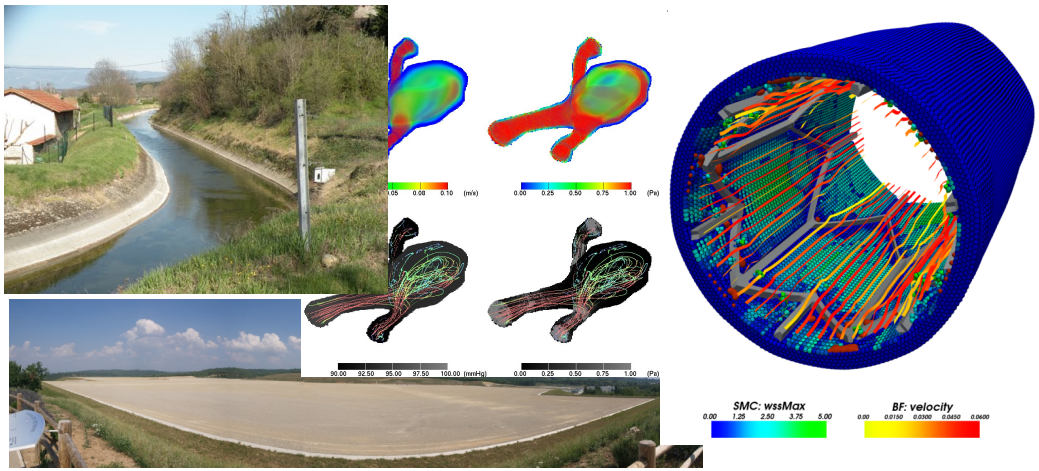
MAPPER Seasonal School

- The MAPPER project will organize its first seasonal school this winter.
- 1-2 february 2012, London, United Kingdom
- Lecture and practical sessions multiscale modelling, coupling tools, and running DMC simulations on e-infrastructures.
- Fore more info, please contact one of the chairs (or send me a mail at d.groen@ucl.ac.uk).



Modelling distributed multiscale simulation performance: an application to nanocomposites

Derek Groen, James Suter, Peter Coveney

University College London

E-Science DMC workshop 2011, Dec 5th 2011,Stockholm

Overview

- Introduction
- Overview of the multiscale scenario
- Current status
- Performance predictions
- Discussion/Conclusion/Future work

