Bioinformatics Measurements with High Performance Computing

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High-performance computing (HPC) is an important domain of the computer science field. For more than 30 years, it has allowed finding solutions to problems and enhanced progress in many scientific areas such as bioinformatics and drug design. The binding of small molecule ligands to large protein targets is central to numerous biological processes. The accurate prediction of the binding modes between the ligand and protein (the docking problem) is of fundamental importance in modern structure-based drug design. The interactions between the receptor and ligand are quantum mechanical in nature, but due to the complexity of biological systems, quantum theory cannot be applied directly. Consequently, most methods used in docking and computational drug discovery are more empirical in nature and usually lack generality. Quantum mechanical phenomena, such as the formation of a covalent bond between the protein and the ligand upon binding during the transition state of the reaction, cannot be predicted and/or evaluated using these empirical methods. In the field of molecular modeling, docking is a method which predicts the preferred orientation of one molecule to a second when bound to each other to form a stable complex. Knowledge of the preferred orientation in turn may be used to predict the strength of association or binding affinity between two molecules using, for example, scoring functions. Docking is frequently used to predict the binding orientation of small molecule drug candidates to their protein targets in order to in turn predict the affinity and activity of the small molecule. Hence docking plays an important role in the rational design of drugs. Given the biological and pharmaceutical significance of molecular docking, considerable efforts have been directed towards improving the methods used to predict docking. Each docking program makes use of one or more specific search algorithms, which are the methods used to predict the possible conformations of a binary complex. An overview of current docking techniques is presented with a description of applications including a benchmark for docking on IBM HPC platform, also mathematical algorithm will be presented. The present benchmark is made from an existing test set (CCDC/Astex Validation Set) on typical HPC system. Selected examples were docked with GOLD software.