

Xiantao Li

Curriculum vitae

Professor of Mathematics | The Pennsylvania State University

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Academic Appointments

2016–present — Professor of Mathematics, The Pennsylvania State University.

2010–2016 — Associate Professor of Mathematics, The Pennsylvania State University.

2005–2010 — Assistant Professor of Mathematics, The Pennsylvania State University.

2004–2005 — Postdoctoral Fellow, Institute for Mathematics and its Applications, University of Minnesota.

2002–2004 — Research Associate, Program in Applied and Computational Mathematics, Princeton University.

Education

2002 — PhD in Applied Mathematics, University of Wisconsin–Madison.

1998 — BS in Mathematics, Peking University, Beijing, China.

Honors and Awards

2007 — Alfred P. Sloan Research Fellowship in Mathematics.

Research Areas

Overall Research Focus

Numerical analysis and scientific computing; multiscale and reduced-order modeling; stochastic dynamics and data assimilation; machine learning; molecular and materials simulation, including electronic structure, quantum transport, and heat transport.

Current Research Directions

Differential equations and scientific computing. Numerical analysis and quantum algorithms for ODEs, PDEs, and SDEs; multilevel methods for observable estimation; fluid dynamics in collaboration with mechanical engineering researchers.

Nonunitary dynamics and quantum control. Dilation methods for nonunitary dynamics in physics; simulation and optimal control of open quantum systems, including non-Markovian dynamics.

Materials and molecular simulation. Quantum algorithms for density functional theory and electronic structure in materials science, and for molecular and protein dynamics.

Machine learning and optimization. Quantum algorithms for machine learning, sampling, and optimization.

Hardware implementation and error mitigation. Error mitigation, circuit implementation, and benchmarking, with access to IBM, IonQ, and Quantinuum platforms.

Research Leadership and Affiliations

Co-Director, Center for Computational Mathematics and Applications ([CCMA](#)), Penn State.

Member, Advisory Committee, ICDS [Quantum Hub](#), Penn State.

Faculty Member, Center for Theory of Emergent Quantum Matter ([C-TEQ](#)), Penn State (2025–present).

Affiliate, Institute for Computational and Data Sciences ([ICDS](#)), Penn State.

Additional affiliations: Center for Advanced Data Assimilation and Predictability Techniques, Penn State.

Research Support since 2015

Amounts below are total award amounts; co-PI awards are identified as team awards.

[2026–2029](#) | NSF 2552687 | Principal Investigator | \$300,000. From Quantum Dynamics to Intelligent Actions: A Framework for Quantum-Accelerated Simulation in Reinforcement Learning.

Awarded [2025](#) | ICDS Quantum SuperSEED | Co-Principal Investigator | \$199,440 total project award. Open Quantum Systems Beyond Markovianity: Building a Cross-Disciplinary Community for Quantum Simulation and Computing. PI: Zhen Bi.

[2024–2027](#) | NSF DMS-2411120 | Principal Investigator | \$300,000. Improving Quantum Speedup for Solving Differential Equations.

[2023–2027](#) | NSF CCF-2312456, FET Small | Co-Principal Investigator | \$600,000 total project award. An Integrated Framework for the Optimal Control of Open Quantum Systems: Theory, Quantum Algorithms, and Applications. PI: Chunhao Wang.

[2022–2023](#) | ICDS Seed Grant | Principal Investigator | \$30,000. Machine-Learning with Quantum Speedup.

[2021–2025](#) | NSF DMS-2111221 | Principal Investigator | \$395,391. Optimal Control of Open Quantum Systems.

[2020–2023](#) | NSF DMS-1953120 | Principal Investigator | \$120,000. Data-Driven Reduced-Order Modeling of Ab Initio Molecular Dynamics.

[2018–2021](#) | NSF DMS-1819011 | Principal Investigator | \$200,000. Stochastic Constitutive Models for Nano-Scale Heat Transport.

[2016–2019](#) | NSF DMS-1619661 | Co-Principal Investigator | \$300,867 total project award. Data-Driven Modeling of Equilibrium and Non-Equilibrium Statistics. PI: John Harlim.

