e-infrastructure

CAPACITIES

Distributed Multiscale Computing, the MAPPER project

10.02.2012

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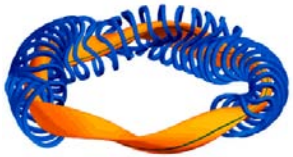
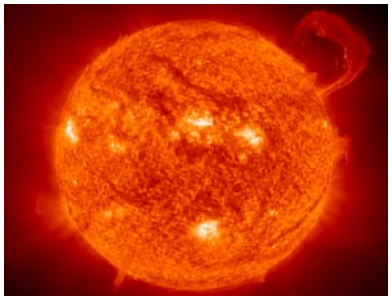
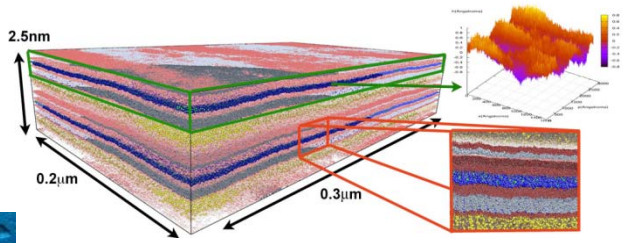
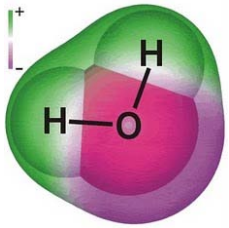
Nature is Multiscale

