



Multiscale materials modelling  
on High Performance Computer  
Architectures

## College on Multiscale Computational Modeling of Materials for Energy Applications

Trieste, 4-15 July 2016

**Training Materials**



This work is licensed under  
a Creative Commons Attribution-NonCommercial 3.0 Unported License  
<http://creativecommons.org/licenses/by-nc/3.0/>

Copyright © 2012-2013 Consorzio Interuniversitario (CINECA)  
Copyright © 2012-2013 Karlsruhe Institute of Technology (KIT)

## Table of contents

1	Exercise 1: Start a workflow polymer electronics on the Live CD .....	3
	Preparation .....	3
	Run a predefined workflow: polymer workflow .....	3
2	Exercise 2: Edit and submit a Pair Finder workflow on the Live CD .....	3
	Preparation .....	3
	Loading, modifying and starting a predefined workflow .....	3

## 1 Exercise 1: Start a polymer electronics workflow on the Live CD

### Preparation

A prerequisite is a PC or a laptop with minimum 1 GB of RAM and a bootable DVD drive. Access to the internet is not necessary. The Live CD contains a self-contained local installation of the MMM@HPC infrastructure (server and client components) capable to execute several applications for demonstration and training purposes. It will not touch the system installed on the hard disk, and it can be run also using a virtual machine (VM) player. For this exercise the version from May 2013 of the Live CD available with the handouts and for download as image under [www.multiscale-modelling.eu](http://www.multiscale-modelling.eu) is mandatory.

After booting up the system, please read and accept the license at the start of the desktop. After that start the UNICORE Rich Client clicking on its icon on the panel. Then start the UNICORE Rich Client (URC) by clicking on the UNICORE icon on the desktop panel. Use the default keystore file and default password ("321") to login.

### Run a predefined workflow: polymer workflow

This is a fragment of a workflow modelling the morphology of a material for polymer electronics. You will find the workflow in the workflow editor in the right pane of the URC right after starting up the URC. First you may inspect the model and other parameters opening each of the workflow steps (GridBeans), accessing the properties by a double click. After this you press the green play button to start the workflow. In the dialogue which pops up you then select the workflow engine "@WORKFLOW" and press the "Finish" button. The workflow is then executed by the selected workflow engine. The overall progress of the workflow run is displayed in the new tab on the right pane. During the workflow run you can monitor the results at each step using the Grid Browser on the upper left pane. In particular you can visualise molecular structures with Jmol by simple double clicking on the XYZ or CML files or right-clicking and selecting "open in editor".

See also the video "Getting started polymer workflow" directly on the desktop.

## 2 Exercise 2: Edit and submit a Pair Finder workflow on the Live CD

### Preparation

The preparation is the same as for Exercise 1.

### Loading, modifying and starting a predefined workflow

This is a fragment of the much more complex and resource consuming OLED workflow. Once a workflow project has been created it can be shared with other people. To import a workflow project go to the "File" menu and select the "Import" entry. An import dialog appears. Select as folder "General" and select the entry "Existing Projects into workspace". Then click on the "Next" button. You move to the next import step. Select the directory or the zip file containing the workflow project you want to import. For this exercise you can open the file '/root/Desktop/Pairfinder-Workflow-Exercise.zip'. Also

select the “Copy projects into workspace” checkbox for a tight integration. After clicking on the “Finish” button the imported workflow project is available in the Navigator view. A double click on ImportWorkflow.flow in the Navigator window will open the workflow project in the workflow editor.

The Pairfinder workflow fragment consists of two steps. The first step converts morphology from the PDB into CML format. In the second step, pairs of molecules are searched and represented using CML. For this workflow to work we need the morphology in PDB format. To specify the morphology double click on the Open Babel red/orange symbol and go to the tab “Files”. Then in the upper pane “Imports” select as input alq3-25-morphology.pdb from the /root directory. After this save the changes with Ctrl+S or clicking on the “save” icon in the toolbar and then close the GridBean GUI. After this press the play button. In the dialogue select the workflow engine "@WORKFLOW" and press the "Finish" button. The workflow is then executed by the selected workflow engine. The overall progress of the workflow run is displayed in the new tab on the right pane.