[2015–2018](#) | NSF DMS-1522617 | Principal Investigator | \$215,000. Modeling Complex Properties of Material Interfaces: From Quantum and Atomic to Macroscopic Scales.

[2026](#) | IonQ | \$10,000 in-kind quantum-computing credits.

Teaching and Educational Contributions

Selected Courses and Working Seminars

Graduate courses: numerical analysis; numerical methods for ordinary differential equations; numerical methods for partial differential equations.

Special-topics courses in quantum computing and quantum algorithms, Department of Mathematics, Penn State.

Designed and piloted MATH 225, Mathematical Foundations for Machine Learning, for Penn State's artificial intelligence major (Spring 2026).

Deep Learning Algorithms and Analysis, undergraduate course, Penn State.

Organizer, working seminars on quantum computing and machine learning, Department of Mathematics, Penn State.

Tutorial Lectures and Public Education

Two invited tutorial lectures, “Basic Elements of Quantum Computing, and Their Applications in Solving PDE,” Workshop on Introduction to Classical Numerical Analysis, Fields Institute, Toronto (July 17, 2026).

Tutorial lectures on open quantum systems and their simulation, Quantum Computer Systems (QuCS) Lecture Series.

Invited lecture, “Open Quantum Systems in Quantum Computing,” Workshop on Quantum Algorithms for Scientific Computation, IPAM, UCLA (October 4, 2023).

Public lecture, “What Can Quantum Computing Do for Scientific Computing?”, Ashtekar Frontiers of Science, “Year of Quantum” series, Penn State (February 8, 2025).

Book Manuscripts and Open Educational Resources

Xiantao Li. [A Quantum Path to Partial Differential Equations](#). Book manuscript and lecture notes, 140 pp. (2026). arXiv:2607.09639. Companion website: quantumpde.org.

Xiantao Li. [Mathematical Pathways to Machine Learning: Calculus, Linear Algebra, and Optimization](#). Open textbook manuscript, version 1.0 (August 2026). DOI: 10.5281/zenodo.21752763.

Advising and Mentoring

Mentor to junior faculty members, Department of Mathematics, Penn State.

Postdoctoral Researchers

Current: Sanjeeb Poudel, Postdoctoral Scholar, Penn State (2026–present).

Former: Lina Ma (2014–2017), co-mentored with Chun Liu; Minxin Chen.

Doctoral and Masters Students

Current doctoral students: Hsuan-Cheng Wu; Pegah Mohammadipour; Menghan Wang; Ruizhe (Ray) Qian.

Completed PhDs: Ke Wang (2025); Taehee Ko (2023); Yushuang Luo (2022); He Zhang (2020); Weiqi Chu (2019); Adam Telatovich (2018); Xiaojie Wu (2018); Chao Liang (2014).

Completed MS: Qing Ruan (2009).

Member, PhD student committees in chemistry, physics, aerospace engineering, computer science, electrical and computer engineering, and mathematics, Penn State.

University and Professional Service

University and Departmental Committees

Member, initial committee for development of Penn State’s artificial intelligence major.

Member, faculty hiring committees, Department of Mathematics, Penn State (multiple years).

Member, Graduate Studies Committee, Department of Mathematics, Penn State.

Member, Promotion and Tenure Committee, Eberly College of Science, Penn State.

Member, departmental Promotion and Tenure Committees, Department of Mathematics, Penn State.

Conference Organization and Panels

Minisymposium organizer, SIAM Conference on Computational Science and Engineering (CSE 2027).

Scientific Committee member, SIAM New York–New Jersey–Pennsylvania Section Annual Conference, Rutgers University (October 23–25, 2026).

Co-organizer, Quantum Scientific Computing Workshop, Penn State (October 15, 2026).

Panelist, “Quantum Computing and Life Sciences,” and session chair, Quantum Machine Learning and Life Sciences Workshop, Penn State (May 27, 2026).

Panelist, quantum computing session, ICDS Symposium, Penn State.

Organizer, Symposium on Computational Mathematics for Engineering and Sciences, Penn State (2024).

