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Unveiling the mechanisms behind biomolecules –the role of Grid

Thursday, 19 September 2013 09:00 (30 minutes)

Structural Biology studies the molecular structure of biological molecules and the way molecules interact with each other. This information is crucial to understand how they function inside living cells and how their deregulation can lead to disease. Structures are determined by measuring distances and angles between the millions of atoms inside proteins and other macromolecules.
To obtain structures and dynamical information at high resolution (angstroms magnitude) bench experiments and computational calculations are used synergistically. Computation of the atom-atom interactions required to describe the simplest of dynamics and cellular process increases the demand for computer power and more accurate methods. Grid Infrastructures provide a solution to tackle this bottleneck.
In this talk I will focus firstly on available applications and examples relevant to the Structural Biology community and secondly on the importance of having access to the Grid Infrastructure.

Description of Work

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Wider Impact of this Work

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Session, double-session

KeyNote

Printable Summary

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Session Classification: Plenary Session