Curriculum Vitae

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Research Interest

I am interested in **computational biology** and **scientific computation**, with particular emphasis on biomolecular simulations and fast force-field evaluations.

Education

- Ph.D. and M.S. in Computer Science, University of Illinois at Urbana-Champaign
  1/2000 – 5/2004 (expected), Area: Scientific Computation, Advisor: Robert Skeel
  Ph.D. thesis: *Fast polarizable force field computation in biomolecular simulations*
  Master thesis: *Analysis of a few numerical integration methods for Langevin dynamics*
- Ph.D. candidate in Physics, Ohio State University, 6/1996 – 12/1999
- M.S. in Physics, Peking University, 9/1993–6/1996
  Thesis: *Impurity energy levels in the Haldane gap*
- Double B.S. in Physics and Applied Mathematics, Tsinghua University, 9/1988–7/1993

Research Experience

Theoretical and Computational Biophysics Group, Beckman Institute for Advanced Science and Technology, and Bionumerics Research Group, Department of Computer Science, University of Illinois at Urbana-Champaign, Graduate Research Assistant, 3/2002–present

- Fast polarizable force field computation
  The incorporation of polarization into the next generation force fields in biomolecular modeling and simulation requires fast methods to do very expensive computations. My thesis develops fast algorithms for computing the induced dipole moments in point dipole models. Twofold performance speedup is already achieved against the currently most reliable implementation (AMBER 7.0).

Computational Biology Group, National Center for Supercomputing Applications (NCSA), and Bionumerics Research Group, Department of Computer Science, University of Illinois at Urbana-Champaign, Graduate Research Assistant, 1/2000–3/2002

- Study on numerical integration methods for Langevin dynamics
  The modified equation approach is used to analyze numerical integrators for Langevin equation. My research found out that the popular Brooks-Brünger-Karplus method has weak convergence only of order 1, while some other methods have order 2 and are more accurate.

- Regularized Multigrid solvers
  Studied multigrid method for solving the Poisson–Boltzmann equation. Translated the multigrid solver code from FORTRAN to C. Tested the regularization idea.

Department of Physics, Ohio State University, Graduate Research Assistant, 6/1996–12/1999

- Simulation study of ad-atom/dimmer diffusion on silicon surface
  Developed C++ code from scratch for molecular dynamics simulation of ad-atom/dimmer diffusion, the slow hopping events are accelerated by several orders of magnitudes using the hyperdynamics technique.

Department of Physics, Peking University, Graduate Research Assistant, 9/1994–6/1996

- Impurity energy levels of one dimensional quantum spin system
  Calculated the impurity energy levels in the Haldane gap for quantum spin-1 chains using the Density Matrix Renormalization Group technique, a novel method to compute the lowest eigenvalues of banded matrices of huge size. The result settled a disagreement about the nature of impurity energy levels.

Publications

- Wei Wang, Robert D. Skeel, "Analysis of a few numerical integration methods for Langevin equation," *Molecular Physics*, **101**:2149–2156 (2003)
- Wei Wang, S. Qin, Z. Lu, Z. Su, L. Yu, "Impurity energy levels in the Haldane gap," *Physical Review B*, **53**:40–43 (1996)
- Wei Wang, Robert D. Skeel, "Accelerating the polarizable force field computation in biomolecular dynamics simulation," in preparation.
- Wei Wang, Robert D. Skeel, "How to compute diffusion constant," in preparation.

Presentations

- "Analysis of a few numerical integration methods for Langevin equation," poster, CIMMS-IPAM workshop on Molecular Modeling and Computation: Perspectives and Challenges, California Institute of Technology, Los Angeles, CA, November, 2002.
- "Hyperdynamics simulation of ad-dimmer diffusion on Si-(100) surface," American Physical Society Annual Meeting, Atlanta, GA, March, 1999.
- "Ad-atom diffusion on Si-(100) surface," American Physical Society Annual Meeting, Los Angeles, CA, March, 1998.

Professional Training

- 2003 Summer School on Theoretical and Computational Biophysics, University of Illinois at Urbana-Champaign, June 2–13, 2003
- Mathematics in Nanoscale Science and Engineering Workshop IV: Modeling and Simulation for Materials, University of California at Los Angeles, CA, November, 2002.
- Proceedings of 3rd International Workshop on Methods for Macromolecular Modeling, New York University, New York, NY, 2000

- Midwest NA Day, Indianapolis, IN 2000, and Urbana, IL, May 12, 2001.

Award and Honors

- President Fellowship, Ohio State University, 1996
- Excellent Student Award, Peking University, 1995
- Guang Hua Prize, Peking University, 1994
- Hong Kong Alumni Award, Tsinghua University, 1990
- Excellent Student Award, Tsinghua University, 1990

Professional Membership

- Society for Industrial and Applied Mathematics (SIAM)

References

Robert D. Skeel, Professor
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Michael T. Heath, Professor and Fulton Watson Copp Chair
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