Co-organizer with Chun Liu, SIAM-sponsored Workshop on Dimension Reduction, Penn State (March 22–25, 2015).

Minisymposium organizer, SIAM Conference on Mathematical Aspects of Materials Science (June 2014).

Minisymposium organizer, Multiscale Materials Modeling conference (2014).

Peer Review

Referee for Quantum; Physical Review Letters; PRX Quantum; Communications in Mathematical Physics; Nature Communications; Journal of Computational Physics; Communications in Mathematical Sciences; Applied Numerical Mathematics; Multiscale Modeling and Simulation; Numerische Mathematik; Communications in Computational Physics; Journal of Scientific Computing; and other journals.

Selected Invited Lectures and Presentations

Invited plenary, “A Quantum Perspective on Nonlinear Stochastic Dynamics,” SIAM New York–New Jersey–Pennsylvania Section Annual Conference, Rutgers University (October 25, 2026; scheduled).

Invited lecture, “End-to-End Quantum PDE Algorithms for Direct Observable Estimation,” Quantum Scientific Computing Workshop, Penn State (October 15, 2026).

Keynote lecture, “From Nonlinear Stochastic Differential Equations to Quantum Channels: The Kolmogorov–Lindblad Mapping,” Symposium on Recent Advances on Quantum Algorithms for Differential Equations: Theory and Applications, Institute for Quantum Computing, University of Waterloo / Fields Institute thematic program (August 28, 2026; online).

Keynote lecture, “Making Classical Problems Quantum,” ICDS Symposium quantum program, Penn State (2025).

Earlier Invited Presentations

Virginia tech 2026

University of Maryland 2026

Indiana University 2025

University of South Carolina, November 2024.

“Quantum Simulation Algorithms for Lindblad Dynamics,” Simons Institute, UC Berkeley, October 22, 2024.

SIAM Material Conference, March 2024.

University of California, Berkeley, March 2023.

IPAM, UCLA, March 2023.

Numerical Analysis of Galerkin ROMs (NA G-ROMs) Seminar series, October 2023.

SIAM Annual Meeting, 2022.

Crunch Seminar, Brown University, September 2022.

Computational Mathematics for Quantum Technologies, July 2022.

SIAM Conference on Applications of Dynamical Systems, May 2021.

SIAM meeting on Mathematical Aspects of Material Sciences, May 2021.

INS Colloquia, Shanghai Jiaotong University, September 2020.

Applied Math Seminar, Purdue University, February 2020.

ICIAM The International Congress on Industrial and Applied Mathematics, Valencia, July 2019.

Department Seminar, University of California at Santa Cruz, June 2019.

Workshop on dimension reduction in data and physical sciences, Duke, 2019.

The 13th World Congress in Computational Mechanics, July 2018.

SIAM Annual Meeting 2018, July 2018.

14th National Congress on Computational Mechanics (USNCCM14), July 2017.

SIAM Conference on Applications of Dynamical Systems, May 2017.

SIAM Conference on computational science and engineering, February 2017.

Applied Math Seminar, Colorado State University, November 2017.

SIAM Conference on Mathematical Aspects of Materials Science (MS16), 2016.

Mathematical and Computational Methods in Quantum Chemistry, Yale University, 2016.

Pacific Northwest National Lab, June 2015.

Department of Mathematics, University of California, Berkeley, April 2015.

Department of Mathematics, Duke University, September 2014.

Division of Applied Math, Brown University, October 2014.

SIAM annual meeting, June 2014.

Department of Math, Hong Kong University of Science and Technology, June 2014.

Courant Institute, New York University, November 2013.

SIAM Conference on Mathematical Aspects of Materials Science, June 2013.

The 2nd Pacific Rim Mathematical Association Congress, June 2013.

