e-infrastructure

CAPACITIES

The World Is Multiscale

02/02/12

Peter Coveney

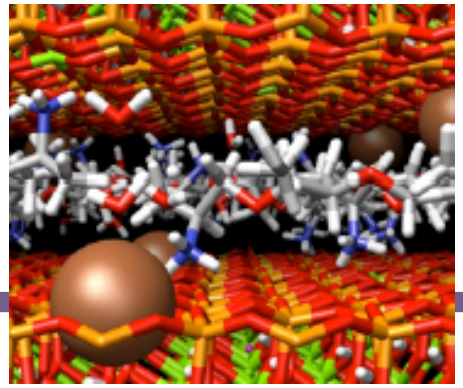
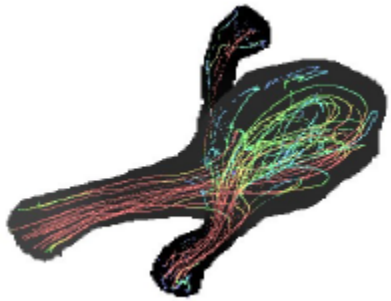
The Mapper project receives funding from the EC's Seventh Framework Programme (FP7/2007-2013) under grant agreement n° RI-261507.

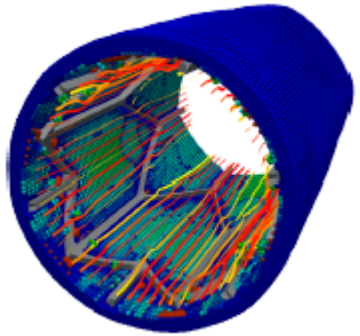
Overview

- Simulating complex multiscale systems
  - + examples.
- Multiscale communities
- Tools for coupling multiscale simulations
- Infrastructure and policy requirements
- Summary and observations

Multiscale systems

- Physical systems are often inherently multiscale.
- Micro- and mesoscopic processes influence the macroscopic behaviour of the system, and vice versa.
- Simulating all processes in a complex system with a single code is often an impossible endeavour.
- High resolution needed to resolve microscopic processes.
- Microscopic accuracy + macroscopic problem size => prohibitive computational and storage demands.