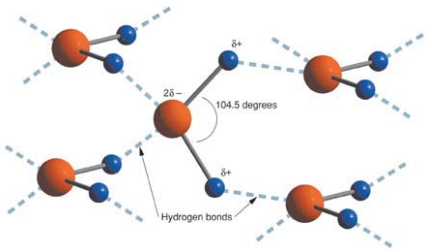
- Natural processes are multiscale

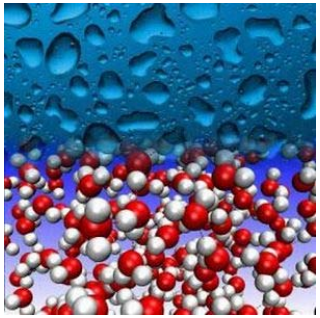










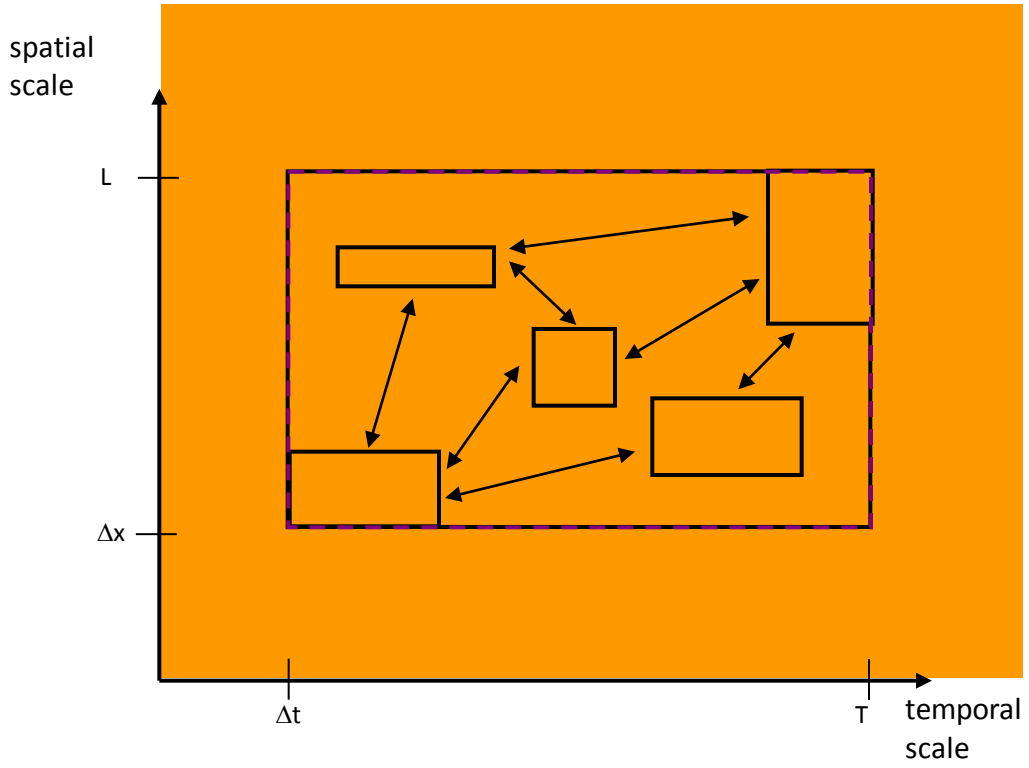


Scale range for biomedical applications

- Temporal
  - Molecular events $O(10^{-6})$ s
  - Human life time $O(10^{9})$ s
  - A range of $\mathbf{10^{15}}$
- Spatial
  - Macro molecules $O(10^{-9})$ m
  - Size of human $O(10^{0})$ m
  - A range of $\mathbf{10^{9}}$

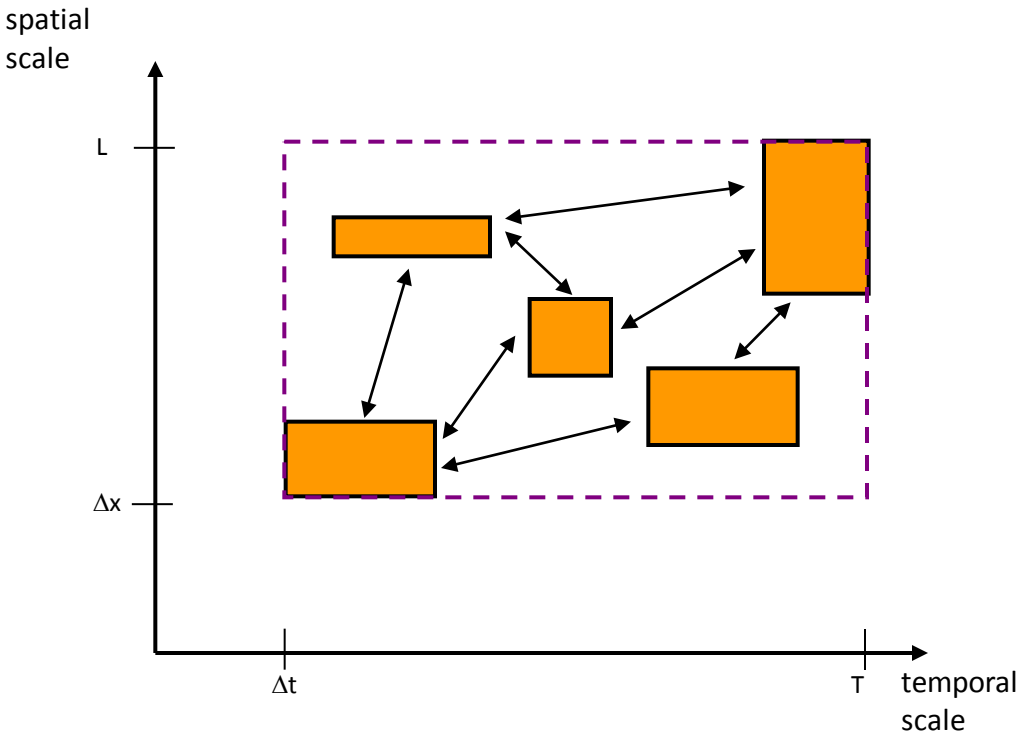
Multi-Scale modeling

- Scale Separation Map
- Nature acts on all the scales
- We set the scales
- And then decompose the multiscale system in single scale sub-systems
- And their mutual coupling



From a Multi-Scale System to many Single-Scale Systems

- Identify the relevant scales
- Design specific models which solve each scale
- Couple the subsystems using a coupling method



Why multiscale models?