Publications

Published and Accepted Papers

1. Zhen Huang, Zhiyan Ding, Ke Wang, Jason Kaye, Xiantao Li, and Lin Lin. Long-time exponential decompositions of non-Markovian Gaussian baths. *Physical Review Research* 8, 043053 (2026). DOI: 10.1103/7765-s8lk.
2. Hsuan-Cheng Wu and Xiantao Li. Universal Dilation of Linear Itô SDEs: Quantum Trajectories and Lindblad Simulation of Second Moments. *Quantum* 10, 2223 (2026). DOI: 10.22331/q-2026-10-01-2223.
3. Guneykan Ozgul, Xiantao Li, Mehrdad Mahdavi, and Chunhao Wang. Quantum Speedups for Sampling and Non-Convex Optimization with Stochastic Oracles. 21st Conference on the Theory of Quantum Computation, Communication and Cryptography (TQC 2026), LIPIcs 389, 8:1–8:25 (2026). DOI: 10.4230/LIPIcs.TQC.2026.8.
4. Xiantao Li. Auxiliary-field quantum Monte Carlo on quantum hardware via unitary dilation. *Physical Review A* 114, 022444 (2026). DOI: 10.1103/9k3q-gd64.
5. Xiantao Li. From Linear Differential Equations to Unitaries: A Moment-Matching Dilation Framework with Near-Optimal Quantum Algorithms. *PRX Quantum* 7, 020350 (2026). DOI: 10.1103/xm61-ytf7.
6. Pinchen Xie, Ke Wang, Anupam Mitra, Yuanran Zhu, Xiantao Li, Wibe Albert de Jong, and Chao Yang. Predicting Open Quantum Dynamics with Data-Informed Quantum-Classical Dynamics. *Physical Review Letters* 136, 010402 (2026). DOI: 10.1103/7lsx-ssjl.
7. Xiantao Li. A Residual-Based Quantum Linear System Algorithm with Dynamic Stopping and Applications to Elliptic PDEs. *ACM Transactions on Quantum Computing*, accepted (2026).
8. Yu Cao, Mingfeng He and Xiantao Li. Dynamically optimal unraveling schemes for simulating Lindblad equations. *Journal of Physics A: Mathematical and Theoretical* 59, 165301 (2026). DOI: 10.1088/1751-8121/ae5afd.
9. Pegah Mohammadipour and Xiantao Li. Reducing circuit depth in Lindblad simulations via step-size extrapolation. *Physical Review A* 112, 062206 (2025). DOI: 10.1103/dzpc-mlp4.
10. Ke Wang and Xiantao Li. Non-Markovian noise mitigation: Practical implementation, error analysis, and the role of spectral properties of the environment. *Physical Review A* 112, 012406 (2025). DOI: 10.1103/db4q-8ny9.
11. Xiantao Li, Exponential Quantum Speedup for Simulating Classical Lattice Dynamics, *Physical Review Letters* 135 (8), 080602, 2025.
12. Xiantao Li, Sangkook Choi, Hyowon Park, and Taehee Ko. Classical optimization algorithms for diagonalizing quantum Hamiltonians. *Physica Scripta* 100, 105101 (2025). DOI: 10.1088/1402-4896/ae09de.
13. Pegah Mohammadipour and Xiantao Li. Direct Analysis of Zero-Noise Extrapolation: Polynomial Methods, Error Bounds, and Simultaneous Physical-Algorithmic Error Mitigation. *Quantum* 9, 1909 (2025). DOI: 10.22331/q-2025-11-14-1909.
14. Hsuan-Cheng Wu, Jingyao Wang and Xiantao Li. Quantum Algorithms for Nonlinear Dynamics: Revisiting Carleman Linearization with No Dissipative Conditions. *SIAM Journal on Scientific Computing* 47, A943–A970 (2025). DOI: 10.1137/24M1665799.
15. Wenhao He, Tongyang Li, Xiantao Li, Zecheng Li, Chunhao Wang, and Ke Wang. Efficient Optimal Control of Open Quantum Systems. 19th Conference on the Theory of Quantum Computation, Communication and Cryptography (TQC 2024), LIPIcs 310, 3:1–3:23 (2024). DOI: 10.4230/LIPIcs.TQC.2024.3.

