High Performance Computational Biology—Past Progress and Future Promise

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Abstract

Biology is awash in data. The amount, complexity and increased need for the rigorous post-processing of these data speak to an increased role for high performance computing (HPC) in biology. Here HPC implies everything from global grid architectures to optimization of specific codes to take advantage of commodity clusters, to Web services needed to optimize and make useful the computer human interface. Currently there is a dearth of literature addressing the role of HPC as applied to problems in computational biology. With HPC becoming more available and the need increasing, this situation is expected to change. This presentation will describe, from a user’s perspective, what is possible with HPC today and what is possible going forward using some representative applications from our own work. Specifically, grid optimization and work flow development for a high throughput genomic annotation pipeline, federation of several cell signaling databases, and new intuitive interfaces to the PDB and other resources.