Jianfeng Lu

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

Phone: (919) 660-2875
EMAIL: jianfeng@math.duke.edu
HOMEPAGE: http://www.math.duke.edu/~jianfeng/

May 17, 2024

Positions

2024 –	**J.B. Duke Distinguished Professor**
2020 –	Professor, Department of Mathematics
2016 – 2020	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
2019 –	Affiliated faculty member of the Rhodes Information Initiative at Duke
2017 –	Affiliated faculty member of the Duke Materials Initiative
2015 –	Affiliated faculty member of the Fitzpatrick Institute of Photonics Duke University
Spring 2021	**Simons Participant and Senior Fellow** Institute of Pure and Applied Mathematics
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 and Recognitions

2023	**Feng Kang Prize**
2023	**Fellow**, American Mathematical Society
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.*

Books, review or expository articles

Thermodynamic limits of electronic systems
with David Gontier and Christoph Ortner, *Density Functional Theory: Modeling, Mathematical Analysis, Computational Methods, and Applications*. ed. Eric Cances and Gero Friesecke, Springer 2023

Recent progresses for evaluating the Kohn-Sham map
with Lin Lin and Lexing Ying, *Density Functional Theory: Modeling, Mathematical Analysis, Computational Methods, and Applications*. ed. Eric Cances and Gero Friesecke, Springer 2023

Proceedings of Conference on Mathematical and Scientific Machine Learning 2020
Proceedings of Machine Learning Research. Volume 107 (co-edited with Rachel Ward)

Mathematical Introduction to Electronic Structure Theory
with Lin Lin, SIAM, June 2019

Numerical Methods for Kohn-Sham density functional theory
with Lin Lin and Lexing Ying, *Acta Numer.* **28**, 405–539 (2019).

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

Multiscale modeling
with Weinan E, *Scholarpedia* **6**(10):11527 (2011).

Preprints

Mixing time of open quantum systems via hypocoercivity
with Di Fang and Yu Tong, 2024

Fully discretized Sobolev gradient flow for the Gross-Pitaevskii eigenvalue problem
with Ziang Chen, Yulong Lu, and Xiangxiong Zhang, 2024

Learning memory kernel in generalized Langevin equations
with Quanjun Lang, 2024

Exact and efficient representation of totally anti-symmetric functions
with Ziang Chen, 2023

Asymptotic analysis for Bloch electrons with Weyl nodes
with Changhe Yang, and Zhennan Zhou, 2023

Convergence of flow-based generative models via proximal gradient descent in Wasserstein space
with Xiuyuan Cheng, Yixin Tan, and Yao Xie, 2023

Diffusion methods for generating transition paths
with Luke Triplett, 2023

Riemannian Langevin Monte Carlo schemes for sampling PSD matrices with fixed rank
Tianmin Yu, Shixin Zheng, Jianfeng Lu, Govind Menon, and Xiangxiong Zhang, 2023

Quantum variational embedding of ground-state energy problems: sum of squares and cluster selection
with Bowen Li, 2023

Accelerate Langevin sampling with birth-death process and exploration component
with Lezhi Tan, 2023

Convergence of stochastic gradient descent under a local Łajasiewicz condition for deep neural networks
with Jing An, 2023

A policy gradient framework for stochastic optimal control problems with global convergence guarantee
with Mo Zhou, 2023

Interpolation between modified logarithmic Sobolev and Poincaré inequalities for quantum Markovian dynamics
with Bowen Li, 2022

Vector-wise joint diagonalization of almost commuting matrices
with Bowen Li and Ziang Yu, 2022

Asymptotic analysis of diabatic surface hopping algorithm in the adiabatic and non-adiabatic limits
with Zhenning Cai and Di Fang, 2022

Optimal artificial boundary conditions based on second-order correctors for three dimensional random elliptic media
with Felix Otto and Lihan Wang, 2021

Finite second moment implies Chern triviality in non-periodic insulators
with Kevin Stubbs, 2021

Structure-preserving numerical schemes for Lindblad equations
with Yu Cao, 2021

Algebraic localization implies exponential localization in non-periodic insulators
with Kevin Stubbs, 2021

Numerical orbital stability of bright solitons in the exciton-polariton system and error estimates
Trang Nguyen, Andreas C. Aristotelous, Jianfeng Lu, and Stephanos Venakidis, 2020

Non-convex planar harmonic maps
Shahar Kovalsky, Noam Aigerman, Ingrid Daubechies, Michael Kazhdan, Jianfeng Lu, and Stefan Steinerberger, 2020

Accelerating Langevin sampling with birth-death
with Yulong Lu and James Nolen, 2019

