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The study of Cytochrome C oxidase on EGEE Grid

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The current project involves Molecular Dynamics calculations on cytochrome c oxidase. CcO is the terminal enzyme of respiratory chains found in the inner mitochondrial membranes or in many bacteria and the last acceptor of electrons from oxidizing processes involving nutrient molecules.

The biophysical interest of this project stems on long standing problems which concern the assignment of difference spectra of isotopically substituted ferryl oxygen.

3. Impact

The Molecular Dynamics calculations on cytochrome c oxidase is a heavily demanding application in terms of the CPU time required. Furthermore, it is demonstrated that the study of the vibrational spectra and dynamics for pumping water molecules from the active site, it presents a perfect example for a Grid application. We performed the domain decomposition of the initial conditions and a large number of sequential jobs have been launched on the Grid.

To this end, the computer codes running on our local clusters were gridified and some scripts were written to make the Grid calculations feasible, automating the management of the large number of jobs.
Some errors occurred in the scheduling of the jobs have been managed resubmitting the failed ones automatically.
The large number of CPUs available on HellasGrid and on Compchem and SEEGrid VOs made it possible to perform the preliminary production runs, while the project is still in progress.

URL for further information:

http://tccc.iesl.forth.gr
http://compchem.unipg.it

4. Conclusions / Future plans

The paper reports our experience in studying the spectroscopy and reaction dynamics of enzymes with classical dynamics on the production EGEE Grid environment using the HellasGrid and CompChem and SEEGrid VOs.

Provide a set of generic keywords that define your contribution (e.g. Data Management, Workflows, High Energy Physics)

Computational Chemistry, Dynamics and Spectroscopy of Proteins, Classical Molecular Dynamics

1. Short overview

Our Grid experience carrying out Molecular Dynamics calculations on the enzyme cytochrome c oxidase (CcO) on EGEE through Compchem VO will be presented and discussed. The biomolecule (CcO) consists of approximately 10000 atoms and the calculations would require years of our local CPU time. Performances and drawbacks of the current status of the Grid will be discussed.

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