CALIFORNIA STATE SCIENCE FAIR
2015 PROJECT SUMMARY

Name(s)

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Project Number

35395

Project Title

Solvemetrix: Implementing a Novel Molecular Dynamics Simulation Package by Using a Heuristic Explicit Solvation Model

Abstract

Objectives/Goals

Molecular dynamics (MD) simulations are among the most useful tools in computational science, with applications in catalyst optimization, drug design, and proteomics. Existing packages such as Nanoscale Molecular Dynamics (NAMD) and AutoDock employ computationally intensive algorithms and scoring functions to calculate molecular trajectories. Solvemetrix attempts to implement a novel heuristic MD simulation package with a similar accuracy to existing software for a fraction of the computational cost by using heuristic methods.

Methods/Materials

A discrete explicit solvent model is used, which leads to more accurate results but requires advanced algorithmic processing. First, an initial state of only solvent molecules is created. Energetics of the pure solvent are computed using Fast-Fourier Transform and Euler rotation matrixes. Then, solvation about a target molecule is modeled using small stochastic steps according to a simple scoring function. Steric effects, dipole moments, dielectric constants, entropy, Brownian motion, and intermolecular forces are all considered in a series of multiplexed matrix operations. Output data is provided at desired time-steps in the form of Protein Data Bank (PDB) files, which allows for efficient construction and visualization of molecular trajectories.

Results

Solvemetrix is approximately 2.5 orders of magnitude faster than NAMD or Autodock, and provides output of a similar caliber. Solvemetrix successfully computed the dimerization states of water-water, water-acetone, benzene-benzene, and benzene-water. In doing so, it only used a fraction of the computational resources and still produced comparable, if not more accurate, output as EFP, CCSD(T), and MP2. Solvemetrix accurately generated a regular ab initio state when simulating the solvation of acetone by 216 water molecules. The minimum energy state was identified after 2,000 iterations and subsequently visualized. Solvemetrix runs in O(n) asymptotic time, which represents a significant advantage over other algorithms which often operates in O(n2) time.

Conclusions/Discussion

Solvemetrix allows us to enhance MD simulations by a faster computational method. It can be used to understand the interactions of complex macromolecules in a shorter amount of time. While Solvemetrix is a work in progress, it represents a new age of high-throughput MD simulation tools with far-reaching applications in science and beyond.

Summary Statement

Solvemetrix attempts to implement a novel heuristic MD simulation package with a similar accuracy to existing software for a fraction of the computational cost by using heuristic methods.

Help Received

Collaborated with Raghu Dhara, a student and researcher at Harvard University.