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

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

Referred journal or conference publications

Regularized Stein variational gradient flow
Ye He, Krishnakumar Balasubramanian, Bharath K. Sriperumbudur, Jianfeng Lu, *Found. Comput. Math.*

One-dimensional tensor network recovery
with Ziang Chen and Anru Zhang, *SIAM J. Matrix Anal. Appl.*

Qubit count reduction by orbital optimization for variational quantum excited states solvers
with Joel Bierman and Yingzhou Li, *J. Chem. Theory Comput.*

Score-based transport modeling for mean-field Fokker-Planck equations
with Yue Wu and Yang Xiang, *J. Comput. Phys.*

Locality of the windowed local density of states
with Terry A. Loring and Alexander Watson, *Numer. Math.*

Deep network approximation: Beyond ReLU to diverse activation functions
Shijun Zhang, Jianfeng Lu, and Hongkai Zhao, *J. Mach. Learn. Res.*

On the convergence of Sobolev gradient flow for the Gross-Pitaevskii eigenvalue problem
with Ziang Chen, Yulong Lu, and Xiangxiong Zhang, *SIAM J. Numer. Anal.*

Representation theorem for multivaraible totally symmetric functions
with Chongyao Chen and Ziang Chen, *Commun. Math. Sci.*

DYNATE: Localizing Rare-Variant Association Regions via Multiple Testing Embedded in an Aggregation Tree
Li, X; Pura, J; Allen, A; Owzar, K; Lu, J; Harms, M; and Xie, J., *Genetic Epidemiology*

A deep learning framework for geodesics under sphereical Wasserstein-Fisher-Rao metric and its application for weighted sample generation
with Yang Jing, Jiaheng Chen, and Lei Li, *J. Sci. Comput.*

Coordinate descent full configuration interaction for excited states
Zhe Wang, Zhiyuan Zhang, Jianfeng Lu, and Yingzhou Li, *J. Chem. Theory Comput.*

Deep equilibrium based neural operators for steady-state PDEs
Tanya Marwah, Ashwini Pokle, Zico Kolter, Zachary Lipton, Jianfeng Lu, and Andrej Risteski, *NeurIPS 2023*

The probability flow ODE is provably fast
with Sitan Chen, Sinho Chewi, Holden Lee, Yuanzhi Li, and Adil Salim, *NeurIPS 2023*

On explicit L^2-convergence rate estimate for underdamped Langevin dynamics
with Yu Cao and Lihan Wang, *Arch. Ration. Mech. Anal.*

Single time-scale actor-critic method to solve the linear quadratic regulartor with convergence guarantees
with Mo Zhou, *J. Mach. Learn. Res.*

Global optimality of Elman-type RNN in the mean-field regime
with Andrea Agazzi and Sayan Mukherjee, *ICML 2023*

On enhancing expressive power via compositions of single fixed-size ReLU network
wiht Shijun Zhang and Hongkai Zhao, *ICML 2023*

Improved analysis of score-based generative modeling: User-friendly bounds under minimal smoothness assumptions
with Hongrui Chen and Holden Lee, *ICML 2023*

Neural network approximations of PDEs beyond linearity: a representational perspective
Tanya Marwah, Zachary Lipton, Jianfeng Lu, and Andrej Risteski, ICML 2023

Edge state dynamics along curved interfaces
with Guillaume Bal, Simon Becker, Alexis Drouot, Clotilde Fermanian Kammerer and Alexander Watson, *SIAM J. Math. Anal.*

HeteRSGD: Tackling heterogeneous sampling costs via optimal reweighted stochastic gradient descent
Ziang Chen, Jianfeng Lu, Huajie Qian, Xinshang Wang, and Wotao Yin, *AISTATS 2023*

Neural network based variational methods for solving quadratic porous medium equations in high dimensions
with Min Wang, *Commun. Math. Statis.*

Convergence of score-based generative modeling for general data distributions
with Holden Lee and Yixin Tan, *ALT 2023*

Improving the accuracy of variational quantum eigensolvers with fewer qubits using orbital optimization
with Joel Bierman and Yingzhou Li, *J. Chem. Theory Comput.*

On the global convergence of randomized coordinate gradient descent for non-convex optimization
with Ziang Chen and Yingzhou Li, *SIAM J. Opt.*

A regularity theory for static Schrödinger equations on $\mathbb{R}^d$ in spectral Barron spaces
with Ziang Chen, Yulong Lu, and Shengxuan Zhou, *SIAM J. Math. Anal.*

Geometry of backflow transformation ansatz for quantum many-body Fermionic wavefunctions
with Hang Huang and Joseph M. Landsberg, *Commun. Math. Sci.*

Convergence for score-based generative modeling with polynomial complexity
with Holden Lee and Yixin Tan, *NeurIPS 2022 (oral)*

