e-infrastructure

CAPACITIES

Distributed Multiscale Simulation of Nanocomposites: Demonstrating a loosely coupled scenario.

02.02.12

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The Mapper project receives funding from the EC's Seventh Framework Programme (FP7/2007-2013) under grant agreement n° RI-261507.

Overview

- Introduction
- Demonstration
  - Technical Overview
  - Application Hosting Environment
  - QosCosGrid Middleware
- End of demonstration
- Explanation of the science + future plans

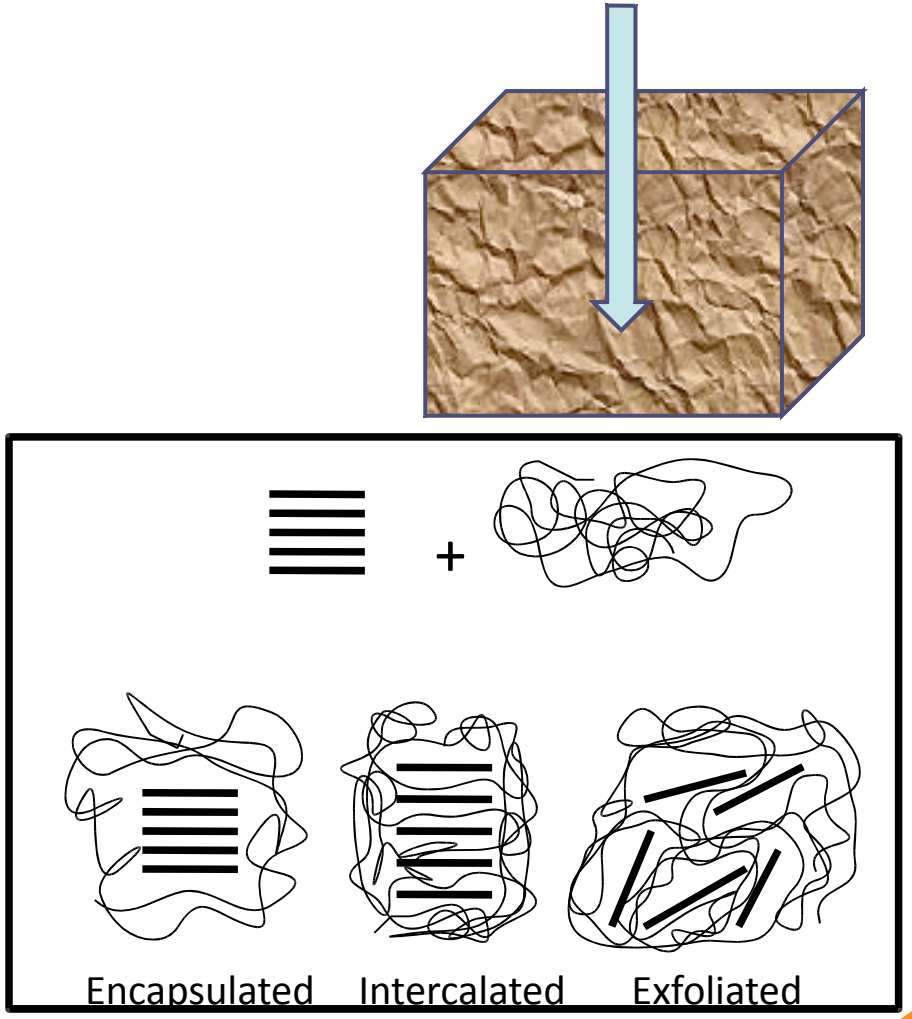
Introduction - nanocomposites

- Mixture of properties of two different materials to give enhanced performance.
- Improved fire retardant properties.
- Similar performance to other composite materials at much lower filler volumes.

