

Michael E. Wall

CURRICULUM VITAE

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Personal Data

Citizenship: USA

Work Address: Mail Stop B256
Center for Nonlinear Studies
Theoretical Division
Computer, Computational, and Statistical Sciences Division
Los Alamos National Laboratory
Los Alamos, NM 87545

Position Research Scientist, Los Alamos National Laboratory

Education B.S. Physics, University of California, San Diego (1989)
Ph.D. Physics, Princeton University (1996)

Professional Appointments

1996-1999 Postdoctoral Fellow, Dept of Biochemistry and Cell Biology and Keck Center for Computational Biology, Rice University
1999-2001 Postdoctoral Research Associate, Chemistry Division, Bioscience Division, and Computer and Computational Sciences Division, Los Alamos National Laboratory
2001-present Research Scientist, Computer, Computational, and Statistical Sciences Division, Los Alamos National Laboratory
2005-present Team Leader, Computational Biology and Bioinformatics
2009-present Executive Committee Member, Center for Nonlinear Studies
2011-2012 Deputy Director (acting), Center for Nonlinear Studies

Honors and Awards

Keck Center for Computational Biology NSF Postdoctoral Fellowship (1996-1998); Robert A. Welch Foundation Postdoctoral Fellowship (1996-1999); Best poster presentation, Keck Center Annual Research Conference on Computational Biology (1997)

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Professional Activities

Cultural exchange: Invited participant, 6th Annual Japanese-American Beckman Frontiers of Science Symposium (Japanese Society for the Advancement of Science, US National Academy of Sciences), Kanagawa, Japan (Dec 2003)

Meeting organization: Annual q-bio Conference on Cellular Information Processing (Santa Fe, 2007-2012); q-bio Summer School on Cellular Information Processing (Los Alamos, 2007-2009); Theory, Simulations, and Computing Capability Workshop on Computational Systems Biology (LANL, Oct 2006)

Referee for over 20 journals and multiple national and international funding agencies.

Organizational review: Member of extramural review panel, Department of Biostatistics, Bioinformatics, and Epidemiology, Medical University of South Carolina (Sep 2008)

Professional society memberships: American Physical Society (1990-present); Biophysical Society (1992-present)

Invited Talks

Telluride workshop on Characterizing Landscapes, 6/14/2012, Telluride, CO, Invited talk: Energy landscapes of protein crystals

OpenEye CUP XIII, 3/5/2012, Santa Fe, NM, Invited talk: Protein dynamics and diffuse X-ray scattering

Department of Biochemistry, University of Otago, 6/21/2011, Invited talk: Use of comparative genomics to improve gene start site annotation

15th International Congress on Molecular Systems Biology, 5/9/2011, Lleida, Spain, Keynote talk: Structure-function relations are subtle in genetic regulatory networks. Session chair.

Telluride workshop on Characterizing Landscapes, 6/14/2010, Telluride, CO, Invited talk: Model of transcriptional activation by MarA in *Escherichia coli*

University of California, Santa Barbara, 6/4/2010, Workshop on Coarse-Grained modeling, Invited talk: Coarse-grained modeling of protein vibrations

University of Nebraska Redox Center, 4/13/2010, Invited talk: Protein dynamics and ligand binding

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Department of Pharmacology, Bioinformatics course, 10/27/2009, University of Colorado, Denver, CO. Invited lecture: Protein Structure.

Department of Pharmacology, 10/26/2009, University of Colorado, Denver, CO. Invited talk: Ligand Binding, Protein Dynamics, and Function Prediction.

Regulation of Protein Phosphorylation: Energy Landscapes, Allostery, and Dynamic Regulation, 12/5-12/7/2008, UC-San Diego, La Jolla, CA. Invited talk: Modulation of the kinase ensemble by second messengers.

Characterizing Landscapes: From Biomolecules to Cellular Networks, 7/7/-7/11/2008, Telluride Science Research Center, Telluride, CA. Invited talk: Ligand-Induced Perturbation of Protein Energy Landscapes.

Workshop on Principles of Biological Computation, 18-21 May 2008, Santa Fe Institute, Santa Fe, NM. Invited talk: Signal transduction using real proteins.

Department of Biochemistry, 4/29/2008, University of Otago, Dunedin, New Zealand. Invited talk: Protein Dynamics and Ligand Binding: Computational Insights into Allostery.

SIMBIOS NIH Center for Biomedical Computing, 4/16/2008, Stanford University, Stanford, CA. Invited talk: Computational Insights into Allostery, with Bioinformatics Applications.

