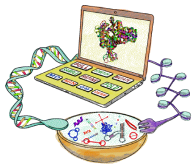

October 8, 2012

Tamar Schlick
Professor of Chemistry, Mathematics, and Computer Science, New York University
http://www.biomath.nyu.edu/

Education

Wayne State Univ., Detroit, MI (B.S., Mathematics, 1982); New York Univ., Courant Institute of Mathematical Sciences, New York, NY (M.S., Applied Mathematics); New York Univ., Courant Institute of Mathematical Sciences, New York, NY (Ph.D., Applied Mathematics, 1987)

Academic Positions

Director of Doctoral Program in Computational Biology (2003–2006); Director of Graduate Program Development, Dept. of Chemistry (2003–2006); Director of Graduate Studies, Dept. of Chemistry, NYU (2000–2003); Associate Investigator, Howard Hughes Medical Institute (1994–2003); Affiliate, Biochemistry Dept., NYU Medical Center (1996–); Professor of Chemistry, Mathematics and Computer Sciences, NYU (1996–); Assistant (until 1992) and Associate (until 1996) Professor of Chemistry and Mathematics, Faculty of Arts and Science and Courant Institute of Mathematical Sciences, NYU (1989–1996); Weizmann Institute Postdoctoral Fellow, Weizmann Institute of Science, Rehovot, Israel (1988); NSF Mathematical Sciences Postdoctoral Fellow, Courant Institute of Mathematical Sciences, NYU (1987–1989)

Honors

SIAM (Society of Industrial and Applied Mathematics) Fellow (2012); Biophysical Society Fellow (2012); Weston Visiting Professor, Department of Structural Biology, Weizmann Institute of Science (Host: Prof. Ada Yonath) (2011); Aspen Health Forum Fellow (2007); APS Fellow (2005); AAAS Fellow (2004); Agnes Fay Morgan Research Award in Chemistry, Iota Sigma Pi National Honor Society (2003); Burroughs Wellcome Visiting Professor, UNC (2000–2001); John Simon Guggenheim Fellow (2000–2001); AWIS Outstanding Woman in Science (2000); Alfred P. Sloan Research Fellow (1993–1995); NYU Distinguished Recent Alumna (1993); NSF Presidential Young Investigator (1991–1996); Whitaker Fellow (1991–1994); Searle Scholar (1991–1994); Whitehead Presidential Fellow, NYU (1991); Marie Curie American Fellow, AAUW (1990–1991); Kurt O. Friedrichs Prize for Outstanding Dissertation in Mathematics, Courant Institute (1988); Jay Krakauer Prize for Outstanding Dissertation in the Sciences, NYU (1988); NSF Mathematical Sciences Postdoctoral Fellow (1987–1989); Dean's Dissertation Fellow, NYU (1986–1987); Phi Beta Kappa, National Honor Society, Graduation with Excellence in Mathematics and French, Outstanding Leadership Award in Univ. Programs, Wayne State Univ. (1982); Wayne State Univ. Merit Scholar (Four-Year Tuition) (1978–1982)

Personal Statement

Following a formal training in applied mathematics, my work has been devoted to developing innovative mathematical and computational tools for biomolecular modeling and simulation and applying them to fundamental biological problems involving protein/nucleic acid complexes associated with biological regulation such as polymerase mechanisms, chromatin organization, and RNA structure and function. My community activities in various editorial boards and advisory committees in mathematics, computational biology, and chemistry reflect my interdisciplinary and educational interests, particularly to enhance and broaden graduate education in applied mathematics and computational biology. I enjoy training and working with young scientists, including to date 38 postdoctoral fellows and 35 research students, as well 19 of undergraduate and high school students, many of which have continued to successful independent scientific careers. My textbook, Molecular Modeling: An Interdisciplinary Guide (Springer-Verlag) has appeared in its second edition in August 2010.