A proximal-gradient algorithm for crystal surface evolution
with Katy Craig, Jian-Guo Liu, Jeremy Marzuola, and Li Wang, *Numer. Math.*

Symmetry breaking in density functional theory due to Dirac exchange for a Hydrogen molecule
with Michael Holst, Houdong Hu, Jeremy L. Marzuola, Duo Song, and John Weare, *J. Nonlinear Sci.*

Posterior computation with the Gibbs zig-zag sampler
Matthias Sachs, Deborshee Sen, Jianfeng Lu, and David Dunson, *Bayesian Anal.*

Quantum orbital minimization method for excited states calculation on quantum computer
with Joel Bierman and Yingzhou Li, *J. Chem. Theory Comput.*

Fast algorithms of bath calculations in simulations of quantum system-bath dynamics
with Zhenning Cai and Siyao Yang, *Comput. Phys. Commun.*

On the closedness and geometry of tensor network state sets
with Thomas Barthel and Gero Friesecke, *Lett. Math. Phys.*

Numerical analysis for inchworm Monte Carlo method: Sign problem and error growth
with Zhenning Cai and Siyao Yang, *Math. Comp.*

Neural-network quantum states for periodic systems in continuous space
Gabriel Pescia, Jiequn Han, Alessandro Lovato, Jianfeng Lu, and Giuseppe Carleo, *Phys. Rev. Research*

Complexity of zigzag sampling algorithm for strongly log-concave distributions
with Lihan Wang, *Statist. Comput.*

Low-rank approximation for multiscale PDEs
with Ke Chen, Shi Chen, Qin Li, and Stephen J. Wright, *Notices Amer. Math. Soc.*

Manifold learning and nonlinear homogenization
with Shi Chen, Qin Li and Stephen J. Wright, *Multiscale Model. Simul.*

Machine Learning for Elliptic PDEs: Fast Rate Generalization Bound, Neural Scaling Law and Minimax Optimality
Yiping Lu, Haoxuan Chen, Jianfeng Lu, Lexing Ying, Jose Blanchet, *ICLR 2022*

A priori generalizaiton error analysis of two-layer neural networks for solving high dimensional Schrödinger eigenvalue problem
with Yulong Lu, *Comm. Amer. Math. Soc.*

Universal approximation of symmetric and anti-symmetric functions
with Jiequn Han, Yingzhou Li, Lin Lin, Jiefu Zhang, and Linfeng Zhang, *Commun. Math. Sci.*

Neural collapse with cross-entropy loss
with Stefan Steinerberger, *Appl. Comput. Harmonic Anal.*

Existence and computation of generalized Wannier functions for non-periodic systems in two dimensions and higher
with Kevin Stubbs and Alexander Watson, *Arch. Ration. Mech. Anal.*

Fast localization of eigenfuncitons via smoothed potentials
with Cody Murphey and Stefan Steinerberger, *J. Sci. Comput.* **90**, 38 (2022).

On the representation of solutions to elliptic PDEs in Barron spaces
with Ziang Chen and Yulong Lu, *NeurIPS 2021 (spotlight)*

Actor-critic method for high dimensional static Hamilton-Jacobi-Bellman partial differential equations based on neural networks
Mo Zhou, Jiequn Han, and Jianfeng Lu, *SIAM J. Sci. Comput.*

Defect resonances of truncated crystal structures
with Jeremy Marzuola and Alexander Watson, *SIAM J. Appl. Math.*

Stable phase recovery from locally stable and conditionally connected measurements
with Cheng Cheng, Ingrid Daubechies, and Nadav Dym, *Appl. Comput. Harmonic Anal.*

Microscopic origins of the crystallographically preferred growth in evaporation-induced colloidal crystals
Ling Li, Carl Goodrch, Haizhao Yang, Katherine R. Phillips, Zian Jia, Hongshun Chen, Lifeng Wang, Jinjin Zhong, Anhua Liu, Jianfeng Lu, Jianwei Shuai, Michael P. Brenner, Frans Spaepen, and Joanna Aizenberg, *Proc. Natl. Acad. Sci. USA*

Deep Network Approximation for Smooth Functions
with Zuowei Shen, Haizhao Yang, and Shijun Zhang, *SIAM J. Math. Anal.*

On explicit L^2-convergence rate estimate for piecewise deterministic Markov processes
with Lihan Wang, *Ann. Appl. Probab.*

Inclusion-exclusion principle for bosonic many-body digrammatics: Algorithm and analysis
with Siyao Yang and Zhenning Cai, *New J. Phys.*

A priori generalization analysis of the deep Ritz method for solving high dimensional elliptic equations
with Yulong Lu and Min Wang, *COLT 2021*