Scientific Motivation

Example application:

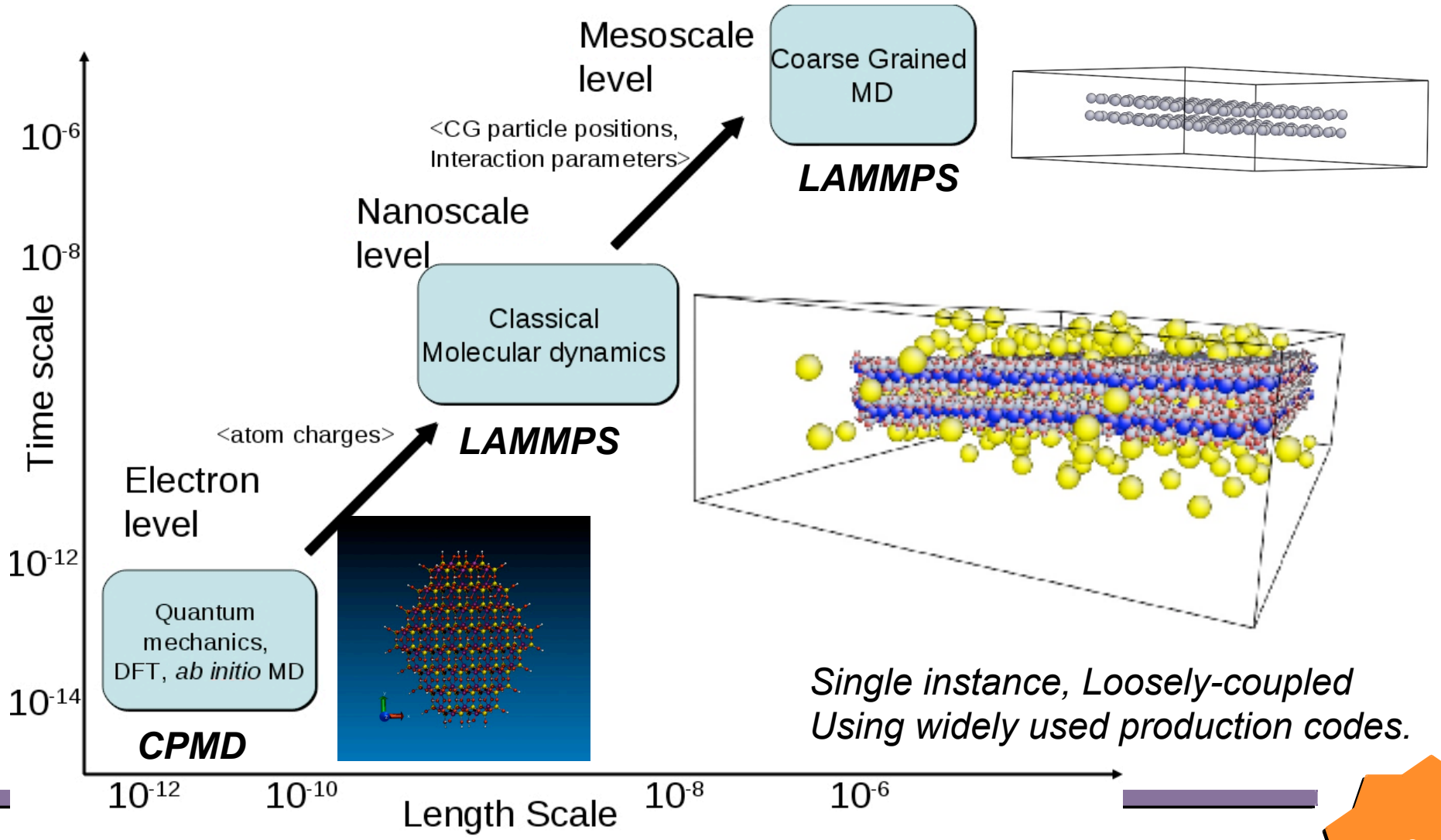
- Problem in oil drilling: Water-based drilling fluid + reactive shale = swelling.
- This is caused by montmorillonite content in the clay.
- We seek to understand the properties of clay-polymer interactions.



Current state

- QM simulations can resolve phenomena at high accuracy for parts of single platelets.
- Atomistic codes can resolve a few platelets for a few nanoseconds at most.
  - Not enough to tackle the problem.
- Course-grained simulations lack the accuracy to directly resolve surface interactions.
- Solution: go distributed multiscale!

Scale Separation Map



Single instance, Loosely-coupled
Using widely used production codes.

