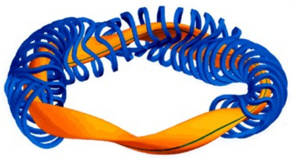
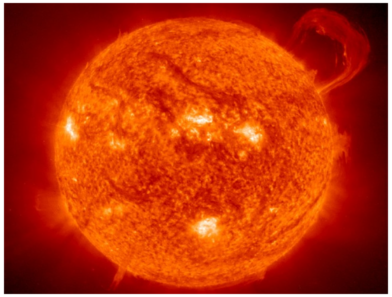
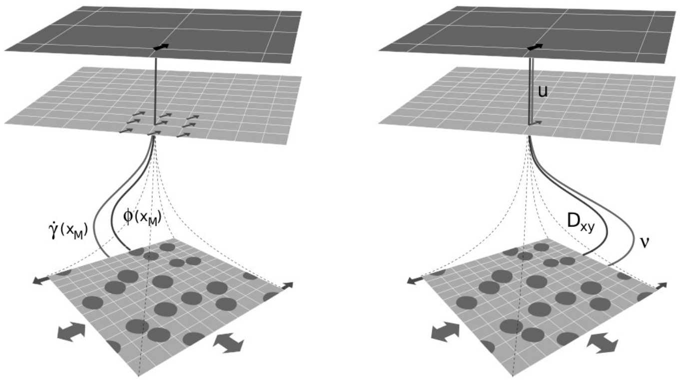
The Mapper project an overview

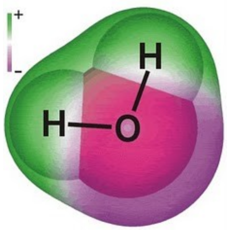
Eric Lorenz

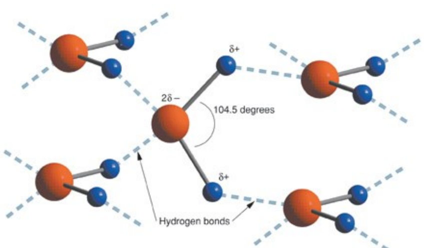
The Mapper project receives funding from the EC's Seventh Framework Programme (FP7/2007-2013) under grant agreement n° RI-261507.

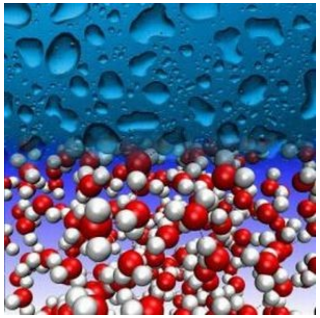
Nature is Multiscale

- Natural processes are multiscale
  - 1 H_2O molecule
  - A large collection of H_2O molecules, forming H-bonds
  - A fluid called water, and, in solid form, ice.

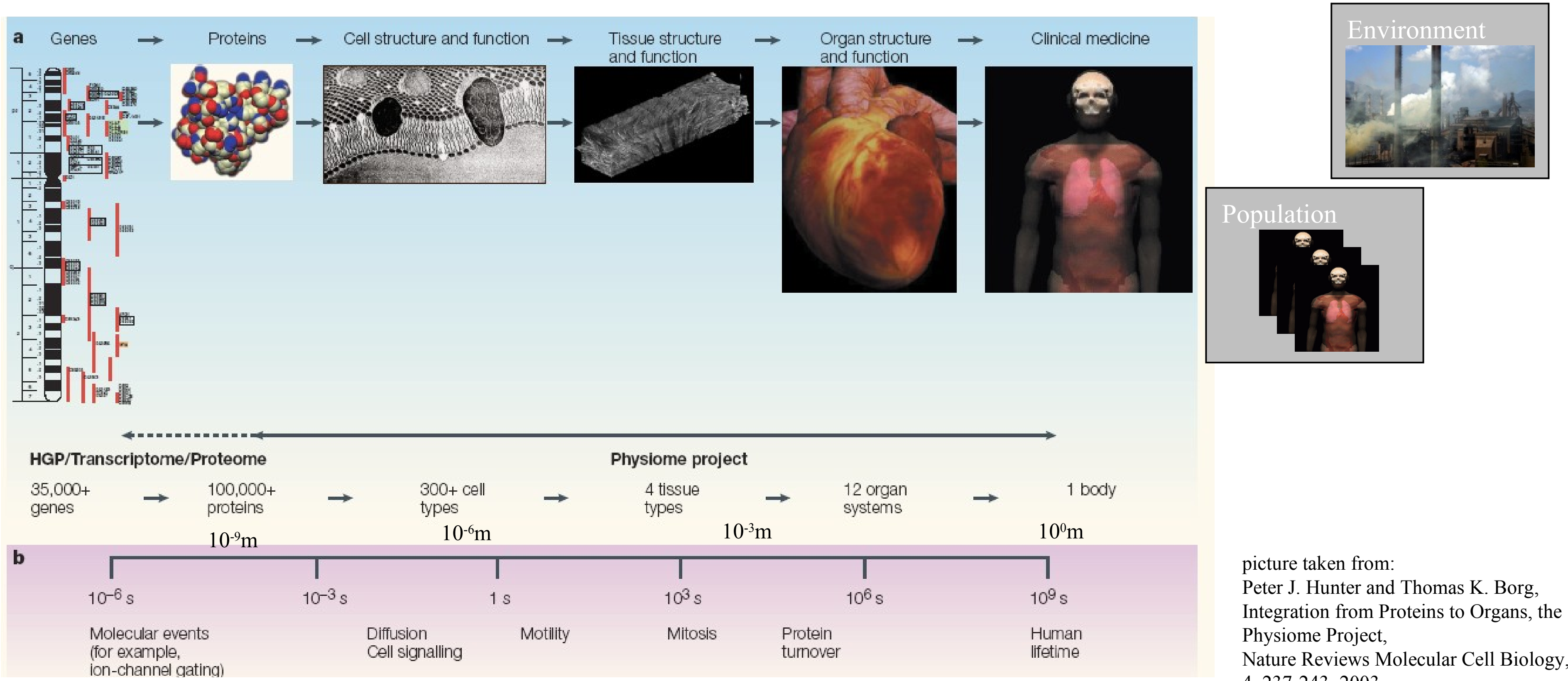







From Molecule to Man

(or, from DNA to Disease to Environment)

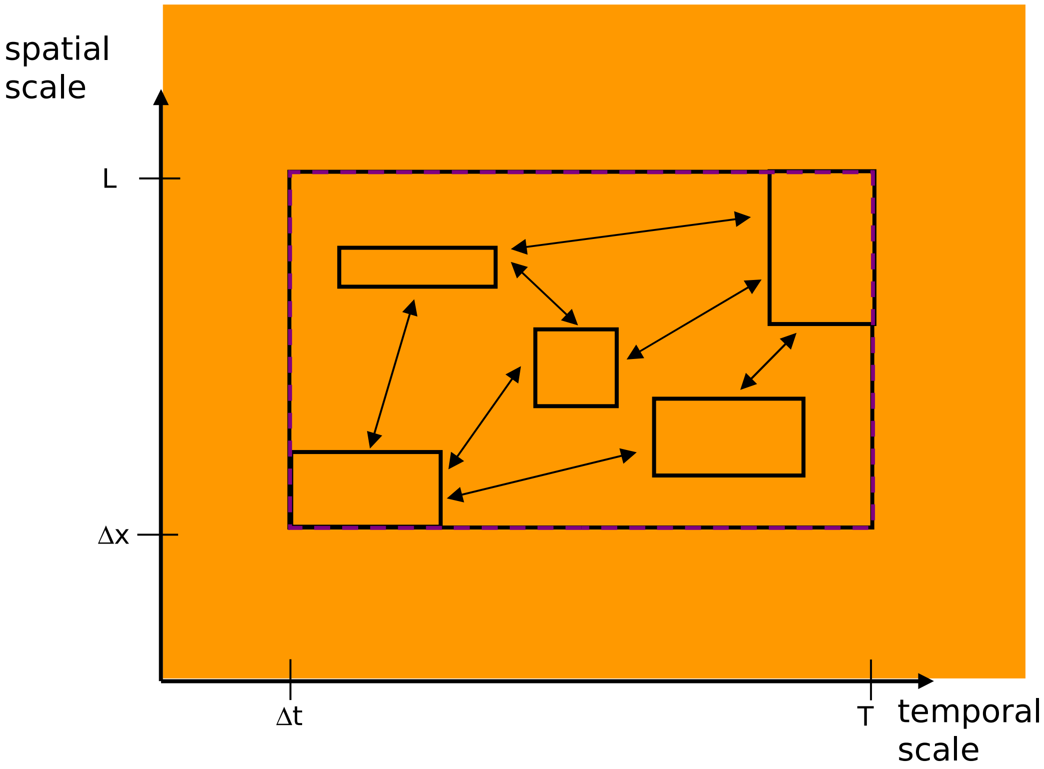


picture taken from:
Peter J. Hunter and Thomas K. Borg, Integration from Proteins to Organs, the Physiome Project, Nature Reviews Molecular Cell Biology, 4, 237-243, 2003

=> Multiscale models in Biomedicine involve biological, chemical and physical processes bridging ranges of scales of **10^9** (spatial) and **10^{15}** (temporal)

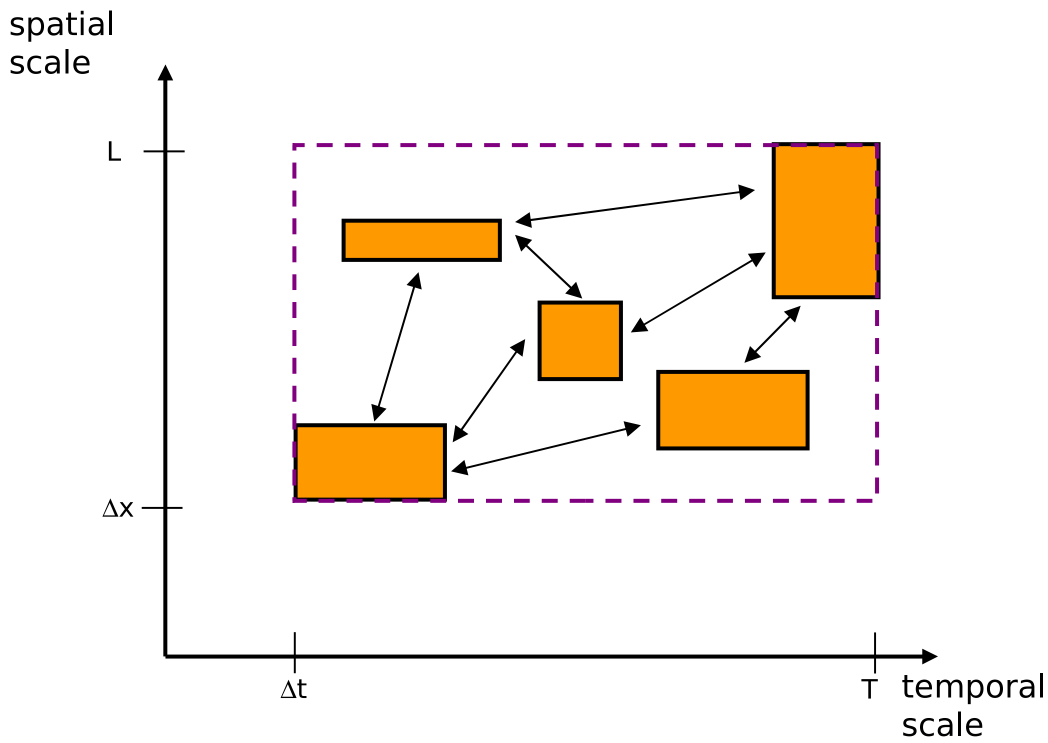
Multi-Scale modeling

- 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



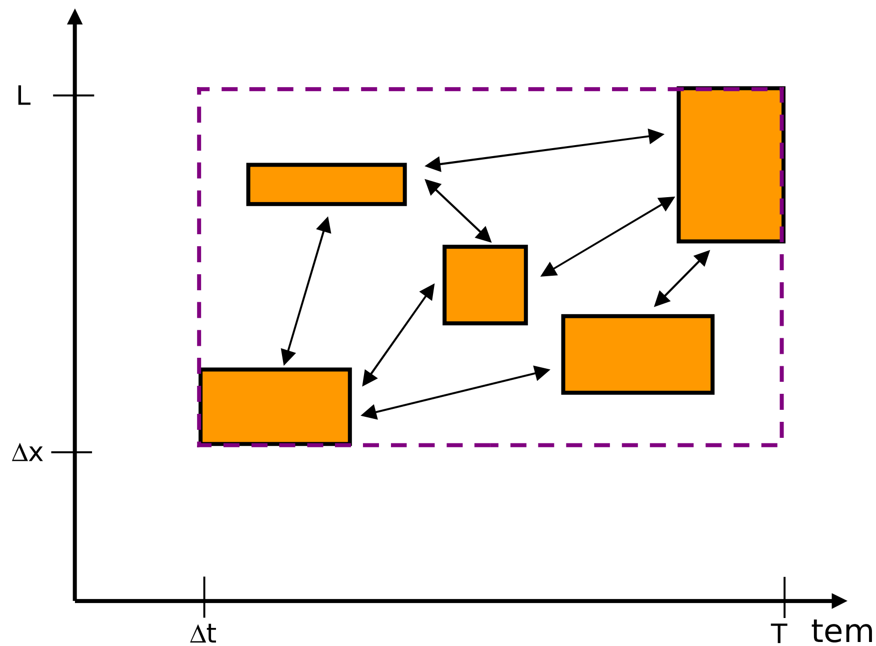
From a Multi-Scale System to many Single-Scale Systems

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



Single Scale Models

- Any model.
- Special case, Cellular Automata, leading to the paradigm of Complex Automata.



