Xiantao Li **Curriculum Vita**

219C McAllister Building
Department of Mathematics Penn State University University Park, PA 16802

(814)8639081
xxl12@psu.edu
www.personal.psu.edu/xxl12

Education

Ph.D. 2002, Applied Mathematics, University of Wisconsin, Madison.
B.S. 1998, Mathematics, Peking University, Beijing, China.

Employment

July 2016 – present
Full Professor
Department of Mathematics, Penn State University

July 2010 – June 2016
Associate Professor
Department of Mathematics, Penn State University

August 2005 – June 2010
Assistant Professor
Department of Mathematics, Penn State University

August 2004 – August 2005
Postdoctoral Fellow
Institute for Mathematics and its Application University of Minnesota, Minneapolis

September 2002 – August 2004
Research Associate
Program in Applied and Computational Mathematics
Princeton University

Other Affiliations at Penn State

Center for Computational and Applied Mathematics (Co-director)
Center for Interdisciplinary Mathematics
PSU Institute for Computational and Data Science
Center for Advanced Data Assimilation and Predictability Techniques

Research Interest

Quantum computing algorithms
Reduced-order modeling; Data assimilation
Analysis of Machine learning algorithms; stochastic algorithms
Open quantum systems; Quantum master equations
Quantum transport

Electron structure calculations
Coarse-graining molecular dynamics; non-Markovian dynamics
Anomalous nano-scale heat conduction; generalized Fourier's Law
Computational mechanics and nano-scale materials

Graduate Students

Former students: Chao Liang; Adam Telatovich; Xiaojie Wu; Weiqi Chu; He Zhang, Yushuang Luo, Taehee Ko.
Current students: Ke Wang, HsuanCheng Wu and Pegah Mohammadipour;

Publications

a. Submitted or published.

1. Ke Wang and Xiantao Li, Non-Markovian Noise Mitigation: Practical Implementation, Error Analysis, and the Role of Environment Spectral Properties, Submitted January 21, 2025, https://arxiv.org/pdf/2501.05019.
2. HsuanCheng Wu and Xiantao Li, Structure-preserving quantum algorithms for linear and nonlinear Hamiltonian systems, https://arxiv.org/pdf/2411.03599.
3. Zhenning Liu, Jin-Peng Liu, Xiantao Li and Chunhao Wang, Toward end-to-end quantum simulation for protein dynamics, https://arxiv.org/pdf/2411.03972.
4. Wu, Wang and Li, Quantum Algorithms for Nonlinear Dynamics: Revisiting Carleman Linearization with No Dissipative Conditions, *SIAM Journal on Scientific Computing,* in press, 2025.
5. He, Li, Li, Li, Wang, Wang, Efficient Optimal Control of Open Quantum Systems, 19th Conference on the Theory of Quantum Computation, Communication and Cryptography (TQC 2024), 2024.
6. Ko, T., Li, X., & Wang, C. Quantum Algorithm for Ground State Properties in Quantum Chemistry with Linear Dependence on the Number of Atoms. 2024 IEEE International Conference on Quantum Computing and Engineering (QCE), Vol 1, pages 669-680. DOI: https://doi.org/10.48550/arXiv.2307.03858,
7. Ding, Z., Li, X., & Lin, L. Simulating Open Quantum Systems Using Hamiltonian Simulations. PRX Quantum, Volume 5, 020332, 2024.
8. 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.
9. Wang, K., & Li, X. Simulation-assisted learning of open quantum systems. *Quantum*. Volume 8, 1407, 2024. DOI: https://doi.org/10.48550/arXiv.2307.03858
10. Ozgul, G., Li, X., Mahdavi, M., & Wang, C. "Stochastic Quantum Sampling for Non-Logconcave Distributions and Estimating Partition Functions." *International Conference on Machine Learning (**ICML**).*2024. DOI:

