

Title: Blue Gene: protein folding and drug discovery

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Abstract:

The IBM Blue Gene project is a large scale multi-year research project to develop a next-generation supercomputer and use it to study the protein folding problem. An overview of the Blue Gene science program will be provided. This program consists of kinetic and thermodynamic simulations of protein folding. Understanding the protein folding problem could significantly change the process of drug discovery. In addition, other areas where Blue Gene could impact the drug discovery process will be discussed. These areas include membrane protein simulations, large-scale molecular docking, and precise binding free energy calculations.