Random coordinate Langevin Monte Carlo
with Zhiyan Ding, Qin Li and Stephen J. Wright, *COLT 2021*

Analysis of a fourth order exponential PDE arising from a crystal surface jump process with Metropolis-type transition rates
with Yuan Gao, Anya E. Katsevich, Jian-Guo Liu, and Jeremy L. Marzuola, *Pure Appl. Anal.*

Convergence of stochastic-extended Lagrangian molecular dynamics method for polarizable force field simulation
with Dong An, Sara Y. Cheng, Teresa Head-Gordon, and Lin Lin, *J. Comput. Phys.*

Temporal-difference learning for nonlinear value function approximation: lazy training and mean field regimes
with Andrea Agazzi, *MSML 2021*

A grid-free approach for simulating sweep and cyclic voltammetry
Alec Coffman, Jianfeng Lu, and Joseph Subotnik, *J. Chem. Phys.*

Complexity of randomized algorithms for underdamped Langevin dynamics
with Yu Cao and Lihan Wang, *Commun. Math. Sci.*

Bloch dynamics with second order Berry phase correction
with Zihang Zhang and Zhennan Zhou, *Asymptotic Anal.*

A low-rank Schwarz method for radiative transport equation with heterogeneous scattering coefficient
with Ke Chen, Qin Li and Stephen J. Wright, *Multiscale Model. Simul*

Numerical methods for stochastic differential equations based on Gaussian mixture
with Lei Li, Jonathan Mattingly and Lihan Wang, *Commun. Math. Sci.*

Random coordinate underdamped Langevin Monte Carlo
with Zhiyan Ding, Qin Li and Stephen J. Wright, *AISTATS 2021*

The iterated projected position algorithm for constructing exponentially localized generalized Wannier functions for periodic and non-periodic insulators in two dimensions and higher
with Kevin Stubbs and Alexander Watson, *Phys. Rev. B* **103**, 075125 (2021).

Global optimality of softmax policy gradient with single hidden layer neural networks in the mean-field regime
with Andrea Agazzi, *ICLR 2021*

Efficient construction of tensor ring representations from sampling
with Yuehaw Khoo and Lexing Ying, *Multiscale Model. Simul.*

Computing edge states without hard truncation
with Kyle Thicke and Alexander Watson, *SIAM J. Sci. Comput.* **43**, B323–B353 (2021).

Efficient sampling from the Bingham distribution
with Rong Ge, Holden Lee, and Andrej Risteski, *ALT 2021*

Optimal artificial boundary condition for elliptic random media
with Felix Otto, *Found. Comput. Math.*

Butterfly-Net: Optimal function representation based on convolutional neural networks
Yingzhou Li, Xiuyuan Cheng, Jianfeng Lu, *Commun. Comput. Phys.* **28**, 1838–1885 (2020).
(Special issue on Machine Learning for Scientific Computing)

Ensemble Kalman inversion for nonlinear problems: Weights, consistency, and variance bounds
with Zhiyan Ding and Qin Li, *Found. Data Sci.* (Special issue on Data Assimilation)

A universal approximation theorem of deep neural networks for expressing distributions
with Yulong Lu, *NeurIPS 2020*

Solving high-dimensional eigenvalue problems using deep neural network: A diffusion Monte Carlo like approach
with Jiequn Han and Mo Zhou, *J. Comput. Phys.*

Continuum limit and preconditioned Langevin sampling of the path integral molecular dynamics
with Yulong Lu and Zhennan Zhou, *J. Comput. Phys.*

Optimal orbital selection for full configuration interaction (OptOrbFCI): Pursuing basis set limit under budget
with Yingzhou Li, *J. Chem. Theory Comput.*

Random sampling and efficient algorithms for multiscale PDEs
with Ke Chen, Qin Li, and Stephen J. Wright, *SIAM J. Sci. Comput.*

Tensor ring decomposition: Energy landscape and one-loop convergence of alternating least squares
with Ziang Chen and Yingzhou Li, *SIAM J. Matrix Anal. Appl.*

Synchronization of Kuramoto oscillators in dense networks
with Stefan Steinerberger, *Nonlinearity* **33**, 5905 (2020).

ELSI – An Open Infrastructure for Electronic Structure Solvers
Victor Wen-zhe Yu, Carmen Campos, William Dawson, Alberto García, Ville Havu, Ben Hourahine, William P Huhn, Mathias Jacquelin, Weile Jia, Murat Keçeli, Raul Laasner, Yingzhou Li, Lin Lin, Jianfeng Lu, Jonathan Moussa, Jose E Roman, Álvaro Vázquez-Mayagoitia, Chao Yang, and Volker Blum
Comput. Phys. Commun. **256**, 107459 (2020).

