

Jianfeng Lu

Mathematics Department
Duke University, Box 90320
120 Science Dr., Durham, NC 27708-0320

Phone: (919) 660-2875

EMAIL: jianfeng@math.duke.edu

HOME PAGE: <http://www.math.duke.edu/~jianfeng/>

May 9, 2018

POSITIONS

- 2016 – **Associate Professor**, Department of Mathematics
2012 – 2016 Assistant Professor, Department of Mathematics
2013 – Secondary appointment in Department of Chemistry
2013 – Secondary appointment in Department of Physics
2015 – Affiliated faculty member of the Fitzpatrick Institute of Photonics
2017 – Affiliated faculty member of the University Program in Materials Science & Engineering
Duke University
- 2016 – 2018 **Faculty Fellow**
Statistical and Applied Mathematical Sciences Institute
- 2009 – 2012 **Courant Instructor**, Courant Institute of Mathematical Sciences
New York University

EDUCATION

- 2009 Ph.D. in APPLIED MATHEMATICS, Princeton University
2005 B.S. in MATHEMATICS, Peking University, China

AWARDS

- 2017 **IMA Prize in Mathematics and its Applications**, Institute of Mathematics and its Applications
2015 **NSF CAREER Award**, National Science Foundation
2013 **Sloan Research Fellowship**, Alfred P. Sloan Foundation
2008 **Porter Ogden Jacobus Fellowship**, Princeton University
The highest honorific fellowship awarded by the Graduate School of Princeton University.

PUBLICATIONS

- Phase space sketching for crystal image analysis based on synchrosqueezed transforms
(with Haizhao Yang), *SIAM J. Imaging Sci.*, in press
- Thermodynamic limit of crystal defects with finite temperature tight binding
(with Huajie Chen and Christoph Ortner), *Arch. Ration. Mech. Anal.*, in press
- Frozen Gaussian approximation for high frequency wave propagation in periodic media
(with Ricardo Delgadillo and Xu Yang), *Asymptotic Anal.*, in press
- A quantum kinetic Monte Carlo method for quantum many-body spin dynamics
(with Zhenning Cai), *SIAM J. Sci. Comput.*, in press

Accelerated sampling by infinite swapping of path integral molecular dynamics with surface hopping (with Zhennan Zhou), *J. Chem. Phys.* **148**, 064110 (2018).

A hybrid global-local numerical method for multiscale PDEs (with Yufang Huang and Pingbing Ming), *J. Sci. Comput.*, in press

A quasinonlocal coupling method for nonlocal and local diffusion models (with Qiang Du, Xingjie Helen Li, and Xiaochuan Tian), *SIAM J. Numer. Anal.*, in press

Point cloud discretization of Fokker-Planck operators for committor functions (with Rongjie Lai), *Multiscale Model. Simul.*, in press

Moderate deviation for random elliptic PDEs with small noise (with Xiaouo Li, Jingchen Liu, and Xiang Zhou), *Ann. Appl. Probab.*, in press

Lindblad equation and its semiclassical limit of the Anderson-Holstein model (with Yu Cao), *J. Math. Phys.* **58**, 122105 (2017).

Trigonometric integrators for quasilinear wave equations (with Ludwig Gauckler, Jeremy Marzuola, Frédéric Rousset, Katharina Schratz), *Math. Comp.*, in press

Cubic scaling algorithms for RPA correlation using interpolative separable density fitting (with Kyle Thicke), *J. Comput. Phys.* **351**, 187–202 (2017).

Fractional stochastic differential equations satisfying fluctuation-dissipation theorem (with Lei Li and Jian-Guo Liu), *J. Stat. Phys.* **169**, 316–339 (2017).

ELSI: A unified software interface for Kohn-Sham electronic structure solvers Victor W.-Z. Yu, Fabiano Corsetti, Alberto García, William P Huhn, Mathias Jacquelin, Weile Jia, Björn Lange, Lin Lin, Jianfeng Lu, Wenhui Mi, Ali Seifitokaldani, Álvaro Vázquez-Mayagoitia, Chao Yang, Haizhao Yang and Volker Blum, *Comput. Phys. Commun.* **222**, 267–285 (2018).

A variation on the Donsker-Varadhan inequality for the principal eigenvalue (with Stefan Steinerberger), *Proc. R. Soc. A.* **473**, 20160877 (2017).

Convergence of phase-field free energy and boundary force for molecular solvation (with Shibin Dai and Bo Li), *Arch. Ration. Mech. Anal.* **227**, 105–147 (2018).