Department of Computational Biology, 11/7/07, University of Pittsburgh Medical Center, Pittsburgh, PA. Invited talk: Computational studies of protein function using dynamics perturbation analysis.

Bioinformatics Research Center, 9/7/07, University of North Carolina, Charlotte, NC. Invited talk: Protein interactions and energy landscapes.

Workshop on Small-Angle X-ray Scattering in Biological Sciences, 5/31/07-6/1/07, Colorado State University, Fort Collins, CO. Invited talk: Large-scale shape changes associated with activation of cGMP-dependent protein kinase.

Department of Microbiology, University of Otago, Dunedin, New Zealand, 12/15/2006. Invited colloquium: Computational modeling of gene regulation in *Escherichia coli*.

Second International Conference of the Biocomputing and Physics of Complex Systems Research Institute (BIFI), University of Zaragoza, Zaragoza, Spain. 8-11 February 2006. Invited talk: Principles of Biochemical Regulation. Session chair.

13th Annual International Meeting on Microbial Genomics, University of Wisconsin, Madison, WI. 11-15 September 2005. Invited talk: Computational Models of Biochemical Regulation.

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The third annual retreat of the Computation and Informatics in Biology and Medicine Training Program, University of Wisconsin, Madison, WI. 15 October 2004. Invited talk: Design principles of genetic regulatory networks.

International Conference on Molecular Systems Biology 2004, 8/21/04-8/25/04, Tahoe City, CA. Invited talk: Design principles of genetic regulatory networks.

Institute for Pure and applied Mathematics, 4/1/04, UCLA, Los Angeles. Invited colloquium: Structure and function of genetic regulatory circuits in *Escherichia coli*.

MIPNETS workshop on Proteins and Signals, 6/25/2003, Liverpool, UK. Invited talk: Mechanisms of Biochemical Regulation. Session chair.

University of Otago, 5/2/2003, Dunedin, New Zealand. Invited talk: Mechanisms of biochemical regulation.

American Physical Society meeting, 3/2/2003, Austin TX. Invited tutorial: Transcriptional Regulatory Networks: Data, Analysis and Modeling

LANL workshop on enabling concepts in systems biology, 9/19/2002, Santa Fe, NM. Invited talk: Integrating systems and structural biology: structural mechanisms in cGMP binding and activation of cGMP-dependent protein kinase

American Chemical Society Rocky Mountain Regional Meeting, 10/14/2002, Albuquerque, NM. Invited talk: Mechanisms associated with cGMP binding and activation of cGMP-dependent protein kinase

Instituto Gulbenkian de Ciencia, 3/11-3/15/2002, Oeiras, Portugal. Institute-sponsored visit; bioinformatics lectures on microarray methods.

APS User Meeting, 10/9/2001, Argonne National Laboratory, Argonne, IL. Invited talk: Diffuse Scattering: Methods for Molecular Structure and Dynamics

LANL/UCSD Workshop, 9/8/2001-9/9/2001, San Diego, CA. Invited talk: Diffuse Scattering and Database Methods

National Center for Genome Resources, March 2001, Santa Fe, NM. Invited seminar: Singular value decomposition analysis of microarray data

Gordon Research Conference on Diffraction Methods in Molecular Biology, Summer 2000, Andover, NH. Invited talk: Harnessing the potential of a structure database

Los Alamos National Laboratory, February 1999, Los Alamos, NM. Invited talk: Refinement of X-ray structures using a database of pairwise interatomic distance probabilities

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School of Biological Sciences, December 1998, Auckland University, Auckland, New Zealand.
Invited talk: Dynamics in Calmodulin

Department of Chemistry, December 1998, Massey University, Palmerston North, New Zealand.
Invited talk: Dynamics in Calmodulin

Department of Biochemistry, December 1998, Otago University, Dunedin, New Zealand. Invited talk: Dynamics in Calmodulin

Gordon Research Conference on Diffraction Methods in Molecular Biology, Summer 1998, Andover, NH. Invited talk: Making sense of diffuse scattering and making use of all the X-rays

Parke-Davis Pharmaceuticals, Spring 1998, Ann Arbor, MI. Two invited talks: Dynamics in calmodulin crystals; Refinement of X-ray structures using a database of pairwise interatomic distance probabilities

Biophysical Society Meeting, Winter 1998, Kansas City, MO. Invited talk: Refinement of X-ray structures using a database of pairwise atomic distance probabilities

Department of Molecular and Cellular Biology, Fall 1997, Brown University, Providence, RI. Invited talk: Dynamics in calmodulin crystals

International Union of Crystallography Meeting, August 1996, Seattle, WA. Invited talk on dissertation research