Hoekstra, A., A. Caiazzo, E. Lorenz, J.-L. Falcone, and B. Chopard, *Complex Automata: Multi-scale Modeling with Coupled Cellular Automata, in Simulating Complex Systems by Cellular Automata, A.G. Hoekstra, J. Kroc, and P.M.A. Sloot, Editors. 2010, Springer Berlin / Heidelberg. p. 29-57.*

Hoekstra, A.G., E. Lorenz, J.-L. Falcone, and B. Chopard, *Towards a Complex Automata Framework for Multi-scale Modeling. International Journal for Multiscale Computational Engineering, 2007.* ***5(6): p. 491-502.***

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.

- Demand:

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

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

Multiscale Speedup

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

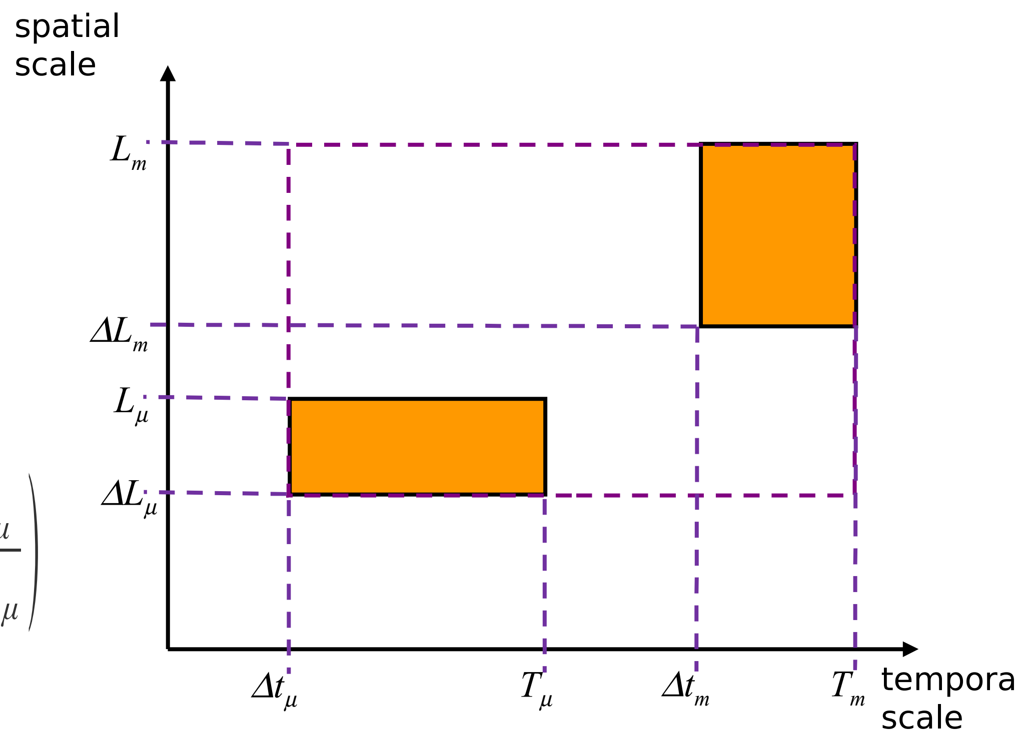
$$T_{ex}^{full} = \left(\frac{L_M}{\Delta x_\mu}\right)^D \left(\frac{T_M}{\Delta t_\mu}\right)$$

- Execution time for multiscale solver

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

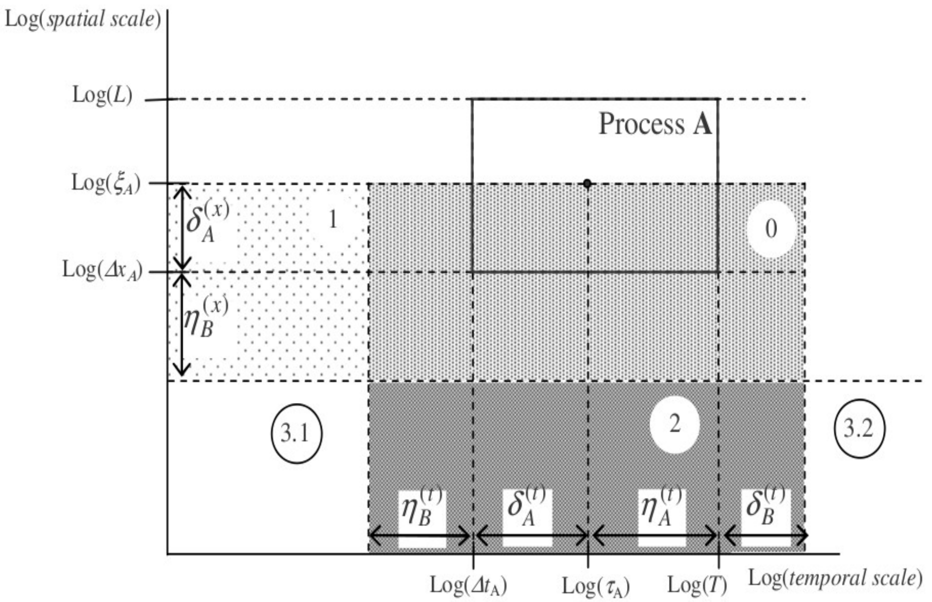
- Multiscale speedup

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



Scale Separation Map

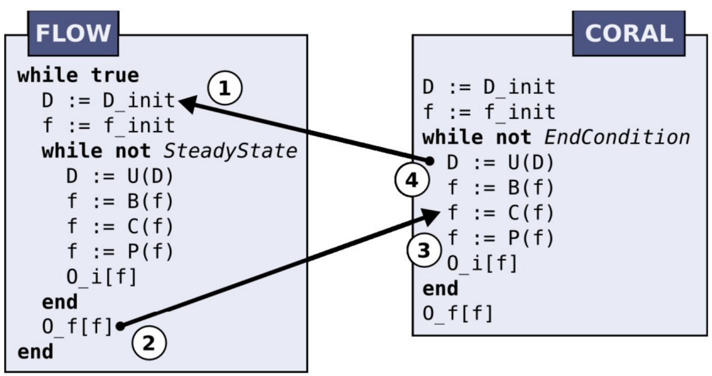
Interaction Regions



Classification

	Time Overlap		Time Separation	
Space Overlap	**Single Domain** Coupling through collision operator. *Snow transport, diffusion/ advection, ...*	**Multi Domain** Coupling through boundary condition. *Fluid structure, grid refinement, ...*	**Single Domain** Coupling through collision operator. *Forest-Savannah-Fire interactions*	**Multi Domain** Coupling through boundary, initial conditions. *Coral Growth, ...*
Space Separation	**Single Domain** Coupling through collision operator. *Algae-Water ecological model, ...*	**Multi Domain** Coupling through boundary condition. *Wave propagation in two media, ...*	**Hierarchical Coupling** Coupling through collision operator and initialization. *Suspension Fluid, ...* **"Physics-Biology Coupling"** Coupling through boundary conditions and initialization. *Oscillating blood flow and endothelial cells, ..*	

=> Coupling Templates



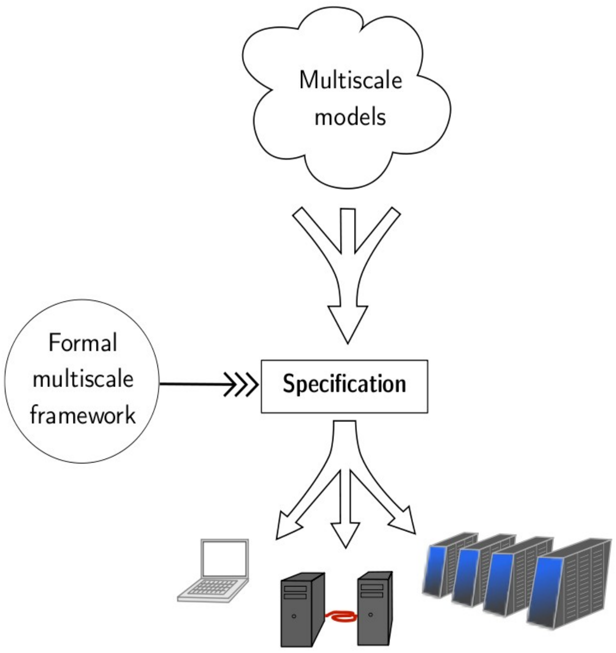
Hoekstra, A., A. Caiazzo, E. Lorenz, J.-L. Falcone, and B. Chopard, *Complex Automata: Multi-scale Modeling with Coupled Cellular Automata, in Simulating Complex Systems by Cellular Automata, A.G. Hoekstra, J. Kroc, and P.M.A. Sloot, Editors. 2010, Springer Berlin / Heidelberg. p. 29-57.*

But what about multiscale computing?

- Inherently hybrid models are best serviced by different types of computing environments
  - capacity <> capability, fast CPU <> GPU, memory <> speed <> network
  - Coupling of existing codes optimized for particular hardware
- 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

MML
Multiscale Modeling Language

- a UML for multiscale modeling
- map an SSM to a MML markup language, and next use that as input to Multiscale computing environments.
- recent multiscale applications require more and more often the coupling of many sub-models, usually originating form different fields of science.
- increasingly important to propose an effective description language
- can help scientists with different background to co-develop a multiscale application.
- MML - a description language aiming at specifying the topology of a multiscale model incl the technical requirements to run each of the submodels



Falcone, J.-L., B. Chopard, and A. Hoekstra, *MML: towards a Multiscale Modeling Language. Procedia Computer Science, 2010.* ***1(1): p. 819-826.***
J. Borgdorff, J.-L. Falcone, E. Lorenz, B. Chopard, A.G.Hoekstra, *in preparation*

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```xml
<?xml version="1.0" standalone="no"?>
<!DOCTYPE model SYSTEM "xmml.dtd">
<model id="Canals" name="Canal system" xmml_version="0.1"
      xmlns:xi="http://www.w3.org/2001/XInclude">
  <description>
    A canal system in France, with possible floods or sedimentation.
  </description>

  <definitions>
    <xi:include href="canal_meta.xml#xpointer(/metadata/*)"/>

    <submodel id="C1D" name="Canal1D" init="yes">
      <timescale delta="10 min" max="1 yr"/>
      <spacescale id="x" delta="1 m" max="3 km"/>

      <ports>
        <in id="flow_left_in" operator="S" datatype="double"/>
        <in id="flow_right_in" operator="S" datatype="double"/>
        <out id="flow_left_out" operator="Oi" datatype="double"/>
        <out id="flow_right_out" operator="Oi" datatype="double"/>
      </ports>
    </submodel>

    <submodel id="J" name="Junction">
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      <spacescale delta="1 dm" max="3 m"/>