- There is simply no hope to computationally track complex natural processes at their finest spatio-temporal scales.
  - Even with the ongoing growth in computational power.

Minimal demand for multiscale methods

$$\frac{\text{cost of multiscale solver}}{\text{cost of fine scale solver}} << 1$$

$$\text{errors in quantities of interest} < tol$$

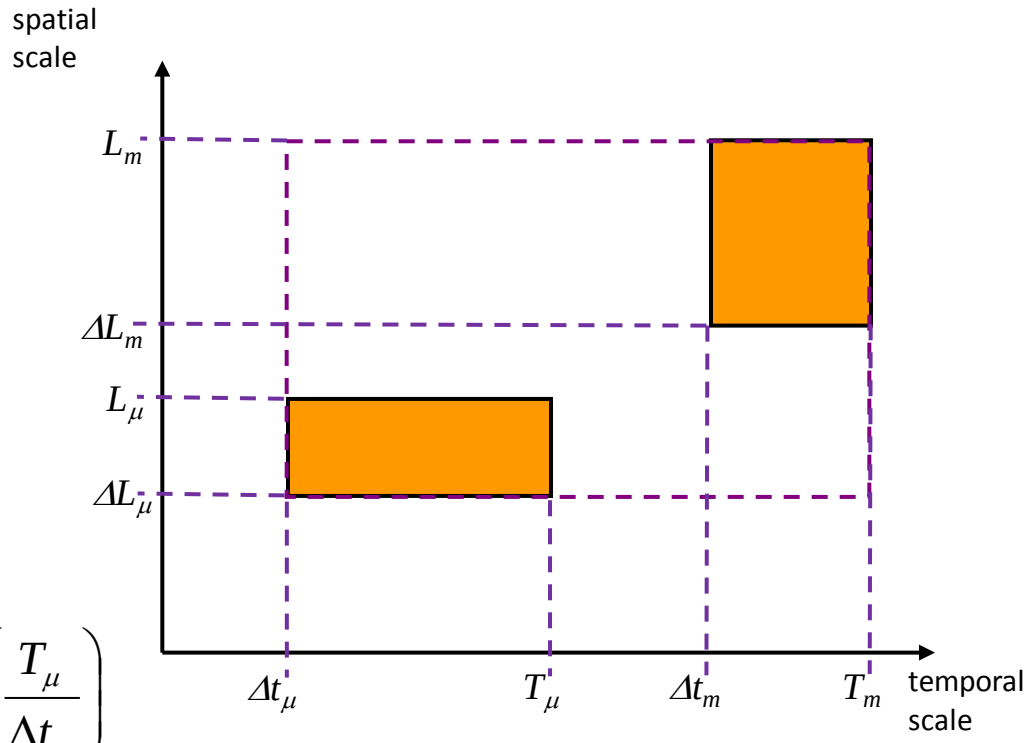
Multiscale Speedup

- 1 microscale and one macroscale process
  - At each iteration of the macroscale, the microscale is called
- Execution time full fine scale solver

$$T_{ex}^{full} = \left(\frac{L_M}{\Delta x_\mu}\right)^D \left(\frac{T_M}{\Delta t_\mu}\right)$$

- Execution time for multiscale solver

$$T_{ex}^{multiscale} = \left(\frac{L_M}{\Delta x_M}\right)^D \left(\frac{T_M}{\Delta t_M}\right)\left(\frac{L_\mu}{\Delta x_\mu}\right)^D \left(\frac{T_\mu}{\Delta t_\mu}\right)$$