CHESS Journal Club, May 1996, Cornell University, Ithaca, NY. Invited talk on dissertation research

Keck Center for Computational Biology Colloquium, September 1995, Rice University, Houston, TX. Invited talk on dissertation research

DCRT Structural Biology Division, 1994, National Institutes of Health, Bethesda, MD. Invited talk on dissertation research

Software and Databases

1. GMV – Genome Majority Vote software to correct gene start site predictions (<http://code.google.com/p/gmv/>)
2. LUNUS – Software for diffuse X-ray scattering from protein crystals (<http://code.google.com/p/lunus/>)
3. SOESA – Structure Optimization and Evaluation using Separations of Atoms (<http://code.google.com/p/soesa/>)

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4. SVDMAN – Singular Value Decomposition Microarray Analysis (<http://code.google.com/p/svdman/>)
5. EcoTFs – *E. coli* Transcription Factors and Signals Database (with William S. Hlavacek, <http://ecotfs.lanl.gov>)

Peer-Reviewed Publications

Journal Articles

1. S.M. Gruner, S.L. Barna, M.E. Wall, M.W. Tate, E.F. Eikenberry. 1993. Characterization of polycrystalline phosphors for area X-ray detectors. Proceedings of the SPIE - The International Society for Optical Engineering 2009:98-108
2. M.W. Tate, E.F. Eikenberry, S.L. Barna, M.E. Wall, J.L. Lowrance, S.M. Gruner. A large-format high-resolution area X-ray detector based on a fiber-optically bonded charge-coupled device (CCD). 1995. Journal of Applied Crystallography 28:196-205
3. R.L. Walter, D.J. Thiel, S.L. Barna, M.W. Tate, M.E. Wall, E.F. Eikenberry, S.M. Gruner and S.E. Ealick. 1995. High-resolution macromolecular structure determination using CCD detectors and synchrotron radiation. Structure 3:835
4. M.E. Wall, S.E. Ealick and S.M. Gruner. 1997. Three-dimensional diffuse X-ray scattering from crystals of *Staphylococcal nuclease*. Proc Natl Acad Sci USA 94:6180-84
5. M.E. Wall, J.B. Clarage and G.N. Phillips, Jr. 1997. Motions of calmodulin characterized using both Bragg and diffuse X-ray scattering. Structure 5:1599-1612
6. M.E. Wall, S. Subramaniam and G.N. Phillips, Jr. 1999. Protein structure determination using a database of interatomic distance probabilities. Protein Sci 8:2720-27.
7. C.S. Tung, M.E. Wall, S.C. Gallagher and J. Trehwella. 2000. A model of troponin-I in complex with troponin-C using hybrid experimental data: the inhibitory region is a β -hairpin. Protein Sci 7:1312-26
8. M.E. Wall, P.A. Dyck and T.S. Brettin. 2001. SVDMAN – singular value decomposition analysis of microarray data. Bioinformatics 6:566-568
9. M.E. Wall, S.H. Francis, J.D. Corbin, K. Grimes, R. Richie-Jannetta, J. Kotera, B.A. Macdonald, R.R. Gibson and J. Trehwella. 2003. Mechanisms associated with cGMP binding and activation of cGMP-dependent protein kinase. Proc Natl Acad Sci USA 100:2380-2385.
10. M.E. Wall, W.S. Hlavacek and M.A. Savageau. 2003. Design principles for regulator gene expression in a repressible gene circuit. J Mol Biol 332:861-876.
11. M.E. Wall, W.S. Hlavacek and M.A. Savageau. 2004. Design of gene circuits: lessons from bacteria. Nat Rev Genet 5:34-42. (Review)
12. D. Ming and M.E. Wall. 2005. Quantifying allosteric effects in proteins. Proteins 59:697-707.
13. M.E. Wall, M.J. Dunlop and W.S. Hlavacek. 2005. Multiple functions of a feed-forward-loop gene circuit. J Mol Biol 349:501-514