      <ports>
        <in id="flow_left_in" operator="S" datatype="double"/>
        <in id="flow_right_in" operator="S" datatype="double"/>
        <in id="flow_top_in" operator="S" datatype="double"/>
        <out id="flow_left_out" operator="Oi" datatype="double"/>
        <out id="flow_right_out" operator="Oi" datatype="double"/>
        <out id="flow_top_out" operator="Oi" datatype="double"/>
      </ports>
    </submodel>

    <submodel id="END" name="End point">
      <timescale delta="10 min" max="1 yr"/>
      <spacescale delta="1 dm" max="3 m"/>
```


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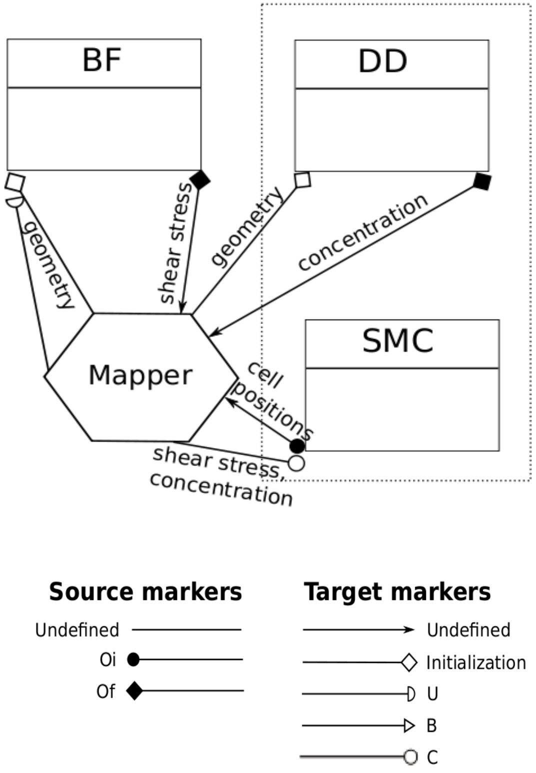

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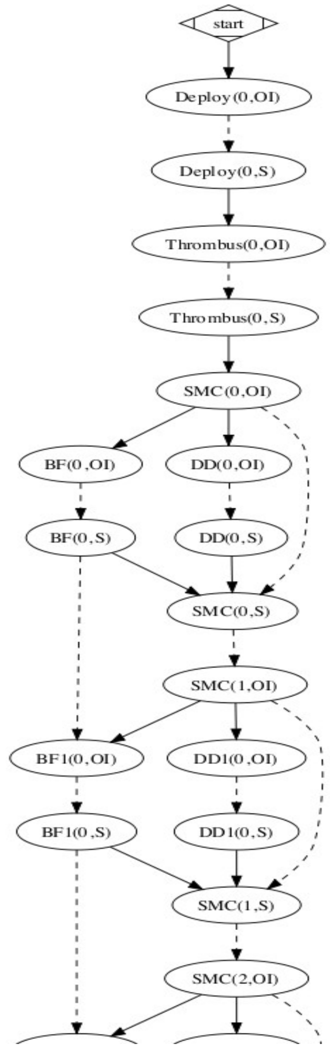

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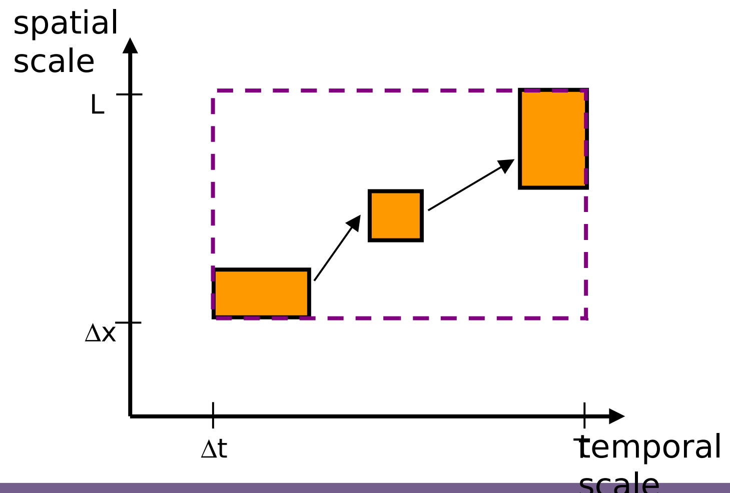
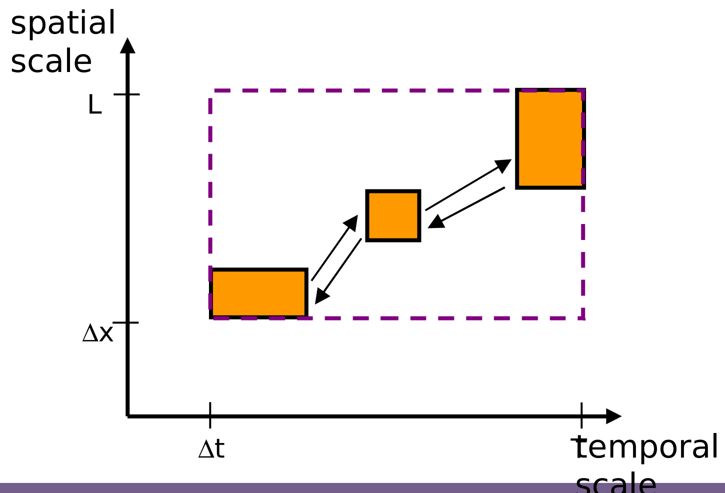
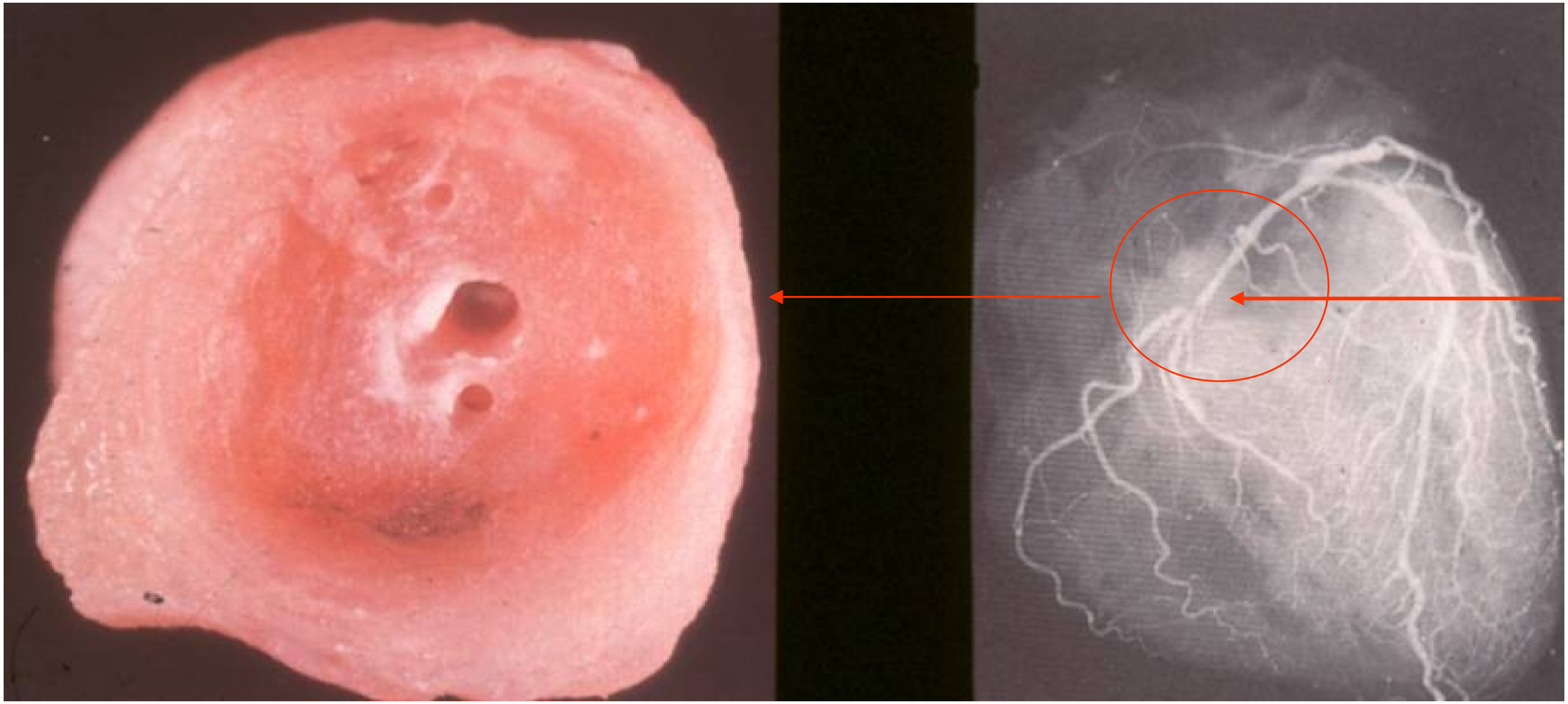
Two Multiscale Computing paradigms

- 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



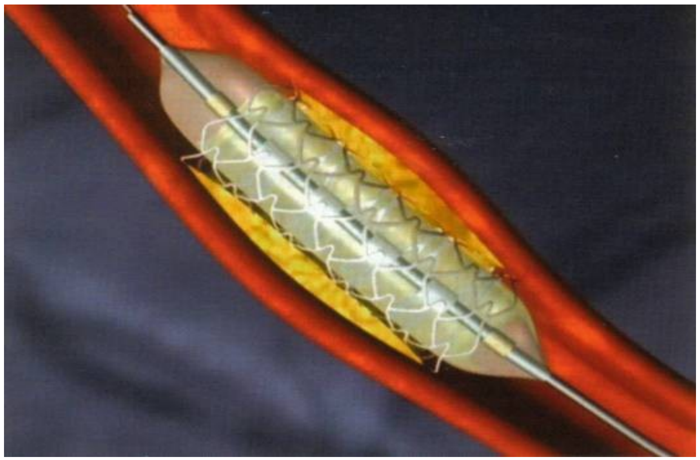


Example for Tight Coupling: Coronary Artery Disease Modeling



Gross appearance Angiogram

Balloon Angioplasty and Stent Implantation



