

Jonathan Weare

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Professional Preparation

University of California, Berkeley, Mathematics and Economics

B.A., 2001

University of California, Berkeley, Mathematics

Ph.D., 2007

Appointments

University of Chicago, Dept. of Statistics, Assistant Professor

2013–

University of Chicago, James Franck Institute, Assistant Professor

2013–

University of Chicago, Computation Institute, Fellow

2011–

University of Marne-la-Vallée / ENPC, Visiting Professor

Feb/Mar 2014

University of Chicago, Dept. of Mathematics, Assistant Professor

2010–2013

New York University, Courant Institute, Courant Instructor

2007–2010

Lawrence Berkeley National Laboratory, Research Assistant

2001–2007

Awards and Honors

Institute for Mathematics and its Applications Prize in Mathematics and its Applications 2015

<https://www.ima.umn.edu/press-room/ima-prize-winner2015>

Department of Energy Early Career Award

2015

<http://science.energy.gov/early-career>

National Science Foundation Postdoctoral Fellowship (declined)

2007

Funding

Principal Investigator:

Early Career Award: Ensemble Simulation Techniques and Fast Randomized Algorithms

Department of Energy, \$820,253, 2015–2020

Analysis and Design of Robust Rare Event Simulation Methods for Protein Folding and Disease Related Aggregation

National Institutes of Health, \$1,740,480, 2013–2018

Long Time Scales and Unlikely Events: Sampling and Coarse Graining Strategies

National Science Foundation, \$175,049, 2011–2015

Co-Principal Investigator:

Research and Training Grant: Computational and Applied Mathematics in Statistical Sciences,

National Science Foundation \$1,749,360, 2016–2021

Interacting Particle Methods for Enhanced Sampling

France and Chicago Collaborating in the Sciences, \$12,000, 2013–2014

The Multifaceted Mathematics Center for Complex Energy Systems (UofC PI)

Department of Energy, \$836,435, 2013–2017

Center for Chemical Innovation: Multiscale Theory and Simulation

National Science Foundation, \$1,650,000, 2011–2015

Synergistic Activities

Organizer:

Society for Industrial and Applied Mathematics, 2016 Materials meeting, Conference organizing committee

International Council for Industrial and Applied Mathematics, 2015 Annual meeting, Rare event simulation mini-symposium

Society for Industrial and Applied Mathematics, 2014 Uncertainty quantification meeting, Data inference mini-symposium

Society for Industrial and Applied Mathematics, 2013 Materials meeting, Computational tools for metastable systems mini-symposium

Midwest Numerical Analysis Day, 2013 Annual workshop

Society of Engineering Science, 2013 Annual meeting, Surface structure and dynamics mini-symposium

International Conference on Industrial and Applied Mathematics, 2011 meeting, Computational chemistry mini-symposium

Reviewer:

Journals in mathematics, scientific computing, surface physics, statistical physics, bio-physics, chemistry, geophysics, statistics, and engineering

University Service:

Co-founder of the *Scientific and Statistical Computing Seminar* which is the only seminar on campus focused on computational and applied mathematics,

<http://www.stat.uchicago.edu/seminars/SSC.seminars.shtml>

Member of the *Physical Sciences Division diversity committee*

Elected member of the *College Council*

Teaching

Undergraduate:

Real analysis

New York University

Calculus

New York University

Mathematical finance

New York University

Math methods for the physical sciences

University of Chicago

Numerical analysis	<i>University of Chicago</i>
Ordinary differential equations	<i>University of Chicago</i>
Complex analysis	<i>University of Chicago</i>
Introductory statistics	<i>University of Chicago</i>
Introductory probability	<i>University of Chicago</i>

Graduate:

Scientific computing	<i>New York University</i>
Monte Carlo methods (new course)	<i>University of Chicago</i>
Stochastic dynamics (new course)	<i>University of Chicago</i>

Mentorship

Undergraduate:

Bradly Stadie	Mathematics, 2013–2014
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Graduate (Ph.D.):

