Gavin E. Crooks

Curriculum Vitae

(2019-05-01)

gavincrooks@gmail.com threeplusone.com

Formerly Senior Scientist at Rigetti Quantum Computing, developing algorithms for near term quantum computers. World expert on non-equilibrium thermodynamics and the physics of information. Extensive experience with modern deep learning, computational biology, statistical analysis of large data sets, information theory, statistical distributions, free energy calculations, software engineering, and algorithm development.

Professional Experience

2019– Quantum Consultant
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

1995–1999 Ph.D. in Theoretical Chemistry
University of California, Berkeley
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

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

46 peer reviewed publications; h-index=31 (⋆); 13000+ citations. (Google Scholar) ORCID: 0000-0002-6870-7956) F: Favorites

[50] Eric C. Peterson, Gavin E. Crooks, and Robert S. Smith. Fixed-depth two-qubit circuits and the monodromy polytope. ArXiv:1904.10541 [PDF]

[49] Gavin E. Crooks. Performance of the quantum approximate optimization algorithm on the maximum cut problem. arXiv:1811.08419 [PDF]

[48] Gavin E. Crooks, Yaneer Bar-Yam, Sergey V. Buldyrev, and H. Eugene Stanley. Comparison of the roughness scaling of the surface topography of Earth and Venus. arXiv:1809.02457 [PDF]

[47] C. M. Wilson, J. S. Otterbach, N. Tezak, Robert S. Smith, Gavin E. Crooks, and Marcus P. da Silva. Quantum Kitchen Sinks: An algorithm for machine learning on near-term quantum computers. arXiv:1806.08321 [PDF]

[46] Gavin E. Crooks and Susanne Still. Marginal and conditional second laws of thermodynamics. *Europhys. Lett.*, 125:40005 (2019). 10.1209/0295-5075/125/40005. 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. 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 [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. 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.*, 113:10263–10268 (2016). 10.1073/pnas.1606273113 [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 [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 [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 [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. 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 [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. 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. [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 [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 [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. 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. [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 [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). 10.1371/journal.pbio.1000137 [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. [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 [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 [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 [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 [PDF] F

★ [23] Gavin E. Crooks. Quantum operation time reversal. *Phys. Rev. A*,

77(3):034101(4) (2008b). 10.1103/PhysRevA.77.034101 [PDF]

⋆⋆ [22] Gavin E. Crooks. Measuring thermodynamic length. *Phys. Rev. Lett.*, 99:100602 (2007a). 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 [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 [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 [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. 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 [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 [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 [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. [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 [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 [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 [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 [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 [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. [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 [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. [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. [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 [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 seperation 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 [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 [PDF]

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Selected Technical notes

http://threeplusone.com/gec/note

[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

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", Unversité 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

FQXi (Foundational Questions Institute)
American Physical Society

Committees

Division Staff Committee, Physical Biosciences, LBL (2012-)
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 (2004-2018)

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.