

Gavin E. Crooks

Curriculum Vitae (2010)

Senior Scientist , Physical Biosciences
Deputy Theory Group Leader, Helios/SERC
Lawrence Berkeley National Laboratory
Berkeley, CA 94720

(510) 219-5039 GECrooks@lbl.gov threeplusone.com

Professional Experience

- 2010- Senior Scientist
Physical Biosciences
Lawrence Berkeley Natl. Lab
- 2005-2010 Divisional Fellow
Physical Biosciences
Lawrence Berkeley Natl. Lab
- 2001-2004 Postdoctoral Fellow
Advisor: Steven E. Brenner
Computational Genomics Research Group
Department of Plant and Microbial Biology
University of California, Berkeley
- 2000-2001 Software Engineer - DoughNET.com

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, Norwich, U.K.
Advisor: R. H. Robinson
Thesis: Characterization of Lipases in Water-in-Oil Microemulsions
- 1989-1992 B.Sc. in Chemistry,
University of East Anglia, Norwich, U.K.

Awards/Honors

- 2002-2004 Sloan/DOE Postdoctoral Fellowship in Computational Molecular Biology.

Publications

28 peer reviewed publications; h-index=13; over 2000 citations. (ISI Web of Science, 2010-06-07)

- [1] D. Greenfield, A. L. McEvoy, H. Shroff, G. E. Crooks, N. S. Wingreen, E. Betzig, and J. Liphardt. Self-organization of the *escherichia coli* chemotaxis network imaged with super-resolution light microscopy. *PLoS Biol.*, 7(6):e1000137, Jun 2009. doi:10.1371/journal.pbio.1000137.
- [2] G. 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, Mar 2009. doi:10.1063/1.3080751.
- [3] E. H. Feng and G. E. Crooks. Far-from-equilibrium measurements of thermodynamic length. *Phys. Rev. E*, 79:012104, Jan 2009. doi:10.1103/PhysRevE.79.012104.
- [4] G. E. Crooks. On the Jarzynski relation for dissipative quantum dynamics. *J. Stat. Mech.: Theor. Exp.*, page P10023, Oct 2008. doi:10.1088/1742-5468/2008/10/P10023.
- [5] E. H. Feng and G. E. Crooks. Length of time’s arrow. *Phys. Rev. Lett.*, 101(9):090602, Aug 2008. doi:10.1103/PhysRevLett.101.090602.
- [6] P. Maragakis, F. Ritort, M. Karplus, C. Bustamante, and G. E. Crooks. Bayesian estimates of free energies from nonequilibrium work data in the presence of instrument noise. *J. Chem. Phys.*, 129:024102, Jul 2008. doi:10.1063/1.2937892.
- [7] G. E. Crooks. Quantum operation time reversal. *Phys. Rev. A*, 77(3):034101(4), Mar 2008. doi:10.1103/PhysRevA.77.034101.
- [8] G. E. Crooks. Measuring thermodynamic length. *Phys. Rev. Lett.*, 99:100602 (4), Sep 2007. doi:10.1103/PhysRevLett.99.100602.
- [9] G. E. Crooks. Beyond Boltzmann-Gibbs statistics: maximum entropy hyperensembles out of equilibrium. *Phys. Rev. E*, 75:041119, Apr 2007. doi:10.1103/PhysRevE.75.041119.
- [10] G. E. Crooks and C. Jarzynski. Work distribution for the adiabatic compression of a dilute and interacting classical gas. *Phys. Rev. E*, 75:021116, Feb 2007. doi:10.1103/PhysRevE.75.021116.
- [11] J. A. Casbon, G. E. Crooks, and M. A. S. Saqi. A high level interface to SCOP and ASTRAL implemented in Python. *BMC Bioinformatics*, 7:10, Jan 2006. doi:10.1186/1471-2105-7-10.
- [12] G. A. Price, G. E. Crooks, R. E. Green, and S. E. Brenner. Statistical evaluation of pairwise protein sequence comparison with the Bayesian bootstrap. *Bioinformatics*, 21(20):3824–3831, Aug 2005. doi:10.1093/bioinformatics/bti627. Erratum: *Bioinformatics* 21:4138 (2005).
- [13] G. E. Crooks, R. E. Green, and S. E. Brenner. Pairwise alignment incorporating dipeptide covariation. *Bioinformatics*, 21(19):3704–3710, Aug 2005. doi:10.1093/bioinformatics/bti616.
- [14] G. E. Crooks and S. E. Brenner. An alternative substitution model of amino acid replacement. *Bioinformatics*, 21(7):975–980, Nov 2005. doi:10.1093/bioinformatics/bti109.
- [15] M. A. Zachariah, G. E. Crooks, S. R. Holbrook, and S. E. Brenner. A generalized affine gap model significantly improves protein sequence alignment accuracy. *Proteins*, 58(2):329–338, Feb 2005. doi:10.1002/prot.20299.
- [16] E. H. Trepagnier, C. Jarzynski, F. Ritort, G. E. Crooks, C. J. Bustamante, and J. Liphardt. Experimental test of hatano and sasa’s nonequilibrium steady-state equality. *Proc. Natl. Acad. Sci. U.S.A.*, 101(42):15038–15041, Oct 2004. doi:10.1073/pnas.0406405101.
- [17] G. E. Crooks, J. Wolfe, and S. E. Brenner. Measurements of protein sequence-structure correlations. *Proteins*, 57(4):804–810, Jun 2004. doi:10.1002/prot.20262.
- [18] G. E. Crooks and S. E. Brenner. Protein secondary structure: Entropy, correlations and prediction. *Bioinformatics*, 20(10):1603–1611, Feb 2004. doi:10.1093/bioinformatics/bth132.