A mean field analysis of deep ResNet and beyond: Towards provably optimization via overparameterization from depth
Yiping Lu, Chao Ma, Yulong Lu, Jianfeng Lu, and Lexing Ying, *ICML 2020*

Solving parametric PDE problems with artificial neural networks
with Yuehaw Khoo and Lexing Ying, *Eur. J. Appl. Math.*, in press

Optimal trapping for Brownian motion: a nonlinear analogue of the torsion function
with Stefan Steinerberger, *Potential Anal.*

Fisher information regularization schemes for Wasserstein gradient flows
with Wuchen Li and Li Wang, *J. Comput. Phys.* **416**, 109449 (2020)

Analysis of a continuum theory for broken bond crystal surface models with evaporation and deposition effects
with Yuan Gao, Jian-Guo Liu, and Jeremy L. Marzuola, *Nonlinearity* **33**, 3816–3845 (2020)

Estimating normalizing constants for log-concave distributions: Algorithms and lower bounds
with Rong Ge and Holden Lee, *STOC 2020*

Variational training of neural network approximations of solution maps for physical models
with Yingzhou Li and Anqi Mao, *J. Comput. Phys.* **409**, 109338 (2020)

Dirac operators and domain walls
with Alexander Watson and Michael I. Weinstein, *SIAM J. Math. Anal.* **52**, 1115–1145 (2020).

A stochastic version of Stein variational gradient descent for efficient sampling
with Lei Li, Yingzhou Li, Jian-Guo Liu, and Zibu Liu, *Comm. App. Math. Comp. Sci.* **15**, 37–63 (2020).

Efficient posterior sampling for high-dimensional imbalanced logistic regression
Deborshee Sen, Matthias Sachs, Jianfeng Lu and David Dunson, *Biometrika*

Tensorization of the strong data processing inequality for quantum chi-square divergence
with Yu Cao, *Quantum* **3**, 199 (2019).

Inchworm Monte Carlo method for open quantum systems
with Zhenning Cai and Siyao Yang, *Comm. Pure Appl. Math.* **73**, 2430–2472 (2020)

Stochastic modified equations for the asynchronous stochastic gradient descent
with Jing An and Lexing Ying, *Inf. Inference*

A dimension-free Hermite-Hadamard inequality via gradient estimates for the torsion function
with Stefan Steinerberger, *Proc. Amer. Math. Soc.* **148**, 673–679 (2020)

Randomized sampling for basis functions construction in generalized finite element methods
with Ke Chen, Qin Li, and Stephen J. Wright, *Multiscale Model. Simul.* **18**, 1153–1177 (2020)

Discontinuous Hamiltonian Monte Carlo for sampling discrete parameters
Akihiko Nishimura, David Dunson, and Jianfeng Lu, *Biometrika* **107**, 365–380 (2020)

Numerical coupling methods of BGK model and Euler equation through linearized Knudsen layer
with Hongxu Chen and Qin Li, *J. Comput. Phys.* **398**, 108893 (2019)

Coordinate-wise descent methods for leading eigenvalue problem
with Yingzhou Li and Zhe Wang, *SIAM J. Sci. Comput.* **41**, A2681–A2716 (2019)

Stop memorizing: A data-dependent regularization framework for intrinsic pattern learning
Wei Zhu, Qiang Qiu, Bao Wang, Jianfeng Lu, Guillermo Sapiro, Ingrid Daubechies, *SIAM J. Math. Data Sci.* **1**, 476–496 (2019)

Exponential decay of Rényi divergence under Fokker-Planck equations
with Yu Cao and Yulong Lu, *J. Stat. Phys.* **176**, 1172–1184 (2019)

Approximating pointwise products of Laplacian eigenfunctions
with Christopher D. Sogge and Stefan Steinerberger, *J. Funct. Anal.* **277**, 3271–3282 (2019)

Coordinate descent full configuration interaction
with Yingzhou Li and Zhe Wang, *J. Chem. Theory Comput.* **15**, 3558–3569 (2019)

Gradient flow structure and exponential decay of the sandwiched Rényi divergence for primitive Lindblad equations with GNS-detailed balance
with Yu Cao and Yulong Lu, *J. Math. Phys.* **60**, 052202 (2019)

Quadrature points via heat kernel repulsion
with Matthias Sachs and Stefan Steinerberger, *Constr. Approx.* **51**, 27–48 (2020)

Asymmetry in crystal facet dynamics of homoepitaxy in a continuum model
with Jian-Guo Liu, Dionisios Margetis, and Jeremy Marzuola, *Phys. D* **393**, 54–67 (2019)