Synergistic Activities

Community Service

Advisory Committee Member/Panelist:
Ad Hoc Member, NIH MFSD study section (Biology, Chemistry & Macromol. Biophysics) (2011); NSF-OCI (OCI, Office of Cyberinfrastructure) Task Force on Grand Challenges and Implications for Cyberscience Communities, National Science Foundation (2010–2012); Simons Foundation Science Series (2010–2012); Chair, Computational Biology Review Panel, Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program (2009); DOE Extreme Biology Workshop, Co-Chair (2009); NIH Pioneer Awards Review Committee (2005, 2006); HHMI-NIBIB Initiative for Interdisciplinary Graduate Research training (2005); NYAS Women Investigators Network (2004–); National Iota Sigma Pi Award Committee (2004–); NIH Computational Biophysics Study Section (2004); NIH Physical Biochemistry Study Section (2003–2004); Philip Morris External Research Program peer Review (2003); NSF's Advanced Computational Infrastructure (PACI) Resource Allocation Committee (2002–); NSF-NPACI

Panel Review Board (2002–); Member-at-Large of the AAAS Section A (Mathematics) (2002–2005); *Faculty of 1000*, Structural Biology/Theory and Simulation (2001–); NIH Special Study Section B, NIGMS (2001); NIH Site Visit panel, Intramural Review of Computational Applications Program (SAIC), NCI (2000); NIH BBCA study section (1999); SIAM Life Sciences Activity Group Steering Committee (1999–); NSF/NIH/DOE panel, *Next Generation Biology: the Role of Next Generation Computing* (1998); NSF Academic Research Infrastructure Program (1996); Burroughs Welcome Fund, Advisory Committee for Interface Program Between the Physical and Biological Sciences (1995–2000); AMS-SIAM Committee on Applied Mathematics (1995–2000); SIAM's representative to the AMS-ASA-AWM-IMS-MAA-NCTM-SIAM Committee on Women in the Mathematical Sciences (1994–2002); NIH RAC Board for the Parallel Structural Biology Project of the San Diego Supercomputing Center and UCSD (1994–); NIH Board of Scientific Counselors, National Library of Medicine (1994–1999); NSF Biophysics Division (1993–1995); NIH Special Review Committee for *Structural Biology as Applied to the Problem of Targeted Drug Design for the Treatment of AIDS* Initiative (1992); NSF Advanced Scientific Computing Postdoctoral Research Associateship Program (1991–1994).

Editorial Boards (selected)
Springer Verlag, Biophysics for Life Sciences series, Advisory Board (2010–); Intl. J. for Multiscale Computational Engineering (2007–, Assoc. Editor); J. Phys. Chem. B (2007–; Advisory Board); Journal of Theoretical Biology (1995–2005); Springer Verlag Lecture Notes in Computational Science and Engineering (1996–); Journal of Computational Physics (1997–); Biophysics J. (2004–2007), Biomedical Computation Review (2005–); **SIAM Multiscale Modeling and Simulation (2005–)**; **SIAM Journal on Scientific Computing (2005–)**; Faculty of 1000, Structural Biology (2001–); **SIAM Life Science Activity Group (2001–)**

Organizer/Co-Organizer
Co-chair of Computational Biology: Then and Today, Weizmann Institute (2013); Fifth International Symposium on Algorithms for Macromolecular Modeling, Co-Organizer (University of Texas, Austin) (2009); *Macromolecular Proteins and Protein Complexes*, Co-Chair, DOE exascale workshop (2009); *3DSig Satellite Meeting of the ISMB Conference*, Scientific Program Advisory Committee (2008); 2007 SIAM conference on *Mathematics for Industry* (Broad theme: Mathematics for Life Sciences) (2007); IMA Year on the Mathematics of Molecular and Cellular Biology, Minneapolis (2007–2008); IMA Special year in Computational Chemistry, Minneapolis (2008–2009); Second SIAM Life Sciences Conference (2004); Fourth International Symposium on Algorithms for Macromolecular Modeling, Leicester, UK (2004); Workshop on Modeling and Simulation for Materials, Institute for Pure and Applied Mathematics (IPAM), UCLA (2002); First SIAM Life Sciences Conference, Boston (2002); Computational Sciences Meeting, Washington, D.C. (2000); Third International Symposium on Algorithms for Macromolecular Modeling, New York (2000); International Conference on Multiscale Methods, Weizmann Institute (2000); Molecular Dynamics Minisymposium, SIAM, Charlotte (1995); Multigrid Techniques with Applications to Molecular Dynamics, Weizmann Institute (1995); Program in Mathematical Biology, MSRI Berkeley (1992)

Collaborators and Other Affiliations
Collaborators: W.A. Beard (NIEHS), S. Grigoryev (PSU), T. Kunkel (NIEHS), N. Leontis (BGSU), B. Sampoli Benitez (Marymount Manhattan College), S. H. Wilson (NIEHS), A. Yonath (Weizmann)