Robert Webber	Statistics, 2015–
Bodhi Vani (A. Dinner co-mentor)	Chemistry, 2015–
Erik Thiede (A. Dinner co-mentor)	Chemistry, 2013–
David Plotkin (D. Abbot co-mentor)	Geosciences, 2012–
Jeremy Tempkin (A. Dinner co-mentor)	Chemistry, 2012–

Postdoctoral:

Zhiyue Lu	Chemistry, 2016–
Charles Matthews	Statistics, 2014–
Brian Van Koten	Statistics, 2014–
Seyit Kale	Chemistry, 2012–2015

Visiting Scholars:

Teresa Pi Torras (<i>École des Ponts ParisTech</i> , T. Lelievre advisor)	Applied Mathematics, 2014
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Submitted Manuscripts

2016

- Ensemble preconditioning for Markov chain Monte Carlo simulation (with C. Matthews and B. Leimkuhler)
- Trajectory stratification of stochastic dynamics (with A. Dinner, J. Mattingly, J. Tempkin, and B. Van Koten)

Publications in Refereed Journals

2016

- Fast randomized iteration: diffusion Monte Carlo through the lens of numerical linear algebra (with L.-H. Lim), *SIAM Reviews: Research Spotlight*, accepted, <http://arxiv.org/abs/1508.06104>

Eigenvector method for umbrella sampling enables error analysis (with E. Thiede, B. Van Koten, and A. Dinner), *Journal of Chemical Physics*, **145**(8), 084115

Multiple time-step dual-Hamiltonian hybrid molecular dynamics Monte Carlo canonical propagation algorithm (with Y. Chen, S. Kale, A. Dinner, and B. Roux), *Journal of Chemical Theory and Computation*, **12**(4), 1449–1458

2015

Sharp entry-wise perturbation bounds for Markov chains (with E. Thiede and B. Van Koten), *Society for Industrial and Applied Mathematics Journal on Matrix Analysis and Applications*, **36**(3), 917–941

The Brownian Fan (with M. Hairer), *Communications in Pure and Applied Mathematics*, **68**(1), 1–60

2014

Finding chemical reaction paths with a multilevel preconditioning protocol (with S. Kale, S. Olaseni, and A. Dinner), *Journal of Chemical Theory and Computation*, **10**(12), 5467–5475

Distinguishing meanders of the Kuroshio using machine learning (with D. Plotkin and D. Abbot), *Journal of Geophysical Research*, **119**(10), 6593–6604

Using multiscale preconditioning to accelerate the convergence of iterative molecular calculations (with J. Tempkin, B. Qui, M. Saunders, B. Roux, and A. Dinner), *Journal of Chemical Physics*, **140**(18), 184114

Improved Diffusion Monte Carlo (with M. Hairer), *Communications in Pure and Applied Mathematics*, **67**(12), 1995–2021

Nucleotide regulation of the structure and dynamics of G-actin (with M. Saunders, J. Tempkin, A. Dinner, B. Roux, and G. Voth), *Biophysical Journal*, **106**(8), 1710–1720

2013

The relaxation of a family of broken-bond crystal-surface models (with J. Marzuola), *Physical Review E*, **88**(3):032403

The theory of ultra coarse graining I, general principles (with J. Dama, A. Sinitskiy, M. McCullagh, B. Roux, A. Dinner, and G. Voth), *Journal of Chemical Theory and Computation*, **9**(5), 2466–2480

On the statistical equivalence of restrained-ensemble simulations with the maximum entropy method (with B. Roux), *Journal of Chemical Physics*, **138**(8):084107

Minimizing memory as an objective for coarse-graining (with N. Guttenberg, J. Dama, M. Saunders, G. Voth, and A. Dinner), *Journal of Chemical Physics*, **138**(9):094111

Extending molecular simulation time scales: Parallel in time integrations for high-level quantum chemistry and complex force representations (with E. Bylaska and J.H. Weare), *Journal of Chemical Physics*, **139**(7):074114

