

Gavin E. Crooks

CURRICULUM VITAE

(2023-04-04)

gavincrooks@gmail.com threeplusone.com

Professional Experience

| | |
|-----------|---|
| 2023– | Lecturer University of California, Berkeley Teaching Chem 220b, Introduction to Stochastic Thermodynamics |
| 2020–2022 | Consultant, Quantum computing and drug discovery Menten AI |
| 2021–2022 | Consultant, Free energy methods and drug discovery InterX |
| 2019–2020 | Visiting Faculty X, the moonshot factory (Google X) |
| 2019–2019 | Visiting Researcher CalTech |
| 2017–2019 | Senior Research Scientist Rigetti Quantum Computing |
| 2010–2016 | Senior Scientist Molecular Biophysics, Lawrence Berkeley Natl. Lab |
| 2012–2016 | Research Physicist Dept. of Physics, University of California, Berkeley |
| 2013–2016 | Founding Member Kavli Energy NanoSciences Institute at Berkeley (Kavli ENSI) |
| 2008–2012 | Deputy Theory Group Leader Helios Solar Energy Research Center (SERC) Lawrence Berkeley Natl. Lab |
| 2004–2010 | Divisional Fellow Physical Biosciences, Lawrence Berkeley Natl. Lab |
| 2001–2004 | Postdoctoral Fellow Dept. of Plant and Microbial Biology, University of California, Berkeley |
| 1999–2001 | Software Developer DoughNET.com, San Francisco |

Education

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| 1995–1999 | Ph.D. in Theoretical Chemistry University of California, Berkeley |
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| | Advisor: David Chandler |
| | Thesis: Excursions in Statistical Dynamics |
| 1992–1993 | M.Sc. in Biocolloid Chemistry |
| | University of East Anglia |
| | Advisor: R. H. Robinson |
| | Thesis: Characterization of Lipases in Water-in-Oil Microemulsions |
| 1990–1991 | International Student |
| | University of Massachusetts, Amherst |
| 1989–1992 | B.Sc. in Chemistry |
| | University of East Anglia |

Awards and Honors

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|------|--|
| 2019 | Fellow of the American Physics Society |
| 2015 | Princeton Center for Theoretical Science Annual Lecturer |
| 2014 | Kavli Scientist-Writer Fellow (Inaugural class) |
| 2012 | Kavli Fellow: Japanese-American Kavli Frontiers of Science Symposium |
| 2011 | Kavli Fellow : National Academy of Sciences / Kavli Frontiers of Science |
| 2010 | Presidential Early Career Awards for Scientist and Engineers (PECASE) |
| 2009 | DOE Office of Science Early Career Scientist and Engineer Award |
| 2005 | Divisional Fellow, Lawrence Berkeley Natl. Lab |
| 2002 | Sloan/DOE Postdoctoral Fellowship in Computational Molecular Biology |

Publications

49 peer reviewed publications; h-index=39 (*); 20000+ citations. ([Google Scholar](#)) ORCID: [0000-0002-6870-7956](#)) [F](#): Favorites

- [49] Grzegorz Nawrocki, Igor Leontyev, Serzhan Sakipov, Mikhail Darkhovskiy, Igor Kurnikov, Leonid Pereyaslavets, Ganesh Kamath, Ekaterina Voronina, Oleg Butin, Alexey Illarionov, Michael Olevanov, Alexander Kostikov, Ilya Ivahnenko, Dhilon S. Patel, Subramanian K. R. S. Sankaranarayanan, Maria G. Kurnikova, Christopher Lock, Gavin E. Crooks, Michael Levitt, Roger D. Kornberg, and Boris Fain. Protein–ligand binding free-energy calculations with ARROW – A purely first-principles parameterized polarizable force field. *J. Chem. Theory Comput* (2022). [10.1021/acs.jctc.2c00930](#) [PDF]
- [48] Leonardo Banchi and Gavin E. Crooks. Measuring analytic gradients of general quantum evolution with the stochastic parameter shift rule. *Quantum*, 5(386) (2021). [10.22331/q-2021-01-25-386](#). arXiv:2005.10299 [PDF]