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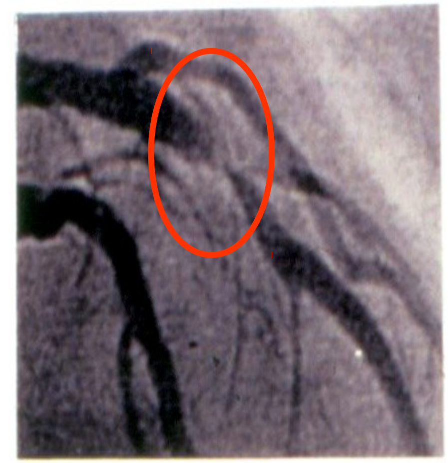
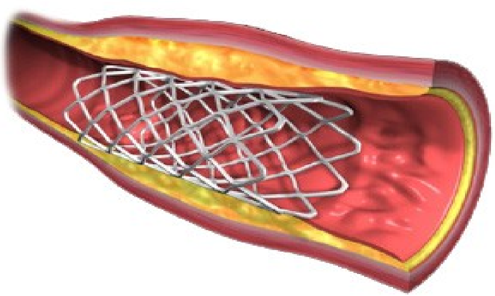
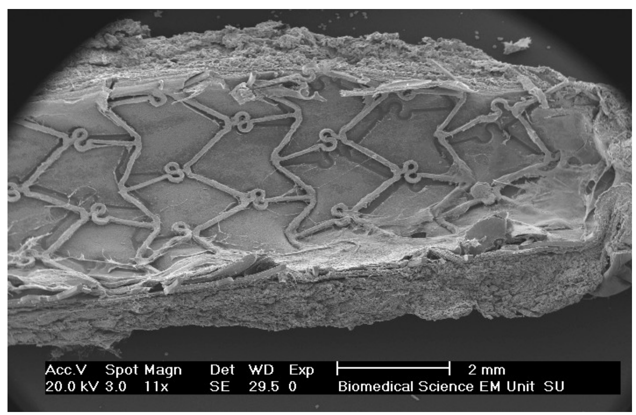
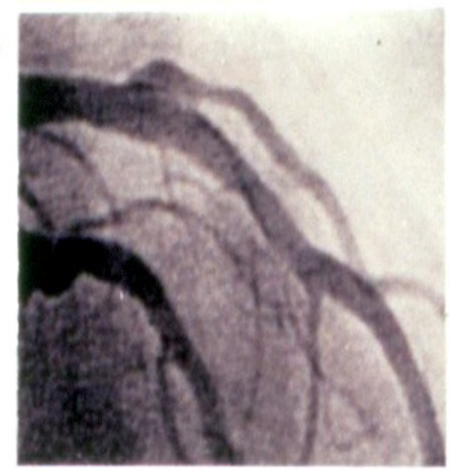




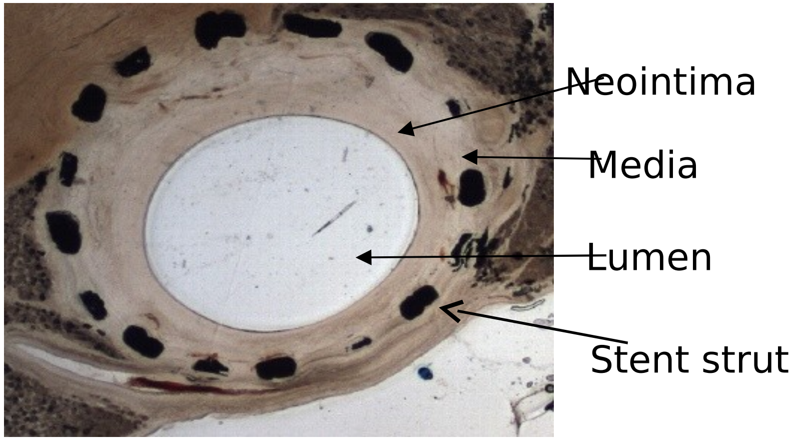


post

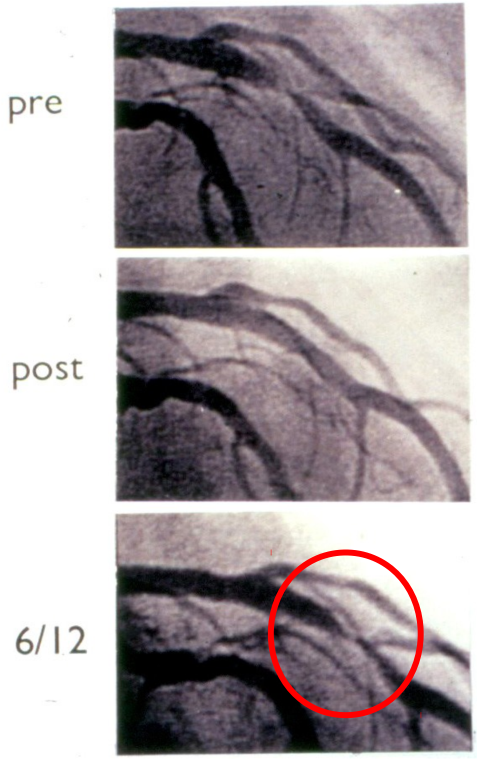


In-stent Restenosis

- Maladaptive response after balloon angioplasty and stenting

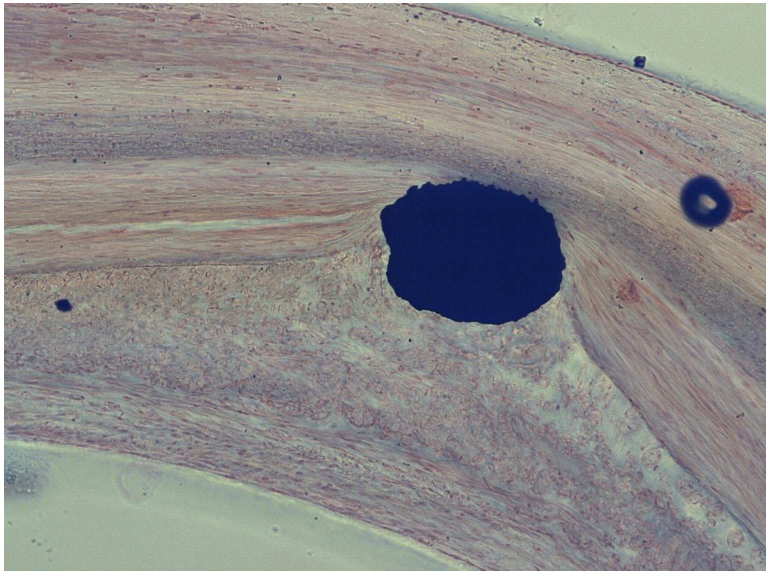


Porcine coronary artery section 28 days post stenting displaying substantial neointima.

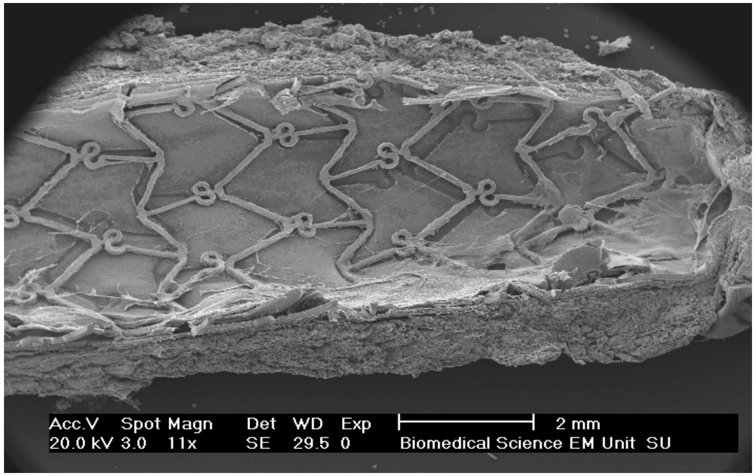


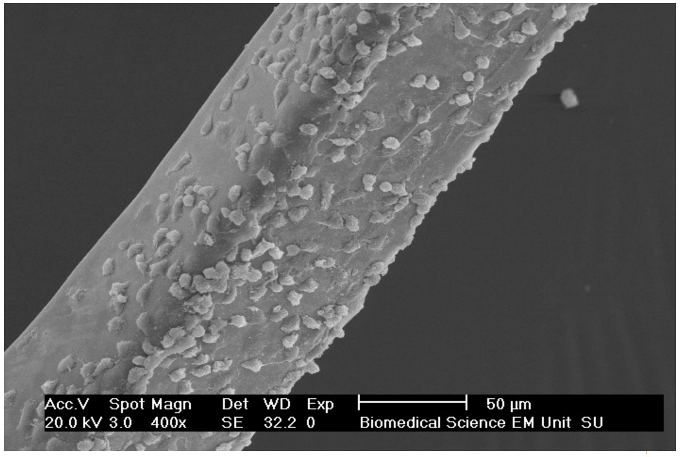
Human angiogram depicting restenosis six months post-PCI.

Detailed information available



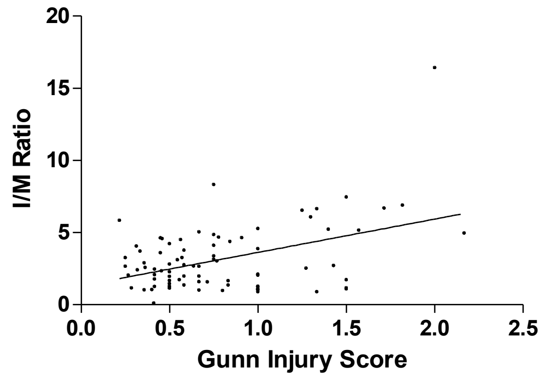
Detail of single stent post showing vessel wall deformation, smooth muscle cell organisation in the neointima and re-endothelialisation



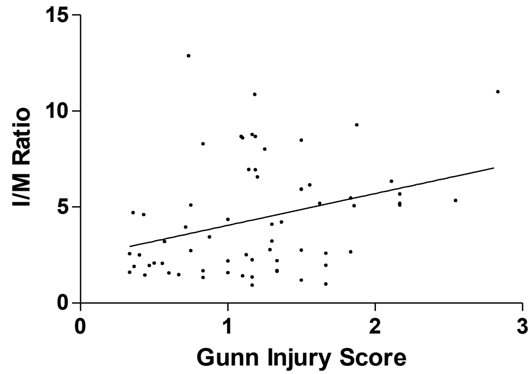


Injury vs. Neointima Area

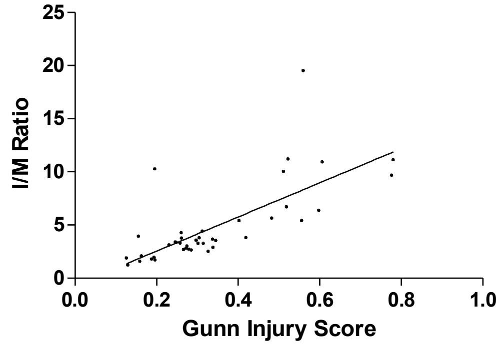
a) 14 Days; N=82, r^2=0.1862



b) 28 Days; N=65, r^2=0.1063

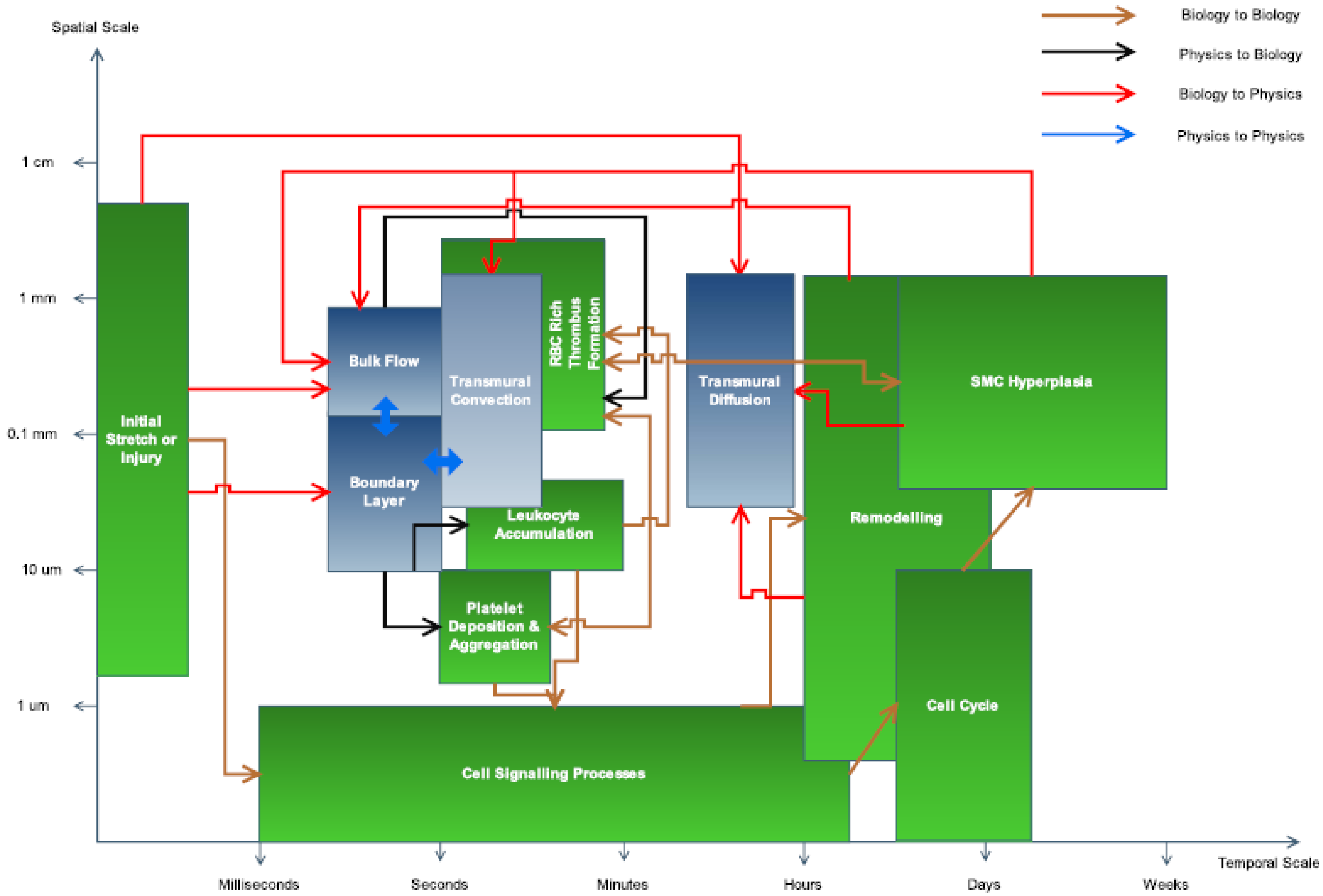


c) 90 Days; N=42, r^2=0.5193

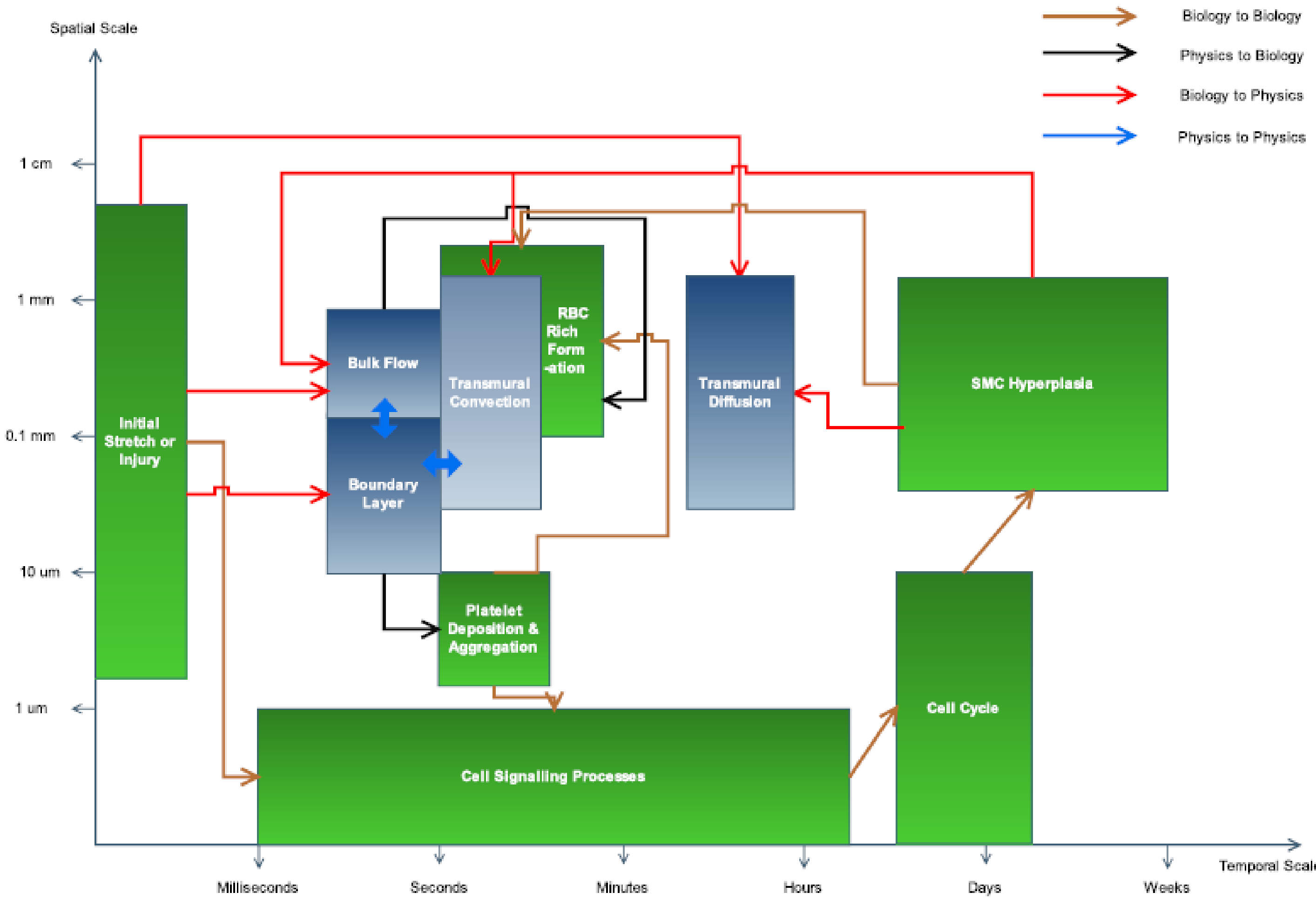


A positive correlation between injury score and intima/media ratio per section is observed at a) 14 days b) 28 days and c) 90 days post-stenting.