Data assimilation in the low noise regime with applications to the Kuroshio (with E. Vanden-Eijnden), *Monthly Weather Review*, **141**(6), 1822–1841

2012

Steered transition path sampling (with N. Guttenberg and A. Dinner), *Journal of Chemical Physics*, **136**:234103

Rare event simulation for small noise diffusions (with E. Vanden-Eijnden), *Communications in Pure and Applied Mathematics*, **65**(12), 1770–1803

An affine-invariant sampler for exoplanet fitting and discovery in radial velocity data (with F. Hou, J. Goodman, D. Hogg, and C. Schwab), *The Astrophysical Journal*, **745**:198

2011

The evolution of a crystal surface: analysis of a 1D step train connecting two facets in the ADL regime (with H. Al Hajj Shehadeh and R.V. Kohn), *Physica D*, **240**, 1771–1784

2010

Ensemble samplers with affine invariance (with J. Goodman), *Communications in Applied Mathematics and Computational Science*, **5**, 65–85

2009

Particle filtering with path sampling and an application to a bimodal ocean current model, *Journal of Computational Physics*, **228**, 4312–4331

Variance reduction for particle filters of systems with time-scale separation (with D. Givon and P. Stinis), *IEEE Transactions on Signal Processing*, **57**, 424–435

2007

Efficient Monte Carlo sampling by parallel marginalization, *Proceedings of the National Academy of Science*, **104**, 12657–12662

Invited Lectures

2016

Purdue University, Joint CS Colloquium and CCAM Seminar USA

University of California, Berkeley, Applied mathematics seminar USA

Institute for Pure and Applied Mathematics, Collective variables in classical mechanics USA

Society for Industrial and Applied Mathematics, 2016 Mathematics of Planet Earth meeting, Geophysical rare events mini-symposium USA

Duke University, Applied math and analysis seminar USA

Frontiers in Applied and Computational Mathematics, 2016 meeting, Molecular dynamics mini-symposium USA

Society for Industrial and Applied Mathematics, 2016 Materials meeting, Electronic structure mini-symposium USA

Society for Industrial and Applied Mathematics, 2016 Materials meeting, Meso-scale modeling mini-symposium USA

New York University, Applied mathematics seminar USA

Rare Event Simulation, 2016 workshop NDL

Imperial College London, Applied mathematics seminar GBR

Illinois Institute of Technology, Applied mathematics seminar USA

2015

- Society for Industrial and Applied Mathematics*, 2015 PDE meeting, Stochastic simulation tutorial USA
- University of Pennsylvania*, AMCS/PICS colloquium USA
- American Mathematical Society*, 2015 Central Fall sectional meeting, Scientific computing mini-symposium USA
- Scientific Computing and Differential Equations*, 2015 Annual meeting, Molecular dynamics mini-symposium DEU
- 2015 Joint Statistical Meeting*, Computational statistics mini-symposium USA
- Casa Matemática Oaxaca*, Free energy methods workshop MEX
- University of Tennessee*, 2015 Barrett memorial lectures USA
- Massachusetts Institute of Technology*, Data assimilation seminar USA
- Institute for Pure and Applied Mathematics*, Machine learning and multibody problems USA

2014

- Rutgers University, Camden*, Applied mathematics seminar USA
- Michigan State University*, Applied mathematics seminar USA
- Institute for Mathematics and its Applications*, Coastal waves workshop USA
- University of Maryland*, Surface physics workshop USA
- Multiscale Computational Methods in Materials Modelling*, 2014 meeting GBR
- International Centre for Mathematical Sciences*, Computational statistical mechanics workshop GBR
- University of Reading*, Data assimilation seminar GBR
- École des Ponts ParisTech*, Series of four lectures on diffusion Monte Carlo FRA
- Centre National de la Recherche Scientifique, Lyon*, Physics seminar FRA
- Collège de France*, PDE seminar FRA