Bold diagrammatic Monte Carlo in the lens of stochastic iterative methods
with Yingzhou Li, *Trans. Math. Appl.* **3**, 1–17 (2019)

Scaling limit of the Stein variational gradient descent: the mean field regime
with Yulong Lu and James Nolen, *SIAM J. Math. Anal.* **51**, 648–671 (2019)

Methodological and computational aspects of parallel tempering methods in the infinite swapping limit
with Eric Vanden-Eijnden, *J. Stat. Phys.* **174**, 715–733 (2019)

Simulated tempering method in the infinite switch limit with adaptive weight learning
with Anton Martinsson, Benedict Leimkuhler and Eric Vanden-Eijnden, *J. Stat. Mech.* **2019**, 013207 (2019)

The full configuration interaction quantum Monte Carlo method through the lens of inexact power iteration
with Zhe Wang, *SIAM J. Sci. Comput.* **42**, B1–B29 (2020)

Solving for high dimensional committor functions using artificial neural networks
with Yuehaw Khoo and Lexing Ying, *Res. Math. Sci.* **6**, 1 (2019)

Analysis of multiscale integrators for multiple attractors and irreversible Langevin samplers
with Konstantinos Spiliopoulos, *Multiscale Model. Simul.* **16**, 1859–1883 (2018)

Learning interacting particle systems: diffusion parameter estimation for aggregation equations
with Hui Huang and Jian-Guo Liu, *Math. Models Methods Appl. Sci.* **29**, 1–29 (2019)

Integrated tempering enhanced sampling method as the infinite switching limit of simulated tempering
Zhiyi You, Liying Li, Jianfeng Lu, and Hao Ge, *J. Chem. Phys.* **149**, 084114 (2018)

A diabatic surface hopping algorithm based on time dependent perturbation theory and semiclassical analysis
with Di Fang, *Multiscale Model. Simul.* **16**, 1603–1622 (2018)

Fundamental limitations for measurements in quantum many-body systems
with Thomas Barthel, *Phys. Rev. Lett.* **121**, 080406 (2018)

Detecting localized eigenstates of linear operators
with Stefan Steinerberger, *Res. Math. Sci.* **5**, 33 (2018)

Stochastic dynamical low-rank approximation method
with Yu Cao, *J. Comput. Phys.* **372**, 564–586 (2018)

A surface hopping Gaussian beam method for high-dimensional transport systems
with Zhenning Cai, *SIAM J. Sci. Comput.* **40**, B1277–B1301 (2018)

Phase space sketching for crystal image analysis based on synchrosqueezed transforms
with Haizhao Yang, *SIAM J. Imaging Sci.* **11**, 1954–1978 (2018)

Thermodynamic limit of crystal defects with finite temperature tight binding
with Huajie Chen and Christoph Ortner, *Arch. Ration. Mech. Anal.* **230**, 701–733 (2018)

Frozen Gaussian approximation for high frequency wave propagation in periodic media
with Ricardo Delgadillo and Xu Yang, *Asymptotic Anal.* **110**, 113–135 (2018)

A quantum kinetic Monte Carlo method for quantum many-body spin dynamics
with Zhenning Cai, *SIAM J. Sci. Comput.* **40**, B706–B722 (2018)

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

A concurrent global-local numerical method for multiscale PDEs
with Yufang Huang and Pingbing Ming, *J. Sci. Comput.* **76**, 1188–1215 (2018)

A quasinonlocal coupling method for nonlocal and local diffusion models
with Qiang Du, Xingjie Helen Li, and Xiaochuan Tian, *SIAM J. Numer. Anal.* **56**, 1386–1404 (2018)

Point cloud discretization of Fokker-Planck operators for committor functions
with Rongjie Lai, *Multiscale Model. Simul.* **16**, 710–726 (2018)

Moderate deviation for random elliptic PDEs with small noise
with Xiaoou Li, Jingchen Liu, and Xiang Zhou, *Ann. Appl. Probab.* **28**, 2781–2813 (2018)

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.* **88**, 717–749 (2019)

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.* **87**, 2189–2232 (2018)

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.* **71**, 1149–1177 (2018)

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.* **3**, 441–472 (2018)

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.* **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)

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)

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)

Teaching

Duke University	**Introduction to Numerical PDEs**, Spring 2013, Spring 2019, Spring 2022, Spring 2023 **Real Analysis**, Fall 2013, Fall 2014, Fall 2017, Fall 2020, Fall 2022 **Analysis and Numerics for High Dimensional PDEs**, Fall 2021 **Computational Methods for Quantum Many-Body Physics** (co-taught with Thomas Barthel), Spring 2020 **Linear Programming**, Spring 2019 **Concentration and Functional Inequalities**, mini-course, Fall 2018 **Stochastic Control and Related Topics**, Fall 2018 **Non-equilibrium Green's function formalism**, mini-course, Spring 2018 **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
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 Colloquia and Plenary Talks

