Hai Minh Nguyen

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OBJECTIVE

A position in the field of computational chemistry with special interests in software development and application.

EDUCATION

PhD, Chemistry
Stony Brook University, 2014

Bachelor of Science, Chemistry
Hanoi University of Science, 2006

COMPUTER SKILLS

Languages:

- Proficient: Python/Cython
- Experience: Javascript, C/C++, FORTRAN

Others:

- git, conda, software continuous integration, parallel programming (MPI, multi-processing)

RELEASED SOFTWARE

Lead developer:

- pytraj (written in Python/Cython): Python API for cpptraj: a data analysis package for biomolecular simulation https://github.com/amber-md/pytraj
- nglview (written in Python/Javascript/HTML): Jupyter widget to interactively view molecular structures and trajectories, https://github.com/arose/nglview

Contributing:

- AMBER program suite (various languages): 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
- MDAnalysis (written in Python): an object-oriented python toolkit to analyze molecular dynamics trajectories, http://www.mdanalysis.org/

EXPERIENCE

Postdoctoral Associate 03/2015-present
Rutgers University

- Developing PHENIX/AMBER interface for protein refinement with alternative conformation
- Explored new Generalized Born solvation models and a Python-based API for recombining Rosetta and Amber force fields for improving structure prediction and design
- Developing conda-build for AMBER suite

Postdoctoral Associate 11/2014-2/2015
Stony Brook University

- Added code and introduced newly optimized Generalized-Born solvation parameters for nucleic acid simulation to AMBER suite program

PUBLICATIONS

Google Scholar statistics (210 citations): http://goo.gl/CpC2zg

Peer Review

1. **Nguyen, H.**; Prez, A.; Bermeo, S.; Simmerling, C., (2015) Refinement of Generalized Born Implicit Solvation Parameters for Nucleic Acids and Their Complexes with Proteins. J Chem Theory Comput.
2. **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)
3. **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.
4. 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.

Software

1. **H. Nguyen**, A. Rose, D. Dotson, M.K. Scherer, nglview v0.5, http://dx.doi.org/10.5281/zenodo.55409
2. **H. Nguyen**, D.R. Roe, J. Swails, D.A. Case, (2016) PYTRAJ v1.0.0.dev1: Interactive data analysis for molecular dynamics simulations. http://dx.doi.org/10.5281/zenodo.44612
3. 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.
4. 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.

AWARDS

- Fellowship for Workshop "From Computational Biophysics to Systems Biology (CBSB12)" (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)