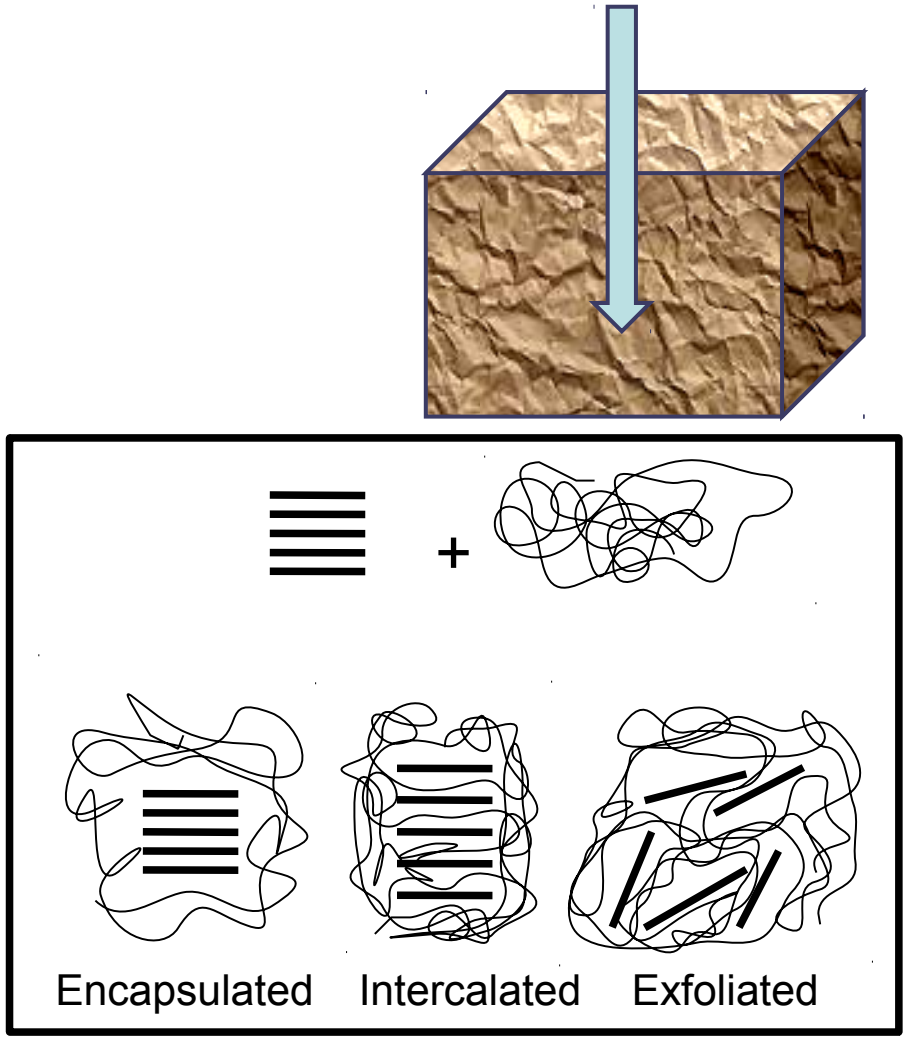
Introduction - nanocomposites

- 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.

