5th EGEE User Forum

Contribution ID : 66

Protein Molecular Dynamics and Free Energy Calculations on the EGEE Production Grid

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Overview :

Atomistic simulations of large biomolecules such as proteins require extensive computational resources. Dynamical and thermodynamical properties can be obtained either by averaging over very long time trajectories or sampling the phase space by running hundreds of short time trajectories. The latter methods are the most appropriate for high throughput computers such as the Grid distributed computers. Algorithms are presented for calculating vibrational spectra of the active site of cytochrome c oxidase as well as free energy landscapes based on thermodynamic perturbation theory.

Analysis :

Proteins are large molecules with thousands of atoms whose motions cover a broad range of time intervals, from a few tens of femtoseconds, the oscillation periods of strong chemical bonds, to milliseconds, the period of large scale conformational changes. The study of dynamics of such complex systems in a broad range of spacial and temporal scales as well as thermodynamic quantities and structural properties remain a challenge for atomistic simulations. Here, we present an algorithm that assists us to harness the current computational Grid infrastructure for carrying out extended samplings of phase space and integrating the classical mechanical equations of motion for long times. A bundle of shell scripts has been written to automatically submit and propagate trajectories in the Grid and to check and store large amounts of intermediate results. We report our last years experience in employing the Enabling Grids for E-sciencE production infrastructure via the CompChem and SEE virtual organizations in investigating the dynamics of enzymes such as Cytochrome c Oxidases.

Impact :

It is demonstrated that by using the thousand of cpus available in EGEE important biophysical/biochemical problems can be solved in a realistic way. Converged thermodynamic quantities can be obtained. Also the availability of flexible scripts can cope with drawbacks of the Grid and make runs stable and long running. Results for Cytochrome c Oxidases have been published [1-3].

[1] V. Daskalakis, S. C. Farantos, C. Varotsis, Assigning vibrational spectra of ferryl-oxo intermediates of Cytochrome c Oxidase by periodic orbits and Molecular Dynamics, J. Am. Chem. Soc. 130(37), 12385-12393, 2008.
[2] Massimiliano Porrini, Vangelis Daskalakis, Stavros C. Farantos, and Constantinos Varotsis, Heme Cavity Dynamics of Photodissociated CO from ba3-Cytochrome c Oxidase: the Role of Ring-D Propionate, J. Phys. Chem. B, 113(35), 12129-12135, 2009.
[3] Vangelis Daskalakis, Stavros C. Farantos, Victor Guallar, and Constantinos Varotsis,
Vibrational Resonances and CuB displacement controlled by proton motion in Cytochrome c Oxidase,
J. Phys. Chem. B, in press, 2009.

Conclusions :

The positive experience gained from running classical dynamics of proteins on the EGEE Grid will be transfered to projects involving Quantum Molecular Dynamics. A highly parallelized Fortran code written for solving the time dependent Schroedinger equation by formulating the Hamiltonian in Cartesian coordinates will be deployed into the Grid [1].

[1] Jaime Suarez, Stavros C. Farantos, Stamatis Stamatiadis, and Lucas Lathouwers, A method for solving the molecular Schroedinger Equation in Cartesian coordinates via angular momentum projection operators, Comp. Phys. Comm., 180:2025-2033, 2009.

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