Graduate and Postdoctoral Advisors: S. Broyde (NYU, doctoral advisor), S. Lifson (deceased, Weizmann Institute, postdoctoral advisor), M. L. Overton (NYU, co-doctoral advisor), C.S. Peskin (NYU, doctoral advisor)

Thesis Advisees and Postdoc Mentees: I. Alberts (Schrodinger), K. Arora (U. Mich.), G. Arya (UCSD), D. Barash (Univ. of Haifa), E. Barth (Kalamazoo), P. Batcho (Los Alamos National Lab), D. Beard (Wisconsin Medical College), M. Bojin (Queens Borough Comm. College), R. Collepardo (postdoc), P. Derreumaux (CNRS, France), S. D'Souza (student), S. Elmetwaly (NYU), M. Foley (student), H. H. Gan (postdoc), L. A. Halvorsen (student), J. Huang (VeraChem, MA), H. Jian (Citicorp, NYC), S. Jung (student), N. Kim (student and postdoc), C. Laing (postdoc), Y. Li (Student), Y. P. Liu (Western Michigan Univ.), A. Luque (NYU), M. Mandziuk (NYU), S. McGuffe (Mem. Sloan-Kettering Cancer Center), B. Mishra (Wall Street, NYC), O. Perisic (ETH, Lausanne), X. Qian (Morgan Stanley, NYC), G. Quarta (student), R. Radhakrishnan (Univ. Pennsylvania), S. Reddy (Columbia), D. Rooklin (student), D. Roy (NYU), B. Sampoli Benitez (Marymount Manhattan College), A. Sandu (Michigan Technological Univ.), D. Strahs (Pace Univ.), J. Sun (Cornell/Weill Medical College), Y. Wang (SD Comm. College), D. Xie (Univ. of Wisconsin-Milwaukee), Y. Xin (Columbia), S. Yagmour (Polytechnic), L. Yang, M. Zahran (NYU), L. Zaslavsky (NIH), Q. Zhang (GlaxoSmithKline)
[Total Postdocs: 32; Total Graduate Students: 15; Note: Some students were also postdocs]

Selected Publications (from 170 total, see http://www.biomath.nyu.edu/)

1. W.L. Hase, D.M. Ludlow, R.J.Wolf, and T. Schlick, "Translational and Vibrational Energy Dependence of the Cross Section for H + C_4H_4 → C_2H_5", *J. Phys. Chem.* **85**, 958–968 (1981).
2. T. Schlick and M. Overton, "A Powerful Truncated Newton Method for Potential Energy Minimization", *J. Comp. Chem.* **8**, 1025–1039 (1987).
3. T. Schlick, C. Peskin, S. Broyde, and M. Overton, "An Analysis of the Structural and Energetic Properties of Deoxyribose by Potential Energy Methods", *J. Comp. Chem.* **8**, 1199–1224 (1987).
4. C.S. Peskin and T. Schlick, "Molecular Dynamics by the Backward-Euler Method", *Comm. Pure Appl. Math.* **42**, 1001–1031 (1989).