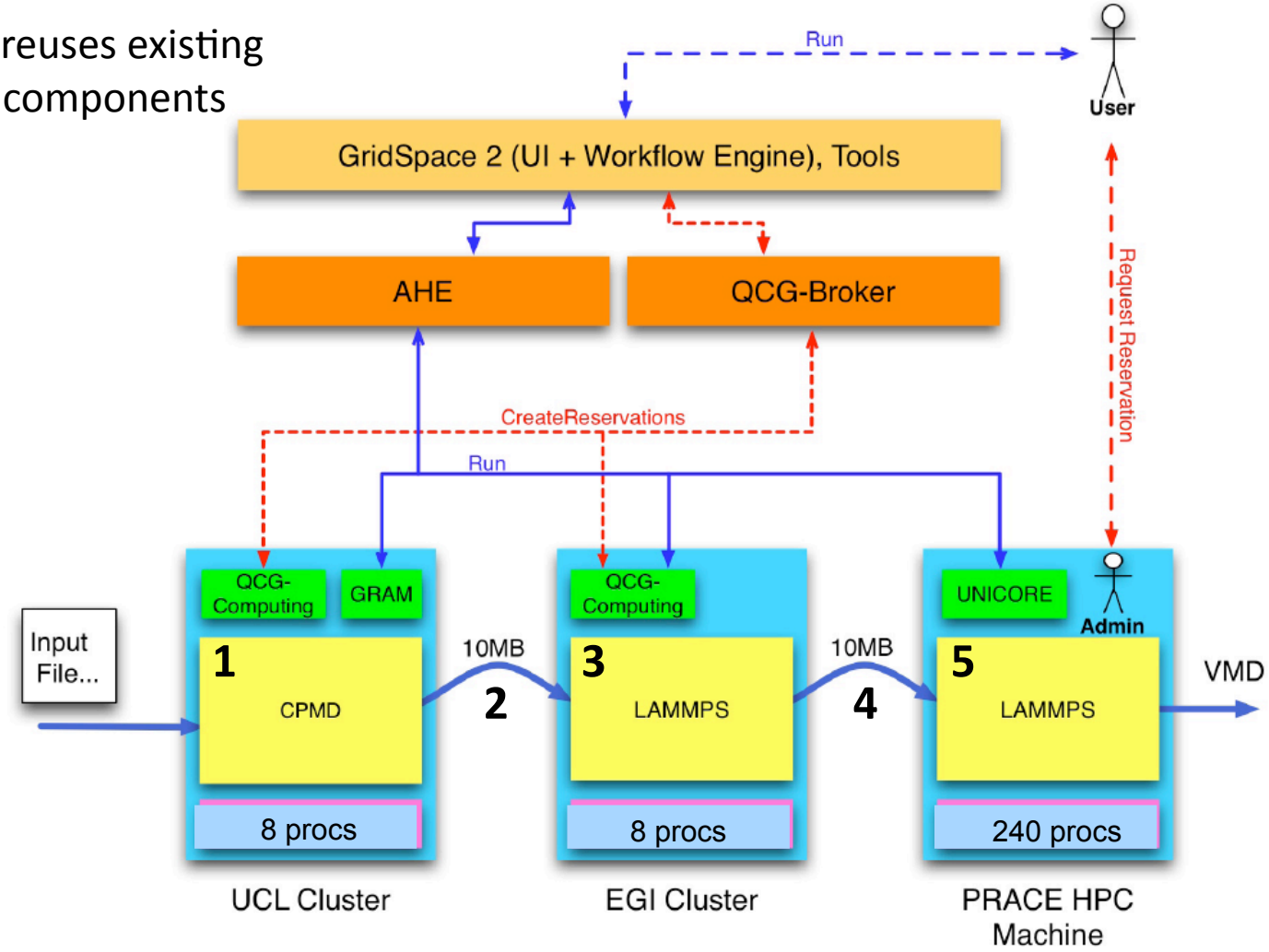
Demonstration

Required functionalities

- Simulation engines (CPMD,LAMMPS).
- Data conversion scripts (Bash, Perl).
- Workflow composition (GridSpace/MAD).
- Advance reservation (QCG Computing).
- File staging (AHE).
- Job submission interface to the heterogeneous e-infrastructure (GS+AHE).