- [47] Eric C. Peterson, Gavin E. Crooks, and Robert S. Smith. Two-qubit circuit depth and the monodromy polytope. *Quantum*, 4:247 (2020). [10.22331/q-2020-03-26-247](https://arxiv.org/abs/1904.10541). arXiv:1904.10541 [PDF]
- [46] Gavin E. Crooks and Susanne Still. Marginal and conditional second laws of thermodynamics. *Europhys. Lett.*, 125(4):40005 (2019). [10.1209/0295-5075/125/40005](https://arxiv.org/abs/1611.04628). arXiv:1611.04628 [PDF] F
- [45] Josh Fass, David A. Sivak, Gavin E. Crooks, Kyle A. Beauchamp, Benedict Leimkuhler, and John D. Chodera. Quantifying configuration-sampling error in Langevin simulations of complex molecular systems. *Entropy*, 20(5):318 (2018). [10.3390/e20050318](https://arxiv.org/abs/1805.03181). BioRxiv 266619 [PDF]
- [44] Grant M. Rotskoff, Gavin E. Crooks, and Eric Vanden-Eijnden. Geometric approach to optimal nonequilibrium control: Minimizing dissipation in nanomagnetic spin systems. *Phys. Rev. E*, 95:012148 (2017). [10.1103/PhysRevE.95.012148](https://arxiv.org/abs/1608.04444) [PDF]
- [43] David A. Sivak and Gavin E. Crooks. Thermodynamic geometry of minimum-dissipation driven barrier crossing. *Phys. Rev. E*, 94(5):052106 (2016). [10.1103/PhysRevE.94.052106](https://arxiv.org/abs/1608.04444). arXiv:1608.04444 [PDF]
- [42] Todd R. Gingrich, Grant M. Rotskoff, Gavin E. Crooks, and Phillip L. Geissler. Near-optimal protocols in complex nonequilibrium transformations. *Proc. Natl. Acad. Sci. U.S.A.* (2016). [10.1073/pnas.1606273113](https://arxiv.org/abs/1606.27311) [PDF]
- [41] Grant M. Rotskoff and Gavin E. Crooks. Optimal control in nonequilibrium systems: Dynamic Riemannian geometry of the Ising model. *Phys. Rev. E*, 92:060102 (2015). [10.1103/PhysRevE.92.060102](https://arxiv.org/abs/1506.0102) [PDF]
- * [40] Srividya Iyer-Biswas, Charles S. Wright, Jonathan T. Henry, Klevin Lo, Stanislav Burov, Yihan Lin, Gavin E. Crooks, Sean Crosson, Aaron R. Dinner, and Norbert F. Scherer. Scaling laws governing stochastic growth and division of single bacterial cells. *Proc. Natl. Acad. Sci. U.S.A.*, 111:15912–15917 (2014a). [10.1073/pnas.1403232111](https://arxiv.org/abs/1403.2321) [PDF]
- * [39] Srividya Iyer-Biswas, Gavin E. Crooks, Norbert F. Scherer, and Aaron R. Dinner. Universality in stochastic exponential growth. *Phys. Rev. Lett.*, 113:028101 (2014b). [10.1103/PhysRevLett.113.028101](https://arxiv.org/abs/1310.2810) [PDF] F
- [38] David A. Sivak, John D. Chodera, and Gavin E. Crooks. Time step rescaling recovers continuous-time dynamical properties for discrete-time Langevin integration of nonequilibrium systems. *J. Phys. Chem. B*, 118:6466–6474 (2014). [10.1021/jp411770f](https://arxiv.org/abs/1301.3800). arXiv:1301.3800 [PDF]
- * [37] David A. Sivak, John D. Chodera, and Gavin E. Crooks. Using nonequilibrium fluctuation theorems to understand and correct errors in equilibrium and nonequilibrium discrete Langevin dynamics. *Phys. Rev. X*, 3:011007 (2013). [10.1103/PhysRevX.3.011007](https://arxiv.org/abs/1301.1007) [PDF]
- * [36] Patrick R. Zulkowski, David A. Sivak, Gavin E. Crooks, and Michael R.

