Jaydeep P. Bardhan

Contact Information

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Education

Massachusetts Institute of Technology, Cambridge, MA **September 2001-June 2006**

Ph. D. in Electrical Engineering and Computer Science (GPA 4.8/5.0).

Advisors: Profs. Jacob K. White and Bruce Tidor

Dissertation Title: "Efficient Numerical Algorithms for Surface Formulations of Mathematical Models for Biomolecule Analysis and Design"

Dissertation selected for publication as a research monograph by VDM Publishing House, Ltd.

Massachusetts Institute of Technology, Cambridge, MA **September 2000-August 2001**

M. Eng. degree in Electrical Engineering and Computer Science (GPA 5.0/5.0).

Master's thesis title: "Calibration of a Microvision System for MEMS Device Characterization"

Advisor: Prof. Stephen D. Senturia

Massachusetts Institute of Technology, Cambridge, MA **September 1996-June 2000**

B.S. in Electrical Engineering (GPA 5.0/5.0).

Academic Experience

Argonne National Laboratory, Biosciences Division
Argonne Scholar **September 2008 - present**

- Developing numerical methods for predicting and analyzing wide-angle X-ray solution scattering (WAXS) of proteins.
- Investigating WAXS of ionic solutions for improving models of ion hydration and interactions.

Rush University Medical Center, Department of Molecular Biophysics and Physiology
Visiting Professor **January 2007 - present**

- Computational studies of drug resistance in escape mutants of HIV-1 membrane-fusion protein gp41 against peptide inhibitors (experimental collaborators: Prof. Fredric Cohen and Dr. Michael Leung).
- Numerical analysis of methods for simulation of electrostatics for permeation of ions through channel proteins.

Argonne National Laboratory, Mathematics and Computer Science Division
Wilkinson Fellow in Scientific Computing **September 2006 - August 2008**

- Developing novel numerical methods for PDE-constrained optimization of electrostatic interactions between biomolecules.
- Numerical analysis of methods for simulating electrostatic interactions within and between molecules in aqueous solution.
- Investigating the role of electrostatic interactions between the serine protease thrombin and co-factors in determining thrombin's specificity for pro-coagulant or anti-coagulant substrates.

M. I. T. Research Laboratory for Electronics, Computational Prototyping Group
Research Assistant **September 2001 - August 2006**

- Developed a hybrid simulation–optimization algorithm for rational drug design; algorithmic performance is more than one order of magnitude better than previous methods.
- Designed a fast boundary element method-based algorithm to rapidly analyze electrostatic interactions between biomolecules and surrounding solvent.
- Developed numerical techniques to discretize biomolecule–solvent interfaces with curved surface elements, and techniques for numerically integrating singular functions over the curved elements.

M. I. T. Microsystems Technology Laboratory, Polychromator Project
Research Assistant **September 2000 - August 2001**

- Designed and calibrated an automated microvision system to test microfabricated programmable diffraction gratings.
- Used automated test system to completely characterize several diffraction gratings; labor savings and reliability improvement are both significant.

Refereed Journal Publications

J. P. Bardhan, R. S. Eisenberg, D. Gillespie. "Discretization of the Induced-Charge Boundary Integral Equation," *in press, Physical Review E.*

S. Park, J. P. Bardhan, B. Roux, L. Makowski, "Simulated X-ray Scattering of Protein Solutions Using Explicit-Solvent Models," *Journal of Chemical Physics*, v.130, 134114 (2009).

J. P. Bardhan, M. Knepley, M. Anitescu. "Bounding Electrostatic Solvation Free Energies Using Boundary-Integral Equations," *Journal of Chemical Physics*, v.130, 104108 (2009). Selected for inclusion in the Virtual Journal of Biological Physics.

J. P. Bardhan, "Numerical Discretization of Boundary Integral Equations for Molecular Electrostatics," *Journal of Chemical Physics*, v.130, 094102 (2009). Selected for inclusion in the Virtual Journal of Biological Physics.

M. D. Altman, J. P. Bardhan, J. K. White, B. Tidor. "Accurate Solution of Multi-Region Continuum Biomolecule Electrostatic Problems Using the Linearized Poisson–Boltzmann Equation with Curved Boundary Elements," *Journal of Computational Chemistry*, v. 30(1), 132-153 (2009).

J. P. Bardhan, "Interpreting the Coulomb-Field Approximation for Generalized-Born Electrostatics Using Boundary-Integral Equation Theory," *Journal of Chemical Physics* v. 129, 144105 (2008). Selected for inclusion in the Virtual Journal of Biological Physics.

J. P. Bardhan, M. D. Altman, D. J. Willis, S. M. Lippow, B. Tidor, J. K. White. "Numerical Integration Techniques for Curved-Element Discretizations of Molecule–Solvent Interfaces," *Journal of Chemical Physics* v.127, 014701 (2007, co-authored). Selected for inclusion in the Virtual Journal of Biological Physics.

