February, 2012
78. Computational Statistical Mechanics Seminar, Courant Institute, February, 2012
79. Applied Mathematics Seminar, UC Berkeley, February, 2012
80. Numerical Analysis Seminar, University of Texas at Austin, October 2011
81. Scientific Computing and Matrix Computations Seminar, UC Berkeley, September, 2011
82. Special PACM Colloquium, Princeton University, March 2011

83. Special Imaging and Computing Seminar, MIT, January 2011
84. Special PACM Colloquium, Princeton University, March 2010
85. Numerical Analysis Seminar, University of Texas at Austin, February 2010
86. Numerical Analysis Seminar, University of Texas at Austin, May 2009