16. Taehee Ko, Xiantao Li and Chunhao Wang. Ground-State Energy and Related Properties Estimation in Quantum Chemistry with Linear Dependence on the Number of Atoms. 2024 IEEE International Conference on Quantum Computing and Engineering (QCE) 1, 669–680 (2024). DOI: 10.1109/QCE60285.2024.00084.
17. Ding, Z., Li, X., & Lin, L. Simulating Open Quantum Systems Using Hamiltonian Simulations. *PRX Quantum*, Volume 5, 020332, 2024.
18. Ding, Z., Ko, T., Yao, J., Lin, L., & Li, X. Random coordinate descent: a simple alternative for optimizing parameterized quantum circuits. *Physical Review Research*, Volume 6, 033029, 2024.
19. Ke Wang and Xiantao Li. Simulation-assisted learning of open quantum systems. *Quantum* 8, 1407 (2024). DOI: 10.22331/q-2024-07-11-1407.
20. Guneykan Ozgul, Xiantao Li, Mehrdad Mahdavi, and Chunhao Wang. Stochastic Quantum Sampling for Non-Logconcave Distributions and Estimating Partition Functions. *Proceedings of the 41st International Conference on Machine Learning*, PMLR 235, 38953–38982 (2024).
21. Jin, S., Li, X., Liu, N. & Yu, Y. Quantum Simulation for Quantum Dynamics with Artificial Boundary Conditions. *SIAM Journal on Scientific Computing* 46, B403–B421 (2024). DOI: 10.1137/23M1563451.
22. Jin, S., Li, X., Liu, N. & Yu, Y. Quantum simulation for partial differential equations with physical boundary or interface conditions. *Journal of Computational Physics* 498, 112707 (2024). DOI: 10.1016/j.jcp.2023.112707.
23. Xiantao Li and Chunhao Wang. Simulating Markovian Open Quantum Systems Using Higher-Order Series Expansion. 50th International Colloquium on Automata, Languages, and Programming (ICALP 2023), *LIPIcs* 261, 87:1–87:20 (2023). DOI: 10.4230/LIPIcs.ICALP.2023.87.
24. Li, X., & Wang, C. (2023). "Efficient Quantum Algorithms for Quantum Optimal Control." *Proceedings of the 40th International Conference on Machine Learning (ICML)*, 202, (pp. 19982-19994).
25. Li and Venturi, The Mori-Zwanzig formulation of deep learning, *Research in the Mathematical Sciences*, 10(23). DOI: <https://doi.org/10.1007/s40687-023-00390-2>, 2023.
26. Ko and Li, A Local Convergence Theory for the Stochastic Gradient Descent Method in Non-Convex Optimization With Non-isolated Local Minima. *J. Mach. Learn.*, 2, 138-160. DOI: 10.4208/jml.230106, 2023.
27. Jin and Li, A Partially Random Trotter Algorithm for Quantum Hamiltonian Simulations, *Communications on Applied Mathematics and Computation*. DOI: <https://doi.org/10.1007/s42967-023-00336-z>, 2023.
28. Taehee Ko and Xiantao Li. Stochastic Algorithms for Self-Consistent Calculations of Electronic Structures. *Mathematics of Computation* 92(342), 1693–1728 (2023). DOI: 10.1090/mcom/3826.
29. Li and Wang, Succinct Description and Efficient Simulation of Non-Markovian Open Quantum Systems, *Communications in Mathematical Physics*, 2023.
30. X. Li, Some error analysis for the quantum phase estimation algorithms, *Journal of Physics A: Mathematical and Theoretical*, 55, 325303, 2022.
31. Shi Jin, Xiantao Li, and Nana Liu. Quantum simulation in the semi-classical regime. *Quantum* 6, 739 (2022). DOI: 10.22331/q-2022-06-17-739.
32. Luo, Y., Li, X. & Hao, W., Stability preserving data-driven models with latent dynamics, *Chaos*, Vol 32, 081103 2022.
33. Luo, Y., Li, X. & Hao, W., Projection based model reduction for the immersed boundary method (IBM), *International Journal for Numerical Methods in Biomedical Engineering*, Vol 38, e3558, 2022.
34. Chu and Li, A Projection-based Reduced-order Method for Electron Transport Problems with Long-range Interactions, *Journal of Chemical Physics*, Volume 155, page 114105, 2021.