Frozen Gaussian approximation with surface hopping for mixed quantum-classical dynamics: A mathematical justification of fewest switches surface hopping algorithms (with Zhennan Zhou), *Math. Comp.*, in press

An asymptotic preserving method for transport equations with oscillatory scattering coefficients (with Qin Li), *Multiscale Model. Simul.* **15** 1694–1718 (2017).

On extending Kohn-Sham density functionals to systems with fractional number of electrons (with Chen Li and Weitao Yang), *J. Chem. Phys.* **146**, 214109 (2017). JCP Editors' Choice

Quasinonlocal coupling of nonlocal diffusions (with Xingjie Helen Li), *SIAM J. Numer. Anal.* **55**, 2394–2415 (2017).

Path integral molecular dynamics with surface hopping for thermal equilibrium sampling of non-adiabatic systems (with Zhennan Zhou), *J. Chem. Phys.* **146**, 154110 (2017).

A cubic scaling algorithm for excited states calculations in particle-particle random phase approximation (with Haizhao Yang), *J. Comput. Phys.* **340**, 297–308 (2017).

A mathematical theory of optimal milestoning (with a detour via exact milestoning) (with Ling Lin and Eric Vanden-Eijnden), *Comm. Pure Appl. Math.*, in press

Wavepackets in inhomogeneous periodic media: Effective particle-field dynamics and Berry curvature Alexander Watson, Jianfeng Lu and Michael I. Weinstein, *J. Math. Phys.* **58**, 021503 (2017).

Weak solution of a continuum model for vicinal surface in the attachment-detachment-limited regime
(with Yuan Gao and Jian-Guo Liu), *SIAM J. Math. Anal.* **49**, 1705–1731 (2017).

Orbital minimization method with ℓ^1 regularization
(with Kyle Thicke), *J. Comput. Phys.* **336**, 87–103 (2017).

Continuum limit of a mesoscopic model of step motion with elasticity on vicinal surfaces
(with Yuan Gao and Jian-Guo Liu), *J. Nonlinear Sci.* **27**, 873–926 (2017).

Ruolin Prize of the 2017 International Consortium of Chinese Mathematicians Best Paper Award

A convergent method for linear half-space kinetic equations
(with Qin Li and Weiran Sun), *ESAIM: Math. Model. Numer. Anal.* **51**, 1583–1615 (2017).

Validity and regularization of classical half-space equations
(with Qin Li and Weiran Sun), *J. Stat. Phys.* **166**, 398–433 (2017).

Dislocation climb models from atomistic scheme to dislocation dynamics
Xiaohua Niu, Tao Luo, Jianfeng Lu, and Yang Xiang, *J. Mech. Phys. Solids* **99**, 242–258 (2017)

Thermalization of particle chains with onsite anharmonicity and comparison with kinetic theory
Christian Mendl, Jianfeng Lu, and Jani Lukkarinen, *Phys. Rev. E* **94**, 062104 (2016)

Preconditioning orbital minimization method for planewave discretization
(with Haizhao Yang), *Multiscale Model. Simul.* **15**, 254–273 (2017)

PEXSI- Σ : A Green's function embedding method for Kohn-Sham density functional theory
(with Xiantao Li and Lin Lin), *Ann. Math. Sci. Appl.*, in press

Removal of canvas patterns in digital acquisitions of paintings
Bruno Cornelis, Haizhao Yang, Alex Goodfriend, Noelle Ocon, Jianfeng Lu, and Ingrid Daubechies
IEEE Trans. Image Process. **26**, 160–171 (2017).

Improved sampling and validation of frozen Gaussian approximation with surface hopping algorithm for non-adiabatic dynamics
(with Zhennan Zhou), *J. Chem. Phys.* **145**, 124109 (2016).

Multiscale implementation of infinite-swap replica exchange molecular dynamics
Tang-Qing Yu, Jianfeng Lu, Cameron F. Abrams, Eric Vanden-Eijnden, *Proc. Natl. Acad. Sci. USA* **113** 11744–11749 (2016).

Gauge-invariant frozen Gaussian approximation method for Schrödinger equation with periodic potentials
(with Ricardo Delgadillo and Xu Yang), *SIAM J. Sci. Comput.* **38**, A2440–A2463 (2016).

Decay estimates of discretized Green's functions for Schrödinger type operators
(with Lin Lin), *Sci. China Math.* **59**, 1561–1578 (2016).

Special issue dedicated to ICIAM 2015

Traction boundary conditions for molecular static simulations
(with Xiantao Li), *Comput. Methods Appl. Mech. Engrg.* **308**, 310–329 (2016).