5. T. Schlick and C.S. Peskin, "Can Classical Equations Simulate Quantum-Mechanical Behavior? A Molecular Dynamics Investigation of a Diatomic Molecule with a Morse Potential", *Comm. Pure Appl. Math.* **42**, 1141–1163 (1989).
6. T. Schlick and W.K. Olson, "Computer Simulations of Supercoiled DNA Energetics and Dynamics", *J. Mol. Biol.* **223**, 1089–1119 (1992).
7. T. Schlick and A. Fogelson, "TNPACK – A Truncated Newton Minimization Package for Large-Scale Problems: I. Algorithm and Usage", *ACM Trans. Math. Softw.* **18**, 46–70 (1992).
8. T. Schlick and A. Fogelson, "TNPACK – A Truncated Newton Minimization Package for Large-Scale Problems: II. Implementation Examples", *ACM Trans. Math. Softw.* **18**, 71–111 (1992).
9. T. Schlick and W.K. Olson, "Trefoil Knotting Revealed by Molecular Dynamics of Supercoiled DNA", *Science* **257**, 1110–1115 (1992).
10. T. Schlick, "Optimization Methods in Computational Chemistry", in *Reviews in Computational Chemistry, Volume 3*, Chapter 1, pp. 1–71, K.B. Lipkowitz and D.B. Boyd, eds., VCH Publishers, New York (1992).
11. T. Schlick, "Modified Cholesky Factorizations for Sparse Preconditioners", *SIAM J. Sci. Comp.* **14**, 424–445 (1993).
12. X. Zou, I.M. Navon, M. Berger, P.K.H. Phua, T. Schlick, and F.X. Le Dimet, "Numerical Experience with Limited-Memory and Truncated Newton Methods", *SIAM J. Opt.* **3**, 582–608 (1993).
13. G. Zhang and T. Schlick, "LIN: A New Algorithm Combining Implicit Integration and Normal Mode Techniques for Molecular Dynamics", *J. Comp. Chem.* **14**, 1212–1233 (1993).
14. G. Zhang and T. Schlick, "The Langevin/Implicit-Euler/Normal-Mode Scheme (LIN)for Molecular Dynamics at Large Timesteps", *J. Chem. Phys.* **101**, 4995–5012 (1994).
15. J. A. Board, Jr., L. V. Kale, K. Schulten, R. D. Skeel, and T. Schlick, "Modeling Biomolecules: Larger Scales, Longer Durations", *IEEE Comp. Sci. Eng.* **1**, 19–30 (1994).
16. G. Zhang and T. Schlick, "Implicit Integration Schemes for Langevin Dynamics", *Mol. Phys.* **84**, 1077–1098(1995).
17. M. Mandziuk and T. Schlick, "Resonance in the Dynamics of Chemical Systems Simulated by the Implicit Midpoint Scheme", *Chem. Phys. Lett.* **237**, 525–535 (1995).
18. T. Schlick, "Pursuing Laplace's Vision On Modern Computers", *Proceedings of the IMA Program in Mathematical Biology*, IMA Volumes in Mathematics and its Applications, Vol. 82, pp. 219–247, J. Mesirov, K. Schulten, and D.W. Sumners, eds., Springer-Verlag, New York (1996).
19. B. Mishra and T. Schlick, "The Notion of Error in Langevin Dynamics: (1) Linear Analysis", *J. Chem. Phys.* **105**, 299–318 (1996).
20. T. Schlick and A. Brandt, "A Multigrid Tutorial with Applications to Molecular Dynamics", *IEEE Comp. Sci. Eng.* **3**, 78–83 (1996).
21. T. Pinou, T. Schlick, B. Li, and H. Dowling, "Addition of Darwin's Third Dimension to Evolutionary Trees", *J. Theor. Bio.* **219**, 505–512 (1996).
22. R. D. Skeel, G. Zhang, and T. Schlick, "A Family of Symplectic Integrators: Stability, Accuracy, and Molecular Dynamics Applications", *SIAM J. Sci. Comp.* **18**, 203–222 (1997).
23. T. Schlick, E. Barth, and M.Mandziuk, "Biomolecular Dynamics at Long Timesteps: Bridging the Time Scale Gap Between Simulation and Experimentation", *Annu. Rev. Biophys. Biomol. Struct.* **26**, 179–220 (1997).
24. T. Schlick, "Geometry Optimization", Contributed chapter to the Encyclopedia of Computational Chemistry (5 volumes), P. von Rague Schleyer, Editor in Chief, and N. L. Allinger, T. Clark, J. Gasteiger, P. A. Kollman, and H. F. Schaefer III, eds., John Wiley & Sons, West Sussex, Vol. 2, pp. 1136–1157 (1998)
25. E. Barth and T. Schlick, "Overcoming Stability Limitations in Biomolecular Dynamics: I. Combining Force Splitting via Extrapolation with Langevin Dynamics in LN", *J. Chem. Phys.* **109**, 1617–1632 (1998).
26. T. Schlick, M. Mandziuk, R. Skeel, K. Srinivas, "Nonlinear Resonance Artifacts in Molecular Dynamics", *J. Comp. Phys.* **140**, 1–29 (1998).
27. L.Y. Zaslavsky and T. Schlick, "An Adaptive Multigrid Technique for Evaluating Long-Range Forces in Biomolecular Simulations", *App. Math. Comp.* **97**, 237–250 (1998).
