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 2010 -- Present
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

Publications

a. Submitted

1. J.Z. Yang, C. Yuan and X. Li, An effective and easy-to-implement boundary condition for molecular dynamics simulations, 2015.
2. L Wu, G Lin and X. Li, The Mori-Zwanzig formalism for coarse-graining molecular dynamics models: A quasi-harmonic approximation, *submitted, 2015.*
3. X. Li and J. Lu, Traction Boundary Conditions for Molecular Static Simulations, *submitted, 2015.*
4. C. Liang, X. Yuan and X. Li, Some New Symplectic Multiple Timestepping Methods for Multiscale Molecular Dynamics Models**,** *submitted, 2015.*

b. Appeared

1. J. Harlim and X. Li, Parametric reduced models for the nonlinear Schrodinger equation, *Physical Review E,* **91,** 053306, *2015.*
2. J. Chen, C. García-Cervera and X. Li, An atomistic/continuum coupling method using

enriched bases, *Multiscale Modeling and Simulations, 2015.*
3. X. Li, Heat conduction in nanoscale materials: A statistical-mechanics derivation of the local heat flux, *Phys. Rev E 90 032112 (2014).*
4. 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.*
5. X. Li, A numerical study of crack initiation in a bcc iron system based on dynamic bifurcation theory, *J. Appl. Phys, (116), 164314 (2014).*
6. 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.*
7. 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*.
8. 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*.
9. 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.
10. 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.
11. 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.*
12. X. Li, A bifurcation study of crack initiation and kinking, *The European Physical Journal B*, The European Physical Journal B, *86, 258, 2013.*
13. 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).*
14. 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
15. X. Li, A coarse-grained molecular dynamics model for crystalline solids, International Journal for Numerical Methods for Engineering, 83, 986--997, 2010.
16. 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.
17. X. Li, Efficient boundary condition for molecular statics models of solids, Physical Review B, 80, 104112, 2009.
18. X. Li, On the stability of boundary conditions for molecular dynamics, Journal of Computational and Applied Mathematics, Volume 231, 493-505, 2009.
19. X. Li, Variational boundary condition for molecular dynamics: Treatment of the loading conditions, Journal of Computational Physics, Volume 227, 10078–10093, 2008.
20. 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.
21. 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.
22. 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.

23. 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.
24. 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.
25. 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.
26. 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.
27. 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.
28. W. E and X. Li, Multiscale modeling for crystalline solids, Handbook of multiscale material modeling, 1, 1491–1596, 2004.
29. 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.
30. 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.
31. 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.
32. 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

1. 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.*
2. Coarse-graining molecular dynamics. *Mathematisches Forschungsinstitut Oberwolfach, Report 21, 2008, page 1148.*
3. 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.*

Research Support

NSF Principal Investigator, **duration:** 06/01, 2006 -- 05/31/2011
(DMS-0609610, Award Amount $126,371)

Alfred P. Sloan Fellowship, **duration:** 09/16, 2007 – 09/15/2011
(Award Amount $45,000)

NSF Principal Investigator, **duration:** 06/01/2010 – 05/31/2013 (DMS-1016582, Award Amount $165,000)

NSF Principal Investigator, **duration:** 09/01/2015 – 08/31/2018 (DMS-1522617, Amount $215,000)

Research Interest

Numerical analysis

Computational mechanics and material defects.

Molecular dynamics modeling and simulations, electron structure calculation

Dimension reduction, uncertainty quantification

Students and Postdocs

- Qing Ruan, MS, 2009
- Chao Liang, PhD 2014
- Xiaojie Wu, PhD Candidate, Current.
- He Zhang, PhD Candidate, Current.
- Lina Ma, Postdoc, Current.

Invited talks and presentations

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.

Teaching and Educational Activities

Undergraduate International Summer Programs

The 5th PSU-PKU summer program for undergraduate students, July 22 – Aug 12, 2013.

The 3rd PSU-PKU summer program for undergraduate students, July 16 – Aug 10, 2010, Penn State University. **Role:** Organizer, lecturer, and research mentor.

The 2nd PSU-PKU summer program for undergraduate students, July 13 -- July 29, 2009, Peking University, China. **Role:** main organizer.

The 1st PSU-PKU summer program for undergraduate students, June 23 -- July 18, 2008, Peking University, China. **Role:** main organizer, lecturer and research mentors.

Regular Courses Taught at Penn State

Calculus II and III; Differential Equations; Numerical Analysis; Numerical methods for ODEs; Functional Analysis; Qualitative Theory of ODEs.

Professional Services

SIAM-sponsored Workshop on Dimension Reduction, held 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.