

## NINA SINGHAL HINRICHS

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### EDUCATION

#### **Stanford University (2001 - 2007), Stanford, CA**

Doctor of Philosophy in Computer Science, September 2007

Thesis: *Algorithms for building models of molecular motion from simulations.*

Advisors: Vijay Pande and Serafim Batzoglou

Master of Science in Computer Science, September 2004

#### **Massachusetts Institute of Technology (1997 - 2001), Cambridge, MA**

Bachelor of Science in Chemical Engineering, May 2001

Bachelor of Science in Mathematics with Computer Science, May 2001

Minor in Economics, May 2001

### WORK AND RESEARCH EXPERIENCE

#### **University of Chicago (2007 - present), Chicago, IL**

Assistant Professor, Department of Computer Science and Department of Statistics.

#### **Stanford University Research Assistant (2002 - 2007), Stanford, CA**

Designed mathematical models to analyze the long timescale behavior of macromolecules from multiple short trajectories. Developed and implemented efficient statistical and Bayesian techniques for error analysis, comparison across models, and iterative procedures to improve models. Advisor - Vijay Pande.

#### **IBM Almaden Research Center (2005 - 2006), Almaden, CA**

Designed, implemented, and verified an iterative algorithm to automatically define metastable kinetic states in the conformational space of a molecule. Advisor - William Swope.

#### **MIT Undergraduate Research Opportunities Program (2000 - 2001), Cambridge, MA**

Investigated the surface properties of various solid models at the molecular level using Monte Carlo computational methods. Applications for this research include studying the efficacy of catalysts as well as areas in atmospheric chemistry. Advisor - Bernhardt Trout.

#### **Akamai Technologies (January 2000), Cambridge, MA**

Designed and implemented models to forecast time dependent internet usage patterns to enhance server reliability and security.

**Corporate Research, Air Products and Chemicals Inc. (Summer 1999), Allentown, PA**

Optimized the process for the large-scale manufacture of an epoxy dispersion by independently designing and executing a series of chemical experiments. Gained experience in the use of a broad range of analytical equipment.

**Bell Laboratories/Lucent Technologies (Summer 1997 and 1998), Allentown, PA**

Developed object-oriented software and mega-widgets for the rapid implementation of multi-platform Graphical User Interfaces. Designed GUIs for a debugger for DSP software.

**TEACHING EXPERIENCE**

Statistical Models and Methods 1 (Winter 2008), University of Chicago

Computational Biology (Spring 2008), University of Chicago

Guest Lecturer, Algorithms in Biology (Autumn 2005), Stanford University  
*Graphical Models for Understanding Protein Kinetics*

Teaching assistant, Design and Analysis of Algorithms (Summer 2004), Stanford University

Teaching assistant, Discrete Structures (Winter 2002), Stanford University

MIT-India Internship Program (Summer 2001), Pune, India  
Taught HTML and JAVA to students at the Kalmadi Shamrao high school.

Tutor, Office of Minority Education (1998-2001), MIT  
Peer tutor and review session leader for courses in chemical engineering, chemistry, and mathematics.

**AWARDS AND HONORS**

National Defense Science and Engineering Graduate Fellowship (2001-2004)  
AT&T/Lucent Technology Merit Scholarship (1997-2001)  
Tau Beta Pi (2000)  
National Merit Scholar (1997)  
AP Scholar with Distinction (1997)  
US National Mathematics Award (1997)

**PUBLICATIONS**

**N. S. Hinrichs** and V. S. Pande. Bayesian metrics for the comparison of Markovian state models for molecular dynamics simulations. (In review, 2007).

- N. S. Hinrichs**. Algorithms for building models of molecular motion from simulations. Ph.D. Dissertation, Stanford University (2007).
- P. M. Kasson, A. Zomorodian, S. Park, **N. Singhal**, L. J. Guibas, and V. S. Pande. Persistent voids: a new structural metric for membrane fusion. *Bioinformatics*, 23(14), 1753-1759 (2007).
- N. S. Hinrichs** and V. S. Pande. Calculation of the distribution of eigenvalues and eigenvectors in Markovian state models for molecular dynamics. *Journal of Chemical Physics*, 126, 244101 (2007).
- J. D. Chodera\*, **N. Singhal**\*, V. S. Pande, K. A. Dill, and W. C. Swope. Automatic discovery of metastable states for the construction of Markov models of macromolecular conformational dynamics. *Journal of Chemical Physics*, 126, 155101 (2007).  
(\* These authors contributed equally to this work)
- P. M. Kasson, N. W. Kelley, **N. Singhal**, M. Vrljic, A. T. Brunger, and V. S. Pande. Ensemble molecular dynamics yields submillisecond kinetics and intermediates of membrane fusion. *Proceedings of the National Academy of Sciences*, 103(32), 11916 (2006).
- N. Singhal** and V. S. Pande. Error analysis and efficient sampling in Markovian state models for protein folding. *Journal of Chemical Physics*, 123, 204909 (2005).
- N. Singhal**, C. D. Snow, and V. S. Pande. Using path sampling to build better Markovian state models: Predicting the folding rate and mechanism of a tryptophan zipper beta hairpin. *Journal of Chemical Physics*, 121(1), 415 (2004).