Mar 2024	Pennsylvania State University
Nov 2023	Massachusetts Insitute of Technology
Oct 2023	The 21st Annual Meeting of China Society of Industrial and Applied Mathematics, Kunming (remote participation)
Sep 2023	School of Industrial and Systems Engineering, Georgia Tech
Jul 2023	The 13th Annual Meeting of Chinese Computational Mathematics Society, Nanjing
Feb 2023	Princeton University
Nov 2022	University of Michigan
Oct 2021	Duke Kunshan University
Sep 2021	44th SIAM Southeastern Atlantic Section Conference (SIAM-SEAS)

Recent Seminar Talks

2023	MIT
2022	Harvard University
2021	University of California, Berkeley; IMA, University of Minnesota; University of Edinburgh

Recent Invited Conference Presentations

May 2024	Interacting Particle Systems: Analysis, Control, Learning and Computation, ICERM
Mar 2024	Machine Learning in Electronic Structure Theory, IMSI, University of Chicago

Feb 2024	Scientific Machine Learning: Theory and Algorithms, Brin Research Center, University of Maryland
Oct 2023	Workshop on Quantum Algorithms for Scientific Computation, IPAM
Nov 2022	Applied Analysis: from the calculus of variations to materials science, finance and data science – a celebration of the science of Bob Kohn, Flatiron Institute
Aug 2022	Computational Mathematics for Quantum Technologies, University of Bath
Mar 2022	Workshop on Multiscale Approaches in Quantum Mechanics, IPAM
Nov 2021	Workshop on Deep Learning and Partial Differential Equations, Newton Institute, University of Cambridge
Oct 2021	Workshop on Sampling Algorithms and Geometries on Probability Distributions, Simons Institute, University of California, Berkeley
Aug 2021	IMA Workshop on the Mathematical Foundation and Applications of Deep Learning, Purdue University

Students & Postdocs [· · ·] indicates first position after Duke, if known

PhD students

Charlio Xu, 2014 – 2017 [private sector]
Kyle Thicke, 2015 – 2019 [TU Munich]
Jeffrey LaComb, 2016 – 2019 [Drexel University]
Yu Cao, 2016 – 2020 [Courant Institute]
Zhe Wang, 2016 – 2020 [private sector]
Kevin Stubbs, 2016 – 2021 [IPAM & UC Berkeley]
Lihan Wang, 2017 – 2021 [Carnegie Mellon University]
Mo Zhou, 2018 – 2023 [UCLA]
Ziang Chen, 2019 – 2023 [MIT]
Yixin Tan, 2019 – current
Joel Bierman, 2020 – current

Postdoctoral scholars

Zhennan Zhou, 2014 – 2017 [Assistant Professor at BICMR, Peking University]
Haizhao Yang, 2015 – 2017 [Assistant Professor at National University of Singapore]
Zhenning Cai, 2016 [Assistant Professor at National University of Singapore]
Yingzhou Li, 2017 – 2020 [Assistant Professor at UC Berkeley]
Yulong Lu (co-mentored with Jonathan Mattingly), 2017 – 2020 [Assistant Professor at UMass Amherst]
Alexander Watson, 2017 – 2020 [postdoctoral scholar at University of Minnesota]
Mathias Sachs (SAMSI postdoc, co-mentored with Jonathan Mattingly), 2017 – 2020 [postdoctoral scholar at University of British Columbia]
Min Wang, 2019 – 2022 [Assistant Professor at University of Houston]
Holden Lee (co-mentored with Rong Ge), 2020 – 2022 [Assitant Professor at Johns Hopkins University]
Bowen Li, 2021 – 2024 [Assistant Professor at City University of Hong Kong]
Shijun Zhang (co-mentored with Hongkai Zhao), 2022 – 2024 [Assistant Professor at Hongkong Polytechnic University]
Jing An, 2022 – present
Quanjun Lang, 2023 – present (co-mentored with Jonathan Mattingly)