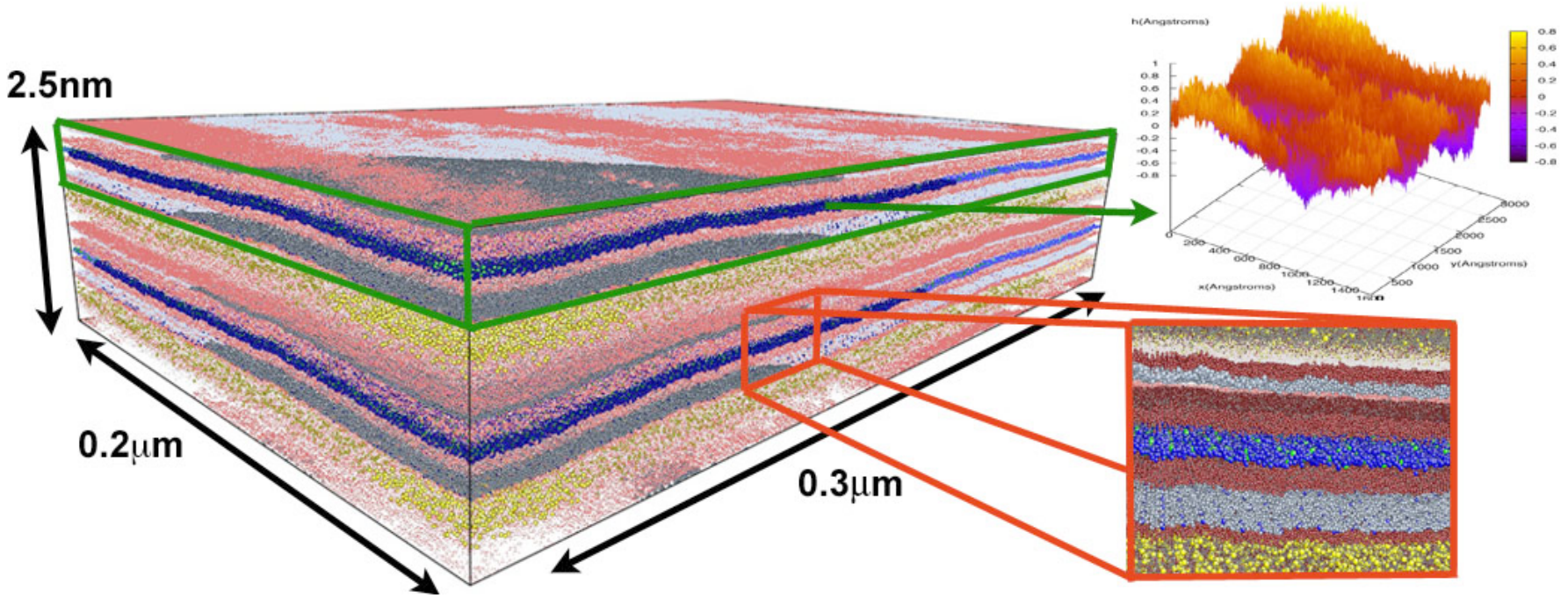


Aim of our work

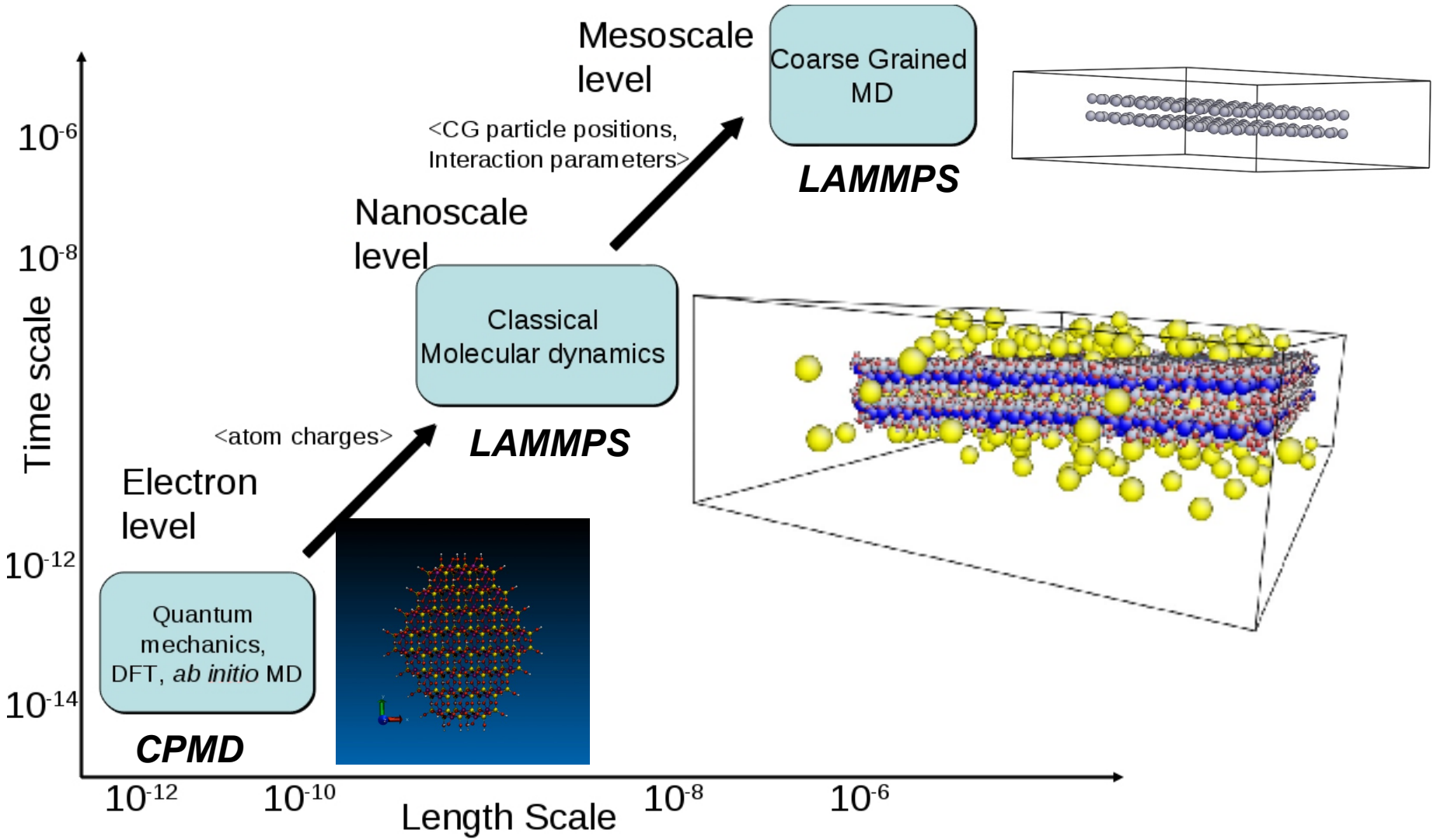
- Predict which combination of clay/nanoparticles, polymer and processing conditions will create the best nano-composite for the properties of interest.
- i.e., we do preliminary in-silico testing, providing input as to what to construct and test in reality.