https://doi.org/10.48550/arXiv.2310.11445

11. Jin, S., Li, X., Liu, N., & Yu, Y. Quantum Simulation for Quantum Dynamics with Artificial Boundary Conditions. *SIAM Journal on Scientific Computing*. Volume 46, B403-B421, 2024. DOI: https://doi.org/10.48550/arXiv.2304.00667
12. Li, X. (Author), & Wang, C. (2023). "Simulating Markovian open quantum systems using higher-order series expansion." *the International Colloquium on Automata, Languages, and Programming. **(ICALP)***, 261, (pp. 87:1-87:20). Schloss Dagstuhl -- Leibniz-Zentrum f{\"u}r Informatik. DOI: https://doi.org/10.4230/LIPIcs.ICALP.2023.87
13. 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).
14. Jin, S., Li, X. (Author), Liu, N., & Yu, Y. (2023). Quantum simulation for partial differential equations with physical boundary or interface conditions. ***Journal of Computational Physics**, 498*, 112707. DOI: https://doi.org/10.1016/j.jcp.2023.112707
15. Li, **Enabling Quantum Speedup of Markov Chains using a Multi-level Approach**, preprint, 2022.
16. 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.*
17. 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.
18. Li and Wang, **Simulating Markovian open quantum systems using higher-order series expansion**, 50th International Colloquium on Automata, Languages, and Programming (ICALP 2023), Volume 87, 1-20, 2023.
19. 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.
20. Ko and Li, Stochastic Algorithms for Self-consistent Calculations of Electronic Structures**,** Mathematics of Computation, 92, 1693-1728. DOI: 10.48550/arXiv.2107.01454 **2023.**
21. Xie, C., Chen, J. & Li, X, A machine-learning method for time-dependent wave equations over unbounded domains, preprint, **2021**.
22. Li and Wang, Succinct Description and Efficient Simulation of Non-Markovian Open

Quantum Systems, Communications in Mathematical Physics, 2023.

23. X. Li, Some error analysis for the quantum phase estimation algorithms, ***Journal of Physics A: Mathematical and Theoretical***, **55,** 325303, **2022.**
24. Jin, X. Li, and N. Liu, Hamiltonian simulation in the semi-classical regime, ***Quantum***, Vol*, pp 739,* **2022***.*
25. Luo, Y., Li, X. & Hao, W., Stability preserving data-driven models with latent dynamics, **Chaos**, Vol **32**, 081103 **2022.**
26. 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**.
27. 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.**
28. Zhang, Harlim and Li, Error Bounds of the Invariant Statistics in Machine Learning of Ergodic Ito Diffusions, ***Physica D***, Volume 427, page 133022, **2021.**
29. 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**.
30. 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****.*
31. H. Zhang, J. Harlim and Xiantao Li, Linear Response Based Parameter Estimation in the Presence of Model Error, **Journal of Computational Physics**, **2021**.
32. 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**.
33. X. Li, On Markovian Embedding Procedures for the Non-Markovian Stochastic Schrodinger Equation**, Physics Letters A, Vol 387, 127036, 2021**.
34. S. Jin and X. Li, Random Batch Algorithms for Quantum Monte Carlo simulations**, Communications in Computational Physics,** Vol 28, 1907-1936*,* **2021.**

35. Francesca Grogan, H Lei, N A Baker and X Li, Data-driven molecular modeling with the generalized Langevin equation ***J. Computational Physiscs***, Vol 41, 109633, **2020**.

36. 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**.

37. 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**.

38. Jingze Li and Xiantao Li, Exponential Integrators for Stochastic Schrödinger Equation, ***Phyical Review E***, Vol 101, 013312, **2020**.

39. With Xiaojie Wu, Absorbing boundary conditions for the time-dependent Schrodinger-type equations in R^3, ***Phys. Rev E***, Vol 101, 013304, **2020**.

40. 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**.

41. Adam Telatovich and X, Li, The strong convergence of operator-splitting methods for the Langevin dynamics model, *ArXiv, 2018.*

42. X. Li, Absorbing Boundary Conditions for Time-dependent Schr\"{o}dinger equations: A Density-matrix Formulation**, *Journal of Chemical Physic****s, (150) 114114, ****2019***.

43. He Zhang, J. Harlim and X. Li, A Parameter Estimation Method Using Linear Response Statistics: Numerical Scheme**, *Chao****s, (29) 033101, ****2019***.

44. Cheng Yuang, Zhijian Yang, and Xiantao Li, An effective and easy-to-implement boundary condition for molecular dynamics simulati**ons,** *Communications in Computational Physics,* (26) 192-205, **2019**.

