Hai M. Nguyen

Postdoctoral Associate

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Education

PHD, Chemistry 2007 - 2014

Stony Brook University

B.Sc, Chemistry 2002 - 2006

Hanoi College of Science

Work History

Postdoctoral Associate Mar 2015 - Present

Rutgers University

- Co-developing visualization package for Molecular Dynamics simulation (NGLView)
- Developing Python interface for a series of programs in Amber suite
- Exploring properties of modified DNA and RNA
- Exploring new Generalized Born solvation models and a Python-based API for recombining Rosetta and Amber force fields for protein prediction and design
- Improving interface between AMBER (simulation package) and Phenix (Software suite for the automated determination of macromolecular structures)

Postdoctoral Associate Oct 2014 - Feb 2015

Stony Brook University

- Developing force field for implicit solvent model
- Implementing newly parameter-optimized implicit solvent for nucleic acid in AMBER suit program

Research Assistant Jan 2008 - Aug 2014

Stony Brook University

- Developing force field for implicit solvent model
- Improving Generalized-Born model's parameters for nucleic acid
- Applying implicit solvent to study protein folding
- Validating ff14SB force field
- Improving Generalized-Born model's parameters for protein
- Improving salt bridge description for HIV-1 protease simulation
- Testing effect of different Generalized-Born models to protein folding

Computational skills

- Programming languages
  - Efficient: Python/Cython
  - Familiar: C/C++, Fortran, JavaScript, R
- High Performance Computing Resources (Bluegene, Kraken, Bluewater)
- Parallel programming experience: MPI, multiprocessing
- Software engineering experience: git (version control) and continuous integration (very experienced)
- AMBER, Phenix
- Lead developer: **pytraj**, a Python package for data analysis for molecular dynamics simulation, https://github.com/Amber-MD/pytraj

- Contributing:
  - **AMBER** program suite: biomolecular simulation program, http://ambermd.org/
  - **cpptraj** (written in C++): Biomolecular simulation trajectory/data analysis, https://github.com/Amber-MD/cpptraj
  - **parmed** (written in Python): Parameter/topology editor and molecular simulator, https://github.com/ParmEd/ParmEd
  - **nglview** (written in Python, Javascript): Jupyter notebook viewer for biomolecular simulation, https://github.com/arose/nglview
  - **MDAnalysis** (written in Python): an object-oriented python toolkit to analyze molecular dynamics trajectories, http://www.mdanalysis.org/

Publications

Google Scholar statistics: https://goo.gl/o8qVU2

1. D.A. Case, R.M. Betz, W. Botello-Smith, D.S. Cerutti, T.E. Cheatham, III, T.A. Darden, R.E. Duke, T.J. Giese, H. Gohlke, A.W. Goetz, N. Homeyer, S. Izadi, P. Janowski, J. Kaus, A. Kovalenko, T.S. Lee, S. LeGrand, P. Li, C. Lin, T. Luchko, R. Luo, B. Madej, D. Mermelstein, K.M. Merz, G. Monard, **H. Nguyen**, H.T. Nguyen, I. Omelyan, A. Onufriev, D.R. Roe, A. Roitberg, C. Sagui, C.L. Simmerling, J. Swails, R.C. Walker, J. Wang, R.M. Wolf, X. Wu, L. Xiao, D.M. York and P.A. Kollman (2016), **AMBER 2016**, University of California, San Francisco.
2. Alexander Rose; **Hai Nguyen ;** David Dotson (2016). nglview v0.4. Zenodo. **10.5281/zenodo.46373**
3. **H Nguyen**, DR Roe, J Swails, DA Case (2016), PYTRAJ v1.0.0.dev1: Interactive data analysis for molecular dynamics simulations. http://dx.doi.org/10.5281/zenodo.44612
4. **Nguyen, H.**; Pérez, A.; Bermeo, S.; Simmerling, C., Refinement of Generalized Born Implicit Solvation Parameters for Nucleic Acids and Their Complexes with Proteins. *J Chem Theory Comput* **2015**. [http://pubs.acs.org/doi/abs/10.1021/acs.jctc.5b00271]
5. A. Case, J.T. Berryman, R.M. Betz, D.S. Cerutti, T.E. Cheatham, III, T.A. Darden, R.E. Duke, T.J. Giese, H. Gohlke, A.W. Goetz, N. Homeyer, S. Izadi, P. Janowski, J. Kaus, A. Kovalenko, T.S. Lee, S. LeGrand, P. Li, T. Luchko, R. Luo, B. Madej, K.M. Merz, G. Monard, P. Needham, **H. Nguyen**, H.T. Nguyen, I. Omelyan, A. Onufriev, D.R. Roe, A. Roitberg, R. Salomon-Ferrer, C.L. Simmerling, W. Smith, J. Swails, R.C. Walker, J. Wang, R.M. Wolf, X. Wu, D.M. York and P.A. Kollman (2015), **AMBER 2015**, University of California, San Francisco. [ambermd.org/doc12/Amber15.pdf]
6. **Nguyen, H.*;** Maier, J.*; Huang, H; Perrone, V; Simmerling, C., (**2014**) Folding simulations for proteins with diverse topologies are accessible in days with a physics-based force field and implicit solvent. *Journal of the American Chemical Society* (*co-1st authors) [http://pubs.acs.org/doi/pdfplus/10.1021/ja5032776]
7. **Nguyen, H**.; Roe, D. R.; Simmerling, C., (**2013**) Improved Generalized Born Solvent Model Parameters for Protein Simulations. *Journal of Chemical Theory and Computation*, *9* (4), 2020-2034. [http://pubs.acs.org/doi/abs/10.1021/ct3010485]
8. Shang, Y., **Nguyen, H.**, Wickstrom, L., Okur, A., and Simmerling, C. (**2011**) Improving the description of salt bridge strength and geometry in a Generalized Born model, *Journal of Molecular Graphics and Modeling 29*, 676-684. [http://www.ncbi.nlm.nih.gov/pmc/articles/pmid/21168352/]

