Folding@Home: Advances in biophysics and biomedicine from world-wide grid computing

Vijay S. Pande
Departments of Chemistry and of Structural Biology
Stanford University, Stanford, CA 94305

Abstract

Simulations of biological molecules offer a lot of promise to complement and extend current experiments in the areas of biophysics and biomedicine. However, there are some serious limitations that must be overcome before computational methods are universally accepted. For example, one must be able to examine experimentally relevant timescales (microseconds to seconds) that are thousands to billions of times longer than most typical simulations (nanoseconds). How can one surmount such fundamental computational barriers? I will discuss our solutions to this problem, which combine novel physical chemistry theory and computational paradigms. In addition, I will discuss recent applications of these methods to fundamental questions in biophysics and biomedical applications, including protein folding, protein-protein association, protein-ligand binding, and protein misfolding & aggregation.