Fast algorithm for periodic density fitting for Bloch waves
(with Lexing Ying), *Ann. Math. Sci. Appl.* **1**, 321–339 (2016).

Half-space kinetic equations with general boundary conditions
(with Qin Li and Weiran Sun), *Math. Comp.* **86**, 1269–1301 (2017).

Combining 2D synchrosqueezed wave packet transform with optimization for crystal image analysis
(with Benedikt Wirth and Haizhao Yang), *J. Mech. Phys. Solids* **89**, 194–210 (2016).

Sparsifying preconditioner for soliton calculations
(with Lexing Ying), *J. Comput. Phys.* **315**, 458–466 (2016).

Localized density matrix minimization and linear scaling algorithms
(with Rongjie Lai), *J. Comput. Phys.* **315**, 194–210 (2016).

Crystal image analysis using 2D synchrosqueezed transforms
(with Haizhao Yang and Lexing Ying), *Multiscale Model. Simul.* **13**, 1542–1572 (2015).

Gentlest ascent dynamics for calculating first excited state and exploring energy landscape of Kohn-Sham density functionals
(with Chen Li and Weitao Yang), *J. Chem. Phys.* **143**, 224110 (2015).

Compression of the electron repulsion integral tensor in tensor hypercontraction format with cubic scaling cost
(with Lexing Ying), *J. Comput. Phys.* **302**, 329–335 (2015).

Orbital-free density functional theory of out-of-plane charge screening in graphene
(with Vitaly Moroz and Cyrill B. Muratov), *J. Nonlinear Sci.* **25**, 1391–1430 (2015).

Analysis of the divide-and-conquer method for electronic structure calculations
(with Jingrun Chen), *Math. Comp.* **85**, 2919–2938 (2016).

Diffusion approximations of linear transport equations: Asymptotics and numerics
(with Qin Li and Weiran Sun), *J. Comput. Phys.* **292**, 141–167 (2015).

Numerical scheme for a spatially inhomogeneous matrix-valued quantum Boltzmann equation
(with Christian Mendl), *J. Comput. Phys.* **291**, 303–316 (2015).

Quantitative canvas weave analysis using 2D synchrosqueezed transforms
Haizhao Yang, Jianfeng Lu, William P. Brown, Ingrid Daubechies, and Lexing Ying,
IEEE Signal Process. Mag. **32**, 55–63 (2015).

Emergence of step flow from atomistic scheme of epitaxial growth in 1 + 1 dimensions
(with Jian-Guo Liu and Dionisios Margetis), *Phys. Rev. E* **91**, 032403 (2015).

Efficient rare event simulation for failure problems in random media
(with Jingchen Liu and Xiang Zhou), *SIAM J. Sci. Comput.* **37**, A609–A624 (2015).

Classification of whale vocalizations using the Weyl transform
Yin Xian, Andrew Thompson, Qiang Qiu, Loren Nolte, Douglas Nowacek, Jianfeng Lu, Robert Calderbank,
2015 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP), 773–777 (2015).

Density matrix minimization with ℓ_1 regularization
(with Rongjie Lai and Stanley Osher), *Commun. Math. Sci.* **13**, 2097–2117 (2015).

Strang splitting methods for a quasilinear Schrodinger equation - convergence, instability and dynamics
(with Jeremy L. Marzuola), *Commun. Math. Sci.* **13**, 1051–1074 (2015).

Reactive trajectories and the transition path processes
(with James Nolen), *Probab. Theory Relat. Fields* **161**, 195–244 (2015).

Stability of a force-based hybrid method with planar sharp interface
(with Pingbing Ming), *SIAM J. Numer. Anal.* **52**, 2005–2026 (2014).

Excitation energies from particle-particle random phase approximation: Davidson algorithm and benchmark studies
Yang Yang, Degao Peng, Jianfeng Lu, and Weitao Yang, *J. Chem. Phys.* **141**, 124104 (2014).

Nonexistence of a minimizer for Thomas-Fermi-Dirac-von Weizsäcker model
(with Felix Otto), *Comm. Pure Appl. Math.* **67**, 1605–1617 (2014).

Exact dynamical coarse-graining without time-scale separation
(with Eric Vanden-Eijnden), *J. Chem. Phys.* **141**, 044109 (2014).

A variational perspective on cloaking by anomalous localized resonance
(with Robert V. Kohn, Ben Schweizer, and Michael I. Weinstein), *Comm. Math. Phys.* **328**, 1–27 (2014).