Technical components

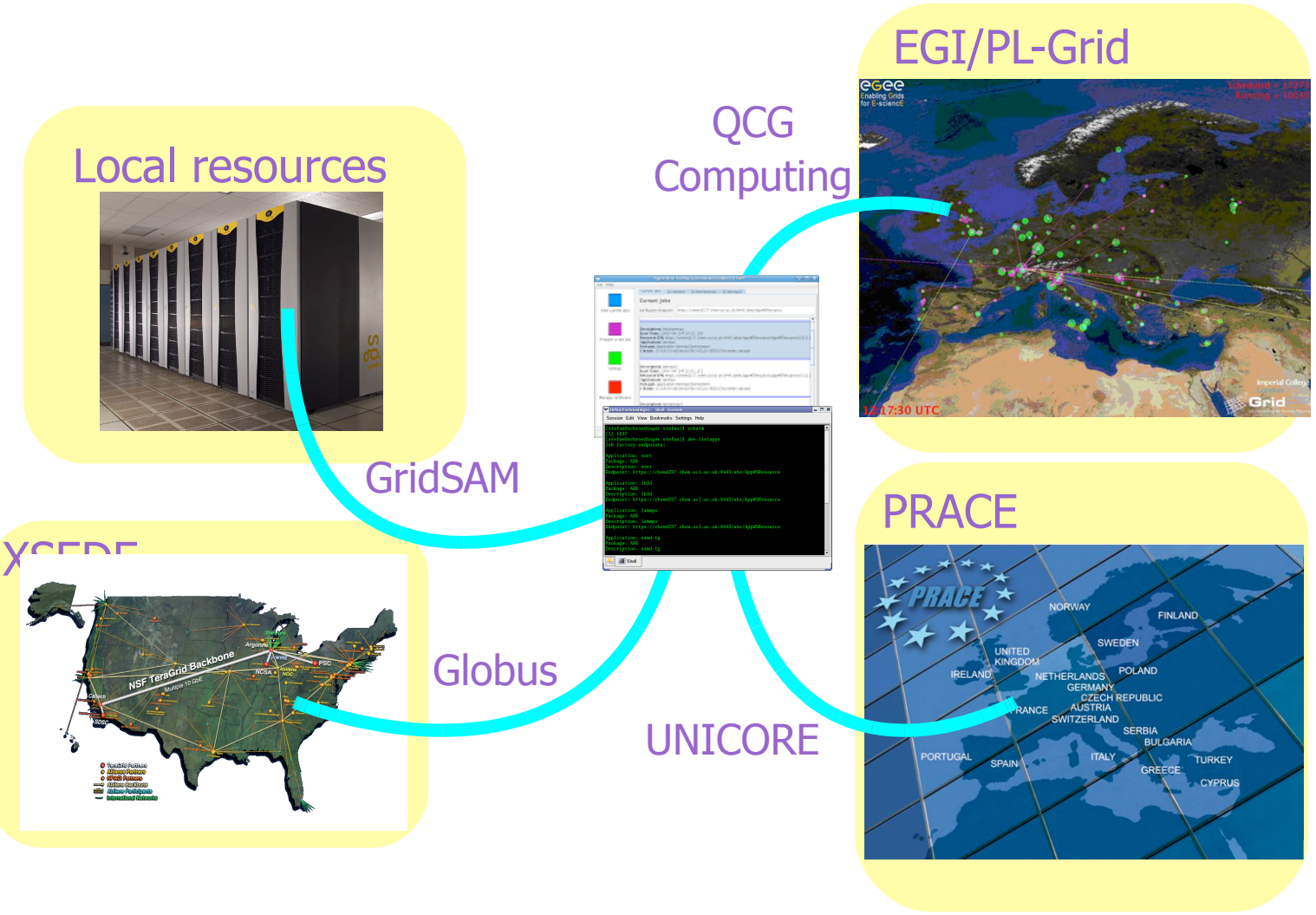
MAPPER reuses existing software components



Application Hosting Environment

- AHE is a tool for building Science Gateways
  - Lightweight hosting environment for running unmodified applications on grid and local resources.
  - Community model: expert user installs and configures an application and uses the AHE to share it with others.
  - Simple clients with very limited dependencies.
  - No intrusion onto target grid resources.
  - One of the TeraGrid approved science gateways.