45. Weiqi Chu and Xiantao Li, The Mori-Zwanzig formalism for the derivation of a fluctuating heat conduction model from molecular dynamics, **Communications in Mathematical Science**s, Vol 17, 539, **2019.**

46. L Ma, X Li and C Liu, Coarse-graining Langevin dynamics using reduced-order techniques**, *Journal of Computational Physics****, (380) 170-190, ****2019***.

47. 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.***

48. Xiaojie Wu and X. Li, Stable absorbing boundary conditions for molecular dynamics in general domains**,** *Computational Mechanics,* ***2018****.*

49. X. Li, L Lin and J Lu, PEXSI-Σ: A Green's function embedding method for Kohn-Sham density functional theory, ***Annals of Mathematical Sciences and Applications****,* in press 3(2), 417, **2018**.

50. 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.

51. J. Harlim, X. Li and H. Zhang, A Parameter Estimation Method Using Linear Response Statistics**,** *Journal of Statistical Physics, Vol 168, 146-170,* ***2017****.*

52. 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****.*

53. 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***.

54. H Lei, X. Li and N Baker, Data-driven parameterization of the generalized Langevin equation, Proceedings of the National Academy of Sciences, *1609587113,* ***2016****.*

55. Zhen Li, Xin Bian, and George Em Karniadakis, Incorporation of memory effects in coarse-grained modeling via the Mori-Zwanzig formalism, Journal of Chemical Physics, 143, 243128 (2015).

56. 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***.

57. X. Li and J. Lu, Traction Boundary Conditions for Molecular Static Simulations, *Computer Methods in Applied Mechanics and Engineering, Vol 308, 310--329,* ***2016****.*

58. J. Harlim and X. Li, Parametric reduced models for the nonlinear Schrodinger equation, *Physical Review E,* **91,** 053306, ***2015****.*

59. J. Chen, C. García-Cervera and X. Li, An atomistic/continuum coupling method using

enriched bases**,** *Multiscale Modeling and Simulations,* ***2015****.*

60. X. Li, Heat conduction in nanoscale materials: A statistical-mechanics derivation of the local heat flux**,** *Phys. Rev E 90 032112* ***(2014).***

61. 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****.*

62. X. Li, A numerical study of crack initiation in a bcc iron system based on dynamic bifurcation theory**,** *J. Appl. Phys, (116), 164314* ***(2014).***

63. 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.*

64. X. Li and P.B. Ming, A study on the quasiconinuum approximations of a one-dimensional fracture model, SIAM, Multiscale Modeling and Simulation, *12, 1379-1400, 2014*.

65. 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*.

66. 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.

67. 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.

68. 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.*

69. X. Li, A bifurcation study of crack initiation and kinking, *The European Physical Journal B*, The European Physical Journal B, *86, 258, 2013.*

70. 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).*

71. 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

72. X. Li, A coarse-grained molecular dynamics model for crystalline solids, International Journal for Numerical Methods for Engineering, 83, 986--997, 2010.

73. 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.

74. X. Li, Efficient boundary condition for molecular statics models of solids, Physical Review B, 80, 104112, 2009.

75. X. Li, On the stability of boundary conditions for molecular dynamics, Journal of Computational and Applied Mathematics, Volume 231, 493-505, 2009.

76. X. Li, Variational boundary condition for molecular dynamics: Treatment of the loading conditions, Journal of Computational Physics, Volume 227, 10078–10093, 2008.

77. W. Wang, X. Li and C.W. Shu, the Discontinuous Galerkin method for the multiscale modeling of dynamics of crystalline solids, SIAM: Multiscale Modeling and Simulation, Volume 7, no.1, 294- 320, 2008.

78. 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.

79. 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.

80. 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.

81. 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.

82. 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.

83. W. E and X. Li, Analysis of the heterogeneous multiscale method for gas dynamics, Methods of

Analysis and Applications, Volume 11(3), 1 – 16, 2004.

84. 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.

85. W. E and X. Li, Multiscale modeling for crystalline solids, Handbook of multiscale material modeling, 1, 1491–1596, 2004.

86. 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.