35. Zhang, Harlim and Li, Error Bounds of the Invariant Statistics in Machine Learning of Ergodic Ito Diffusions, *Physica D*, Volume 427, page 133022, 2021.
36. Lei, H. & Li, X., Petrov-Galerkin methods for the construction of non-Markovian dynamics preserving nonlocal statistics, *Journal of Chemical Physics*, Vol 154, 184108, 2021.
37. Weiqi Chu and Xiantao Li, Nonlinear Constitutive Models for Nano-scale Heat Conduction, *SIAM Journal of Multiscale Modeling and Simulation*, Volume, 19, 533-549, 2021.
38. H. Zhang, J. Harlim and Xiantao Li, Linear Response Based Parameter Estimation in the Presence of Model Error, *Journal of Computational Physics*, 2021.
39. X. Li, On Markovian Embedding Procedures for the Non-Markovian Stochastic Schrödinger Equation, *Physics Letters A*, Vol 387, 127036, 2021.
40. He Zhang, J Harlim and X Li, Computing linear response statistics using orthogonal polynomial based estimators: An RKHS formulation, *Foundation of Data Science*, Volume 2, 443-485, 2020.
41. Shi Jin and Xiantao Li. Random Batch Algorithms for Quantum Monte Carlo Simulations. *Communications in Computational Physics* 28, 1907–1936 (2020). DOI: 10.4208/cicp.OA-2020-0168.
42. Francesca Grogan, Huan Lei, Xiantao Li, and Nathan A. Baker. Data-driven molecular modeling with the generalized Langevin equation. *Journal of Computational Physics* 418, 109633 (2020). DOI: 10.1016/j.jcp.2020.109633.
43. W. Chu and Xiantao Li, A reduced-order modeling approach for electron transport in molecular junctions, *J. Chem. Theory Comput*, Vol 16, 3746-3756, 2020.
44. Q. Du, Xiantao Li and L. Yuan, Analysis of coarse-grained lattice models and connections to nonlocal interactions, *CSIAM Trans. Appl. Math*, Vol 1, 155-185, 2020.
45. Jingze Li and Xiantao Li, Exponential Integrators for Stochastic Schrödinger Equation, *Physical Review E*, Vol 101, 013312, 2020.
46. Xiaojie Wu and Xiantao Li. Absorbing boundary conditions for the time-dependent Schrödinger-type equations in $\mathbb{R}^3$, *Phys. Rev E*, Vol 101, 013304, 2020.
47. X. Li, The Computation of Local Stress in ab initio Molecular Simulations, *Modelling and Simulation in Materials Science and Engineering (MSMSE)*, Vol 27, 065016, 2019.
48. Xiantao Li. Absorbing boundary conditions for time-dependent Schrödinger equations: A density-matrix formulation. *Journal of Chemical Physics* 150, 114111 (2019). DOI: 10.1063/1.5079326.
49. He Zhang, J. Harlim and X. Li, A Parameter Estimation Method Using Linear Response Statistics: Numerical Scheme, *Chaos*, (29) 033101, 2019.
50. Cheng Yuang, Zhijian Yang, and Xiantao Li, An effective and easy-to-implement boundary condition for molecular dynamics simulations, *Communications in Computational Physics*, (26) 192-205, 2019.
51. Weiqi Chu and Xiantao Li, The Mori-Zwanzig formalism for the derivation of a fluctuating heat conduction model from molecular dynamics, *Communications in Mathematical Sciences*, Vol 17, 539, 2019.
52. L Ma, X Li and C Liu, Coarse-graining Langevin dynamics using reduced-order techniques, *Journal of Computational Physics*, (380) 170-190, 2019.
53. Weiqi Chu and Xiantao Li, On the asymptotic behavior of the kernel function of the Generalized Langevin equation -- a one-dimensional lattice model. *J. Statistical Physics.*, 170, page 378, 2018.
54. Xiaojie Wu and X. Li, Stable absorbing boundary conditions for molecular dynamics in general domains, *Computational Mechanics*, 2018.