Nanomaterials: the need for multiscale

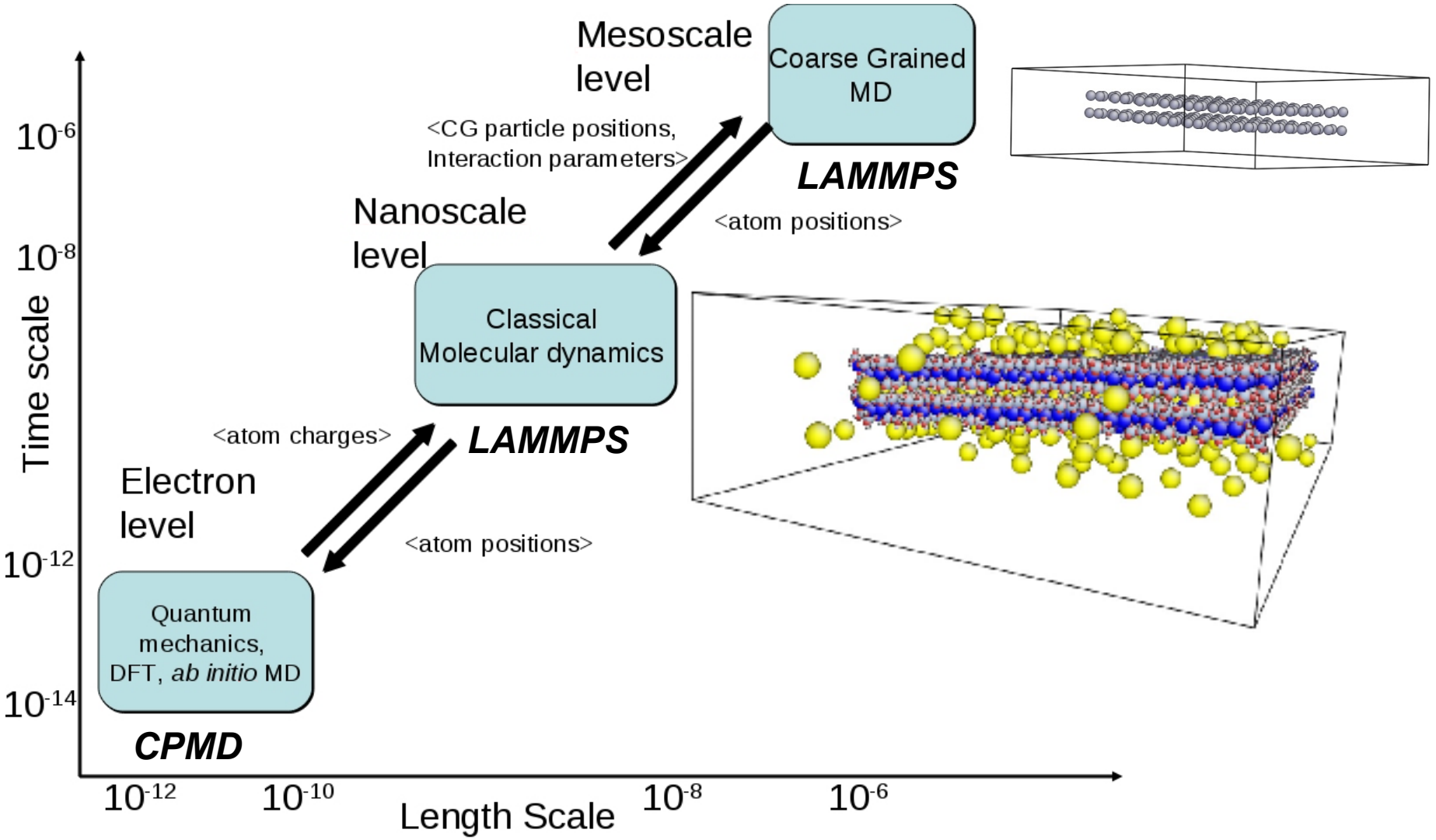
- To accurately resolve the behavior of clay-polymer interactions, we need to simulate a large number of very thin platelets at high resolution.
- No single code is able to do this (many resort to periodic boundary conditions on short length scales or using smaller sheets).
- Solution: Use a distributed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



