Hai Minh Nguyen

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EDUCATION

Doctor of Philosophy, Chemistry
Stony Brook University, 2014
Advisor: Carlos Simmerling

Bachelor of Science, Chemistry
Hanoi University of Science, 2006

EXPERIENCE

Postdoctoral Associate 03/2015-present
Rutgers University, PI: David A. Case

- Developing PHENIX/AMBER interface for protein refinement with alternative conformation
- Applied new Generalized Born solvation models and a Python-based API for recombining Rosetta and Amber force fields for improving structure prediction and design
- Developing softwares (pytraj, nglview) for molecular dynamics simulation data analysis and visualization

Postdoctoral Associate 11/2014-2/2015
Stony Brook University, PI: Carlos Simmerling

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

Research Assistant 2018-2014
Stony Brook University, PI: Carlos Simmerling

- Developed solvent model for protein and nuleic acid simulations
- Developed and validated force field
- Improved salt bridge description for HIV-1 protease simulation

COMPUTER SKILLS

Languages:

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

Others:

- GIT, software continuous integration, parallel programming (MPI, multiprocessing), AMBER, VMD, PyRosetta, rdkit, docker, Linux, OSX

RELEASED SOFTWARE

Lead developer:

- pytraj: Python API for cpptraj: a data analysis package for biomolecular simulation
  https://github.com/Amber-MD/pytraj
- pymdgx: Python API for mdgx simulation package
  https://github.com/Amber-MD/pymdgx
- nglview: Jupyter widget to interactively view molecular structures and trajectories,
  https://github.com/arose/nglview

Contributing:

- AMBER program suite: biomolecular simulation program, http://ambermd.org
- cpptraj: Biomolecular simulation trajectory/data analysis, https://github.com/Amber-MD/cpptraj
- parmed: Parameter/topology editor and molecular simulator, https://github.com/ParmEd/ParmEd
- MDAnalysis: an object-oriented python toolkit to analyze molecular dynamics trajectories, http://www.mdanalysis.org/

PUBLICATIONS

Google Scholar statistics: 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.
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.

CONTRIBUTED TALKS

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

SELECTED POSTERS

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 ICBDD 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 ICBDD 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

ACADEMIC REFERENCES

David A. Case
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