Jianfeng Lu

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

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January 27, 2017

POSITIONS

2016 –	**Associate Professor,** Department of Mathematics
2012 – 2016	Assistant Professor, Department of Mathematics
2013 –	Secondary appointment in Department of Physics
2013 –	Secondary appointment in Department of Chemistry
2015 –	Affiliated member of the Fitzpatrick Institute of Photonics
	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

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

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.*, in press

Continuum limit of a mesoscopic model of step motion on vicinal surfaces
(with Yuan Gao and Jian-Guo Liu), *J. Nonlinear Sci.*, in press

A convergent method for linear half-space kinetic equations
(with Qin Li and Weiran Sun), *Math. Model. Numer. Anal.*, in press

Validity and regularization of classical half-space equations
(with Qin Li and Weiran Sun), *J. Stat. Phys.*, in press

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.*, in press

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 nonadiabatic 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.*, in press

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.*, in press

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.*, in press

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).

SelInv - 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

Path integral molecular dynamics with surface hopping for thermal equilibrium sampling of non-adiabatic systems
(with Zhennan Zhou), 2017

Fractional stochastic differential equations satisfying fluctuation-dissipation theorem
(with Lei Li and Jian-Guo Liu), 2016

A variation on the Donsker-Varadhan inequality for the principal eigenvalue
(with Stefan Steinerberger), 2016

Kohn-Sham density functionals with fractional number of electrons
(with Chen Li and Weitao Yang), 2016

Wavepackets in inhomogeneous periodic media: Effective particle-field dynamics and Berry curvature
(with Alexander Watson and Michael I. Weinstein), 2016

A cubic scaling algorithm for excited states calculations in particle-particle random phase approximation
(with Haizhao Yang), 2016

Moderate deviation for random elliptic PDEs with small noise
(with Xiaoou Li, Jingchen Liu, and Xiang Zhou), 2016

An asymptotic preserving method for transport equations with oscillatory scattering coefficients
(with Qin Li), 2016

A mathematical theory of optimal milestoning (with a detour via exact milestoning)
(with Ling Lin and Eric Vanden-Eijnden), 2016

A hybrid global-local numerical method for multiscale PDEs
(with Yufang Huang and Pingbing Ming), 2016

Thermodynamic limit of crystal defects with finite temperature tight binding
(with Huajie Chen and Christoph Ortner), 2016

Quasinonlocal coupling of nonlocal diffusions
(with Xingjie Helen Li), 2016

Multiscale integrators for stochastic differential equations and irreversible Langevin samplers
(with Konstantinos Spiliopoulos), 2016

Convergence of phase-field free energy and boundary force for molecular solvation
(with Shibin Dai and Bo Li), 2016

Orbital minimization method with ℓ^1 regularization
(with Kyle Thicke), 2016

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

Frozen Gaussian approximation for high frequency wave propagation in periodic media
(with Ricardo Delgadillo and Xu Yang), 2015

Teaching

Duke University	**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 **Real Analysis**, Fall 2013, Fall 2014 **Introduction to Numerical PDEs**, Spring 2013 **Elementary Differential Equations**, Fall 2012, Fall 2014
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 (upcoming); Max Planck Institute Leipzig (upcoming); Stanford University (upcoming); University of Wisconsin at Madison (upcoming)
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

Apr 2017	(upcoming) Selected topics in transport phenomena: deterministic and probabilistic aspects, University of Maryland
Apr 2017	(upcoming) Quantum Control Theory: Mathematical Aspects and Physical Applications, TU Munich, Institute for Advanced Study
Mar 2017	(upcoming) Dynamics and geometry from high dimensional data, Center of Nonlinear Analysis, Carnegie Mellon University
Jan 2017	(upcoming) 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
  Dangxing Chen (UNC Chapel Hill), 2015 – 2017 (expected), co-advised with Jingfang Huang.
  Charlio Xu, 2014 – 2017 (expected)
  Kyle Thicke, 2015 – current
  Yu Cao, 2016 – current
  Jeffrey LaComb, 2016 – current
  Kevin Subbs, 2016 – current
  Zhe Wang, 2016 – current

Postdoctoral scholars
  Zhennan Zhou, 2014 – current
  Haizhao Yang, 2015 – current
  Zhenning Cai, 2016 (now Assistant Professor at National University of Singapore)

Undergraduate mentoring
  Leslie Lei, PRUV Fellow, Summer 2013 – Spring 2014 (now PhD student at Stanford University)
  Fuchsia Chen, PRUV Fellow, Summer 2015
  Austin Ferguson, MathBio REU student, Summer 2015
  Jeremy Tay, Research Independent Study, Fall 2015
  Matthew Gherman, PRUV Fellow, Summer 2016

SERVICE

Editorial board
  Communications in Mathematical Sciences, Associate Editor (2017 – 2020)

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.;   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

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

Mini-workshop on mixed quantum-classical dynamics
(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, 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. Spiliopoulous)
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

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

Member of AMS and SIAM