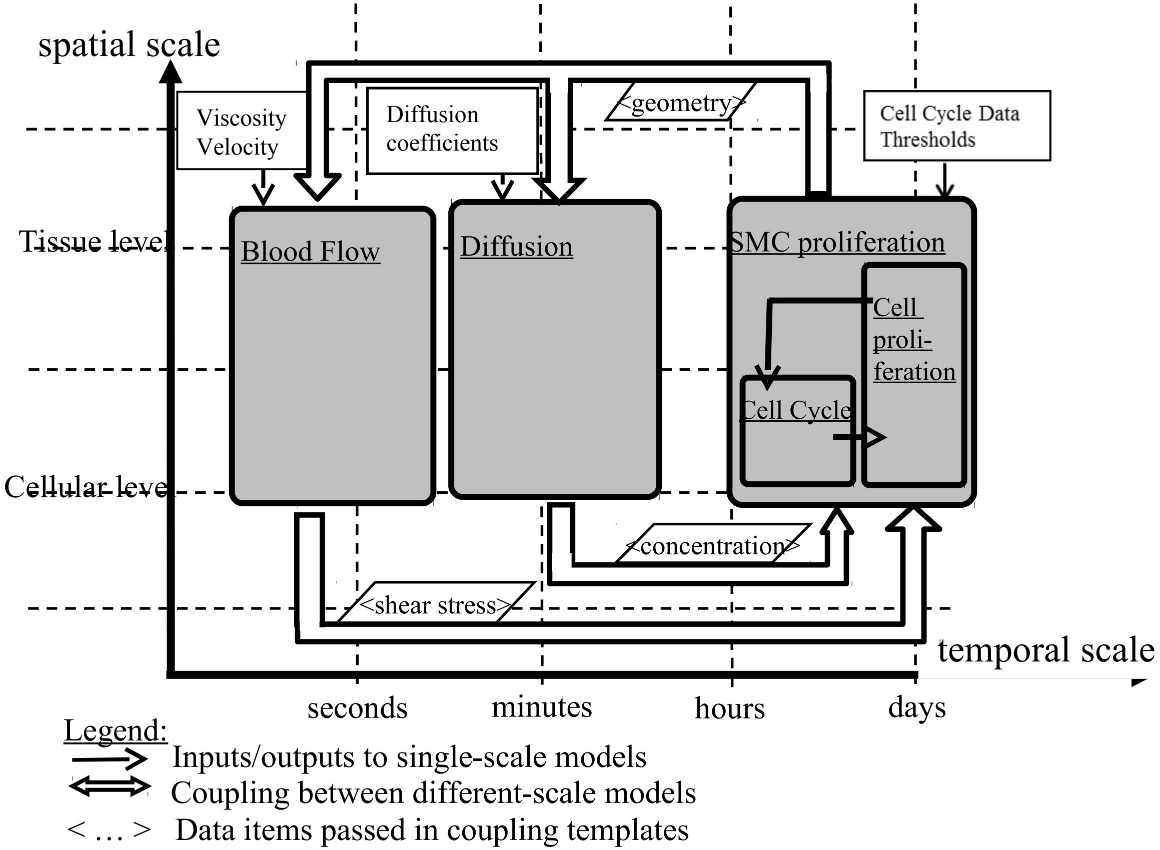
Comprehensive Scale Separation Map

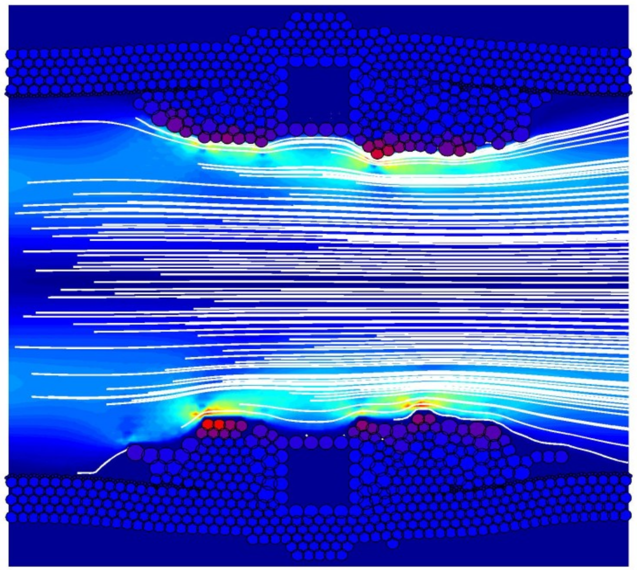


Simplified Scale Separation Map



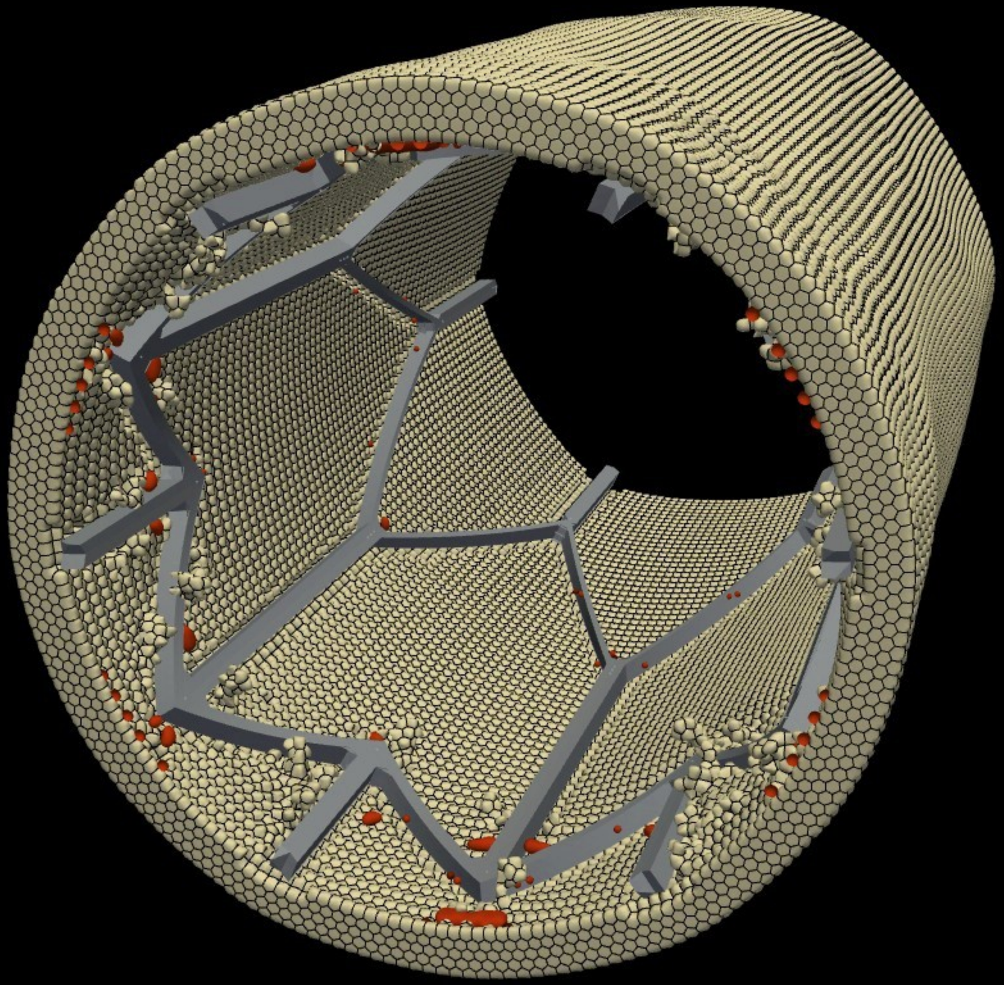
Simplified Scale Separation Map for ISR, and 2D Results





Some 3D results

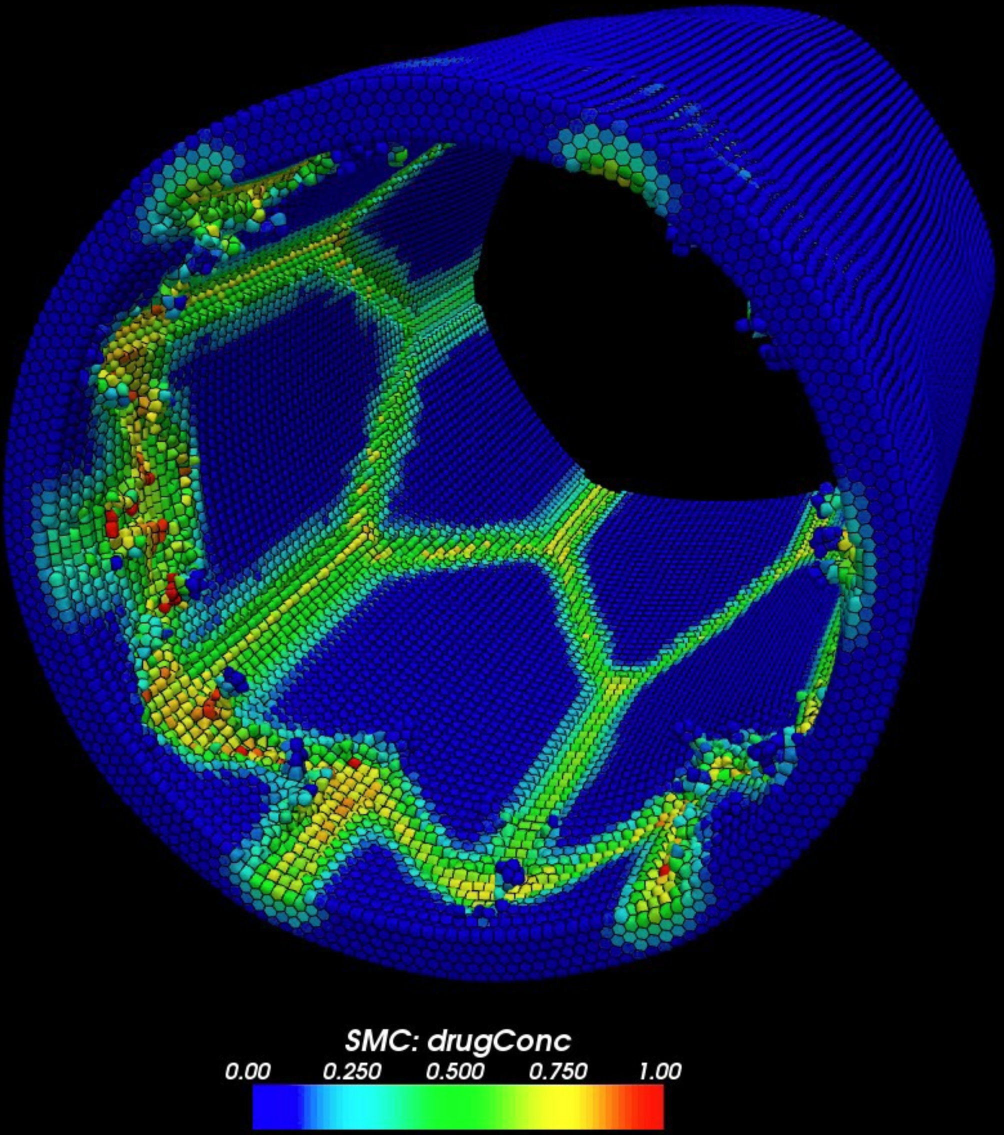
SMCs
Stent
Thrombus



Visualisations:
-- SMC Voronoi tesselation
- fill space with virtual cells
- selective edge smoothing
– Stent: hull triangulation
– Thrombus: isosurfaces

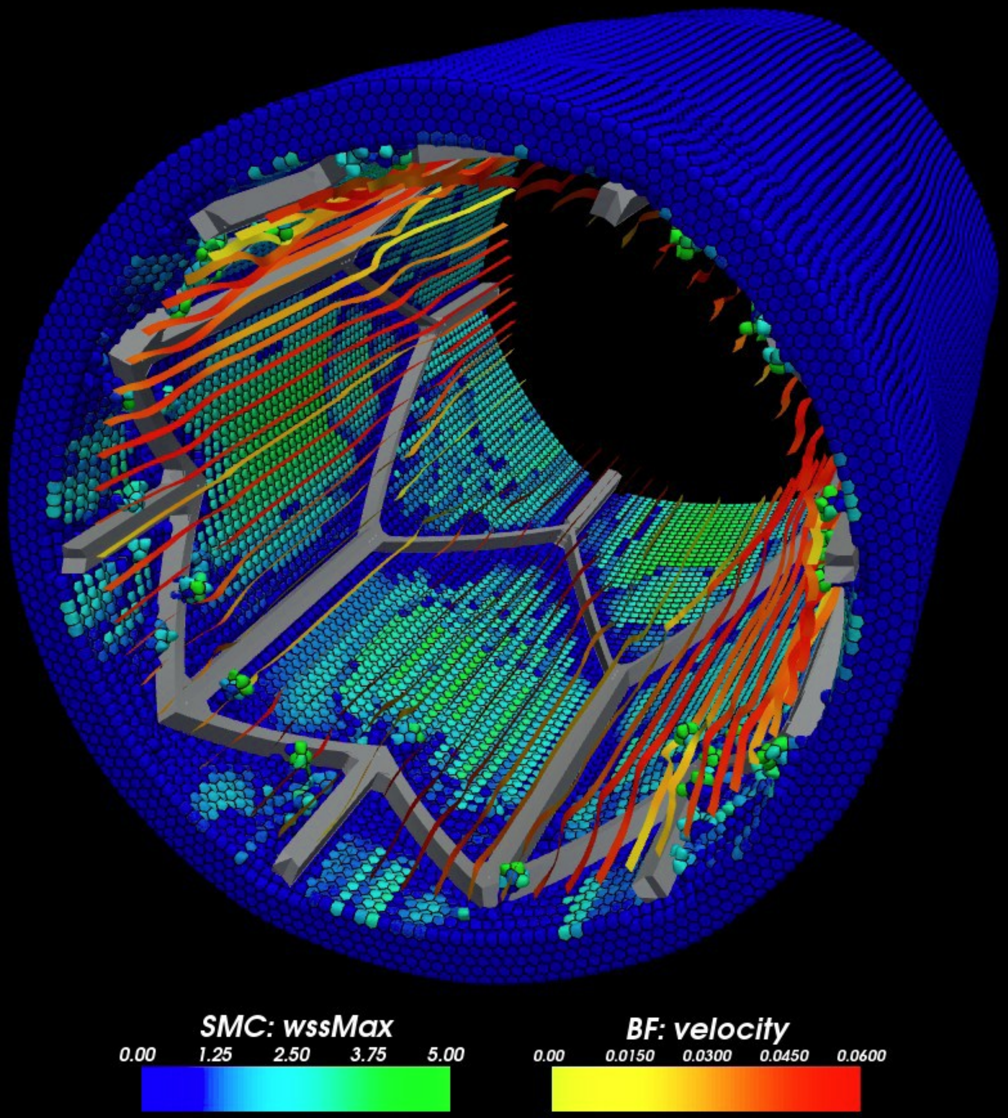
Some 3D results

Drug concentration coloring



Some 3D results

SMCs (WSS color scale
Stent
Flow (Ribbons, color scale)

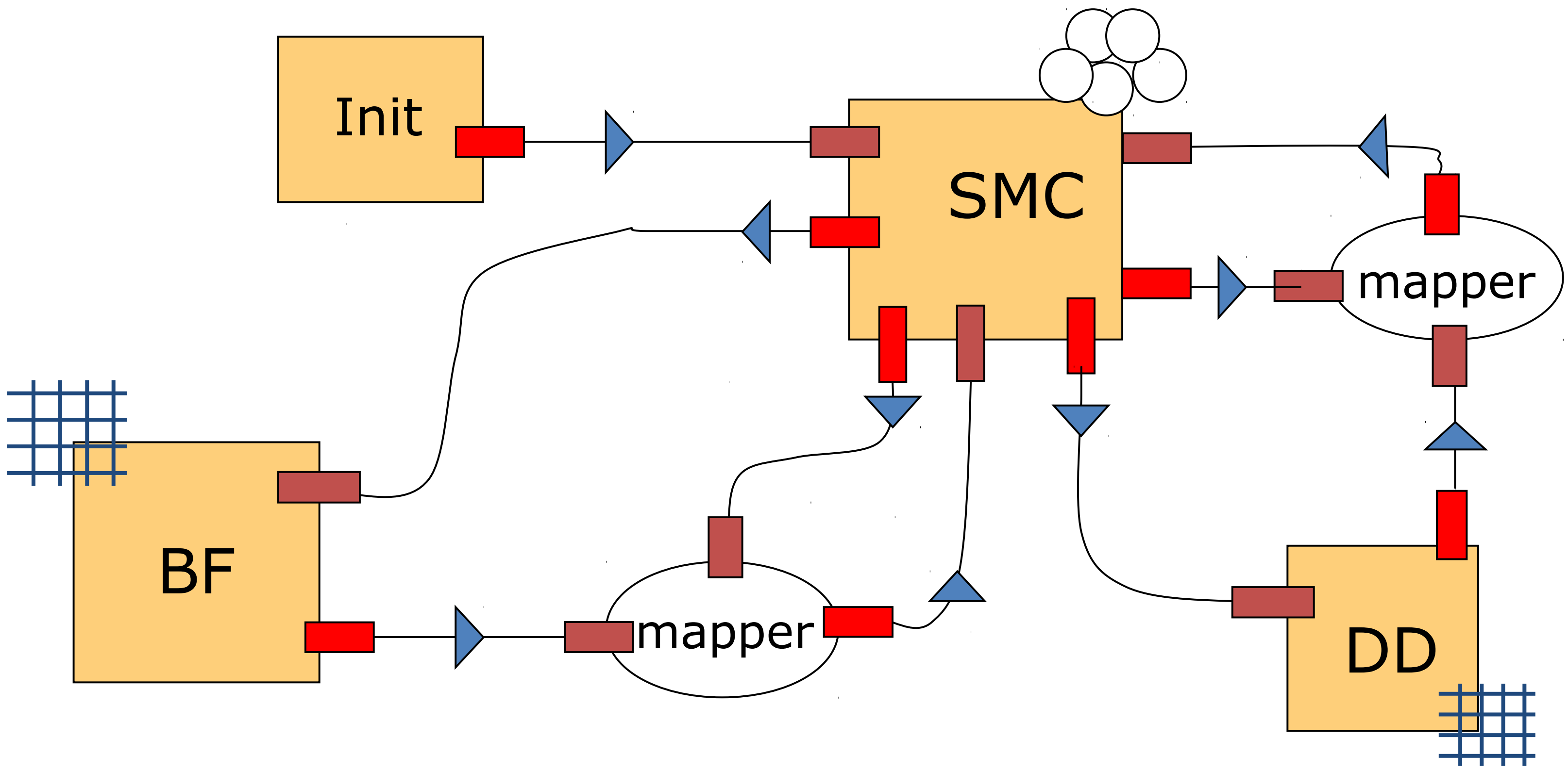


MUSCLE, a Complex Automata Framework

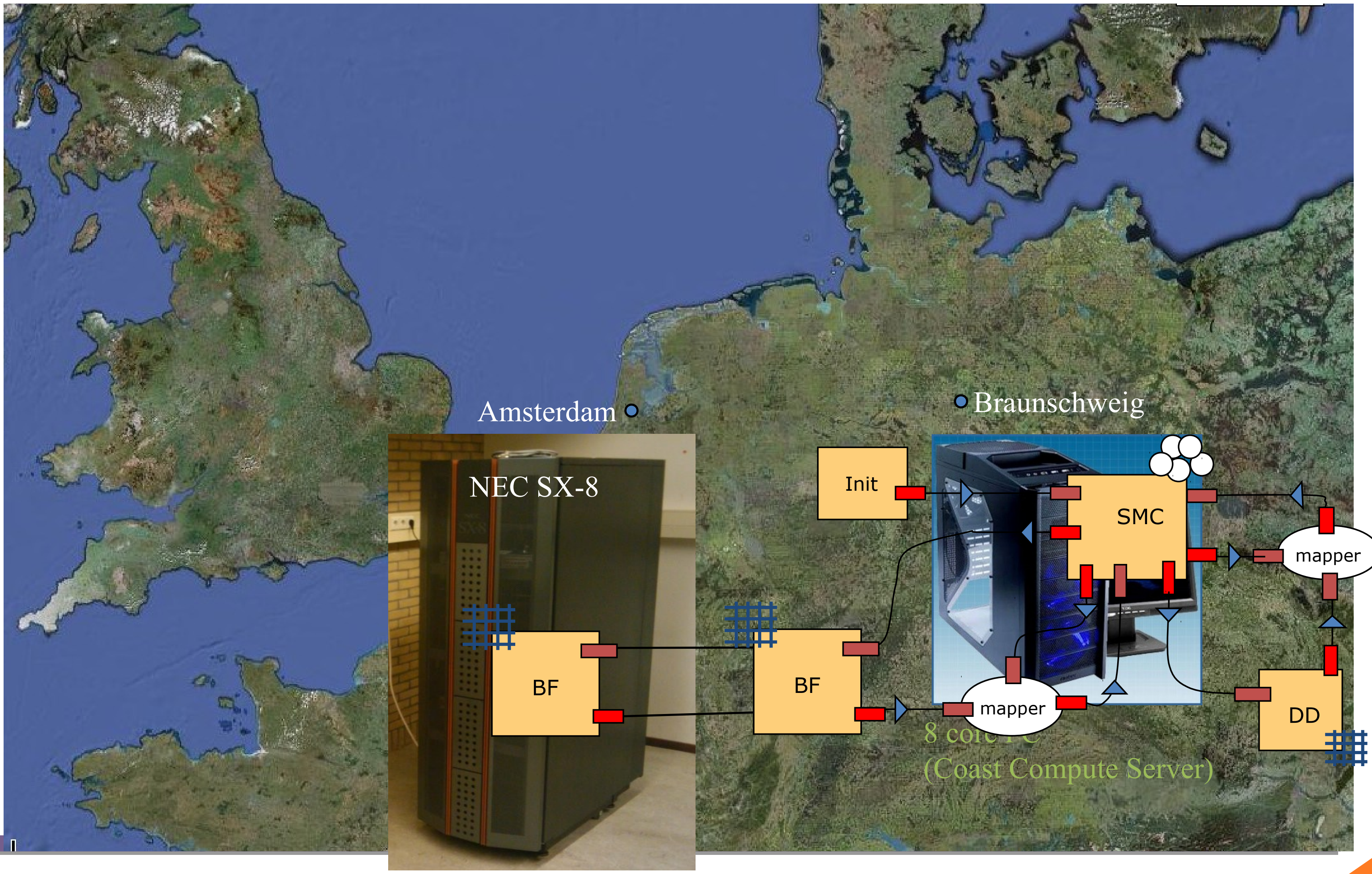
- A software environment for CxA simulations.
- The **MU**lti**S**cale **C**oupling **L**ibrary and **E**nvironment (MUSCLE)
  - Based on JADE: Java platform for multi agent based simulation
  - Single scale models are wrapped into agents
  - Agents communicate via smart conduits
  - Conduits model the multiscale couplings
    - Simple interpolation, or full blown models by themselves.
