

Study of a Highly Accurate and Fast Protein-Ligand Docking Algorithm Based on Molecular Dynamics

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Abstract

Few methods use molecular dynamics simulations based on atomically detailed force fields to study the protein-ligand docking process because they are considered too time demanding despite their accuracy. In this paper we present a docking algorithm based on molecular dynamics simulations which has a highly flexible computational granularity. We compare the accuracy and the time required with well-known, commonly used docking methods like AutoDock, DOCK, FlexX, ICM, and GOLD. We show that our algorithm is accurate, fast and, because of its flexibility, applicable even to loosely coupled distributed systems like desktop grids for docking.

Keywords: *Force field based methods, docking accuracy, desktop grid computing.*