55. Xiantao Li, Lin Lin, and Jianfeng Lu. PEXSI- Σ : A Green's function embedding method for Kohn-Sham density functional theory. *Annals of Mathematical Sciences and Applications* 3(2), 441–472 (2018). DOI: 10.4310/amsa.2018.v3.n2.a3.
56. Xiaojie Wu and X. Li, Simulations of Micron-scale Fracture using Atomistic-based Boundary Element Method, *Modelling and Simulation in Materials Science and Engineering* 25.8 (2017): 085008.
57. J. Harlim, X. Li and H. Zhang, A Parameter Estimation Method Using Linear Response Statistics, *Journal of Statistical Physics*, Vol 168, 146-170, 2017.
58. L Ma, X. Li and C Liu, Fluctuation-Dissipation Theorem Consistent Approximation of the Langevin Dynamics Model, *Communications in Mathematical Sciences*, Vol 15, 1171—1181, 2017.
59. L. Ma, X. Li and C. Liu, Derivation and approximation of coarse-grained dynamics from Langevin dynamics, *Journal of Chemical Physics*, Vol 145, 204117, 2016.
60. H Lei, X. Li and N Baker, Data-driven parameterization of the generalized Langevin equation, *Proceedings of the National Academy of Sciences*, 1609587113, 2016.
61. L. Ma, X. Li and C. Liu, From Generalized Langevin Equations to Brownian Dynamics and Embedded Brownian Dynamics, *J. Chemical Physics*, Vol 145, 114102, 2016.
62. X. Li and J. Lu, Traction Boundary Conditions for Molecular Static Simulations, *Computer Methods in Applied Mechanics and Engineering*, Vol 308, 310–329, 2016.
63. Zhen Li, Xin Bian, Xiantao Li, and George Em Karniadakis. Incorporation of memory effects in coarse-grained modeling via the Mori-Zwanzig formalism. *Journal of Chemical Physics* 143, 243128 (2015). DOI: 10.1063/1.4935490.
64. J. Harlim and X. Li, Parametric reduced models for the nonlinear Schrödinger equation, *Physical Review E*, 91, 053306, 2015.
65. J. Chen, C. García-Cervera and X. Li, An atomistic/continuum coupling method using enriched bases, *Multiscale Modeling and Simulations*, 2015.
66. X. Wu and X. Li, On Consistent Definitions of Momentum and Energy Fluxes for Molecular Dynamics Models with Multi-body Interatomic Potentials, *Modelling and Simulation in Materials Science and Engineering*, 23, 015003, 2015.
67. J.Z. Yang, C. Mao, X. Li and C. Liu, On the Cauchy-Born Approximation at Finite Temperature, *Computational Materials Science*, 99, 21-28, 2015.
68. X. Li, Heat conduction in nanoscale materials: A statistical-mechanics derivation of the local heat flux, *Phys. Rev E* 90 032112 (2014).
69. X. Li, A numerical study of crack initiation in a bcc iron system based on dynamic bifurcation theory, *J. Appl. Phys.*, (116), 164314 (2014).
70. M. Chen, X Li and C. Liu, Computation of the Memory Functions in the Generalized Langevin Models for Collective Dynamics of Macromolecules, *J. Chemical Physics*, Vol 141 064112, 2014.
71. X. Li and P.B. Ming, A study on the quasicontinuum approximations of a one-dimensional fracture model, *Multiscale Modeling and Simulation*, 12, 1379-1400, 2014.
72. J.Z. Yang, X. Wu and X. Li, Accurate Evaluations of Strain and Stress in Atomistic Simulations of Crystalline Solids, *Modelling and Simulation in Materials Science and Engineering*, 22, Page 045008, 2014.
73. X. Li, Coarse-graining molecular dynamics models using an extended Galerkin projection, *International Journal for Numerical Methods in Engineering*, Vol 99, pages 157-182, 2014.
74. X. Li and P. Ming, On the effect of ghost force in the quasicontinuum method: dynamic problems in one dimension, *Commun. Comput. Phys.*, 15 (2014), pp. 647-676.