- DeWeese. Geometry of thermodynamic control. *Phys. Rev. E*, 86(4):041148 (2012). [10.1103/PhysRevE.86.041148](https://doi.org/10.1103/PhysRevE.86.041148). arXiv:1208.4553 [PDF]
- ★★ [35] Susanne Still, David A. Sivak, Anthony J. Bell, and Gavin E. Crooks. Thermodynamics of prediction. *Phys. Rev. Lett.*, 109(12):120604 (2012). [10.1103/PhysRevLett.109.120604](https://doi.org/10.1103/PhysRevLett.109.120604). [PDF] F
- ★★ [34] David A. Sivak and Gavin E. Crooks. Thermodynamic metrics and optimal paths. *Phys. Rev. Lett.*, 108(19):190602 (2012a). [10.1103/PhysRevLett.108.190602](https://doi.org/10.1103/PhysRevLett.108.190602) [PDF] F
- ★ [33] David A. Sivak and Gavin E. Crooks. Near-equilibrium measurements of nonequilibrium free energy. *Phys. Rev. Lett.*, 108(15):150601 (2012b). [10.1103/PhysRevLett.108.150601](https://doi.org/10.1103/PhysRevLett.108.150601) [PDF] F
- ★ [32] Jerome P. Nilmeier, Gavin E. Crooks, David D. L. Minh, and John D. Chodera. Nonequilibrium candidate Monte Carlo is an efficient tool for equilibrium simulation. *Proc. Natl. Acad. Sci. U.S.A.*, 108(45):E1009–E1018 (2011). [10.1073/pnas.1106094108](https://doi.org/10.1073/pnas.1106094108). Erratum: *Proc. Natl. Acad. Sci. U.S.A.* 109:9665 (2012) [PDF]
- [31] Gavin E. Crooks. On thermodynamic and microscopic reversibility. *J. Stat. Mech.: Theor. Exp.*, page P07008 (2011). [10.1088/1742-5468/2011/07/P07008](https://doi.org/10.1088/1742-5468/2011/07/P07008). [PDF]
- [30] Gavin E. Crooks and David A. Sivak. Measures of trajectory ensemble disparity in nonequilibrium statistical dynamics. *J. Stat. Mech.: Theor. Exp.*, page P06003 (2011). [10.1088/1742-5468/2011/06/P06003](https://doi.org/10.1088/1742-5468/2011/06/P06003) [PDF]
- ★★ [29] Derek Greenfield, Ann L. McEvoy, Hari Shroff, Gavin E. Crooks, Ned S. Wingreen, Eric Betzig, and Jan Liphardt. Self-organization of the *escherichia coli* chemotaxis network imaged with super-resolution light microscopy. *PLoS Biol.*, 7(6):e1000137 (2009) [PDF]
- [28] Gavin E. Crooks. Comment regarding “On the Crooks fluctuation theorem and the Jarzynski equality” [*J. Chem. Phys.* 129, 091101 (2008)] and “Nonequilibrium fluctuation-dissipation theorem of Brownian dynamics” [*J. Chem. Phys.* 129, 144113 (2008)]. *J. Chem. Phys.*, 130(10):107101 (2009). [10.1063/1.3080751](https://doi.org/10.1063/1.3080751). [PDF]
- ★ [27] Edward H. Feng and Gavin E. Crooks. Far-from-equilibrium measurements of thermodynamic length. *Phys. Rev. E*, 79:012104 (2009). [10.1103/PhysRevE.79.012104](https://doi.org/10.1103/PhysRevE.79.012104) [PDF]
- [26] Gavin E. Crooks. On the Jarzynski relation for dissipative quantum dynamics. *J. Stat. Mech.: Theor. Exp.*, page P10023 (2008a). [10.1088/1742-5468/2008/10/P10023](https://doi.org/10.1088/1742-5468/2008/10/P10023) [PDF]
- ★★ [25] Edward H. Feng and Gavin E. Crooks. Length of time’s arrow. *Phys. Rev. Lett.*, 101(9):090602 (2008). [10.1103/PhysRevLett.101.090602](https://doi.org/10.1103/PhysRevLett.101.090602) [PDF] F