2013

- Technical University of Eindhoven*, Stochastic modeling of multiscale systems workshop NLD
- University of Warwick*, Computational coarse-graining workshop GBR
- Scientific Computing and Differential Equations*, 2013 meeting, Multiscale modeling mini-symposium ESP
- Free University Berlin*, Molecular kinetics workshop DEU
- Society for Industrial and Applied Mathematics*, 2013 Materials meeting, Molecular simulation mini-symposium USA
- Banff International Research Station*, Geophysical data-assimilation workshop CAN
- American Geophysical Union*, Fall meeting, Statistical mechanics mini-symposium USA
- American Geophysical Union*, Fall meeting, Data assimilation mini-symposium USA

2012

- University of Arizona*, Applied mathematics colloquium USA
- Institute for Pure and Applied Mathematics*, Modeling of materials defects workshop USA
- University of Chicago*, James Frank Institute seminar USA
- Society for Industrial and Applied Mathematics*, 2012 Annual meeting, Modeling of rare events mini-symposium USA
- American Institute of Mathematical Sciences*, 2012 Annual meeting, Stochastic climate modeling mini-symposium USA
- Lorenz Center*, Multiscale simulation workshop NLD
- University of Maryland*, PDE seminar USA
- Northwestern University*, Applied mathematics colloquium USA
- University of Delaware*, Probability seminar USA
- University of California, Berkeley*, Applied mathematics seminar USA
- Society for Industrial and Applied Mathematics*, 2012 Uncertainty quantification meeting, Stochastic PDE mini-symposium USA
- Society for Industrial and Applied Mathematics*, 2012 Uncertainty quantification meeting, Implicit sampling mini-symposium USA
- University of North Carolina, Chapel Hill*, Applied math/Analysis seminar USA
- North Carolina State University*, Numerical analysis seminar USA
- Duke University*, Applied math and analysis seminar USA
- Statistical and Applied Mathematical Sciences Institute*, Rare event simulation workshop USA
- University of Illinois, Urbana–Champaign*, Probability seminar USA

2011

- University of Warwick*, Multiscale systems workshop USA
- Illinois Institute of Technology*, Applied mathematics colloquium USA
- National Institute for Mathematical and Biological Synthesis*, Modeling of intracellular movements workshop USA
- University of Chicago*, Statistics colloquium USA
- University of Chicago*, Computations in science seminar USA
- University of Chicago*, Computational molecular science symposium USA
- Archimedes Center for Modeling, Analysis, and Computation*, Mathematical modeling of materials workshop GRC
- University of Maryland*, Monte Carlo methods tutorial USA
- Society for Industrial and Applied Mathematics*, 2011 Computational science and engineering meeting, Stochastic numerical methods mini-symposium USA

2010

<i>University of Warwick</i> , Stochastic analysis seminar	GBR
<i>University of California, Berkeley</i> , Applied mathematics seminar	USA
<i>Society for Industrial and Applied Mathematics</i> , 2010 Annual meeting, Stochastic numerical methods mini-symposium	USA
<i>National Center for Atmospheric Research</i> , Data assimilation and climate research workshop	USA
<i>Cornell University</i> , Scientific computing and numerics seminar	USA
<i>Princeton University</i> , PACM colloquium	USA
<i>Harvard University</i> , Applied mathematics seminar	USA
<i>University of Michigan, Anne Arbor</i> , Applied mathematics seminar	USA
<i>California Institute of Technology</i> , Applied mathematics colloquium	USA
2009	
<i>University of Chicago</i> , CAMP seminar	USA
<i>University of California, Berkeley</i> , Applied mathematics seminar	USA
<i>Brown University</i> , Applied mathematics seminar	USA
<i>New York University</i> , Applied mathematics seminar	USA
<i>Society for Industrial and Applied Mathematics</i> , 2008 Computational science and engineering meeting, Data assimilation mini-symposium	USA
2008	
<i>Statistical and Applied Mathematical Sciences Institute</i> , Sequential Monte Carlo workshop	USA
2007	
<i>New York University</i> , Applied mathematics seminar	USA
<i>Mathematical Sciences Research Institute</i> , Dynamical systems working group	USA
<i>Brown University</i> , Applied mathematics seminar	USA