- [19] G. E. Crooks, G. Hon, J.-M. Chandonia, and S. E. Brenner. Weblogo: A sequence logo generator. *Genome Research*, 14:1188–1190, 2004. doi:10.1101/gr.849004.
- [20] G. E. Crooks and D. Chandler. Efficient transition path sampling for nonequilibrium stochastic dynamics. *Phys. Rev. E*, 64:026109, Jul 2001. doi:10.1103/PhysRevE.64.026109.
- [21] B. Ostrovsky, G. Crooks, M. A. Smith, and Y. 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, Apr 2001. doi:10.1016/S0167-8191(00)00081-8.
- [22] G. E. Crooks. Path-ensemble averages in systems driven far from equilibrium. *Phys. Rev. E*, 61(3):2361–2366, Mar 2000. doi:10.1103/PhysRevE.61.2361.
- [23] G. E. Crooks, B. Ostrovsky, and Y. Bar-Yam. The mesostructure of polymer collapse and fractal smoothing. *Phys. Rev. E*, 60(4):4559–4563, Oct 1999. doi:10.1103/PhysRevE.60.4559.
- [24] G. E. Crooks. Entropy production fluctuation theorem and the nonequilibrium work relation for free energy differences. *Phys. Rev. E*, 60(3):2721–2726, Sep 1999. doi:10.1103/PhysRevE.60.2721.
- [25] G. E. Crooks. Nonequilibrium measurements of free energy differences for microscopically reversible Markovian systems. *J. Stat. Phys.*, 90(5-6):1481–1487, Mar 1998. doi:10.1023/A:1023208217925.
- [26] G. E. Crooks and D. Chandler. Gaussian statistics of the hard-sphere fluid. *Phys. Rev. E*, 56(4):4217–4121, Oct 1997. doi:10.1103/PhysRevE.56.4217.
- [27] G. 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, Nov 1995. doi:10.1002/bit.260480304.
- [28] G. 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, Oct 1995. doi:10.1002/bit.260480111.

Selected Invited Presentations

“Nonequilibrium thermodynamics at the nanoscale”, Workshop on the Theory and Simulation of Nanoscale Materials for Solar Energy Applications, Molecular Foundry, Lawrence Berkeley National Laboratory (2009)

“Length of time’s arrow”, BioStruct09, Unraveling the structure of biomolecules: from nonequilibrium statistical mechanics to mechanical manipulation, Area CNR di Sesto Fiorentino, Florence, Italy. (2009)

“Length of time’s arrow”, Berkeley Mini Statistical Mechanics Meeting (2009)

“Non-equilibrium thermodynamics of small systems”, D.E. Shaw Research, New York (2008)

“The shape of work: Non-equilibrium estimates of free energy”, Xth Linz Winter Workshop, Linz, Austria, (2008)

“There and back again: The statistical dynamics of trajectories”, Second workshop on the computational worldview and the sciences, California Institute of Technology (2007)

“Measuring free energy”, Conference on finite time thermodynamics, University of California, San Diego (2006)

“Measuring free energy”, University of Barcelona, Spain, 2006

“Measuring free energy”, Theory of single molecule force experiments and simulations, CECAM, Lyon (2006).

“Beyond Boltzmann-Gibbs statistics: Maximum entropy hyperensembles out-of-equilibrium” , International conference: “Work,dissipation , and fluctuations in non-equilibrium physics”, Université Libre de Bruxelles, (2006).

“Statistical dynamics of protein evolution”, Berkeley Mini Statistical Mechanics Meeting (2005)

“Quantum heat and quantum work”, Workshop on stochastic and deterministic dynamics in equilibrium and nonequilibrium systems Erwin Schroedinger Institute, Vienna, Austria (2004)

“Protein structure: Entropy, correlations and prediction”, University of California, San Francisco (2004)

“Statistical dynamics far from equilibrium.”, Lawrence Berkeley National Laboratory (2002)

“Statistical dynamics far from equilibrium” , Los Alamos National Laboratory (1999)