- ★ [24] P. Maragakis, Felix Ritort, M. Karplus, Carlos Bustamante, and Gavin E. Crooks. Bayesian estimates of free energies from nonequilibrium work data in the presence of instrument noise. *J. Chem. Phys.*, 129:024102 (2008). [10.1063/1.2937892](https://doi.org/10.1063/1.2937892) [PDF] F
- ★ [23] Gavin E. Crooks. Quantum operation time reversal. *Phys. Rev. A*, 77(3):034101(4) (2008b). [10.1103/PhysRevA.77.034101](https://doi.org/10.1103/PhysRevA.77.034101) [PDF]
- ★★ [22] Gavin E. Crooks. Measuring thermodynamic length. *Phys. Rev. Lett.*, 99:100602 (2007a). [10.1103/PhysRevLett.99.100602](https://doi.org/10.1103/PhysRevLett.99.100602). arXiv:0706.0559 [PDF] F
- ★★ [21] Gavin E. Crooks. Beyond Boltzmann-Gibbs statistics: maximum entropy hyperensembles out of equilibrium. *Phys. Rev. E*, 75:041119 (2007b). [10.1103/PhysRevE.75.041119](https://doi.org/10.1103/PhysRevE.75.041119) [PDF]
- ★★ [20] Gavin E. Crooks and Christopher Jarzynski. Work distribution for the adiabatic compression of a dilute and interacting classical gas. *Phys. Rev. E*, 75:021116 (2007). [10.1103/PhysRevE.75.021116](https://doi.org/10.1103/PhysRevE.75.021116) [PDF]
- [19] J. A. Casbon, Gavin E. Crooks, and M. A. S. Saqi. A high level interface to SCOP and ASTRAL implemented in Python. *BMC Bioinformatics*, 7:10 (2006). [10.1186/1471-2105-7-10](https://doi.org/10.1186/1471-2105-7-10) [PDF]
- ★ [18] G. A. Price, Gavin E. Crooks, R. E. Green, and Steven E. Brenner. Statistical evaluation of pairwise protein sequence comparison with the Bayesian bootstrap. *Bioinformatics*, 21(20):3824–3831 (2005). [10.1093/bioinformatics/bti627](https://doi.org/10.1093/bioinformatics/bti627). Erratum: *Bioinformatics* 21:4138 (2005) [PDF]
- [17] Gavin E. Crooks, R. E. Green, and Steven E. Brenner. Pairwise alignment incorporating dipeptide covariation. *Bioinformatics*, 21(19):3704–3710 (2005). [10.1093/bioinformatics/bti616](https://doi.org/10.1093/bioinformatics/bti616) [PDF]
- [16] Gavin E. Crooks and Steven E. Brenner. An alternative substitution model of amino acid replacement. *Bioinformatics*, 21(7):975–980 (2005). [10.1093/bioinformatics/bti109](https://doi.org/10.1093/bioinformatics/bti109) [PDF]
- ★ [15] M. A. Zachariah, Gavin E. Crooks, S. R. Holbrook, and Steven E. Brenner. A generalized affine gap model significantly improves protein sequence alignment accuracy. *Proteins*, 58(2):329–338 (2005). [10.1002/prot.20299](https://doi.org/10.1002/prot.20299) [PDF]
- ★★ [14] E. H. Trepagnier, Christopher Jarzynski, Felix Ritort, Gavin E. Crooks, Carlos Bustamante, and Jan Liphardt. Experimental test of Hatano and Sasa’s nonequilibrium steady-state equality. *Proc. Natl. Acad. Sci. U.S.A.*, 101(42):15038–15041 (2004). [10.1073/pnas.0406405101](https://doi.org/10.1073/pnas.0406405101). [PDF]
- ★ [13] Gavin E. Crooks, J. Wolfe, and Steven E. Brenner. Measurements of protein sequence-structure correlations. *Proteins*, 57(4):804–810 (2004a). [10.1002/prot.20262](https://doi.org/10.1002/prot.20262) [PDF] F
- ★★ [12] Gavin E. Crooks and Steven E. Brenner. Protein secondary structure: Entropy, correlations and prediction. *Bioinformatics*, 20(10):1603–1611 (2004).