Mathematical theory of solids: From quantum mechanics to continuum models (invited expository paper)
(with Weinan E), *Discrete Contin. Dyn. Syst. Ser. A* **34** 5085–5097 (2014).

Analysis of the time reversible Born–Oppenheimer molecular dynamics
(with Lin Lin and Sihong Shao), *Entropy* **16**, 110–137 (2014).
Special issue on Molecular Dynamics Simulation, edited by Giovanni Ciccotti, Mauro Ferrario, and Christof Schütte

The landscape of complex networks: Critical nodes and a hierarchical decomposition
(with Weinan E and Yuan Yao), *Methods Appl. Anal.* **20**, 383–404 (2013).
Special issue dedicated to Professor Stanley Osher on the occasion of his 70th birthday.

Seismic modeling using the frozen Gaussian approximation,
(with Sergey Fomel and Xu Yang), SEG Technical Program Expanded Abstracts 2013, pp. 4677–4682.

Infinite swapping replica exchange molecular dynamics leads to a simple simulation patch using mixture potentials
(with Eric Vanden-Eijnden), *J. Chem. Phys.* **138**, 084105 (2013).

Convergence of a force-based hybrid method for atomistic and continuum models in three dimension
(with Pingbing Ming), *Comm. Pure Appl. Math.* **66**, 83–108 (2013).

The Kohn–Sham equation for deformed crystals
(with Weinan E), *Mem. Amer. Math. Soc.* **221**, no. 1040 (2013).

Asymptotic analysis of the quantum dynamics: Bloch–Wigner transform and Bloch dynamics
(with Weinan E and Xu Yang), *Acta Math. Appl. Sin. Engl. Ser.* **29**, 465–476 (2013).

Stability and the continuum limit of the spin-polarized Thomas–Fermi–Dirac–von Weizsäcker model
(with Weinan E), *J. Math. Phys.* **53**, 115615 (2012).
Special issue dedicated to Professor Peter Constantin on the occasion of his 60th birthday.

Optimized local basis function for Kohn–Sham density functional theory
(with Weinan E, Lin Lin, and Lexing Ying), *J. Comput. Phys.* **231**, 4515–4529 (2012).

Frozen Gaussian approximation for general linear strictly hyperbolic system: formulation and Eulerian methods
(with Xu Yang), *Multiscale Model. Simul.* **10**, 451–472 (2012).

Adaptive local basis set for Kohn–Sham density functional theory in a discontinuous Galerkin framework I: Total energy calculation
(with Weinan E, Lin Lin, and Lexing Ying), *J. Comput. Phys.* **231**, 2140–2154 (2012).

Convergence of frozen Gaussian approximation for high frequency wave propagation
(with Xu Yang), *Comm. Pure Appl. Math.* **65**, 759–789 (2012).

Multiscale modeling (invited mini-review article)
(with Weinan E), *Scholarpedia* **6**(10):11527 (2011).

Markov state models based on milestoning
(with Frank Noé, Marco Sarich, Christof Schütte, and Eric Vanden-Eijnden),
J. Chem. Phys. **134**, 204105 (2011).

A fast parallel algorithm for selected inversion of structured sparse matrix with application to 2D electronic structure calculations
(with Weinan E, Lin Lin, Chao Yang, and Lexing Ying), *SIAM J. Sci. Comput.* **33**, 1329–1351 (2011).

Fast construction of hierarchical matrix representation from matrix–vector multiplication
(with Lin Lin and Lexing Ying), *J. Comput. Phys.* **230**, 4071–4087 (2011).

Frozen Gaussian approximation for high frequency wave propagation
(with Xu Yang), *Commun. Math. Sci.* **9**, 663–683 (2011).

Synchrosqueezed wavelet transforms: a tool for empirical mode decomposition
(with Ingrid Daubechies and Hau-Tieng Wu), *Appl. Comp. Harmonic Anal.* **30**, 243–261 (2011).

Effective Maxwell equations from time-dependent density functional theory
(with Weinan E and Xu Yang), *Acta Math. Sin.* **32**, 339–368 (2011).
Special issue dedicated to Professor Hua Loo-Keng on his 100th birth anniversary.

The electronic structure of smoothly deformed crystals: Wannier functions and the Cauchy-Born rule
(with Weinan E), *Arch. Ration. Mech. Anal.* **199**, 407–433 (2011).

