

Dmitry A. Kondrashov

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EDUCATION Ph.D. Applied Mathematics, Biochemistry minor, May 2005
University of Arizona, Tucson, AZ, USA

M.S. Applied Mathematics, May 1999
University of Arizona, Tucson, AZ, USA

B.A., Natural Science (Chemistry), *cum laude*, May 1996
Simon's Rock College of Bard, Great Barrington, MA, USA

EMPLOYMENT *Postdoctoral Trainee* **University of Wisconsin**
Computation and Informatics in **Madison, WI, USA**
Biology and Medicine **2005–**

Development and application of coarse-grained simulation methods for protein dynamics. Work under direction of Dr. George Phillips in Biochemistry with Dr. Qiang Cui of Chemistry as secondary mentor.

Graduate Teaching Assistant **University of Arizona**
Department of Mathematics **Tucson, AZ, USA**
2001-02 1998-99

Independently taught sections of the following courses: Introduction to Statistics (Math 160), Mathematics in Modern Society (Math 105), Elements of Calculus (Math 123). Led discussion section for Principles of Analysis (Math 527A and B), served as grader for Methods of Applied Mathematics (Math 583B) and Multi-variable Calculus (Math 223).

Staff Research Assistant **Los Alamos National Lab**
Theoretical Biology and Biophysics **Los Alamos, NM, USA**
Summer 1999

Worked on a summer research project with Dr. Angel García. Wrote a Molecular Dynamics program to simulate a minimalist model of a protein. Analyzed the thermodynamic properties of the system such as its folding transition, free energy plots, as well as folding kinetics.

Applications Chemist **Millipore Corp.**
Bedford, MA, USA
1996–1997

Ran a part of Millipore's Gas Applications Lab. Responsibilities included conducting tests of various purification devices using APIMS (Atmospheric Pressure Ionization Mass Spec) and other analytical instruments, data analysis and writing reports and presentations.

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- PUBLICATIONS** Kondrashov, D.A., Roberts, S.A, Weichsel, A., and Montfort, W.R. “Protein functional cycle viewed at atomic resolution: conformational change and mobility in nitrophorin 4 as a function of pH and NO binding”, *Biochemistry* **43**: 13637-13647 (2004).
- Kondrashov, D.A. and Phillips, G.N., Jr. “Molecular mastication mechanics”, *Structure* **13**: 836-837 (2005).
- Kondrashov, D.A., Cui, Q., and Phillips, G N., Jr. “Optimization and evaluation of a coarse-grained model of protein motion using X-ray crystal data”, *Biophysical Journal*, **91**: 2760-2767 (2006).
- Kondrashov, D.A., Van Wynsberghe, A.W., Bannen, R.M., Cui, Q. and Phillips, G.N., Jr. “Protein structural variation in computational models and crystallographic data,” *Structure*, accepted.
- McCoy, J.G., Bitto, E., Bingman, C.A., Wesenberg, G.E., Bannen, R.M., Kondrashov, D.A., Phillips, G.N., Jr. “Structure and dynamics of UDP-glucose pyrophosphorylase from *Arabidopsis thaliana* with bound UDP-glucose and UTP”, *Journal of Molecular Biology*, accepted.
- Kondrashov, D.A., Zhang, W., Aranda, R. IV, Stec, B., and Phillips, G.N, Jr. “Sampling of the native conformational ensemble of myoglobin via structures in different crystalline environments ,” submitted.
- Kondrashov, D.A. and Montfort, W.R. “Nonequilibrium dynamics simulations of nitric oxide release: comparative study of nitrophorin and myoglobin,” submitted.
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- HONORS & AWARDS** Faculty of 1000 recommended paper “Optimization and evaluation of a coarse-grained model of protein motion using X-ray crystal data” (see above)
- CIBM Postdoctoral Fellowship, University of Wisconsin – Madison, 2005 –
- BIO5 Institute Graduate Fellowship, University of Arizona, 2004
- Predoctoral Fellowship from NSF-IGERT grant to the Biology, Mathematics and Physics Initiative, University of Arizona, 1999–01, 02–03
- Graduate Fellowship from Mathematics Dept, University of Arizona, 1997 – 98
- Acceleration to Excellence Scholarship, Simon’s Rock College, 1992–93
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- SERVICE** Referee for *Biopolymers* 2006-
- Session chair and ad hoc co-organizer, Steenbock Symposium on Protein Dynamics, University of Wisconsin, May 2006. This symposium attracted about 100 participants from around the nation who were interested in coarse-grained modeling of macromolecules.
- Organizer of a workshop for high school students on mathematics and biology, University of Arizona, November 2003. Day long presentation on mathematical modeling in molecular biology.
- Organizer of graduate mathematics day, University of Arizona, May 2001. Day long mini-conference for pure and applied mathematics graduate students.
- Volunteer tutor, Berkshire Farm Center and Services for Youth, Canaan, NY, 1995-96. Participated in weekly tutoring sessions for juveniles in residential facility.

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- SELECTED TALKS AND PRESENTATIONS “Harmonic models of protein motion and their evaluation using X-ray crystal data”, invited talk at Institute for Experimental and Theoretical Biophysics, Russian Academy of Sciences, Pushchino, Russia, July 14, 2006
- “Optimization, validation, and application of coarse-grained models of residue interaction”, talk at 32nd Steenbock Symposium on Dynamics of Proteins and Macromolecules, Madison, WI, May 20, 2006
- “Coarse-grained models of residue interaction in protein structures”, invited talk at University of British Columbia, Pacific Institute for Mathematical Sciences, Mathematical Biology Seminar, March 29, 2006
- “Modeling and simulation of ligand escape from protein: nitrophorin and myoglobin”, talk at Society for Industrial and Applied Mathematics Annual Meeting, Portland, OR, July 10-16, 2004
- “Loop dynamics and function in nitrophorin 4”, Kondrashov, D.A., Roberts, S.A., Weichsel, A., Watkins, J.C. and Montfort, W.R. poster at Biophysical Society Meeting, Baltimore, MD, February 15-19, 2004
- “The effects of temperature and pressure on thermodynamics and kinetics of folding in a minimalist protein model”, Kondrashov D.A. and Garcia A.E., poster at Dynamics Days 2000 meeting, Santa Fe, NM, January 2000
- SKILLS Computational Tools: C, perl, MATLAB, UNIX, OS X
Programming Experience: Discrete Molecular Dynamics code in C, Elastic Network Models in perl, scientific computing using MATLAB
Molecular Simulations: extensive experience with AMBER, VMD
Structural Biology: collection, processing and refinement of protein X-ray data