75. X. Li, A bifurcation study of crack initiation and kinking, *The European Physical Journal B*, 86, 258, 2013.
76. J. Z. Yang, X. Wu and X. Li, A generalized Irving-Kirkwood formula for the calculation of stress in molecular dynamics models, *Journal of Chemical Physics*, 137, 134104 (2012).
77. X. Li, An atomistic-based boundary element method for the reduction of the molecular Statics Models. *Computer Methods in Applied Mechanics and Engineering*. 225, 1-13, 2012
78. X. Li, A coarse-grained molecular dynamics model for crystalline solids, *International Journal for Numerical Methods for Engineering*, 83, 986–997, 2010.
79. X. Li, J. Z. Yang, and W. E, A multiscale coupling method for crystalline solids with application to dynamics of crack propagation, *Journal of Computational Physics*, 229, 3970-3987, 2010.
80. X. Li, Efficient boundary condition for molecular statics models of solids, *Physical Review B*, 80, 104112, 2009.
81. X. Li, On the stability of boundary conditions for molecular dynamics, *Journal of Computational and Applied Mathematics*, Volume 231, 493-505, 2009.
82. X. Li, Variational boundary condition for molecular dynamics: Treatment of the loading conditions, *Journal of Computational Physics*, Volume 227, 10078–10093, 2008.
83. W. Wang, X. Li and C.W. Shu, the Discontinuous Galerkin method for the multiscale modeling of dynamics of crystalline solids, *Multiscale Modeling and Simulation*, Volume 7, no.1, 294- 320, 2008.
84. X. Li and W. E, Variational boundary conditions for molecular dynamics simulations of crystalline solids at finite temperature: Treatment of the thermal bath, *Physical Review B*, Volume 76, Article no. 104107, 2007.
85. W. E, B. Engquist, X. Li, W. Ren and E. Vanden-Eijnden, the heterogeneous multiscale method: A Review, *Communication in Computational Physics*, Volume 2, 367 – 450, 2007.
86. J. Z. Yang and X. Li, Comparative study of boundary conditions for molecular dynamics simulations of solids at low temperature, *Physical Review B*, Volume 73, Article no. 224111, 2006.
87. X. Li and W. E, Variational boundary conditions for molecular dynamics simulations of solids at low temperature, *Communications in Computational Physics*, Volume 1, no.1, 135 – 175, 2006.
88. X. Li and W. E, Multiscale modeling for the dynamics of solids at finite temperature, *Journal of the Mechanics and Physics of Solids*, Volume 53, 1650 – 1685, 2005.
89. Weinan E and Xiantao Li. Analysis of the heterogeneous multiscale method for gas dynamics. *Methods and Applications of Analysis* 11(4), 557–572 (2004). DOI: 10.4310/MAA.2004.v11.n4.a7.
90. W. E, X. Li and E. Vanden-Eijnden, Some recent progress on multiscale modeling, *Lecture Notes in Computational Science and Engineering*, Volume 39, 3–22, 2004.
91. W. E and X. Li, Multiscale modeling for crystalline solids, *Handbook of multiscale material modeling*, 1, 1491–1596, 2004.
92. X. Li, J. G. Wohlbier, S. Jin and J. Booske, An Eulerian method for computing multi-valued solutions of the Euler-Poisson equations, *Physical Review E*, Volume 70, Article no. 016502, 2004.
93. Laurent Gosse, Shi Jin and Xiantao Li. Two moment systems for computing multiphase semiclassical limits of the Schrödinger equation. *Mathematical Models and Methods in Applied Sciences* 13(12), 1689–1723 (2003). DOI: 10.1142/S0218202503003082.
94. S. Jin and X. Li, Multi-phase Computations for semiclassical limits of Schrödinger Equation and related problems: Whitham vs Wigner, *Physica D*, Volume 182, 46-85, 2003.
95. F. Bouchut, S. Jin and X. Li, Numerical solutions of pressure-less gas equations, *SIAM Journal of Numerical Analysis*, Volume 41, 135-158, 2003.

Preprints and Submitted Manuscripts

96. Hsuan-Cheng Wu and Xiantao Li. From Nonlinear Stochastic Differential Equations to Quantum Channels: The Kolmogorov–Lindblad Mapping. arXiv:2608.09903 (2026).
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