28. H. Jian, T. Schlick, and A. Vologodskii, "Internal Motion of Supercoiled DNA: Brownian Dynamics Simulations of Site Juxtaposition", *J. Mol. Biol.* **284**, 287–296 (1998). **[Figure featured on journal cover]**.
29. D. Xie and T. Schlick, "Efficient Implementation of the Truncated Newton Method for Large-Scale Chemistry Applications", *SIAM J. Opt.* **10**, 132–154 (1999).
30. T. Schlick, "Computational Molecular Biophysics Today: A Confluence of Methodological Advances and Complex Biomolecular Applications", *J. Comp. Phys.* **151**, 1–8 (1999).
31. A. Sandu and T. Schlick, "Resonance Analysis in Force Splitting Methods for Biomolecular Dynamics", *J. Comp. Phys.* **151**, 74–113 (1999).
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33. D. Xie, A. Tropsha, and T. Schlick, "An Efficient Projection Protocol for Chemical Databases: Singular Value Decomposition Combined With Truncated-Newton Minimization", *J. Chem. Inf. Comp. Sci.* **40**, 167–177 (2000).
34. D. Beard and T. Schlick, "Inertial Stochastic Dynamics: I. Long-Timestep Methods for Langevin Dynamics", *J. Chem. Phys.* **112,** 7313–7322 (2000).
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36. D. Beard and T. Schlick, "Modeling Salt-Mediated Electrostatics of Macromolecules: The Algorithm DiSCO (Discrete Surface Charge Optimization) and Its Application to the Nucleosome", *Biopolymers* **58**, 106–115 (2001). **[Figure featured on journal cover]**.
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42. L. Yang, S. Broyde, W. Beard, S. Wilson, and T. Schlick, "Polymerase β Simulations Reveal That Arg258 Rotation Is A Slow Step Rather Than Large Subdomain Motions *Per Se*", *J. Mol. Biol.* **317**, 651–671 (2002).
43. P. Batcho, D. A. Case, and T. Schlick, "Optimized Particle-Mesh Ewald/Multiple-Timestep Integration for Molecular Dynamics Simulations", *J. Chem. Phys.* **115**, 4003–4018 (2001).
44. T. Schlick, "Time-Trimming Tricks for Dynamic Simulations: Splitting Force Updates to Reduce Computational Work", *Structure* **9**, R45–R53 (Invited Ways & Means article) (2001).
45. X. Qian and T. Schlick, "Efficient Multiple-Timestep Integrators with Distance-Based Force Splitting for Particle-Mesh-Ewald Molecular Dynamics Simulations", *J. Chem. Phys.* **116**, 5971–5983 (2002). [Erratum in *J. Chem. Phys.* **117**, 1927 (2002)].
46. L. Yang,W. Beard, S.Wilson, B. Roux, S. Broyde, and T. Schlick, "Local Deformations Revealed by Dynamics Simulations of DNA Polymerase β with DNA Mismatches at the Primer Terminus", *J. Mol. Biol.* **321**, 459–478 (2002).
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53. N. Kim, N. Shiffeldrim, H. H. Gan, and T. Schlick, "Candidates for Novel RNA Topologies", *J. Mol. Biol.* **341**, 1129–1144 (2004).
54. T. Schlick, "The Critical Collaboration Between Art and Science: Applying *An Experiment on a Bird in an Air Pump* to the Ramifications of Genomics on Society", *Leonardo* **38** (4), 323–329 (2005).
55. J. Sun, Q. Zhang, and T. Schlick, "Electrostatic Mechanism of Nucleosomal Array Folding Revealed by Computer Simulation", *Proc. Natl. Acad. Sci.* **102**, 8180–8185 (2005).
56. J. Gevertz, H. H. Gan, and T. Schlick, "*In Vitro* RNA Random Pools are Not Structurally Diverse: A Computational Analysis", *RNA* **11**, 853–863 (2005).
57. U. Laserson, H. H. Gan and T. Schlick, "Predicting Candidate Genomic Sequences that Correspond to Synthetic Functional RNA Motifs", *Nuc. Acids Res.* **33**, 6057–6069 (2005).
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62. T. Schlick, "Mathematical and Biological Scientists Assess the State-of-the-Art in RNA Science at an IMA Workshop *RNA in Biology, Bioengineering and Biotechnology"*, *Intl. J. Mult. Sci. Eng.*, **8**: 369–378 (2010).
63. M. Foley and T. Schlick, "Simulations of DNA Pol λ R517 Mutants Indicate 517's Crucial Role in Ternary Complex Stability and Suggest DNA Slippage Origin", *J. Amer. Chem. Soc.* **130**: 3967–3977 (2008).
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73. T. Schlick, R. Collepardo-Guevara, L. A. Halvorsen, S. Jung, and X. Xiao, "Biomolecular Modeling and Simulation: A Field Coming of Age", *Quart. Rev. Biophys.*, **44**: 191–228 (2011).
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