[10.1093/bioinformatics/bth132](https://doi.org/10.1093/bioinformatics/bth132) [PDF] F

- ★★ [11] Gavin E. Crooks, G. Hon, J.-M. Chandonia, and Steven E. Brenner. Weblogo: A sequence logo generator. *Genome Research*, 14:1188–1190 (2004b). [10.1101/gr.849004](https://doi.org/10.1101/gr.849004) [PDF]
- ★★ [10] Gavin E. Crooks and D. Chandler. Efficient transition path sampling for nonequilibrium stochastic dynamics. *Phys. Rev. E*, 64:026109 (2001). [10.1103/PhysRevE.64.026109](https://doi.org/10.1103/PhysRevE.64.026109) [PDF]
- [9] B. Ostrovsky, Gavin E. Crooks, M. A. Smith, and Yaneer Bar-Yam. Cellular automata for polymer simulation with application to polymer melts and polymer collapse including implications for protein folding. *Parallel Computing*, 27(5):613–641 (2001). [10.1016/S0167-8191\(00\)00081-8](https://doi.org/10.1016/S0167-8191(00)00081-8) [PDF]
- ★★ [8] Gavin E. Crooks. Path-ensemble averages in systems driven far from equilibrium. *Phys. Rev. E*, 61(3):2361–2366 (2000). [10.1103/PhysRevE.61.2361](https://doi.org/10.1103/PhysRevE.61.2361). [PDF] F
- ★ [7] Gavin E. Crooks, B. Ostrovsky, and Yaneer Bar-Yam. The mesostructure of polymer collapse and fractal smoothing. *Phys. Rev. E*, 60(4):4559–4563 (1999). [10.1103/PhysRevE.60.4559](https://doi.org/10.1103/PhysRevE.60.4559) [PDF]
- ★★ [6] Gavin E. Crooks. Entropy production fluctuation theorem and the nonequilibrium work relation for free energy differences. *Phys. Rev. E*, 60(3):2721–2726 (1999). [10.1103/PhysRevE.60.2721](https://doi.org/10.1103/PhysRevE.60.2721). [PDF] F
- ★★ [5] Gavin E. Crooks. Nonequilibrium measurements of free energy differences for microscopically reversible Markovian systems. *J. Stat. Phys.*, 90(5-6):1481–1487 (1998). [10.1023/A:1023208217925](https://doi.org/10.1023/A:1023208217925). [PDF] F
- ★★ [4] Gavin E. Crooks and D. Chandler. Gaussian statistics of the hard-sphere fluid. *Phys. Rev. E*, 56(4):4217–4121 (1997). [10.1103/PhysRevE.56.4217](https://doi.org/10.1103/PhysRevE.56.4217) [PDF] F
- [3] G. D. Rees, K. Carlile, Gavin E. Crooks, T. R.-J. Jenta, L. A. Price, and B. H. Robinson. Lipases in water-in-oil microemulsions, organogels and Winsor II systems: Aspects of reactivity and separation science. In F.X. Malcata, editor, *Engineering of/with Lipases.*, pages 577–595. Kluwer Academic Press (1996) [PDF]
- [2] Gavin E. Crooks, G. D. Rees, B. H. Robinson, M. Svensson, and G. R. Stephenson. Comparison of hydrolysis and esterification behavior of *Humicola lanuginosa* and *Rhizomucor miehei* lipases in AOT-stabilized water-in-oil microemulsions: II. Effect of temperature on reaction kinetics and general considerations of stability and productivity. *Biotechnol. Bioen.*, 48(3):190–196 (1995a). [10.1002/bit.260480304](https://doi.org/10.1002/bit.260480304) [PDF]
- ★★ [1] Gavin E. Crooks, G. D. Rees, B. H. Robinson, M. Svensson, and G. R. Stephenson. Comparison of hydrolysis and esterification behavior of *Humicola lanuginosa* and *Rhizomucor miehei* lipases in AOT-stabilized water-in-oil

microemulsions: I. Effect of pH and water content on reaction kinetics. *Biotechnol. Bioen.*, 48(1):78–88 (1995b). [10.1002/bit.260480111](https://doi.org/10.1002/bit.260480111) [PDF]

Books

Field guide to continuous probability distributions (2019) [PDF | Amazon]
<http://threeplusone.com/gud>

Selected Technical notes

<http://threeplusone.com/notes>

- [014] Gates, States, and Circuits: Notes on the circuit model of quantum computing [PDF]
- [009] On Measures of Entropy and Information [PDF]
- [007] Field Guide to Continuous Probability Distributions [PDF]
- [004] Inequalities Between the Jensen-Shannon and Jeffreys Divergences [PDF]
- [002] Logistic Approximation to the Logistic-Normal Integral [PDF]