- Multiscale speedup

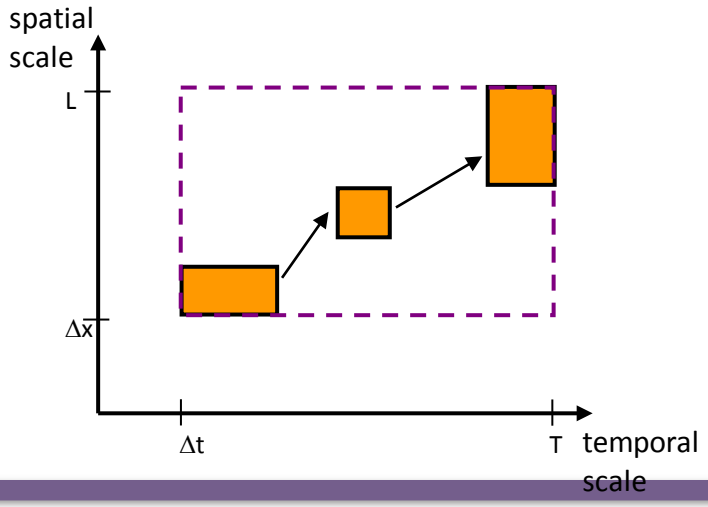
$$S^{multiscale} = \frac{T_{ex}^{full}}{T_{ex}^{multiscale}} = \left(\frac{\Delta x_M}{L_\mu}\right)^D \left(\frac{\Delta t_M}{T_\mu}\right)$$

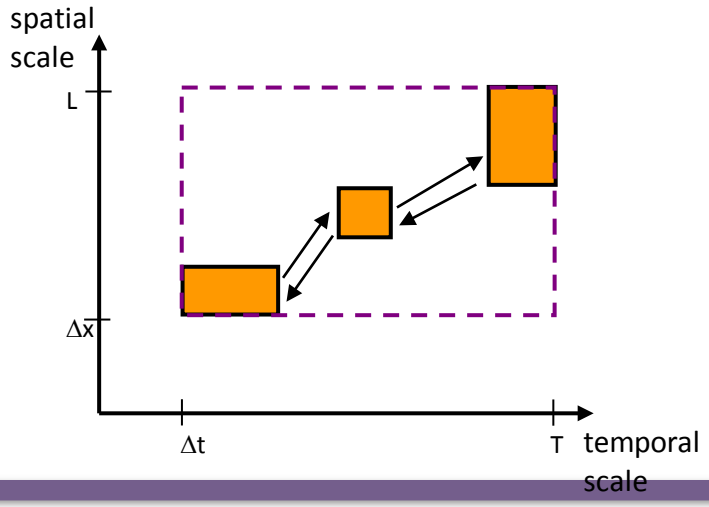
But what about multiscale computing?

- Inherently hybrid models are best serviced by different types of computing environments
- When simulated in three dimensions, they usually require large scale computing capabilities.
- Such large scale hybrid models require a distributed computing ecosystem, where parts of the multiscale model are executed on the most appropriate computing resource.
- Distributed Multiscale Computing

Two Multiscale Computing paradigms

- Loosely Coupled
  - One single scale model provides input to another
  - Single scale models are executed once
  - workflows
- Tightly Coupled
  - Single scale models call each other in an iterative loop
  - Single scale models may execute many times
  - Dedicated coupling libraries are needed





Multiscale APPlications on European e-infRastructures

(proposal number 261507)