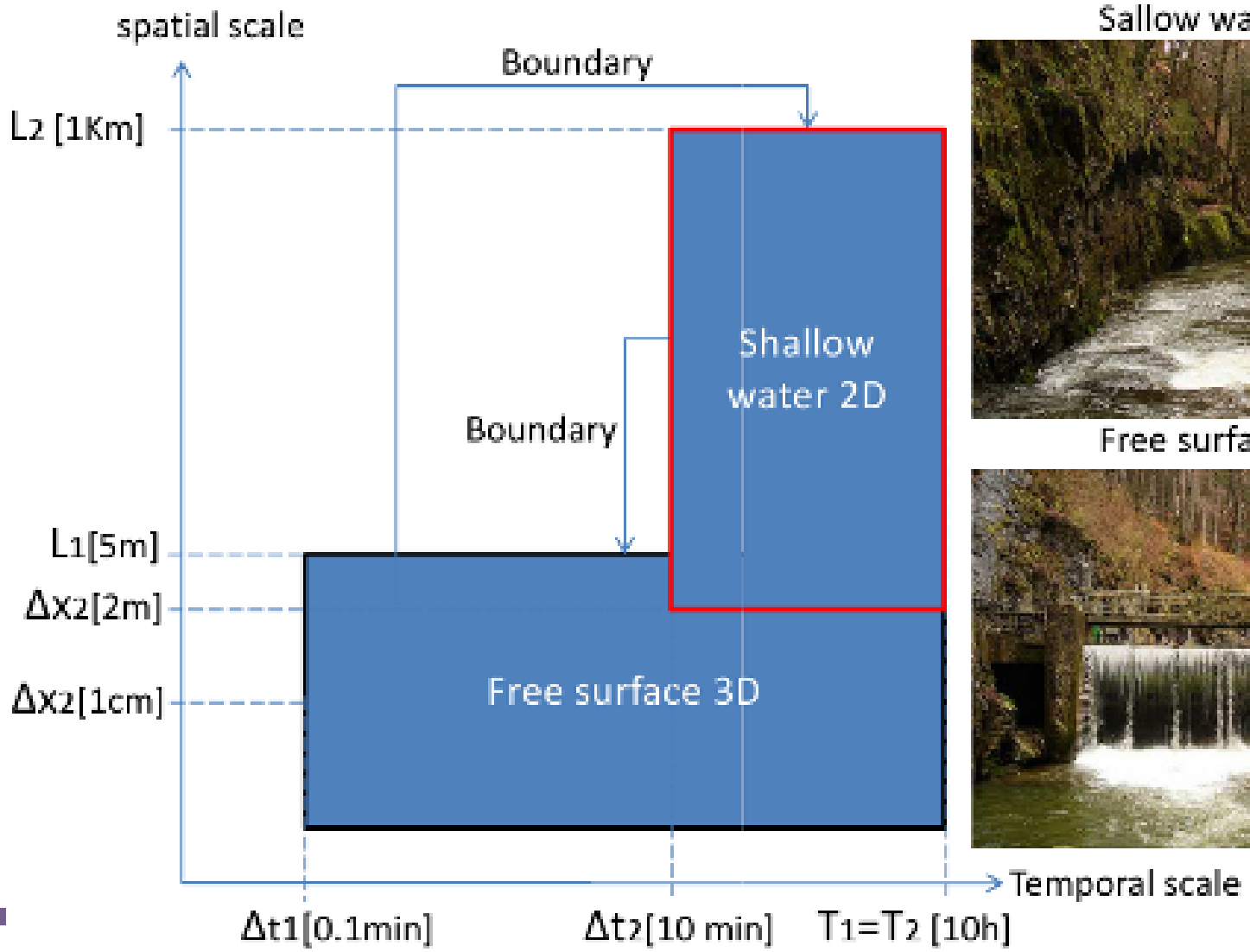
Multiscale systems

- Multiscale methods allow researchers to simulate systems by taking the best of both worlds.
- Microscopic detail in the most critical subsections of the problem.
- Efficiency and problem size advantages of macroscopic simulations.
- Wide range of applications
  - e.g. simulating relevant processes in the human body...

Overview

- Two-way “tight” coupling between subcodes.
  - e.g. continuum-particle hybrid coupling. R. Delgado-Buscalioni and P. V. Coveney, Phys. Rev. E 67, 046704 (2003)
  - Typically performed using specialized coupling tools.
- One-way “loose” coupling between subcodes.
  - Typically performed using workflow managers.
    - e.g. GridSpace, Swift or Kepler.