SellInv - an algorithm for selected inversion of a sparse symmetric matrix
(with Weinan E, Lin Lin, Juan Meza, Chao Yang, and Lexing Ying),
ACM Trans. Math. Software **37**, article no. 40 (2011).

The electronic structure of smoothly deformed crystals: Cauchy-Born rule for nonlinear tight-binding model
(with Weinan E), *Comm. Pure Appl. Math.* **63**, 1432–1468 (2010).

Localized basis of eigen-subspaces and operator compression
(with Weinan E and Tiejun Li), *Proc. Natl. Acad. Sci. USA* **107**, 1273–1278 (2010).

Fast algorithm for extracting the diagonal of the inverse matrix with application to the electronic structure analysis of metallic systems
(with Roberto Car, Weinan E, Lin Lin, and Lexing Ying), *Commun. Math. Sci.* **7**, 755–777 (2009).

Pole-based approximation of the Fermi-Dirac function
(with Weinan E, Lin Lin, and Lexing Ying), *Chin. Ann. Math. Ser. B* **30**, 729–742 (2009).

Special issue dedicated to Professor Andrew Majda on the occasion of his 60th birthday.

Multipole representation of the Fermi operator with application to the electronic structure analysis of metallic systems
(with Roberto Car, Weinan E, and Lin Lin), *Phys. Rev. B* **79**, 115133 (2009).

A linear scaling subspace iteration algorithm with optimally localized non-orthogonal wave functions for Kohn-Sham density functional theory
(with Weinan E, Carlos J. García-Cervera, and Yulin Xuan), *Phys. Rev. B* **79**, 115110 (2009).

Sequential multiscale modelling using sparse representation
(with Weinan E, Carlos J. García-Cervera, and Weiqing Ren), *Commun. Comput. Phys.* **4**, 1025–1033 (2008).
Special issue dedicated to Professor Xiantu He on the occasion of his 70th birthday.

Electronic structure for elastically deformed solids,
Mathematisches Forschungsinstitut Oberwolfach Report **21**, 1123–1125 (2008).

A sub-linear scaling algorithm for computing the electronic structure of materials
(with Weinan E and Carlos J. García-Cervera), *Commun. Math. Sci.* **5**, 999–1024 (2007).

The continuum limit and QM-continuum approximation of quantum mechanical models of solids
(with Weinan E), *Commun. Math. Sci.* **5**, 679–696 (2007).

Seamless multiscale modelling via dynamics on fiber bundles
(with Weinan E), *Commun. Math. Sci.* **5**, 649–663 (2007).

The elastic continuum limit of the tight binding model
(with Weinan E), *Chin. Ann. Math. Ser. B* **28**, 665–675 (2007).

Uniform accuracy of the quasicontinuum method
(with Weinan E and Jerry Z. Yang), *Phys. Rev. B* **74**, 214115 (2006).

PREPRINTS

Solving for high dimensional committor functions using artificial neural networks
(with Yuehaw Khoo and Lexing Ying), 2018

Stochastic dynamical low-rank approximation method
(with Yu Cao), 2018

On discrete Wigner transforms
(with Zhenning Cai and Kevin Stubbs), 2018

Fundamental limitations for measurements in quantum many-body systems
(with Thomas Barthel), 2018

Learning interacting particle systems: diffusion parameter estimation for aggregation equations
(with Hui Huang and Jian-Guo Liu), 2018

Randomized sampling for basis functions construction in generalized finite element methods
(with Ke Chen, Qin Li, and Stephen J. Wright), 2018

Methodological and computational aspects of parallel tempering methods in the infinite swapping limit
(with Eric Vanden-Eijnden), 2017

The full configuration interaction quantum Monte Carlo method in the lens of inexact power iteration
(with Zhe Wang), 2017

Bold diagrammatic Monte Carlo in the lens of stochastic iterative methods
(with Yingzhou Li), 2017

Detecting localized eigenstates of linear operators
(with Stefan Steinerberger), 2017

Solving parametric PDE problems with artificial neural networks
(with Yuehaw Khoo and Lexing Ying), 2017

A diabatic surface hopping algorithm based on time dependent perturbation theory and semiclassical analysis
(with Di Fang), 2017

Discontinuous Hamiltonian Monte Carlo for sampling discrete parameters
Akihiko Nishimura, David Dunson, and Jianfeng Lu, 2017

Asymmetry in crystal facet dynamics of homoepitaxy in a continuum model
(with Jian-Guo Liu, Dionisios Margetis, and Jeremy Marzuola), 2017

A surface hopping Gaussian beam method for high-dimensional transport systems
(with Zhenning Cai), 2017

