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Bio

2002:	PhD in Physics, Michigan State University, East Lansing, MI, USA
2003-2004:	Research Associate, Department of Physics, Syracuse University, Syracuse, NY, USA
2005	Research Associate, Department of Physics, Michigan Technological University, Houghton, MI, USA
2005-2008	Research Associate, John von Neumann Institute for Computing, Research Centre, Jülich, Jülich, Germany
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Current Work

I am interested in the behavior of complex system. Currently, I am investigating the statistics and mechanism of protein folding, protein-protein interactions, and formation of large biomolecular assemblies. Our simulations of the C-terminal fragment of the designed protein Top7, for example, showed an interesting folding mechanism via a non-native intermediate [1].

My work also includes the parallelization of existing programs and the development and implementation of new methods—in particular methods that can take advantage of high-performance computer systems. To make modern computational methods available to a broader audience, I built, for example, a Python module for the protein simulation package SMMP [2]. I would like to discuss experiences of using Python on HPC systems, in particular the BlueGene/P. Possible topics for collaboration include the development of a Python frame-work on BlueGene/P and other ways to make HPC more user friendly.

Processes in biological systems cover many orders of magnitude in both time and space. One way of dealing with the different scales is to use multi-scale models that represent the physical system at different levels of details. I have started to look into multi-scale systems and am interested in discussing the methodology and implementations. Possible topics for collaboration include studying the cell membrane and aggregation.

References

1. Mohanty, S. et al. Simulation of Top7-CFr: A transient helix extension guides folding. PNAS 105, 8004(2008).
2. Meinke, J.H. et al. SMMP v. 3.0—Simulating proteins and protein interactions in Python and Fortran. Comp. Phys. Comm (2007).