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Assessing the materials properties of clay-polymer nancomposites: A MAPPER use case on EGI-EUDAT-PRACE

Wednesday, 18 September 2013 11:20 (20 minutes)

Printable Summary

In this talk we present the design, implementation, deployment and first results from our distributed multi-scale simulations of clay-polymer nanocomposites. Our simulations rely especially on large computational resources as found in EGI and PRACE. We perform quantum-mechanical, atomistic and coarse-grained molecular dynamics simulations of montmorillonite clay sheets interaction with different polymers, both in a charged and uncharged setting. In addition to discussing the scientific aspects of our problem, we will also present our computational approach, and what facilities it requires in terms of hardware, software, and modes of computing. The simulations were made possible on a joint infrastructure of EGI, EUDAT and PRACE by a pilot activity that involved these e-infrastructures and various scientific communities.

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