Selected Invited Presentations

- 2021 Harvard SPS Chilloquium
The Length of Time's Arrow
- 2021 Living Histories
- 2020 Berkeley Statistical Mechanics Meeting
–Berkeley, CA
Approximate bound on the energy-speed-accuracy tradeoff from thermodynamic geometry

- 2019 QHACK
– Xanadu, Toronto
The space of 2-qubit gates
- 2019 Statistical Physics of Complex Systems
– Nordita, Stockholm, Sweden
Thermodynamic control of molecular machines
- 2019 Manoa Symposium on Physics of Adaptive Computation
– University of Hawai'i at Manoa
On the thermodynamic tradeoff between power, error rate, and speed
- 2019 Workshop on Thermodynamic Computing
– Computing Community Consortium (CCC)
Introduction to modern non-equilibrium stochastic thermodynamics
- 2016 Information Engines at the Frontiers of Nanoscale Thermodynamics
– Telluride Science Research Conference.
Thermodynamics of strongly coupled systems
- 2016 Rutgers - 115th Statistical Mechanics Conference
Riemannian Geometry of Thermodynamic Control
- 2016 UC Davis - Physics Colloquium
Optimal Thermodynamic Control and the Dynamic Riemannian Geometry of Ising magnets
- 2016 The Scripps Research Institute
Thermodynamic control of molecular machines
- 2016 University of Hawai'i at Manoa - Physics Seminar
Optimal control of microscopic non-equilibrium thermodynamic systems
- 2015 M.I.T. - Physics Colloquium (Guest of the Physics Graduate Student Council)
Optimal Thermodynamic Control & The Geometry of Ising magnets
- 2015 U. of Maryland, College Park - Statistical Physics Seminar
Optimal Thermodynamic Control & The Geometry of Ising magnets
- 2015 Edgestream Partners, Princeton
Optimal Thermodynamic Control and the Geometry of Information
- 2015 N.I.H. - Statistical Physics Seminar
Optimal Thermodynamic Control & The Geometry of Ising magnets
- 2015 Stonybrook University - Laufer Center lecture
Optimal Thermodynamic Control & The Geometry of Ising magnets
- 2015 Memorial Sloan Kettering Cancer Center
Optimal thermodynamic control & The thermodynamic cost of nostalgia

- 2015 Princeton Center for Theoretical Science Annual Lecturer
The Fluctuations of Dissipation
The Ambiguity of Time's Arrow
The Geometry of Thermodynamics
Entropy, Information and Maxwell's demon
- 2015 CalTech
Optimal Thermodynamic Control and the Geometry of Ising magnets
- 2014 Pacific Northwest National Laboratory
Optimal Thermodynamic Control: Riemannian Geometry of Ising magnets
- 2014 Symposium on Statistical Mechanics in Physics, Chemistry, and Biology. MIT.
Riemannian Geometry and Optimal Thermodynamic Control
- 2014 Shortcuts to Adiabaticity, Optimal Quantum Control, and Thermodynamics.
– Telluride Science Research Conference.
Thermodynamic Geometry of the Ising Model
- 2014 Higgs Centre Workshop on Viewpoints on Emergent Phenomena in Nonequilibrium Systems, U. of Edinburgh
Far-from-equilibrium Statistical Dynamics: Past, Present & Future
- 2013 Frontiers of Physics and Information Processing 2013, Kyoto University.
Geometry of Thermodynamics & The Thermodynamics of Prediction
- 2013 University of Tokyo
Molecular Machines, Optimal Response, and the Cost of Nostalgia.
- 2013 U.C. Santa Cruz, Condensed Matter Seminar
Molecular machines and the thermodynamic cost of nostalgia
- 2012 Japanese-American Kavli Frontiers of Science Symposium, Beckman Center, Irvine, CA
The dynamics of disorder: From Clausius to Jarzynski
- 2012 Condensed Matter Seminar, Physics, U.C. Berkeley
Thermodynamic control of molecular scale systems
- 2012 Lawrence Berkeley National Laboratory
The dynamics of disorder
- 2012 The James Franck Institute (JFI), U. Chicago
Optimal thermodynamic control and molecular machines
- 2012 University of Southern California
Thermodynamic control and molecular machines
- 2011 University College London, Physics Colloquia.
Statistical thermodynamics and the breaking of time-symmetry