Analysis of multiscale integrators for multiple attractors and irreversible Langevin samplers
(with Konstantinos Spiliopoulos), 2016

Bloch dynamics with second order Berry phase correction
(with Zhennan Zhou), 2015

An isoperimetric problem with Coulomb repulsion and attraction to a background nucleus
(with Felix Otto), 2015

TEACHING

Duke University	Non-equilibrium Green's function formalism , mini-course, Spring 2018 Real Analysis , Fall 2013, Fall 2014, Fall 2017 Elementary Differential Equations , Fall 2012, Fall 2014, Fall 2017 Locality in Quantum Systems , mini-course, Fall 2016 Applied Computational Analysis , Spring 2016 Functional Analysis , Fall 2015 Variational Methods in Quantum Mechanics , mini-course, Fall 2014 Introduction to Numerical PDEs , Spring 2013
New York University	Chaos and Dynamical System , Spring 2012 Calculus I , Fall 2009, Fall 2011 Calculus II , Fall 2010, Spring 2011 Mechanics , Spring 2010
Summer School	Putting the Theory Back in Density Functional Theory: A summer school IPAM, UCLA, Aug 2016

LBNL/MSRI Summer School on Electronic Structure Theory
(co-organized with Lin Lin and James A. Sethian)
Mathematical Sciences Research Institute, Berkeley, Jul 2016

Topics in Computational Quantum Chemistry,
Summer School in Applied Mathematics,
Peking University, China, Jul 2015

Topics in Many Body Quantum Mechanics,
Summer School in Applied Mathematics,
Peking University, China, Jul 2014

Mathematical Introduction to Quantum Mechanics,
Summer School in Applied Mathematics,
Peking University, China, Jul 2012

Introduction to Multiscale Modelling
Summer School in Applied Mathematics,
Fudan University, China, Aug 2008

RECENT COLLOQUIUM TALKS

- FEB 2017 Stanford University
- OCT 2016 University of North Carolina at Charlotte
- OCT 2015 Statistics Department, University of Chicago
- OCT 2015 Rensselaer Polytechnic Institute
- MAY 2014 Applied Math Colloquium, Pennsylvania State University
- FEB 2014 Indiana University

RECENT SEMINAR TALKS

- 2017 New York University; Max Planck Institute Leipzig; Stanford University; University of Toronto; University of Wisconsin at Madison; Technische Universität München
- 2016 University of Maryland; Yale University
- 2015 Brown University; Georgia Institute of Technology; Max Planck Institute; Purdue University; University of California, Berkeley; University of California, Irvine; University of California, Los Angeles; University of North Carolina, Chapel Hill; University of Southern Carolina; WWU Münster
- 2014 Beijing Computational Science Research Center; Chinese Academy of Sciences; Max Planck Institute Leipzig; Michigan State University; New York University; North Carolina State University; Peking University; Stanford University; University of Michigan
- 2013 Lawrence Berkeley National Laboratory; University of Chicago; University of North Carolina at Chapel Hill; University of North Carolina at Charlotte

RECENT INVITED CONFERENCE PRESENTATIONS

- MAY 2018 QMC Transition Workshop, SAMSI
- MAY 2018 Transport and Localization in Random Media, Columbia University
- OCT 2017 Stochastic Sampling and Accelerated Time Dynamics on Multidimensional Surfaces, IPAM, UCLA
- JUL 2017 Density Functional Theory and Beyond: Analysis and Computation, Mathematics Institute, University of Warwick
- MAY 2017 SAMSI Optimization Transition Workshop, SAMSI
- APR 2017 Selected topics in transport phenomena: deterministic and probabilistic aspects, University of Maryland
- APR 2017 Quantum Control Theory: Mathematical Aspects and Physical Applications, TU Munich, Institute for Advanced Study
- MAR 2017 Dynamics and geometry from high dimensional data, Center of Nonlinear Analysis, Carnegie Mellon University
- JAN 2017 Big Data Meets Computation, IPAM, UCLA
- MAY 2016 Mathematical and Computational Methods in Quantum Chemistry, Yale University
- MAY 2016 Minisymposium on Computational Techniques for Multiscale Materials Modeling,
Minisymposium on Numerical Methods in Multiscale Materials Modelling
Minisymposium on Efficient Numerical Methods and Analytical Techniques for Defect Problems,
SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia
- APR 2016 Boundary Value Problems and Multiscale Coupling Methods for Kinetic Equations, University of Wisconsin-Madison, Madison
- FEB 2016 Computation of Quantum Systems in Cold-matter Physics and Chemistry, Fields Institute, University of Toronto, Toronto
- NOV 2015 Analysis and Computation in Kinetic Theory, Stanford University, Stanford
- AUG 2015 International Conference on Numerical Mathematics and Scientific Computing (ICIAM 2015 Satellite Conference), Nanjing, China
- AUG 2015 Minisymposium on Analysis, Modeling, and Numerical Methods for High Frequency Waves,
Minisymposium on Energy-Driven Pattern Formation,
Minisymposium on Modeling, Simulation and Analysis of Interface and Defect Problems in Solids,
ICIAM 2015, Beijing, China
- AUG 2015 Workshop on Multiscale Modelling and Analysis in Materials Sciences (ICIAM 2015 Satellite Conference), Shanghai, China
- JUN 2015 Workshop on Mathematical Methods in Quantum Molecular Dynamics, Oberwolfach, Germany
- MAY 2015 Groups and interactions in data, networks and biology, Carnegie Mellon University, Pittsburgh
- OCT 2014 Symposium on Mathematical Theory and Computational Techniques for Multiscale Material Modeling, Multiscale Materials Modeling 2014, Berkeley