87. S. Jin, L. Gosse and X. Li, On two moment systems for computing multiphase semiclassical limits of the Schroedinger equation, International Journal Of Mathematical Models qnd Methods in Applied Sciences, Volume 3(12), 1689-1723, 2003.

88. S. Jin and X. Li, Multi-phase Computations for semiclassical limits of Schroedinger Equation and related problems: Whitham vs Wigner, Physica D, Volume 182, 46-85, 2003.

89. F. Bouchut, S. Jin and X. Li, Numerical solutions of pressure-less gas equations, SIAM Journal of Numerical Analysis, Volume 41, 135-158, 2003.

c. Book chapters and conference proceedings

90. Introduction to molecular dynamics simulations. *Lecture Notes Series, Multiscale Modeling and Analysis for Materials Simulation, Institute for Mathematical Sciences, National University of Singapore: Volume 22, 95-146, 2011.*
91. Coarse-graining molecular dynamics. *Mathematisches Forschungsinstitut Oberwolfach, Report 21, 2008, page 1148.*
92. Interface conditions for coupled atomistic and continuum models of solids for dynamics problems at finite temperature. *Material Research Society Proceedings, Paper no. 0978-GG06-02, 2006.*

Recent Research Support

NSF PI, 2024-2027 (DMS, Award Amount, $300,000).
NSF Co-PI, 2023 – 2026 (FET, Award Amount $600,000)
Penn State Institute of Computational and Data Science Grant
2022-2023) $30,000.

NSF Principal Investigator, 2021--2024 (DMS- 2111221, Award Amount $395,391).
NSF Principal Investigator, 2020--2023 (DMS- 1953120, Award Amount $120,000).
NSF Principal Investigator, 2018--2021 (DMS-1819011, Award Amount $200,000).
NSF Co-Principal Investigator, 2016--2019 (DMS-1619661, Award Amount $300,867).
NSF Principal Investigator, 2015--2018 (DMS-1522617, Award Amount $215,000)

Research Interest

Quantum Computing

Machine learning

Molecular modeling and simulations

Dimension reduction

Computational mechanics and material defects.

Numerical analysis

Students and Postdocs

- Qing Ruan, **MS, 2009**
- Chao Liang, **PhD 2014**
- Xiaojie Wu, **PhD 2018**
- Adam Telatovich, **PhD 2018**.
- Weiqi Chu, **PhD 2019**.
- He Zhang, PhD 2020.
- Yushuang Luo, PhD 2022.
- Taehee Ko, PhD 2023.
- Ke Wang, PhD Candidate, Current
- HsuanCheng Wu, PhD Candidate, Current
- Pegah Mohammadipour, PhD Candidate, Current
- Lina Ma, Postdoc, 2015-2017.

Invited talks

University of South Carolina, November, 2024.
Simon's Institute, October 2024.
SIAM Material Conference, March 2024.

University of California, Berkeley, March, 2023
IPAM-UCLA, March and October 2023.
Numerical Analysis of Galerkin ROMs (NA G-ROMs) Seminar series, Oct 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, Sep 2020.
Applied Math Seminar, Purdue University, Feb 2020.
ICIAM The International Council for Industrial and Applied Math, 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 System, May 2017.
SIAM Conference on computational science and engineering, Feb 2017.
Applied Math Seminar, Colorado State University, Nov 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, Nov 2013.
SIAM Conference on Mathematical Aspects of Materials Science, June 2013.
The 2nd Pacific Rim Mathematical Association Congress, June 2013.
The International Conference on Applied Mathematics, April 2012.

Professional Services

Symposium organizer Symposium on Computational Mathematics for Engineering and Sciences at Penn State, 2024.

SIAM-sponsored Workshop on Dimension Reduction (March 22-25, 2015 at Penn State). Organized with colleague Chun Liu.

Mini-symposium organizer for the SIAM Conference on Mathematical Aspects of Materials Science, June 2014.

Mini-symposium organizer for the multiscale material modeling meeting (MMM 2014).

Manuscript reviewer for Journal of Computational Physics, Communication in Mathematical Science, Journal of Applied Numerical Mathematics, SIAM Multiscale Modeling and Simulation, Journal Numerische Mathematik, Communications of Computational Physics, Journal of Scientific Computing etc.