Large Scale Biomolecular Modeling with IBM Blue Gene

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Abstract

"How does a protein fold and interact with other molecules?" still remains largely a mystery in molecular biology despite extensive studies from both experimental and theoretical approaches. In this talk, I will present some of our recent work with massively parallel computer simulations using IBM Blue Gene, including single mutation effects on protein misfolding and aggregation, nanoscale dewetting transition in protein complex folding, water nanopore design with carbon nanotubes, influenza antigen-antibody and antigen-receptor binding, as well as protein-nanoparticle interactions. These large scale simulations reveal detailed molecular mechanisms on protein folding/misfolding, protein-protein and protein-nanoparticle interactions. This talk will also briefly describe the IBM Blue Gene Project, including its hardware, system software, and application science programs.