- OCT 2014 Conference on Nonlinearity, Transport, Physics, and Patterns, The Fields Institute for Research in Mathematical Sciences, Toronto
- JUN 2014 Multiscale materials modeling: mathematical and computational aspects, International Center for Applied Computational Mechanics, Rensselaer Polytechnic Institute, Troy
- MAR 2014 KI-Net: Mathematical and Numerical Methods for Complex Quantum Systems, University of Illinois at Chicago, Chicago
- MAR 2014 Model-Data Integration in Physical Systems, Isaac Newton Institute for Mathematical Sciences, University of Cambridge, United Kingdom

STUDENTS & POSTDOCS

PhD students

Charlio Xu, 2014 – 2017
Kyle Thicke, 2015 – current
Yu Cao, 2016 – current
Jeffrey LaComb, 2016 – current
Kevin Stubbs, 2016 – current
Zhe Wang, 2016 – current
Lihan Wang, 2017 – current

Postdoctoral scholars

Zhennan Zhou, 2014 – 2017 (now Assistant Professor at BICMR, Peking University)
Haizhao Yang, 2015 – 2017 (now Assistant Professor at National University of Singapore)
Zhenning Cai, 2016 (now Assistant Professor at National University of Singapore)
Yingzhou Li, 2017 – current
Yulong Lu (co-mentored with Jonathan Mattingly), 2017 – current
Alexander Watson, 2017 – current
Mathias Sachs (SAMSI postdoc, co-mentored with Jonathan Mattingly), 2017 – current

Undergraduate mentoring

Leslie Lei, PRUV Fellow, Summer 2013 – Spring 2014 (now graduate student at Stanford)
Fuchsia Chen, PRUV Fellow, Summer 2015 (now graduate student at Harvard)
Austin Ferguson, MathBio REU, Summer 2015
Jeremy Tay, Research Independent Study, Fall 2015
Matthew Gherman, PRUV Fellow, Summer 2016
Ji Won Park, DOMath, Summer 2017
Junmo Ryang, DOMath, Summer 2017
Shengtong Zhang (Tsinghua Univ.), Undergraduate Internship, Summer 2017
Mo Zhou (Tsinghua Univ.), Undergraduate Internship, Summer 2017
Qinyi Zhu (Nankai Univ.), Undergraduate Internship, Summer 2017

SERVICE

Editorial service

Communications in Mathematical Sciences, Associate Editor (2017 – 2020)
Springer Book Series on *Mathematics of Molecular Modeling*, Series Editor (2017 –)

Journal and book refereeing

Adv. Comput. Math.; Appl. Comp. Harmonic Anal.; Arch. Ration. Mech. Anal.; Comm. Pure Appl. Math.; Commun. Comput. Phys.; Commun. Math. Sci.; Comput. Math. Appl.; Comput. Methods Appl. Mech. Eng.; ESAIM: COCV; IEEE Signal Processing Lett.; IEEE Trans. Signal Proc.; J. Amer. Math. Soc.; J. Chem. Phys.; J. Chem. Theory Comput.; J. Comput. Phys.; J. Mech. Phys. Solids; J. Nonlinear Sci.; J. Stat. Phys.; Math. Method. Appl. Sci.; Math. Phys. Anal. Geom.; Multiscale Model. Simul.; Phys. Rev. B; Proc. Natl. Acad. Sci. USA; Proc. R. Soc. A; Res. Math. Sci.; Sci. China Math.; SIAM J. Appl. Math.; SIAM J. Imaging Sci.; SIAM J. Math. Anal.; SIAM J. Numer. Anal.; SIAM J. Sci. Comput.

