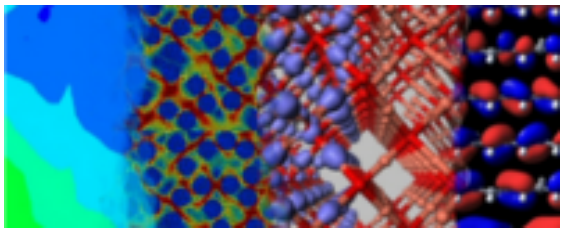

Contribution ID: **22** Type: **Poster**

BigDFT GridBean within the UNICORE framework, a component for fully automated workflows

Thursday, November 8, 2012 5:55 PM (10 minutes)

Density functional theory (DFT) is the fundamental theory used to describe the quantum laws that governs the interactions between atoms and molecules within a molecular system. Realistic simulations requires a large amount of resources, which most often exceed the available resources given at a local site. These simulations belong to a certain class of High Performance Computing (HPC) and can only take place in the world of large scale computing involving several applications linked together via a Grid infrastructure. Furthermore these simulations requires the use of hybrid machines, that is machine composed of both CPU and GPU accelerators. In this work we describe the work accomplished so far in the GridBean development for a DFT code, that is used within the UNICORE frame work. This GridBean, which we call BigDFTGridBean is then used within UNICORE to create workflows in a Grid computing infrastructure replacing laborious and tedious codes manipulations.

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Session Classification: Poster Session