MMM@HPC Bologna Training Course

Date: 13th September 2013

Time: 9.00-15.30

Location: Hotel I Portici, Via Indipendenza 69, 40121 Bologna – Italy.

Registration deadline: 31st August 2013

Introduction

Multiscale modeling has become the method of choice to treat advanced materials computationally. This approach has been adopted recently in the MMM@HPC project, developing tools and services to integrate well established physical sub-models, implemented in highly efficient computer codes, on different size- and time-scales as steps in extendable generic workflows. To accomplish the integration of the sub-models numerous reusable application interfaces, GridBeans, have been implemented to date and used in workflows to model materials for various applications, such as organic light emitting diodes. The UNICORE middleware, which has been selected as basis for the implementation, has been broadly and productively deployed in large computing infrastructures such as PRACE (http://www.prace-ri.eu) and XSEDE (https://www.xsede.org). In order to implement a particular multiscale model the user selects and combines those GridBeans that are required into a workflow using the graphical interface of the UNICORE Rich Client. Then the simulation is carried out on distributed computing resources by simple submission from the client. Using the freely accessible repository of existing GridBeans provided by the MMM@HPC project, users can incorporate a wide range of sub-models commonly used in materials science to tailor new workflows for materials science applications.

Course Outline

This training course will provide a comprehensive introduction to the following topics:

1. Basic usage of the UNICORE Rich Client;
2. Setting up and running single-step simulations using GridBeans;
3. Editing and running a pre-constructed workflow model;
4. Constructing a multi-step workflow model from available GridBeans;
5. How to construct your own GridBean.

Target Audience

The training course is aimed at PhD students and postdoctoral researchers working in the fields of computational materials science or computational nanoscience and who want to apply the techniques described in their own research. Previous experience with modeling and computer simulations (for example with quantum chemistry, molecular dynamics, coarse grain models or finite-element analysis) would be a benefit.

Fee and registration

The training course is free but places are limited so registration is necessary and this should be done when registering for the main workshop. In addition, since limited access will be given to one of Cineca's supercomputers, for security reasons we must know in advance who will attend the course. Thus, even if

places are available, we cannot guarantee access to the course unless students register with us first before the deadline. Successful applicants will be asked to sign a user agreement before the start of the course.

Requirements

Personal laptop with Windows, Linux or Mac operating systems with wireless capability.

Contact information

For further information please contact the course secretariat via corsi@cineca.it.

References

[1] Stefan Bozic, Ivan Kondov, Velimir Meded, and Wolfgang Wenzel, "UNICORE based Workflows for the Simulation of Organic Light-Emitting Diodes", UNICORE Summit 2012 Proceedings, May 30-31, 2012, Dresden, Germany, 2012, IAS Series, Vol. 15, pp. 15-25, Jülich 2012.

[2] Ivan Kondov, Robert Maul, Stefan Bozic, Velimir Meded, and Wolfgang Wenzel, "UNICORE-Based Integrated Application Services for Multiscale Materials Modeling", UNICORE Summit 2011 Proceedings, 7 - 8 July, Torun, Poland, 2011; IAS Series, Vol. 9, pp. 1-10, Jülich 2011.