- 2011 Setting Time Aright: An international and inter-disciplinary meeting, Foundational Questions Institute, Norway and Denmark.
Whither time's arrow?
- 2010 Multiscale Molecular Modeling: Molecular Dynamics, Computational Statistical Mechanics, and Simulation Algorithms, University of Edinburgh.
Near equilibrium measurements of non-equilibrium free energies
- 2009 Workshop on the Theory and Simulation of Nanoscale Materials for Solar Energy Applications, Molecular Foundry, Lawrence Berkeley National Laboratory
Nonequilibrium thermodynamics at the nanoscale
- 2009 BioStruct09, Unraveling the structure of biomolecules: from nonequilibrium statistical mechanics to mechanical manipulation, Florence, Italy.
Length of time's arrow
- 2009 Berkeley Mini Statistical Mechanics Meeting
Length of time's arrow
- 2008 D.E. Shaw Research, New York
Non-equilibrium thermodynamics of small systems
- 2008 Xth Linz Winter Workshop, Linz, Austria.
The shape of work: Non-equilibrium estimates of free energy
- 2007 Second workshop on the computational worldview and the sciences, CalTech
There and back again: The statistical dynamics of trajectories
- 2006 Conference on finite time thermodynamics, University of California, San Diego
Measuring free energy
- 2006 University of Barcelona, Spain
Measuring free energy
- 2006 Theory of single molecule force experiments and simulations, CECAM, Lyon
Measuring free energy
- 2006 International conference: "Work, dissipation, and fluctuations in non-equilibrium physics", Université Libre de Bruxelles
Beyond Boltzmann-Gibbs statistics: Maximum entropy hyperensembles
- 2005 Berkeley Mini Statistical Mechanics Meeting
Statistical dynamics of protein evolution
- 2004 Workshop on stochastic and deterministic dynamics in equilibrium and nonequilibrium systems, Erwin Schrödinger Institute, Vienna, Austria
Quantum heat and quantum work
- 2004 University of California, San Francisco
Protein structure: Entropy, correlations and prediction

- 2002 Lawrence Berkeley National Laboratory
Statistical dynamics far from equilibrium
- 1999 Los Alamos National Laboratory
Statistical dynamics far from equilibrium

Academic Activities

AD HOC REVIEWER

| | | |
|------------------------|----------------------------|--------------------------|
| Physics Review Letters | Physics Review E | European Physics Letters |
| J. Physics A | J. Statistical Mechanics | J. Statistical Physics |
| Nucleic Acids Research | J. Chem. Physics | Bioinformatics |
| Biophysical Journal | Proc. Natl. Acad. Sci. USA | Nature Physics |

PROFESSIONAL SOCIETIES

Fellow, American Physical Society
Foundational Questions Institute (FQXi)
American Association for the Advancement of Science (AAAS)
Berkeley Institute for the Theoretical Sciences (BITS)

COMMITTEES

Division Staff Committee, Physical Biosciences, LBL (2012-2016)
Faculty Recruitment, U.C. Berkeley, Dept. of Physics. (2012)

TEACHING

Princeton Center for Theoretical Science Annual Lecturer (Spring 2015)
Thermodynamics and Statistical Mechanics (Graduate) (Fall 2013)
Mentor for Google's Summer of Code (2015)
Mentor for Rails Girl's Summer of Code (2016)

FEATURED OPEN SOURCE

WebLogo: Sequence Logos Redrawn (2004-2022)

<https://github.com/WebLogo/weblogo>

<http://weblogo.threeplusone.com>

A popular bioinformatics application for visualizing patterns in DNA or protein sequences.

QuantumFlow: A Quantum Algorithms Development Toolkit (2018)

<https://github.com/rigetticomputing/quantumflow>

<http://quantumflow.readthedocs.io>

Implements a simulation of a quantum computer with TensorFlow, so that we can train quantum machine learning algorithms with stochastic gradient descent, analogous to training deep neural networks.