  - Compatible with different software, programming languages and hardware
  - Distributed communication
  - Open source (http://muscle.berlios.de/)

J. Hegewald; M. Krafczyk; J. Tölke; A.G. Hoekstra and B. Chopard: *An Agent-Based Coupling Platform for Complex Automata*, in M.T. Bubak; G.D. van Albada; J.J. Dongarra and P.M.A. Sloot, editors, *Computational Science - ICCS 2008: 8th International Conference, Krakow, Poland, Proceedings, Part II*, in series *Lecture Notes in Computer Science*, vol. 5102, pp. 227-233. Springer, Berlin, Heidelberg, June 2008. 978-3-540-69386-4.

CxA for ISR: Connection Scheme



Distributed MultiScale Computing



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;

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

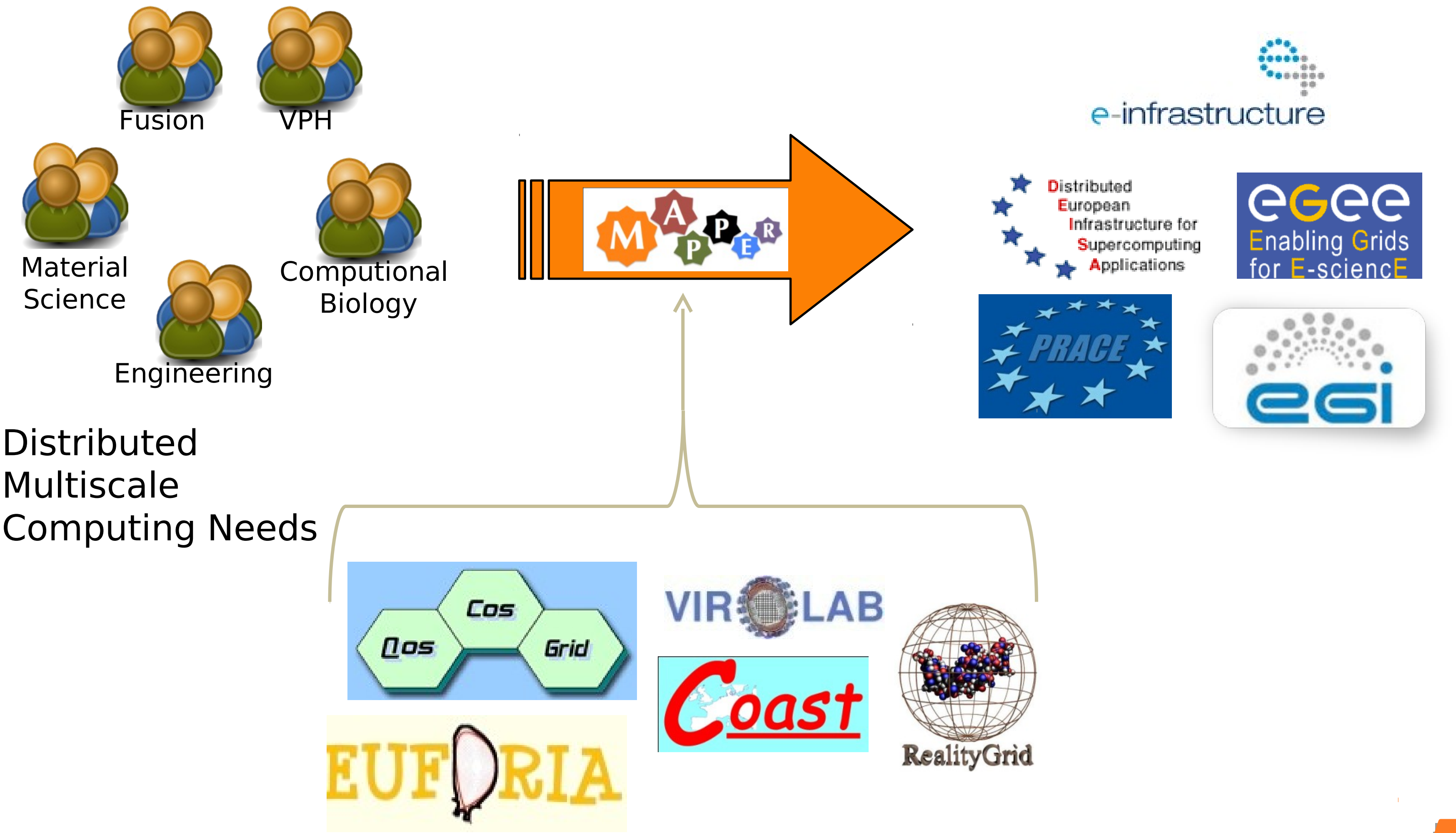
Ludwig-Maximilians-Universität München

University of Geneva

Chalmers Tekniska Högskola

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

Motivation: user needs



Overview

MAPPER Applications

- Fusion, Physiology, Systems Biology
- Nano Material Science, Engineering

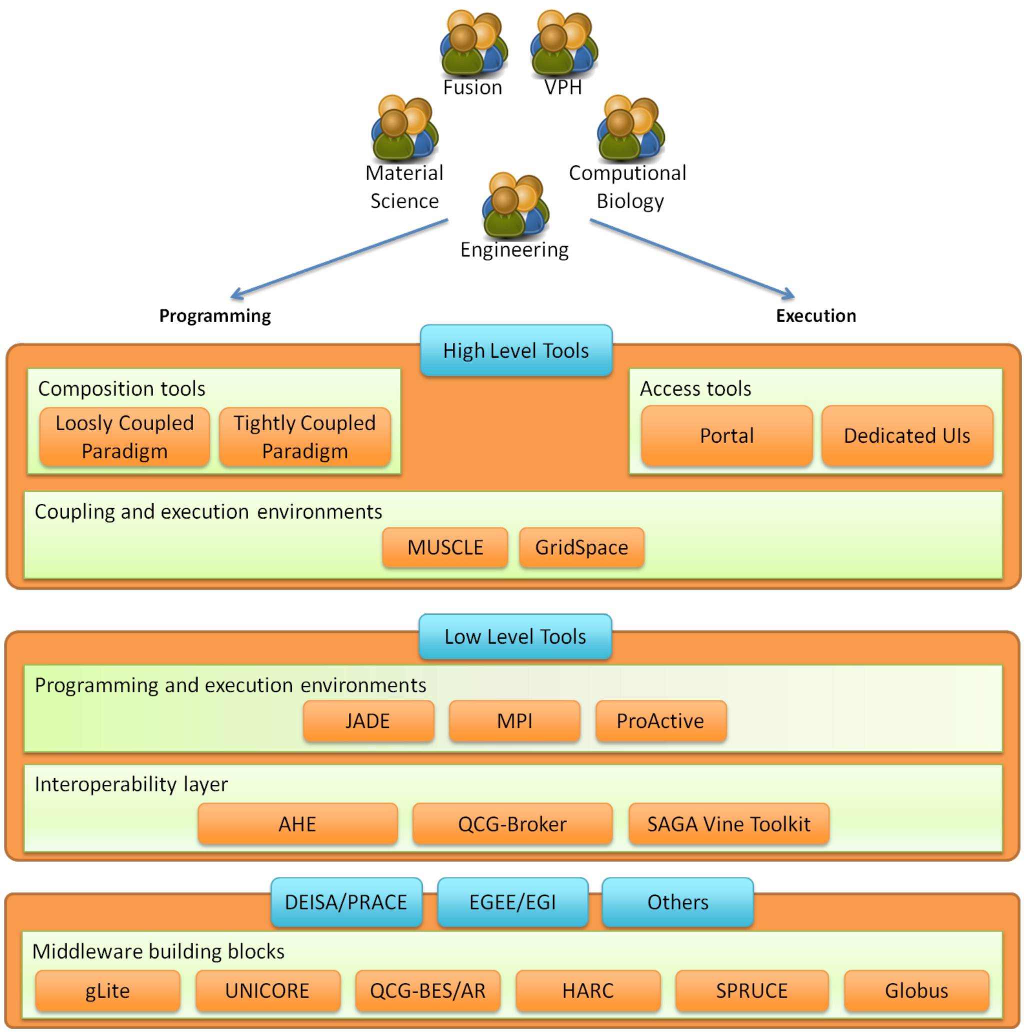
MAPPER environment

- 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

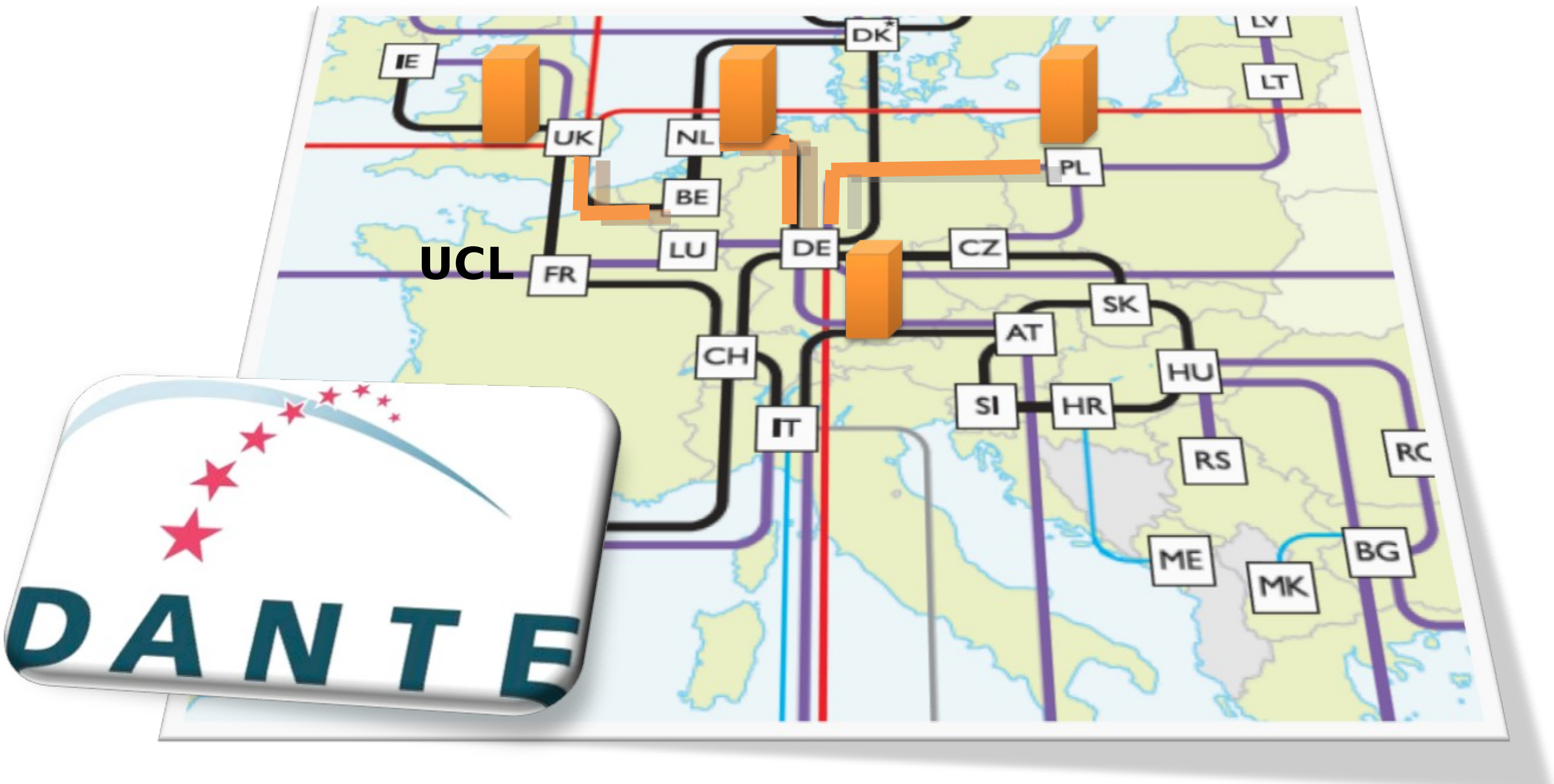
