# Jianfeng Lu

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# **Positions**

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
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### Education

2009	Ph.D. in Applied Mathematics, Princeton University
2005	B.S. in Mathematics, Peking University, China

# Awards and Recognitions

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, in press

Recent progresses for evaluating the Kohn-Sham map with Lin Lin and Lexing Ying, in press

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).

### Referred journal or conference publications

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.*, in press

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.*, in press

Posterior computation with the Gibbs zig-zag sampler

Matthias Sachs, Deborshee Sen, Jianfeng Lu, and David Dunson, Bayesian Anal., in press

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

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

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

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

Neural-network quantum states for periodic systems in continuous space

Gabriel Pescia, Jiequn Han, Alessandro Lovato, Jianfeng Lu, and Giuseppe Carleo, Phys. Rev. Research, in press

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

Low-rank approximation for multiscale PDEs

with Ke Chen, Shi Chen, Qin Li, and Stephen J. Wright, Notices Amer. Math. Soc., in press

Manifold learning and nonlinear homogenization

with Shi Chen, Qin Li and Stephen J. Wright, Multiscale Model. Simul., in press

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., in press

Universal approximation of symmetric and anti-symmetric functions

with Jiequn Han, Yingzhou Li, Lin Lin, Jiefu Zhang, and Linfeng Zhang, Commun. Math. Sci., in press

Neural collapse with cross-entropy loss

with Stefan Steinerberger, Appl. Comput. Harmonic Anal., in press

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., in press

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), in press

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., in press

Defect resonances of truncated crystal structures

with Jeremy Marzuola and Alexander Watson, SIAM J. Appl. Math., in press

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

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*, in press

Deep Network Approximation for Smooth Functions

with Zuowei Shen, Haizhao Yang, and Shijun Zhang, SIAM J. Math. Anal., in press

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

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

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., in press

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., in press

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., in press

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

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

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*, in press

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

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.*, in press

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.*, in press

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.*, in press (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., in press

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

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

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

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

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.*, in press

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*, in press

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*, in press

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, SLAM J. Sci. Comput. 40, B1277–B1301 (2018)

Phase space sketching for crystal image analysis based on synchrosqueezed transforms with Haizhao Yang, SLAM 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  $\ell^1$  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 nona-diabatic 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, SLAM 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  $\ell_1$  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, SLAM 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**

Improved analysis of score-based generative modeling: User-friendly bounds under minimal smoothness assumptions

with Hongrui Chen and Holden Lee, 2022

Convergence of score-based generative modeling for general data distributions with Holden Lee and Yixin Tan, 2022

Improving the accuracy of variational quantum eigensolvers with fewer qubits using orbital optimization with Joel Bierman and Yingzhou Li, 2022

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, 2022

One-dimensional tensor network recovery with Ziang Chen and Anru Zhang, 2022

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

Neural network based variational methods for solving quadratic porous medium equations in high dimensions with Min Wang, 2022

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

Single time-scale actor-critic method to solve the linear quadratic regulartor with convergence guarantees with Mo Zhou, 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

Edge state dynamics along curved interfaces

with Guillaume Bal, Simon Becker, Alexis Drouot, Clotilde Fermanian Kammerer and Alexander Watson, 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

On the global convergence of randomized coordinate gradient descent for non-convex optimization with Ziang Chen and Yingzhou Li, 2021

Locality of the windowed local density of states with Terry A. Loring and Alexander Watson, 2021

On explicit  $L^2$ -convergence rate estimate for underdamped Langevin dynamics with Yu Cao and Lihan Wang, 2019

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

### Teaching

Duke University Real Analysis, Fall 2013, Fall 2014, Fall 2017, Fall 2020

Computational Methods for Quantum Many-Body Physics (co-taught with Thomas

Barthel), Spring 2020

Linear Programming, Spring 2019

Introduction to Numerical PDEs, Spring 2013, 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

Nov 2022	University of Michigan
Oct 2021	Duke Kunshan University
SEP 2021	44th SIAM Southeastern Atlantic Section Conference (SIAM-SEAS)
Nov 2020	Center for Mathematics and Artificial Intelligence, George Mason University
Oct 2020	Peking University
SEP 2020	MATH-IMS Joint Applied Mathematics Colloquium, Chinese University of Hong Kong
Jul 2020	SIAM/CAIMS Annual Meeting
Apr 2020	Shanghai Jiaotong University

# RECENT SEMINAR TALKS

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

2020 JFI, University of Chicago; Chinese Academy of Science

# RECENT INVITED CONFERENCE PRESENTATIONS

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
DEC 2020	Recent Progress in Applied and Computational PDEs, Peking University
SEP 2020	Hausdorff School on MCMC: Recent developments and new connections, Hausdorff Center for Mathematics, Bonn
Apr 2020	PDE and Inverse Problem Methods in Machine Learning, IPAM, UCLA

# Students & Postdocs $[\cdots]$ indicates first position after Duke, if known

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PhD students
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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 - current

Yixin Tan, 2019 – current

Ziang Chen, 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 - present

Jing An, 2022 – present

Shijun Zhang, 2022 – present (co-mentored with Hongkai Zhao)

### Service

### Editorial service

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, NeurIPS2021

#### 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 Processing Lett.; IEEE Trans.

nal 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 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

### Outreach activity

Judge for Alibaba Global Mathematics Contest, 2021–2022

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