AHE – Bridging the Gap



AHE

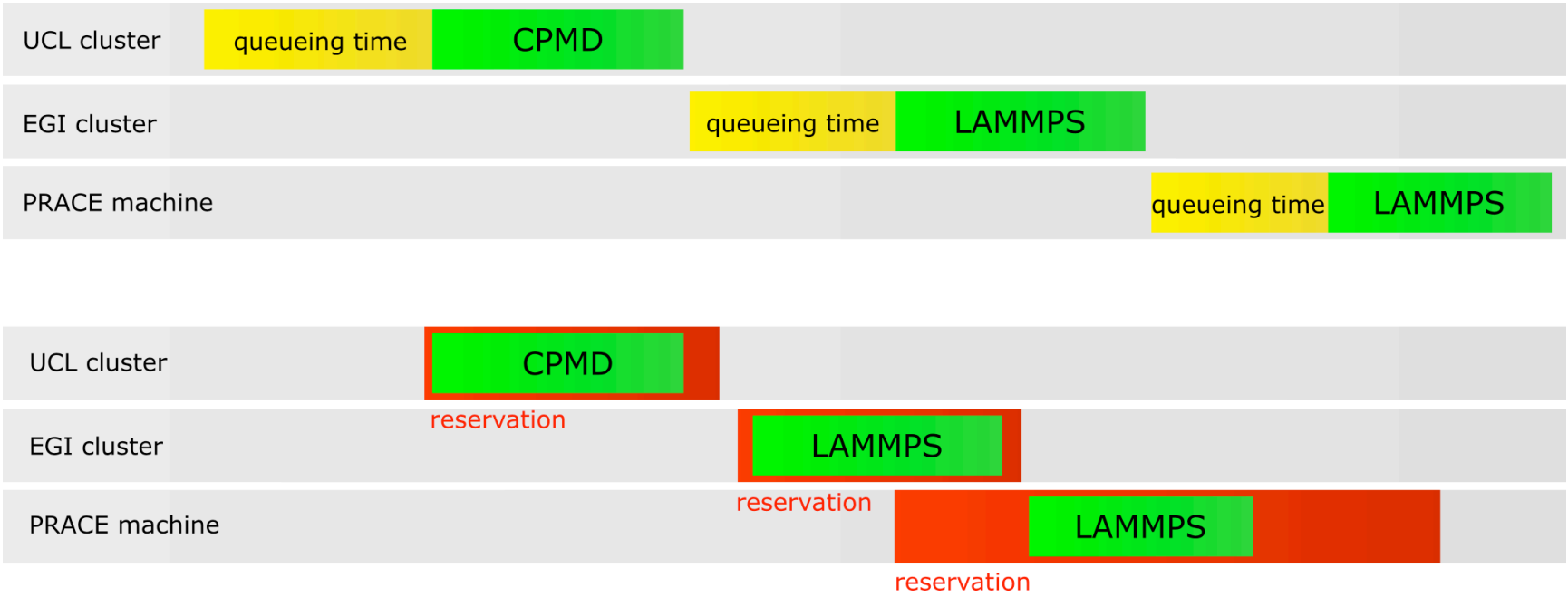
- AHE is used by several international communities.
  - The two main AHE publications have been cited at least 80 times since 2007.
- Client is easy to install
  - No other middleware required.
- Version 3.0 will support:
  - Urgent computing using SPRUCE.
  - Mechanisms to hide the complexity of certificate management to the user.