Lecture Notes in Mathematics, Springer; Princeton University Press

2011 top referee award for the journal Proceedings of the Royal Society A

Grant proposal refereeing

European Research Council
National Science Foundation (ad hoc review and review panels)
Conference proposals of Banff International Research Station

Conference organization

Workshop on Mathematical and Numerical Aspects of Quantum Dynamics
(co-organized with Eitan Tadmor)
CSCAMM, University of Maryland, June 2018

42nd SIAM Southeastern Section Conference (SIAM-SEAS 2018)
(co-organized with Xiuyuan Cheng, Alina Chertock, Greg Forest, Mansoor Haider, and Katie Newhall)
UNC Chapel Hill, March 2018

SAMSI Workshop on trends and advances in Monte Carlo sampling algorithms
(co-organized with David Dunson, Ben Leimkuhler, Mauro Maggioni)
SAMSI and Duke University, December 2017

Quantum dynamics focus meeting: the FGA-SH method
(co-organized with Sara Bonella and Giovanni Ciccotti)
CECAM, EPFL, Lausanne, May 2017

Workshop on Mathematical and Physical Aspects of Topologically Protected States
(co-organized with Shi Jin and Michael I. Weinstein)
Columbia University, May 2017

Workshop on Optimization under Uncertainty and Data-Driven Science and Engineering
(co-organized with Wilkins Aquino, Robert Calderbank, Drew Kouri, and Michael Zavlanos)
Duke University, April 2017

KI-Net Young Researchers Workshop
(co-organized with Jacob Bedrossian, Alina Chertock, and Zhennan Zhou)
Duke University, November 2016

Algorithms and Applications for Excited State Electronic Structure Theories
(co-organized with Wei Cai, Lin Lin, Limin Liu, and Chi-Yung Yam)
Beijing Computational Science Research Center, August 2016

Mathematical and Computational Methods in Quantum Chemistry
(co-organized with Victor Batista, Shi Jin, Qin Li, and Weitao Yang),

Yale University, May 2016

Collective Dynamics in Biological and Social Systems
(co-organized with Alina Chertock and Jian-Guo Liu),
Duke University, November 2015

Summer Program on Electronic Structure Analysis and Computation
(co-organized with Lexing Ying),
Shanghai Jiao Tong University, China, Summer 2011

Minisymposia/symposia organization

Recent Advances in Stochastic Processes and Stochastic Computation
(with J. Nolen and K. Spiliopoulos)
AMS Fall Southeastern Sectional Meeting 2016

Mathematics and Algorithms for Ground State Electronic Structure Theory (with G. Friesecke and L. Lin),
Microscopic, Mesoscale and Macroscale Models in Mechanics (with D. Margetis),
SIAM Conference on Mathematical Aspects of Materials Science 2016 (SIAM MS16)

PDEs for Defects Problems in Materials Science (with Y. Xiang),
SIAM Conference on Analysis of Partial Differential Equations 2015 (SIAM PD15)

Analysis and Algorithm for Coupling of Kinetic and Fluid Equations (with W. Sun),
Rare Events in Complex Physical Systems (with M. Cameron, T. Li, J. Weare and X. Zhou),
Mathematical and Numerical Aspects of Electronic Structure Theory (with L. Lin),
8th International Congress on Industrial and Applied Mathematics (ICIAM 2015)

Mathematical Theory and Computational Techniques for Multiscale Materials Modeling
(with C. Linder, C.J. Garcia-Cervera, D. Kochmann, X. Li, W. Ren and Y. Xiang),
Multiscale Materials Modeling 2014 (MMM2014)

Efficient Simulation of Rare Events (with J. Liu and X. Zhou),
SIAM Conference on Uncertainty Quantification 2014 (SIAM UQ14)

Multiscale Simulation of Materials (with M. Luskin and C. Ortner)
SIAM Conference on Mathematical Aspects of Materials Science 2013 (SIAM MS13)

Outreach activity

SAMSI E&O Undergraduate Workshop, February 26–27, 2018

Faculty advisor for student research program at North Carolina School of Science and Mathematics, 2015–2016

Member of NATIONAL OLYMPIAD IN INFORMATICS (NOI) Scientific Committee, Chinese Computer Federation,
2003–2005