Project Overview

University of Amsterdam

University College London

University of Ulster

Poznan Supercomputing and Networking Centre

Akademia Gorniczo-Hutnicza im. Stanislawa Staszica w Krakowie

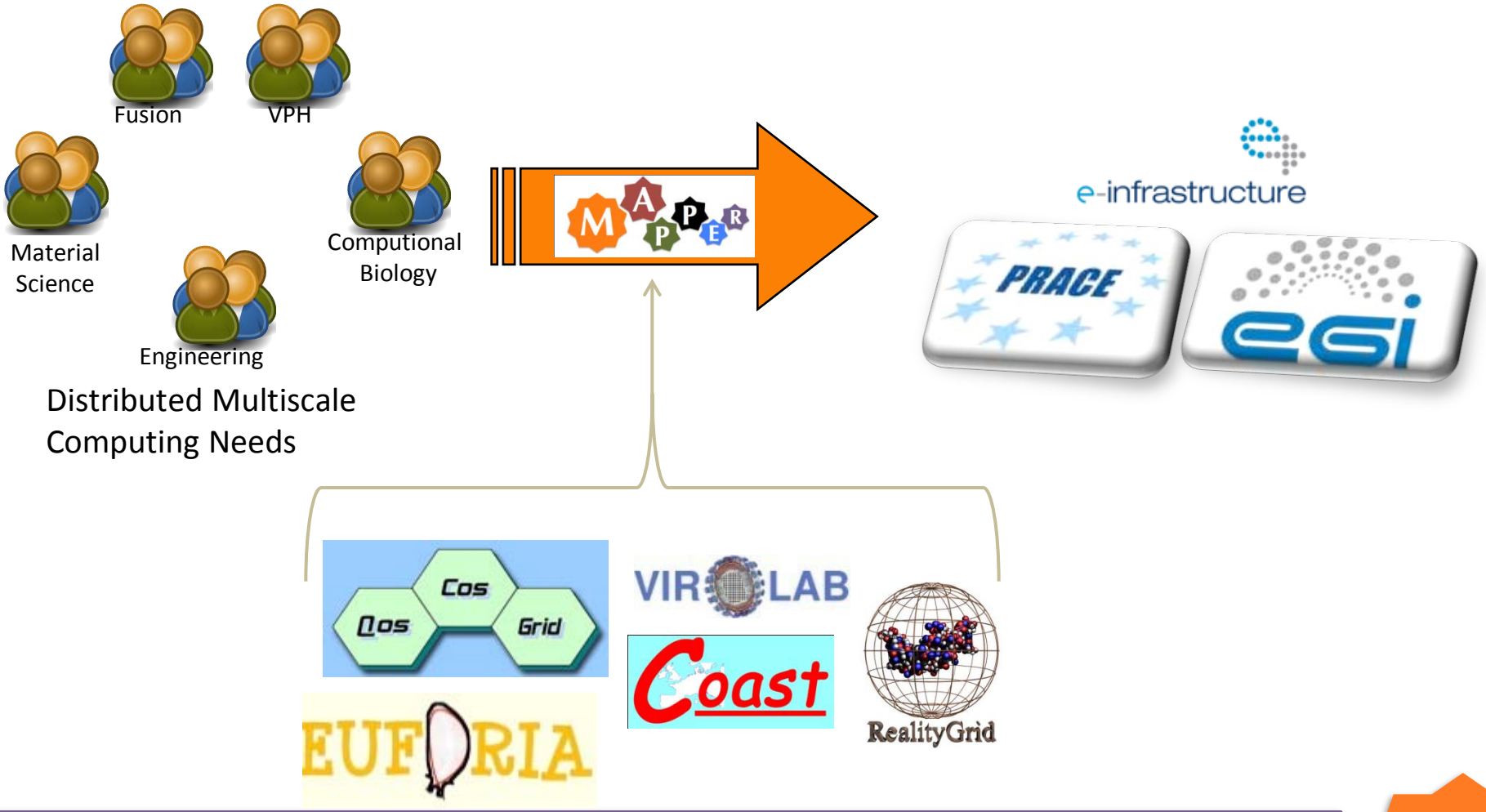
Ludwig-Maximilians-Universität München

University of Geneva

Chalmers Tekniska Högskola

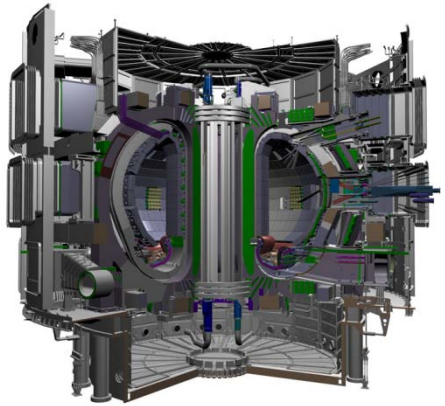
Max-Planck Gesellschaft zur Foerderung der Wissenschaften E.V.