QCG Role in Loosely Coupled Scenario (I)

- Guarantees the requested level of Quality of Service
  - number and characteristics of resources,
  - execution time window

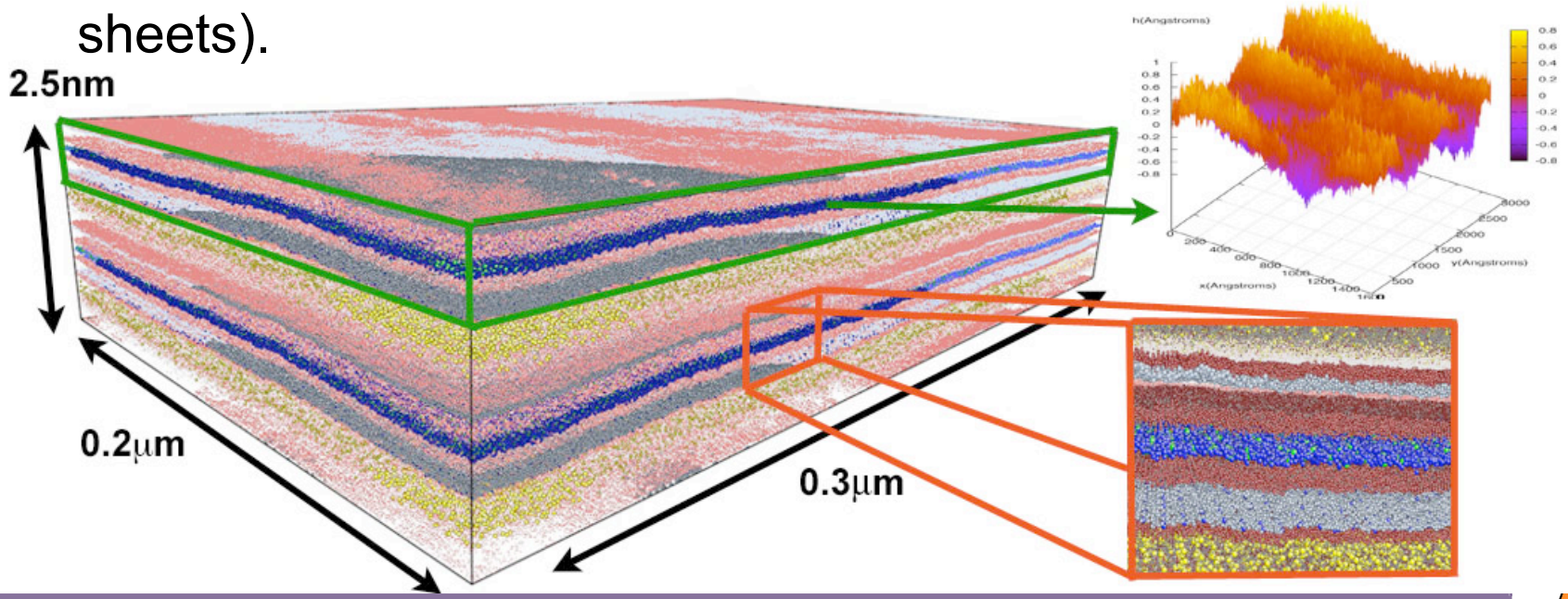
  by using an advance reservation mechanism
    - EGI (PL-Grid, Zeus cluster) and national/campus (UCL, mavrino cluster) infrastructures (QCG-Broker).
- Reduction of the overall completion time of the workflow experiment (QCG-Broker).
- Efficient execution and management of tasks on EGI and UCL resources (QCG-Computing).

QCG Role in Loosely Coupled Scenario (II)



Nanomaterials: the need for multiscale

- To accurately resolve the behavior of clay-polymer interactions, we need to simulate a large number of very thin platelets at high resolution.
- No single code is able to do this (many resort to periodic boundary conditions on short length scales or using smaller sheets).



Nanomaterials science unlocked

- Our distributed multiscale application allows us to address several important science questions, e.g.:
  - Do periodic boundary conditions become limiting at large length scales?
  - How does the clay interact with polymers on the sheet edges and in undulations?
  - How do QM effects influence these interactions?

Plans for the future

- Validate the coupling on a scientific level.
- Scale up the scenario to resolve sufficiently large systems consisting of dozens of accurately resolved clay sheets.
- Investigate the aforementioned science questions.
- Continue our 40.5M core hour PRACE grant on JUGENE into a multi-site allocatiion.

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