M. D. Altman and J. P. Bardhan, B. Tidor, J. K. White, "FFTSVD: A Fast Multiscale Boundary Element Method Solver Suitable for BioMEMS and Biomolecule Simulation," *IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems*, v. 25 (2), pp. 274-284 (2006, co-authored).

J. P. Bardhan, M. D. Altman, B. Tidor, J. K. White. "A 'Reverse-Schur' Approach to Optimization with Linear PDE Constraints: Application to Biomolecule Analysis and Design," *submitted to the Journal of Chemical Theory and Computation* (co-authored).

J. P. Bardhan, S. Park, L. Makowski: "SoftWAXS: A Computational Tool for Modeling Wide-Angle X-ray Solution Scattering from Biomolecules," *to be submitted, Journal of Applied Crystallography.*

Refereed Conference Publications

J. P. Bardhan and M. D. Altman, J. K. White, B. Tidor. "Efficient Optimization of Biomolecule Electrostatic Interactions," IEEE Conference on Decision and Control 2007.

M. D. Altman, J. P. Bardhan, J. K. White, B. Tidor. "A Fast and Accurate Surface Formulation for Biomolecule Electrostatics in Non-ionic Solution", IEEE Conference on Engineering in Medicine and Biology 2005.

J. P. Bardhan, M. D. Altman, S. M. Lippow, B. Tidor, J. K. White, "A Curved Panel Integration Technique for Molecular Surfaces", Nanotech 2005.

J. P. Bardhan, J. H. Lee, M. D. Altman, S. Benson, S. Leyffer, B. Tidor, J. K. White. "Biomolecule Electrostatic Optimization with an Implicit Hessian," Nanotech 2004.

J. P. Bardhan, J. H. Lee, M. D. Altman, B. Tidor, J. K. White. "Fast Methods for Biomolecule Charge Optimization," Nanotech 2003.

E. R. Deutsch, J. P. Bardhan, S. D. Senturia, G. B. Hocker, D. W. Youngner, M. B. Sinclair, M. A. Butler. "A Large-Travel Vertical Planar Actuator with Improved Stability," Transducers 2003.

S. S. Kuo, M. D. Altman, J. P. Bardhan, B. Tidor, J. K. White. "Fast Methods for Biomolecule Electrostatics," International Conference on Computer Aided Design 2002.

Book Chapters and Monographs

M. G. Knepley and J. P. Bardhan, "Modeling of Molecular-Scale Processes," in *Quantitative Modeling of Multiscale Biological Processes*, ed. D. Yuen; Springer Science, to appear.

J. P. Bardhan, "Computational Methods for Biomolecular Analysis and Design," VDM Verlag, to appear.

M. D. Altman and J. P. Bardhan, B. Tidor, J. K. White, "FFTSVD: A Fast Multiscale Boundary Element Method Solver Suitable for BioMEMS and Biomolecule Simulation," in *Design Automation Methods and Tools for Microfluidics-Based Biochips*, ed. K. Chakrabarty and J. Zeng; Springer Netherlands, 2006.

Presentations

- "Computational Modeling Approaches for Biomolecular Analysis and Design," Stanford University, March 12, 2009.
- "Numerical Methods in Molecular Science and Engineering," Toyota Technical Institute, February 25, 2009.
- "Approximating Electrostatic Interactions in Solution Using Boundary-Integral Equation Theory," Institute for Mathematics and its Applications (IMA) at U. Minnesota, Workshop on Solvation and Protein Folding, December 11, 2008.
- "Mathematical Models and Numerical Algorithms in Molecular Science," U. Minnesota Aerospace Engineering and Mechanics Seminar Series, November 7, 2008.
- "Numerical Methods for Molecular Science and Engineering," Rochester Institute of Technology, July 14, 2008.
- "Numerical Algorithms for Approximating Electrostatic Interactions," Rocky Mountain Regional Meeting of the American Chemical Society, June 16, 2008.