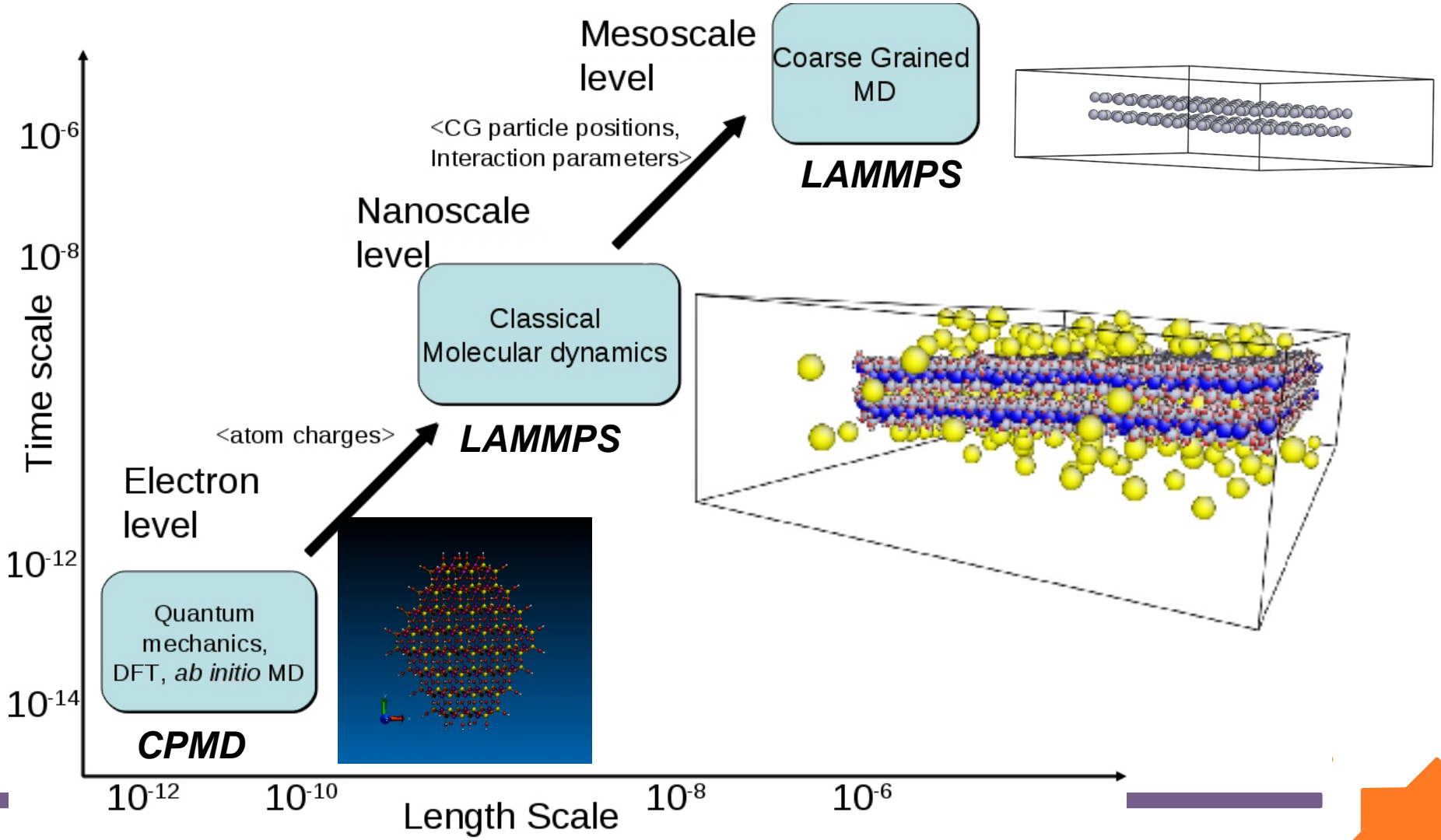
Tightly Coupled Example: Canals



Sallow water 2D

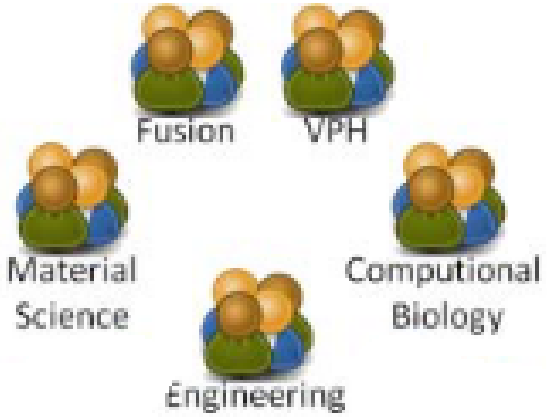
Free surface 3D

Loosely Coupled Example: Nanomaterials

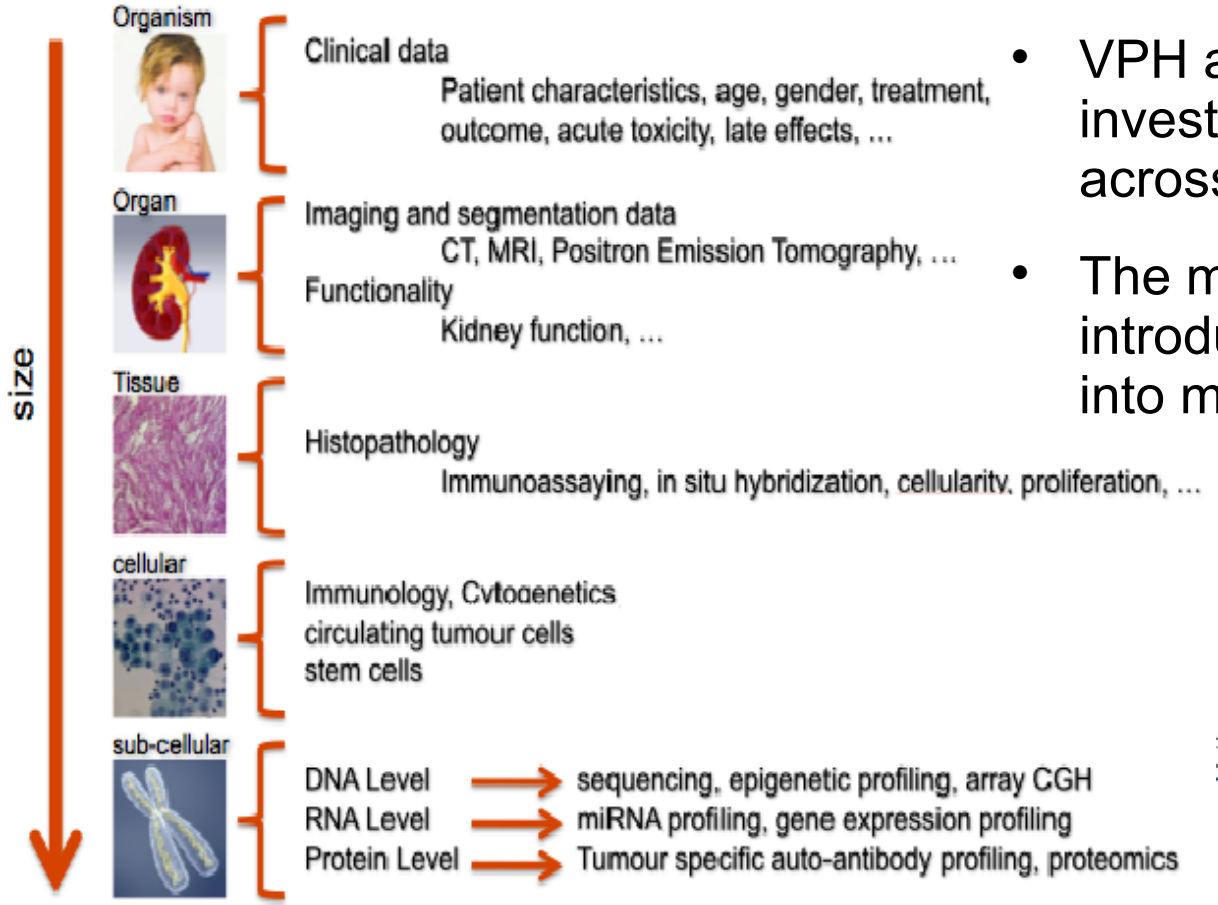


Example Project: MAPPER

- Goal: To make multiscale applications possible on European production e-Infrastructures.
- Duration: Oct. 2010 – Sept. 2013.
- 5 application domains within the project,
  - + cooperation with external communities.
- EU FP7 project with partners throughout Europe.
- http://www.mapper-project.eu



Example Community: Virtual Physiological Human



- €200M initiative in EU-FP7
- VPH aims to enable collaborative investigation of the human body across all relevant scales.
- The main aim of VPH is to introduce *multiscale* methodologies into medical and clinical research.

Coupling frameworks

- Coupling frameworks are tools which enable application developers to combine multiple subcodes into a multiscale simulation.
- These tools come in various forms:
  - All-in-one monolithic simulation codes.
    - The 'old' method with internally hardcoded coupling.
  - Software frameworks with pluggable modules.
  - Module independent coupling tools.

Example Coupling frameworks

- MUSCLE
  - Java-based coupling tool usable across domains.
  - Intended for tight coupling.
- GridSpace
  - Workflow-based tool running as SaaS.
  - Enables loose coupling (but may function as an interface for tight coupling scenarios).
- Both tools will feature in the Seasonal School tutorials.

Other requirements for multiscale simulations

- Infrastructural requirements, e.g.:
  - Suitable compute, storage and network resources.
  - Proper software tools for using and reserving remote resources.
    - Covered by for example the Application Hosting Environment and QosCosGrid Broker.
- Policy requirements, e.g.:
  - Support for automated advance reservation.
  - Uniform interfaces for resource access and accounting.
  - Scientist-friendly application procedures for compute time.
    - e.g., include resource allocations as a part of EU project application procedure, rather than arranging it using additional proposals.

Summary and Observations

- Multiscale simulation and modelling has gained much popularity in recent years.
  - Especially in biology and materials science.
- Each domain prefers its own approach:
  - Some domains generally prefer hand-scripting the coupling (e.g., materials),
  - some prefer domain-specific coupling tools (e.g., astrophysics),
  - and some communities adopt general-purpose solutions (e.g., biology or environmental sciences).
- MAPPER introduces a range of general-purpose tools for multiscale simulations, and aims to enable distributed multiscale simulations on EU production infrastructures.

Peter Coveney

p.v.coveney@ucl.ac.uk

UCL