Undergraduate mentoring

Leslie Lei, PRUV Fellow, Summer 2013 – Spring 2014 [Stanford]
Fuchsia Chen, PRUV Fellow, Summer 2015 [Harvard]
Austin Ferguson, MathBio REU, Summer 2015 [UNC Chapel Hill]
Jeremy Tay, Research Independent Study, Fall 2015 [private sector]
Matthew Gherman, PRUV Fellow, Summer 2016 [UCLA]
Ji Won Park, DOMath, Summer 2017 [Stanford]
Junmo Ryang, DOMath, Summer 2017
Shengtong Zhang (Tsinghua Univ.), Undergraduate Internship, Summer 2017 [Northwestern]
Mo Zhou (Tsinghua Univ.), Undergraduate Internship, Summer 2017 [Duke]
Qinyi Zhu (Nankai Univ.), Undergraduate Internship, Summer 2017 [Berkeley]
Ziang Chen (Peking Univ.), Undergraduate Internship, Summer 2018 [Harvard]
Meng Li (Peking Univ.), Undergraduate Internship, Summer 2018 [Berkeley]
Anqi Mao (Shanghai Jiaotong Univ.), Undergraduate Internship, Summer and Fall 2018 [Courant Institute]
Norah Tan, Research Independent Study, Spring 2021 [MIT]
Ziang Yu (Shanghai Jiaotong U.), Research Intern, Spring & Summer 2021 [U Chicago]
Hongrui Chen (Peking Univ.), Research Intern, Summer & Fall 2022 [Stanford]
Lezhi Tan (Peking Univ.), Research Intern, Summer & Fall 2022 [Stanford]
Alice Ding, PRUV and Research Independent Study, Summer & Fall 2023 [Yale]
Luke Triplett, PRUV and Research Indepdent Study, Summer & Fall 2023 [Berkeley]

Service

Editorial service

Journal of Machine Learning, Editor-in-Chief (2024 –)

Numerical Methods for PDEs, Associate Editor (2022 –)
Kinetics and Related Fields, Associate Editor (2022 –)
SIAM Journal on Mathematical Analysis, Associate Editor (2022 –)
Communications in Computational Physics, Associate Editor (2021 –)
Networks and Heterogenous Media, Editorial Board (2021 –)
Communications of the American Mathematical Society, Associate Editor (2020 –)
Communications in Mathematical Sciences, Associate Editor (2017 –)
CSIAM Transaction on Applied Mathematics, Associate Editor (2019 –)
Journal of Computational Mathematics, Associate Editor (2021 –)
Multiscale Modeling and Simulation, Associate Editor (2019 –)
Springer Book Series on *Mathematics of Molecular Modeling*, Series Editor (2017 –)
Conference Program Committee: MSML2021, 2022; NeurIPS2021, 2022, 2023; ICML2023; ICLR2024

Service to the profession

Vice Chair, SIAM Activity Group in Mathematical Aspects of Materials Science (2019 – 2020)
Member, BIRS Scientific Advisory Board and Equity, Diversity and Inclusion Advisory Board (2023 – 2025)

Journal and book refereeing

Adv. Comput. Math.; Appl. Comp. Harmonic Anal.; Ann. Statist.; 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.; WIREs Comput. Mol. Sci.

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

Lecture Notes in Mathematics, Springer; Princeton University Press; SIAM; CRC Press;

Grant proposal refereeing

European Research Council
National Science Foundation (ad hoc review and review panels)
Research Grant Council of Hong Kong
FWF Austrian Science Fund
Conference proposals of Banff International Research Station
Scientific program proposal of Isaac Newton Institute

Program organization

IMS Program on Multiscale Analysis and Methods for Quantum and Kinetic Problems
IMS, NUS, Spring 2023
Long Program on Tensor Methods and Emerging Applications to the Physical and Data Science
IPAM, UCLA, Spring 2021

Conference organization (recent)

Mathematical and Computational Materials Science Workshop
IMSI, University of Chicago, February 2021

Inaugural conference on Mathematical and Scientific Machine Learning (MSML2020)
(co-chair with Rachel Ward)
Princeton University, NJ (virtually), July 2020

Organizing Committee Member
SIAM Conference on Analysis of Partial Differential Equations (PD19)
La Quinta, CA, December 2019

Workshop on Dimension Reduction in Physical and Data Sciences
Duke University, April 2019

Mini-workshop on Mathematical and Numerical Analysis of Gradient Flows
Duke University, August 2018

MolSSI Workshop / ELSI Conference on Solving or Circumventing Eigenvalue Problems in Electronic Structure Theory (co-organized with Volker Blum, William Huhn, Lin Lin, Alvaro Vazquez-Mayagoitia, and Chao Yang)
Richmond, Virginia, August 2018

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

Minisymposia/symposia organization (recent)

Mathematical perspectives in quantum mechanics and quantum chemistry
(with I. Michael Sigal)

The Eleventh IMACS International Conference on Nonlinear Evolution Equations and Wave Phenomena: Computation and Theory, University of Georgia, April 2019

Outreach activity

Judge for Alibaba Global Mathematics Contest, 2021, 2022, 2023

Judge for Yau College Student Mathematics Contest, 2020

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

Member of AMS and SIAM