Contributed talks

- **Hai Nguyen**, Pytraj, nglview: bring AmberTools to Python ecosystem, **University of California, San Francisco**, 03/2016.
- **Hai Nguyen,** Improved generalized Born solvent model parameters for protein and nucleic acid simulations, **Icahn School of Medicine at Mount Sinai, 08/2014** (invited speaker)
- **Hai Nguyen**, Improved generalized Born solvent model parameters for protein and nucleic acid simulations, **Memorial Sloan Kettering**, 02/2014 (invited speaker)
- **Hai Nguyen**, Implicit solvent developments in AMBER. AMBER developer meeting, **Stony Brook University**, 01/2014.
- **Hai Nguyen**, Improved Generalized Born solvent model parameters for protein and nucleic acid simulations", Hai Nguyen, Carlos Simmerling, **244th ACS conference**, Philadelphia, 08/2012.

Poster presentations

1. **Hai Nguyen,** Daniel R. Roe, Jason Swails, David A. Case, "*Pytraj: Interactive data analysis for molecular dynamics simulations*", **Biophysical Society 60th Annual Meeting,** February 29, 2016.
2. **Hai Nguyen**, James Maier, He Huang, Victoria Perrone, Alberto Perez, Carlos Simmerling, "*Simulating protein and nucleic acid dynamics on the microsecond to millisecond timescale*", **Biophysical Society 59th Annual Meeting**, February 8, 2015.
3. **Hai Nguyen**, James Maier, He Huang, Victoria Perrone, Alberto Perez, Carlos Simmerling, "*Simulating protein and nucleic acid dynamics on the microsecond to millisecond timescale*", **The New York Structural Biology Discussion Group 10th Winter Meeting**, January 21, 2015.
4. **Hai Nguyen**, James Maier, He Huang, Victoria Perrone, Alberto Perez, Carlos Simmerling, "*Simulating protein and nucleic acid dynamics on the microsecond to millisecond timescale*", **Stony Brook University Chemistry Research Day**, October 31, 2014.
5. **Hai Nguyen**, James Maier, He Huang, Victoria Perrone, Alberto Perez, Carlos Simmerling, "*Simulating protein and nucleic acid dynamics on the microsecond to millisecond timescale*", **Stony Brook University ICB&DD 8th Annual Symposium**, October 9, 2014.
6. **Hai Nguyen**, Daniel R. Roe, Lauren Wickstrom, Carlos Simmerling, "Improvement of an Implicit Solvent Model", **workshop "From Computational Biophysics to Systems Biology (CBSB12)"**, Knoxville, June 3, 2012
7. **Hai Nguyen**, Daniel R. Roe, Lauren Wickstrom, Carlos Simmerling, "Improvement of an Implicit Solvent Model", **ACS conference**, Boston, August 24, 2010
8. **Hai Nguyen**, Daniel R. Roe, Carlos Simmerling, "An Improvement of Implicit Solvent Model", Chemistry Research Day, **Stony Brook University**, November 13, 2009
9. **Hai Nguyen**, Daniel R. Roe, Carlos Simmerling, "An Improvement of Implicit Solvent Model", 3rd Annual ICB&DD Symposium, **Stony Brook University**, October 6, 2009
10. **Hai Nguyen**, Daniel R. Roe, Carlos Simmerling, "An Improvement of Implicit Solvent Model", Inaugural Symposium for the Laufer Center for Computational Biology and Genome Sciences, **Stony Brook University**, September 25, 2009

Awards

- Rosetta CADRES GRANTS: Exploring new Generalized Born solvation models and a Python-based API for recombining Rosetta and Amber force fields for improving structure prediction and design

  Aliza Rubenstein, Kristin Blacklock (PI: Sagar Khare); **Hai Nguyen** (PI: David Case), Rutgers University
- Workshop "From Computational Biophysics to Systems Biology (CBSB12)" fellowship (2012)
- Sigma Xi Award (2012)
- Full Scholarship for Excellent Student Award, Hanoi College of Science (2002-2006)
- Outstanding Student Award, Hanoi College of Science (2003, 2004)

Professional Organizations

- AMBER software developer, 2013 – Present (http://ambermd.org)
- MDAnalysis software contributor, 2015 - Present (https://github.com/MDAnalysis)
- Biophysical Society (BPS) Member, 2014 - Present (http://www.biophysics.org/)
- Bioconda Member, 2016 - Present (https://github.com/bioconda)

Other activities

- Presiding session "Computational Approaches to Spectroscopy Analysis", ACS Fall 2012
- Assisting students in AMBER session in Interdisciplinary Boot Camp in Quantitative Biology, Rutgers University, January 2016

References

Dr. David A. Case

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