Motivation: user needs



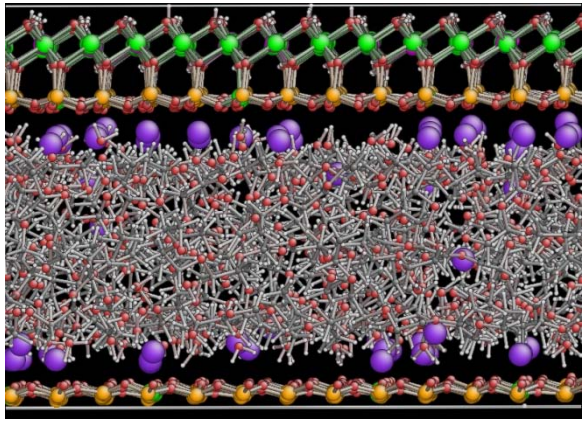
Application Portfolio

virtual physiological human

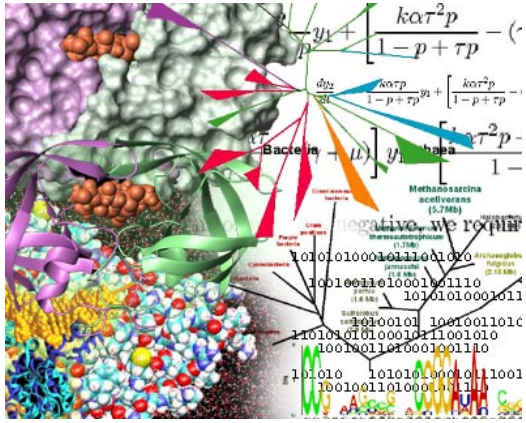


fusion

hydrology



nano material science



computational biology

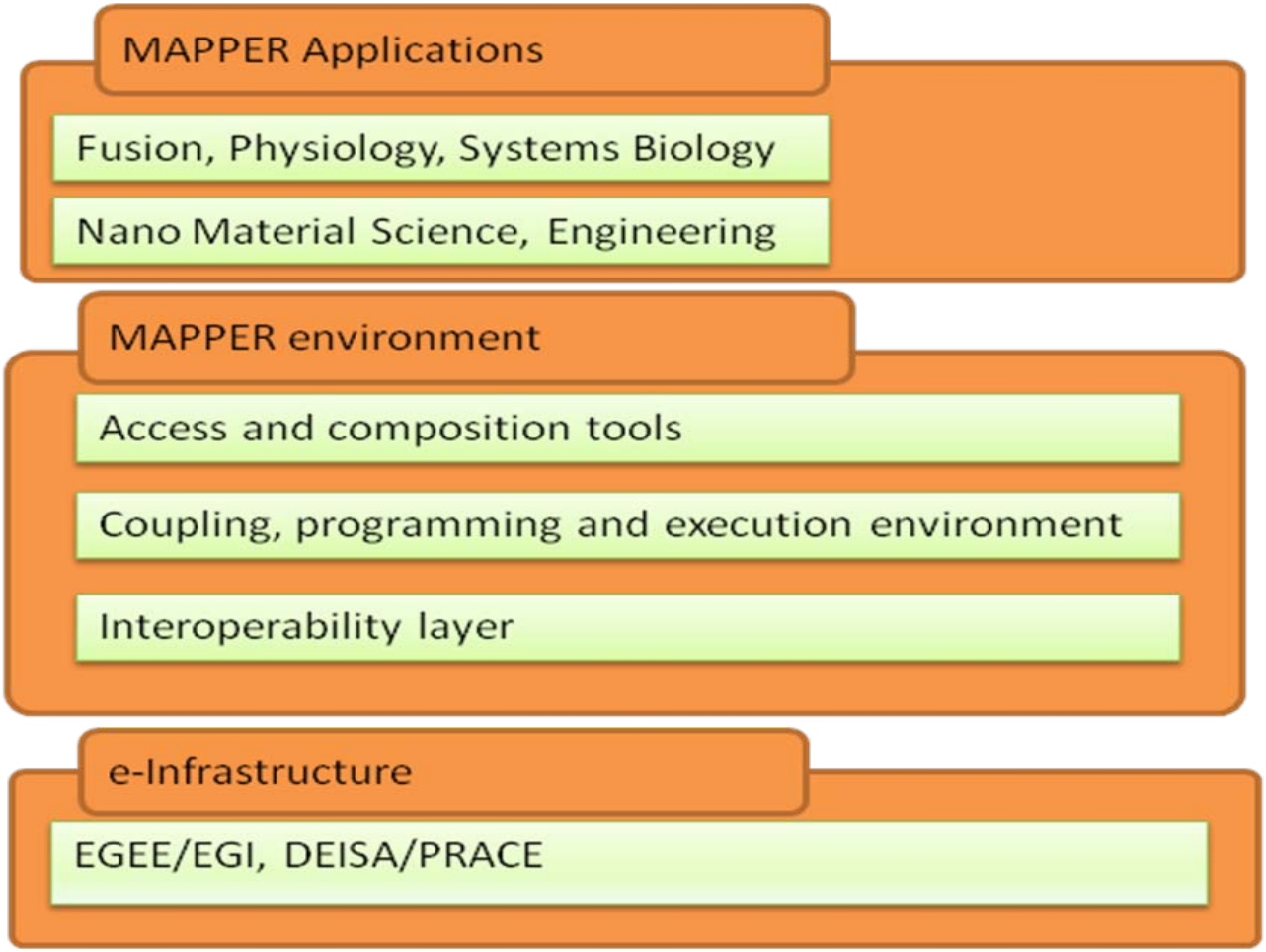
Computational power needed

Table 2: Multiscale characteristics of applications

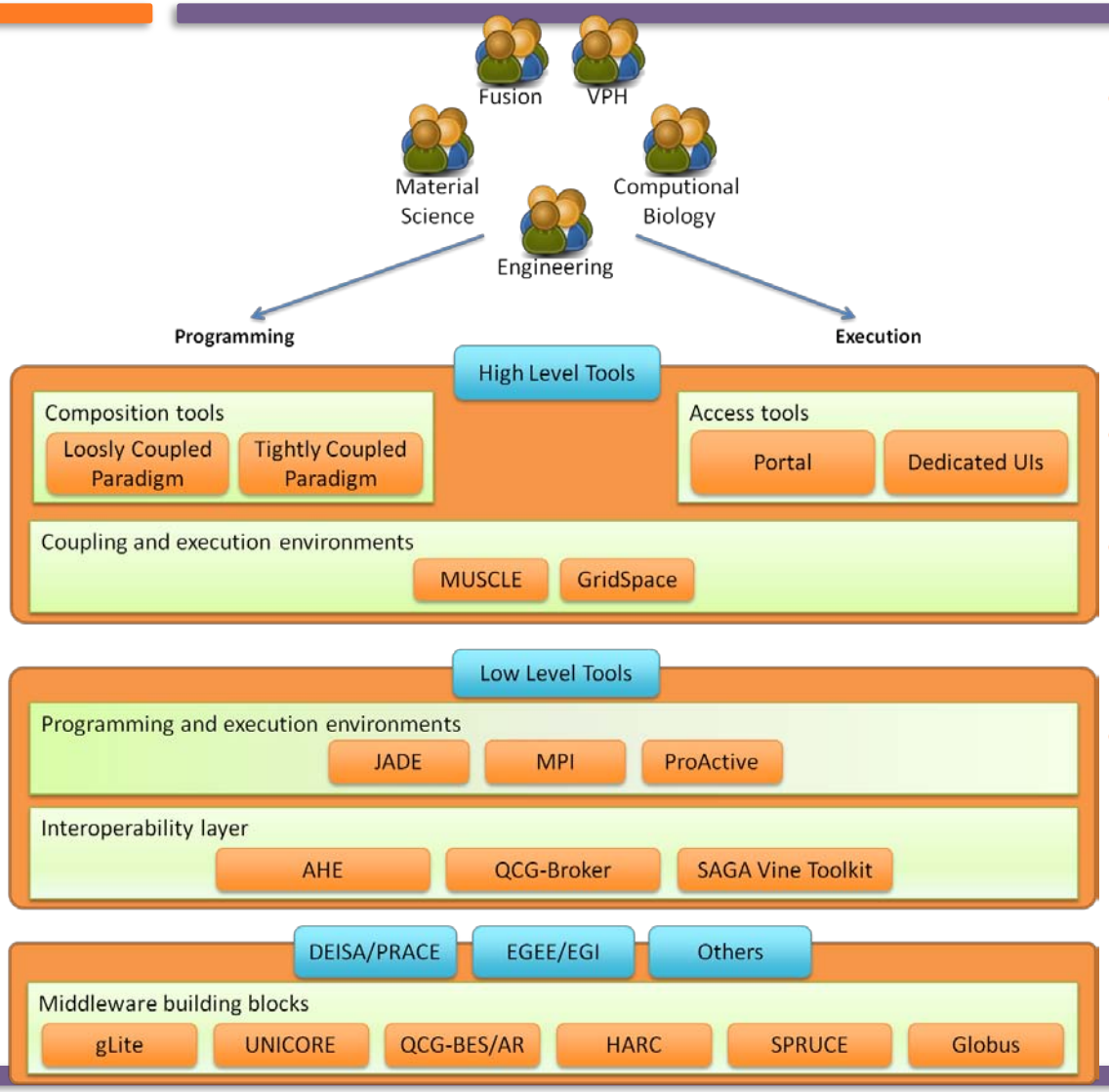
Application	Loosely Coupled	Tightly Coupled	Total number of single scale models	Number of single scale models that require supercomputers
In-stent restenosis		X	5(1)	2
Coupled same-scale and multi-scale hemodynamics		X	3(2)	2
Multi-scale modelling of the BAXS	X		2(3)	1
Edge Plasma Stability	X		3(4)	1
Core Workflow		X	3-10(5)	1-4
Irrigation canals		X	5(6)	1-2
Clay polymers	X		3(7)	2