- "Numerical Methods for Electrostatic Optimization in Molecular Design," SIAM Conference on Optimization, May 13, 2008 (organizer of minisymposium, *Optimization in Molecular Design*).
- "Systems Biology: More than Just ODEs," Johannes Kepler University, Radon Institute for Computational and Applied Mathematics Workshop on Systems Biology, November 6, 2007.
- "Accurate and Efficient Numerical Methods for Simulation and Optimization of Biomolecule Electrostatics," EMBL Hamburg, November 2, 2007.
- "Accurate and Efficient Numerical Methods for Simulation and Optimization of Biomolecule Electrostatics," University of Vienna, October 30, 2007.
- "Accurate and Efficient Numerical Methods for Simulation and Optimization of Biomolecule Electrostatics," Johannes Kepler University, Radon Institute for Computational and Applied Mathematics Workshop on Ion Channels, October 9 2007.
- "Accurate and Efficient Numerical Methods for Simulation and Optimization of Biomolecule Electrostatics," National University of Singapore Symposium on Computational Engineering, July 30 2007.
- "The Importance of Accuracy and Efficiency for Numerical Simulations of Protein Electrostatics," Rush University Medical Center, October 20, 2006 (invited).
- "Accurate and Efficient Numerical Methods for Simulation and Optimization of Biomolecule Electrostatics," National University of Singapore Symposium on Computational Engineering July 28 2006.
- "Efficient Methods for Optimizing Electrostatic Interactions Between Biomolecules," SIAM Conference on Partial Differential Equations, July 10 2006.
- "Numerical Techniques for Biomolecule Analysis and Design," Nanofluidics Group Seminar, Stanford University; October 23, 2005 (invited).
- "Computer-Aided Analysis and Design of Biomolecules," Nanotechnology Seminar, Purdue University; March 10, 2005 (invited).
- "From Biology to Applied Mathematics and Back," Applied Mathematics Seminar, MIT; September 23, 2004 (invited).
- "A Different Look at Modeling Biomolecule Electrostatics," High-Performance Computing Seminar, Computational Systems Biology Initiative, MIT; May 26, 2004 (invited).
- "The Hessian-Implicit Primal-Dual Method" Argonne National Laboratory; December 3, 2002 (invited).

Honors and Awards

- Howes Scholar (2007)
- Wilkinson Fellowship in Scientific Computing (2006 - present)
- Department of Energy Computational Science Graduate Fellowship (2002 - 2006)
- Advanced Micro Devices scholarship (1998 - 2000)
- Member, Eta Kappa Nu
- Member, Tau Beta Pi

Professional Activities

- Reviewer
  - Microfluidics and Nanofluidics
  - ACM Journal on Emerging Technologies in Computing Systems

Teaching Experience

M. I. T., Computational Systems Biology Initiative, Singapore–MIT Alliance
Teaching Assistant **July 2006**

- National University of Singapore course: Introduction to Computational Systems Biology. Course taught by Prof. Paul Matsudaira (MIT) and Prof. Jacob K. White (MIT).
- Participated in the development of intensive laboratory exercises designed to instruct students about the design and analysis of numerical techniques for analysis of biological problems.

M. I. T., Computational Systems Biology Initiative, Singapore–MIT Alliance
Teaching Assistant **July 2005**

- National University of Singapore course: Introduction to Computational Systems Biology. Course taught by Prof. Paul Matsudaira (MIT) and Prof. Jacob K. White (MIT).
- Participated in the development of intensive laboratory exercises designed to instruct students about the design and analysis of numerical techniques for analysis of biological problems.

M. I. T., EECS Department
Teaching Assistant **January 2004 - May 2004**

- Course 6.971: Foundations of Algorithms and Computational Techniques for Systems Biology, taught by Prof. Jacob K. White and Prof. Bruce Tidor.
- Participated in curriculum design.
- Wrote problem sets and solutions, graded problem sets, and held office hours.

Teaching Assistant **September 2001 - December 2001**

- Course 6.002: Introductory Circuits and Signals, taught by Prof. Gerald J. Sussman and Prof. Ron Parker.
- Designed lessons for small groups of students and taught 10 hours of class per week.
- Wrote problem set solutions, designed sets of practice problems and wrote solutions.
- Assisted students during laboratory exercises.
- Held extensive weekly office hours and review sessions.

Industrial Experience

Advanced Micro Devices *K6 CAD Group*, Sunnyvale, CA.

- Designed process migration tools for the K6 microprocessor family.
- Developed experimental flows for circuit model extraction and timing analysis.

Advanced Micro Devices *Design Methodology Group*, Sunnyvale, CA.

- Developed software for design automation, simulation, and design rule checking.
- Projects included tools for automatic repeater insertion and sizing, mask generation, and timing analysis.

Storefront Media, Boston, MA.

- Co-founder of web services company focused on improving consumer experiences at apparel websites.
- Technical lead for presentations to venture capitalists in Boston and San Francisco.
- Lead developer for a project that created on-demand custom client-side Javascript applications, using a database-driven back end.
- Participated in discussions leading to investment by a Boston based incubator.
- Led negotiations between investors and interested third-parties exploring the possible sale of developed technologies.

Advanced Micro Devices *Process Methodology Group*, Sunnyvale, CA.

- Developed numerical simulation tools to aid in the design of the Opteron microprocessor: development focused on timing analysis and parasitic extraction.

PROFICIENCIES

- Software engineering in C, C++, PERL, Python, Scheme, Tcl
- Molecular modeling in CHARMM, NAMD, GAMESS, AmberTools, AutoDOCK