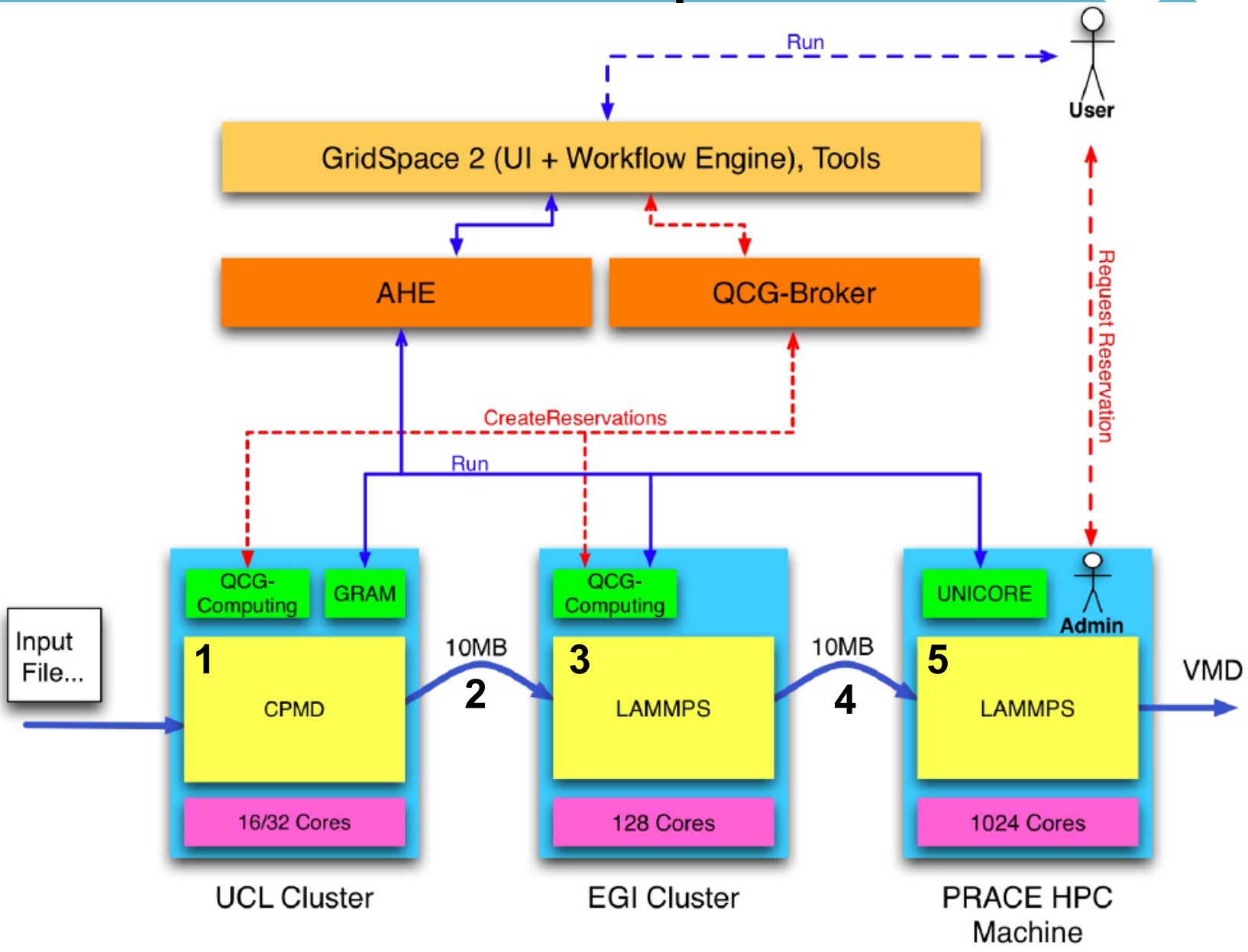
Scale Separation Map



SSM tightly coupled



Technical components



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?

Analyzing performance

- We developed a performance model to model and predict the behavior of MD-based multiscale simulations.
  - Model is partially scale-free (e.g. no new prediction needed for resized problem sizes).
  - Model includes the use and assessment of multiscale efficiency.
- General definition of multiscale efficiency:

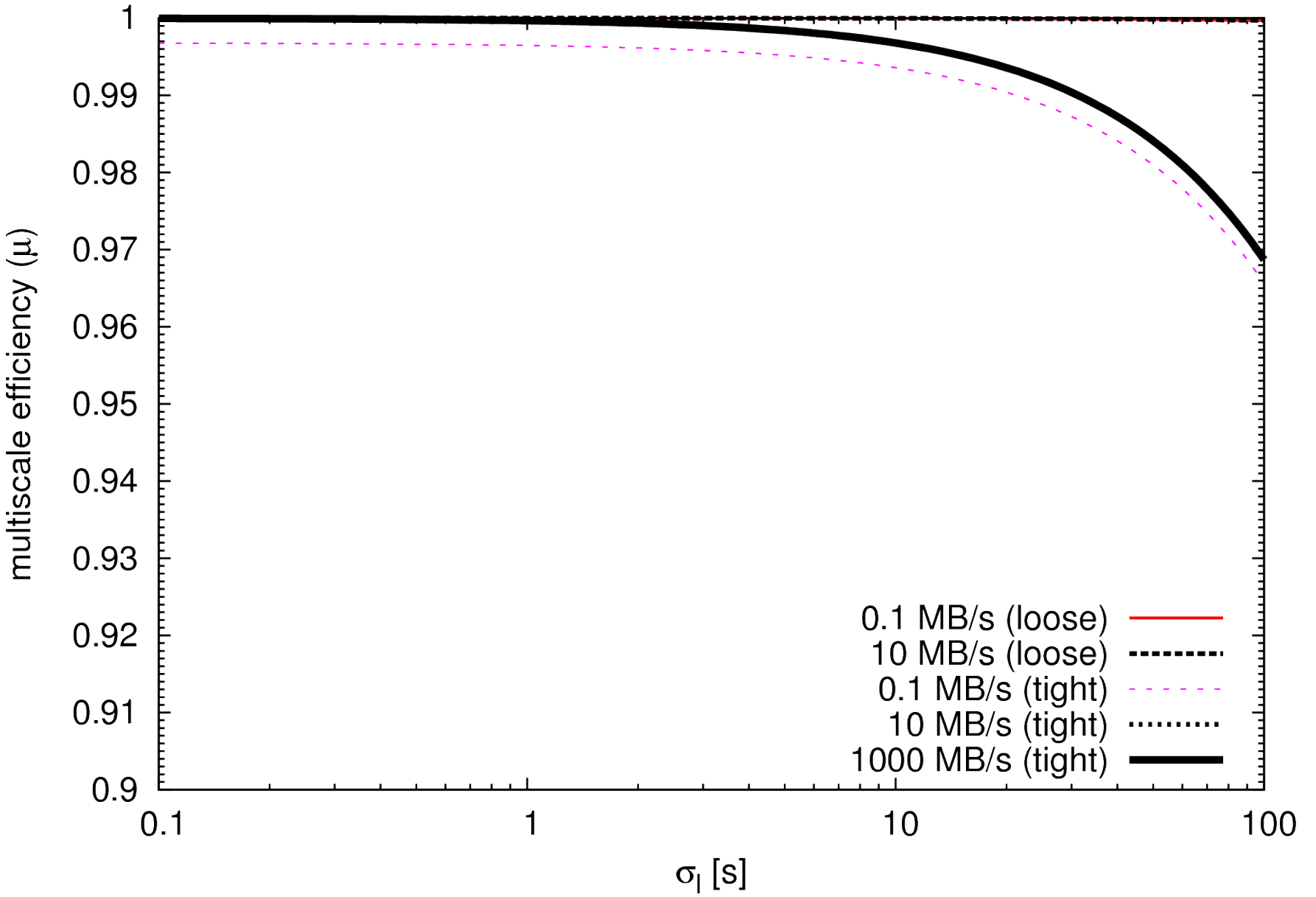
$$\mu = \frac{\text{Time spent on executing each subcode}}{\text{Total time spent on the multiscale simulation}}$$

- In our case:

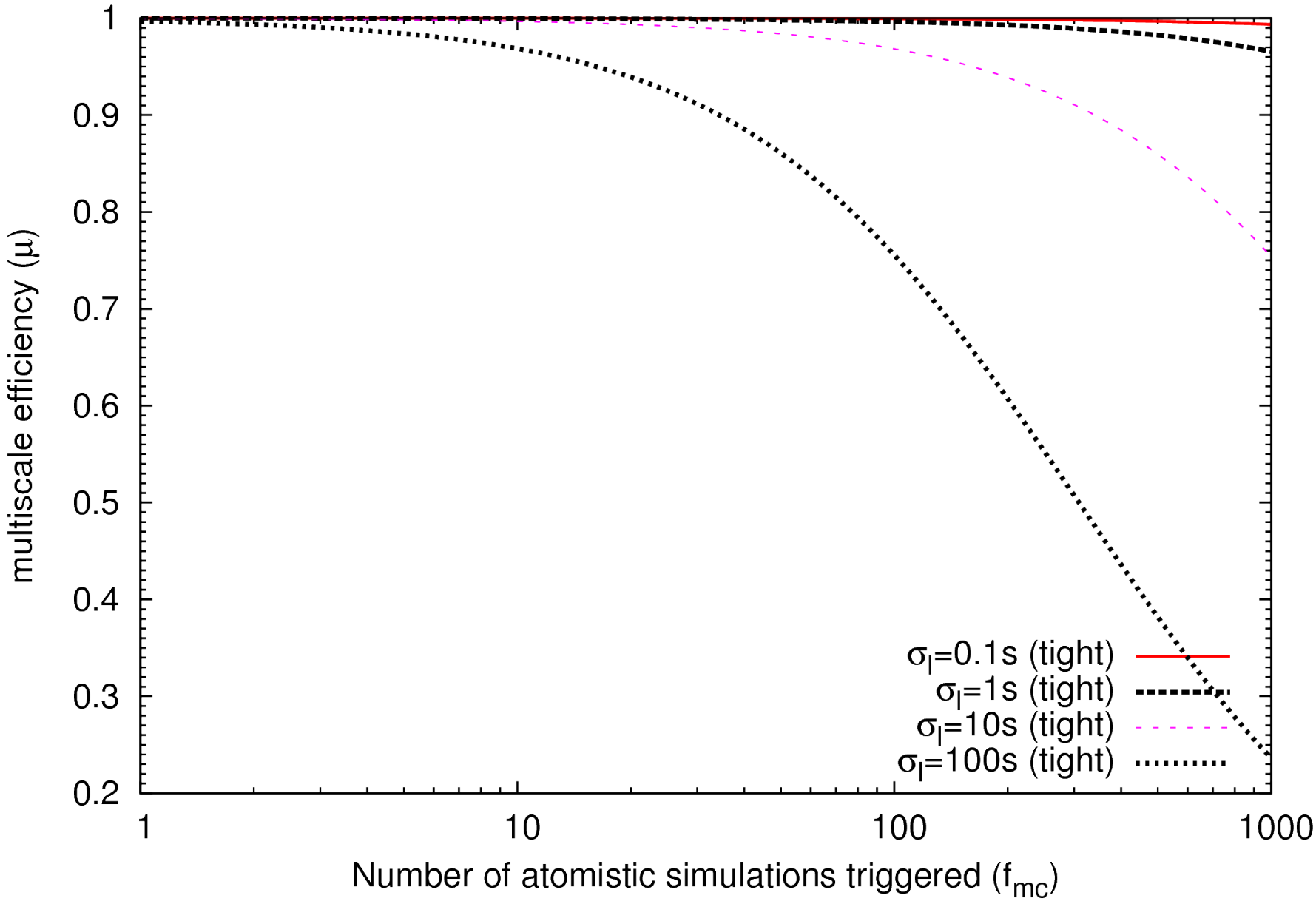
$$\mu = \frac{T_{qm} + T_{atomistic} + T_{course\text{-}grained}}{T_{total}}$$

- Assumptions in our performance model:
  - Duration:
    - QM: 1ps, Atom-MD: 1ns, CG-MD: 50ns.
  - Problem size:
    - QM: 500 atoms, 150k plane waves, 32 cores
    - Atom: 30k (~235 atoms/core), 128 cores.
    - CG: 400k (~390 particles/core), 1024 cores.
  - Internal efficiency:
    - We assume 90% efficiency for all codes.
  - WAN Bandwidth:
    - 10MB/s

Performance predictions



Performance predictions



Current Status

- We have run our first loosely-coupled DMC simulations.
  - Using 8 cores on a local UCL cluster, 8 cores on a Polish EGI site (Reef in Poznan) and 128 cores on a PRACE Tier-1 machine (Huygens at SARA)
- Runs are still in a test setup: we focus now on scaling them up in size and scientific relevance.

Ongoing efforts

- Build a toolkit for flexibly coupling QM, atomistic MD and CG MD on the scientific level.
  - QM-Atom conversion tool in testing, Atom-CG tool in development.
  - Supports a range of problem types and material compositions.
- Test the multiscale simulation on larger scales.
  - First to ~2000 cores on Huygens, then to Tier-0 PRACE facilities.
  - Include replica simulations for better sampling.

Acknowledgements

- Thanks go out to:
  - Stefan Zasada
  - Krzysztof Kurowski
  - Michel Scheerman
  - Axel Berg
  - SARA
  - PSNC

الصندوق القطري لرعاية البحث العلمي
Qatar National Research Fund
Member of Qatar Foundation