  exploiting existing and evolving European e-infrastructure
- Deploy a computational science infrastructure
- Deliver high quality components

  aiming at large-scale, heterogeneous, high performance multi-disciplinary multiscale computing.
- Advance state-of-the-art in high performance computing on e-infrastructures

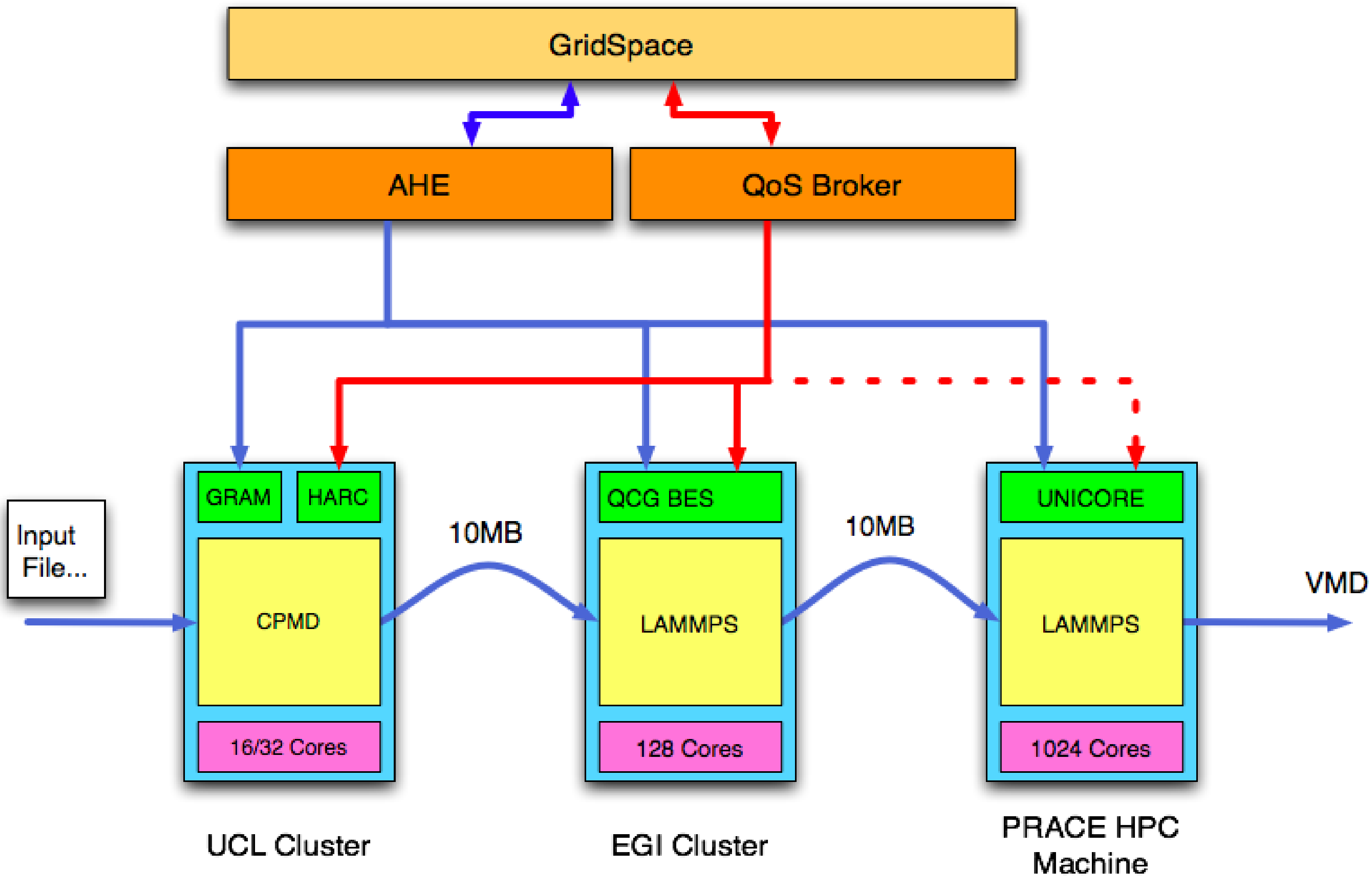
  enable distributed execution of multiscale models across e-Infrastructures,

Computing e-Infrastructure

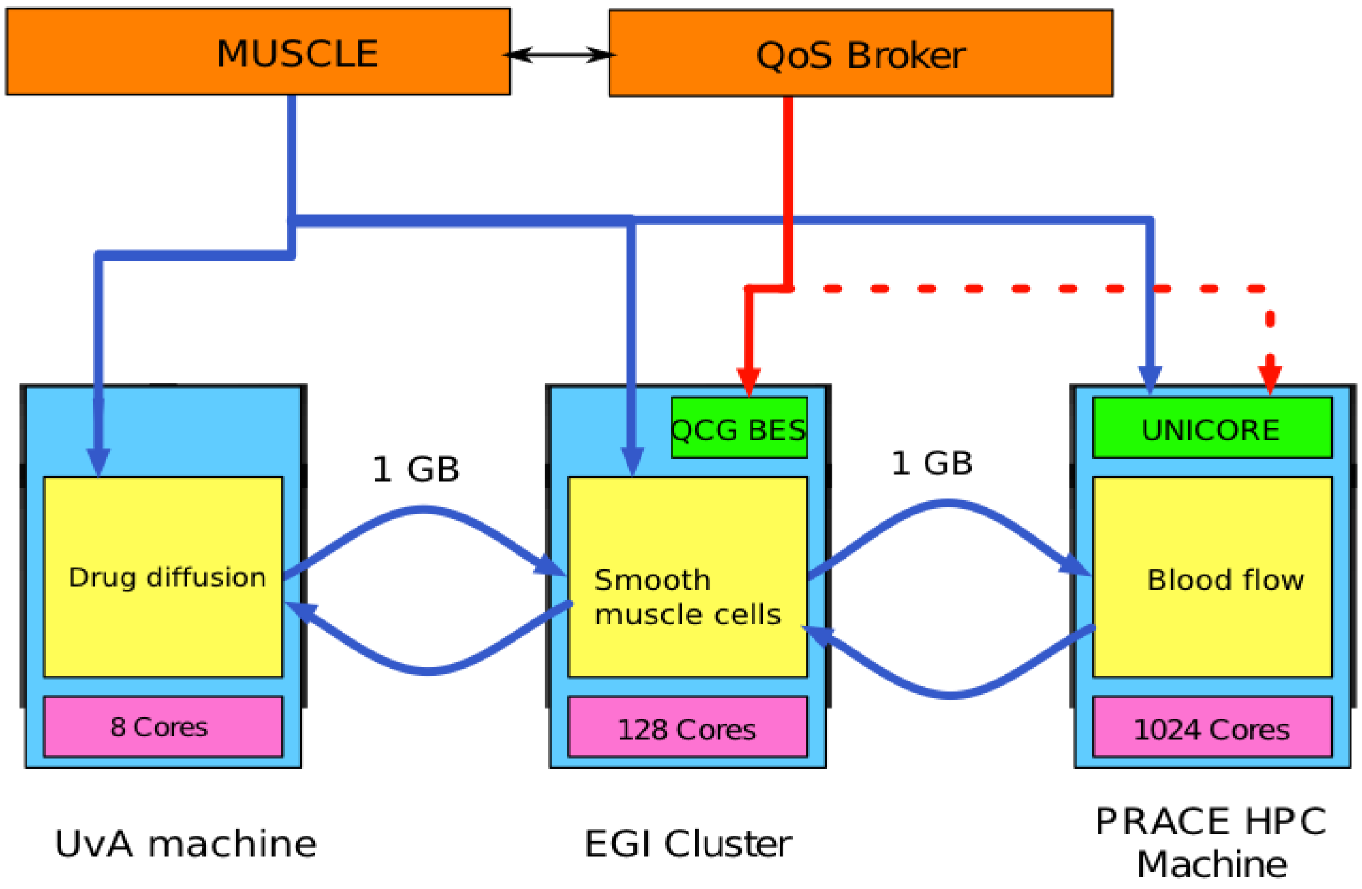
Networking e-Infrastructure



Use case – loosely coupled



Use case – tightly coupled



Conclusion

- Distributed Multiscale Computing
  - A relevant and important paradigm with a potential huge impact on scientific communities
- MAPPER will facilitate DMC
  - Obstacles: Policies
    - Obtaining access to resources
    - Support for advanced reservation and co-allocation
    - Interoperability
    - Allocation management
- MAPPER will open up to external applications in 2012

DMC workshop CFP

1st Workshop on Distributed Multiscale Computing
in conjunction with the IEEE e-Science conference 2011
December 5, 2011, Stockholm, Sweden

This workshop provides a forum for multiscale modelers, framework developers and experts from the distributed infrastructure communities to identify and discuss challenges in and solutions for modeling multiscale systems, as well as their execution on distributed e-infrastructures. With single scale models being well-tested and mature field in many areas, multiscale modeling is now one of the greatest challenges in science today. **We aim to bring together modelers of multiscale problems, developers of multiscale applications and frameworks, as well as experts from infrastructure (HPC, Grid and Cloud) communities.** The DMC workshop will provide the opportunity to present and discuss the latest advances in distributed multiscale computing and to discuss the establishment of distributed multiscale computing standards based on the concepts and techniques presented in the workshop.

The deadline for submitting your paper to the DMC workshop is **July 18th 2011.**

It is expected that the proceedings of the e-Science 2011 workshops will be published by the IEEE Computer Society Press, USA and will be made available online through the IEEE Digital Library.

http://www.computationalscience.nl/dmc2011

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The DMC Workshop Organizers

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