

Capacity and Capability Biomolecular Simulation: Drug discovery and biophysics

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We have entered the petaFLOP/s (10¹⁵ floating point operations/second) era of high-performance computing (HPC). In addition, the hardware trends of multi-core systems and custom accelerators now yield teraFLOP/s (10¹² floating point operations/second) performance for desktop workstations. This new level of performance offers both opportunities and challenges for the computational chemist. At IBM, we have an ongoing research program to explore all aspects of the effective use of HPC systems for computational biology and chemistry applications. In this talk, I will present results illustrating some of our efforts in computer-aided drug discovery and in the biophysics of protein folding. In the drug discovery area, I will discuss a collaboration between IBM and GlaxoSmithKline where BlueGene systems enable high-throughput computation of solvation free energies for a data set of over 250 small molecules with drug-like functional groups. These same computer systems also enable routine microsecond simulations of biomolecular systems -- a capability I will illustrate with simulation results which, in connection with experiment, suggest the presence of specific residual structures in the unfolded ensembles of proteins.