(1) Blood flow, smooth muscle cell proliferation, drug diffusion, thrombus, stent-deployment; Depending on state-of-the-art when starting the project; (2) HemeLB, a lattice-Boltzmann code for blood flow, NEKTAR, a FEM-based code for blood flow in large arteries, CellML models for cellular processes; (3) metabolism (Phase 1), conjugation (Phase 2) and further modification and excretion (transport) (Phase 3) of the target drug/xenobiotic/endobiotic/bile acid; (4) HELENA or equivalent plasma equilibrium code and ILSA or equivalent plasma stability code; (5) HELENA/CHEASE/EQUAL, some combination of ETAIGB/ NEOWES/ NCLASS/ GLF23/ WEILAND/ GEM, some heating modules from ICRH/NBI/ECRH/LH, some particle source modules from NEUTRALS/PELLETS, some MHD modules from SAWTEETH/NTM/ELMs (6) 1D shallow water models, 2D shallow water models, 2D Free surface flow models, 3D Free surface flow models, Sediment transport models; (7) ab initio molecular dynamics code CASTEP, atomistic molecular dynamics code LAMMPS, coarse-grained simulations also using LAMMPS;

Overview


MAPPER Applications
Fusion, Physiology, Systems Biology
Nano Material Science, Engineering
MAPPER environment
Access and composition tools
Coupling, programming and execution environment
Interoperability layer
e-Infrastructure
EGEE/EGI, DEISA/PRACE

Ambition



- Develop computational strategies, software and services
  - for *distributed multiscale simulations* across disciplines
  - exploiting existing and evolving European e-infrastructure
- Deploy a computational science infrastructure
- Deliver high quality components
  - aiming at large-scale, heterogeneous, high performance multi-disciplinary multiscale computing.
- Advance state-of-the-art in high performance computing on e-infrastructures
  - enable distributed execution of multiscale models across e-Infrastructures,

MAPPER Roadmap

- October 1, 2010 – start of project
- Fast track deployment – first year of project
  - Loosely and tightly coupled distributed multiscale simulations can be executed.
- Deep track deployment – second and third year
  - More demanding loosely and tightly coupled distributed multiscale simulation can be executed
  - Programming and access tools available
  - Interoperability available

- Have a good school!