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14. D. Ming and M.E. Wall. 2005. Allostery in a coarse-grained model of protein dynamics. *Phys Rev Lett* 95:198301
15. D. Ming and M.E. Wall. 2006. Interactions in native binding sites cause a large change in protein dynamics. *J Mol Biol* 358:213-223
16. D. Ming, M.E. Wall, and K.Y. Sanbonmatsu. 2007. Domain motions of Argonaute, the catalytic engine of RNA interference. *BMC Bioinformatics* 8:470 (“Highly accessed” designation).
17. D. Ming, M. Anghel, and M.E. Wall. 2008. Hidden structure in protein energy landscapes. *Phys Rev E* 77:021902.
18. D. Ming, J.D. Cohn, and M.E. Wall. 2008. Fast dynamics perturbation analysis for prediction of protein functional sites. *BMC Struct Biol* 8:5.
19. R. G. Martin, E. S. Bartlett, J. L. Rosner, M. E. Wall. 2008. Activation of the *Escherichia coli marA/soxS/rob* regulon in response to transcriptional activator concentration. *J Mol Biol* 380:278-284.
20. D.W. Dreisigmeyer, J. Stajic, I. Nemenman, W.S. Hlavacek, M.E. Wall. 2008. Determinants of bistability in induction of the *Escherichia coli lac* operon. *IET Syst Biol* 5:293-303
21. M. E. Wall, D. A. Markowitz, J. L. Rosner, R. G. Martin. 2009. Model of transcriptional activation by MarA in *Escherichia coli*. *PLoS Computational Biology* 5:e1000614.
22. J. Dunbar, J. D. Cohn, M. E. Wall. 2011. Consistency of gene starts among *Burkholderia* genomes. *BMC Genomics* 12:125.
23. M. E. Wall. 2011. Structure-function relations are subtle in genetic regulatory networks. *Mathematical Biosciences* 231:61-68.
24. M. E. Wall, S. V. Raghavan, J. D. Cohn, J. Dunbar. 2011. Genome majority vote improves gene predictions. *PLoS Computational Biology* 7:e1002284.
25. K.M. Verspoor, J.D. Cohn, K.E. Ravikumar, and M.E. Wall. 2012. Text mining improves prediction of protein functional sites. *PLoS One* 7:e32171.

Conference Proceedings

26. M.J. Dunlop and M.E. Wall. 2005. Robustness in gene circuits: clustering of functional responses. *Proceedings of the 24th American Control Conference* 6:4411-4416
27. M.E. Wall. Ligand binding, protein fluctuations, and allosteric free energy. 2006. *AIP Conference Proceedings* 851:16-33
28. I. Nemenman, G.S. Escola, W.S. Hlavacek, P.J. Unkefer, C.J. Unkefer, M.E. Wall. 2007. Reconstruction of metabolic networks from high-throughput metabolite profiling data: *in silico* analysis of red blood cell metabolism. *Ann NY Acad Sci* 1115:102-115
29. Ravikumar, KE, Liu H, Cohn JD, Wall ME, Verspoor K. 2011. Pattern Learning through Distant Supervision for Extraction of Protein-Residue Associations in the Biomedical Literature. *Machine Learning and Applications and Workshops (ICMLA), 10th International Conference on Machine Learning and Applications.* 2:59–65.

Other Publications

Review Articles

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30. M.E. Wall, S.C. Gallagher and J. Trehwella. 2000. Large-scale shape changes in proteins and macromolecular complexes. *Ann Rev Phys Chem* 51:355-80

Book Chapters

31. M.E. Wall, A. Rechtsteiner, L.M. Rocha. 2003. Singular Value Decomposition and Principal Component Analysis. In *A Practical Approach to Microarray Data Analysis*. D.P. Berrar, W. Dubitzky, M. Granzow, eds. pp. 91-109, Kluwer:Norwell, MA.
32. M.E. Wall. 2009. Methods and software for diffuse X-ray scattering from protein crystals. *Meths Mol Biol* 544:269-279.
33. D. Ming, M.E. Wall. 2012. Predicting binding sites by analyzing allosteric effects. *Meths Mol Biol* 796:423.

Editorials

34. I. Nemenman, W.S. Hlavacek, J.S. Edwards, J.R. Faeder, Y. Jiang, M.E. Wall. 2008. Selected papers from the First q-bio Conference on Cellular Information Processing. *IET Syst Biol* 5:203-205
35. I. Nemenman, W. S. Hlavacek, Y. Jiang, M. E. Wall. 2009. Editorial: Selected papers from the Second q-bio Conference on Cellular Information Processing. *IET Syst Biol* 3:297.
36. I. Nemenman, W. S. Hlavacek, Y. Jiang, M. E. Wall, A. Zilman. 2010. The third q-bio conference on cellular information processing. *IET Systems Biology* 4:331.
37. I. Nemenman, J. R. Faeder, W. S. Hlavacek, Y. Jiang, A. Zilman. 2011. Selected papers from the Fourth Annual q-bio Conference on Cellular Information Processing. *Physical Biology* 8(5):050301.

News Features

38. J.S. Edwards, J.R. Faeder, W.S. Hlavacek, Y. Jiang, I. Nemenman, and M.E. Wall. 2007. q-bio 2007: A Watershed Moment in Modern Biology. *Mol Syst Biol* 3:148