Multiscale APPlications on European e-infRastructures

www.mapper-project.eu

Motivation

- Scientists are often faced with modelling **multiscale, multi discipline** systems
- Simulating such models in three dimensions requires large scale computing capabilities
- Existing modelling frameworks and middleware for distributed simulations do often not suffice

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

Services

- Interoperability services:
  - can be accessed by users and applications
  - form an abstraction layer to grid resources and middleware
  - are responsible for providing access to resources and for synchronizing and distributing applications.
- For example: multiscale simulations can be controlled by a broker developed in the QosCosGrid project

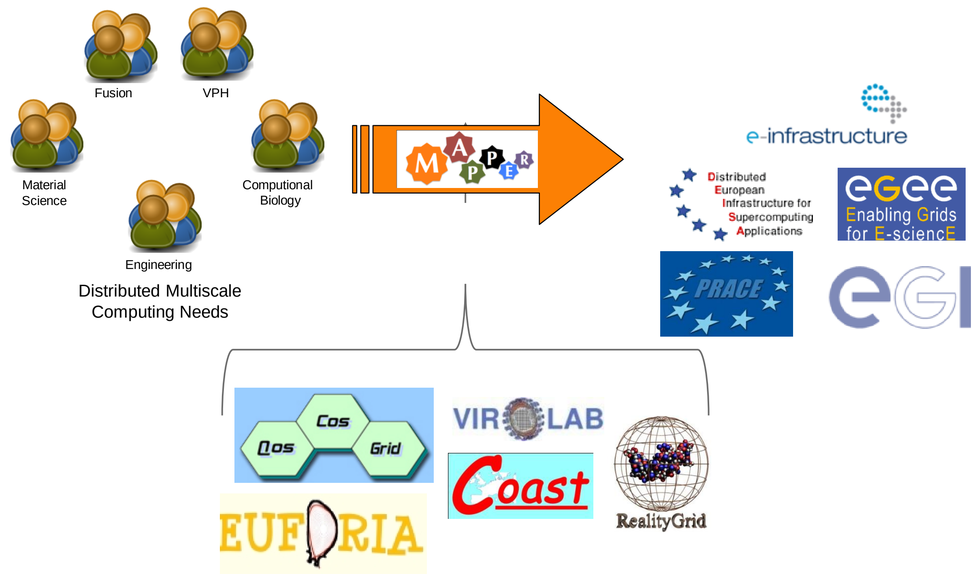


***Figure 1**: A lot of communities have distributed multiscale needs, and there are resources available to do distributed computing. MAPPER wants to make the link by integrating different middleware.*

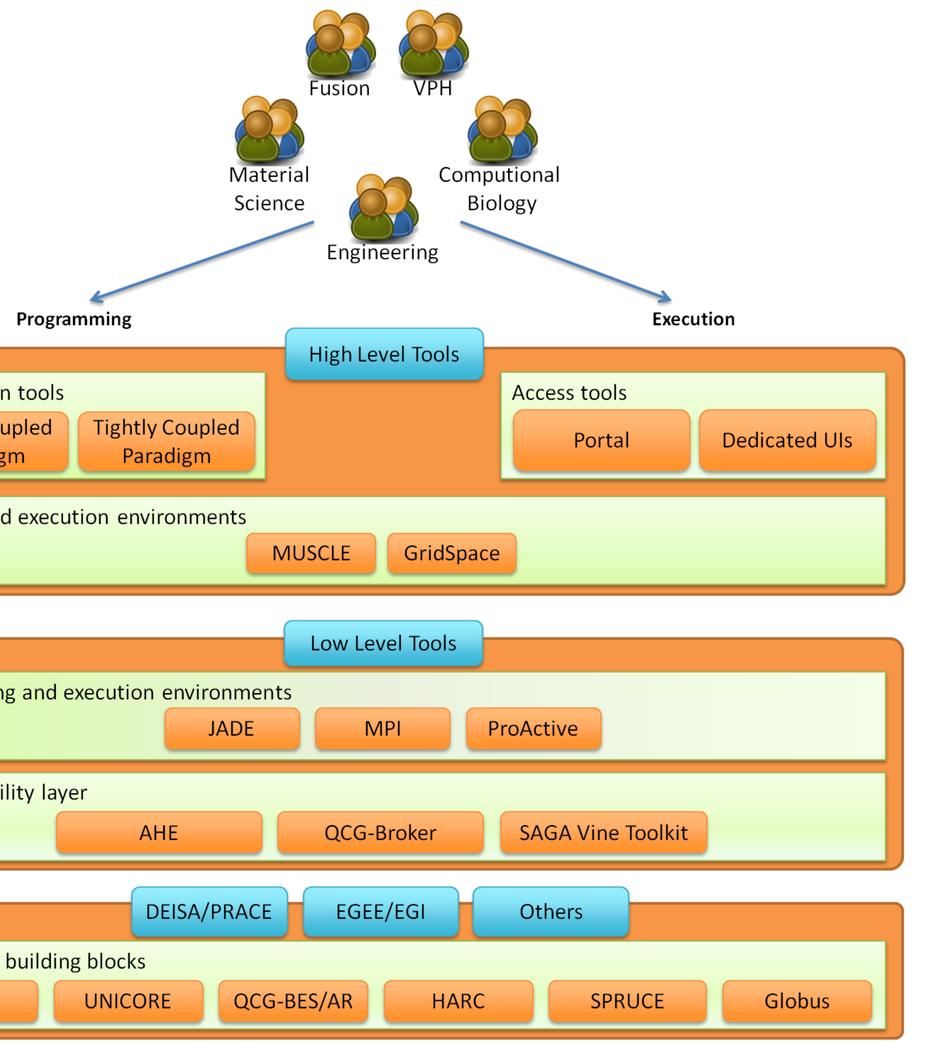


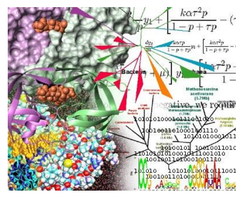
***Figure 2:** Different levels and, within, different implementations of middleware currently available.*

- Many middleware services do not yet interoperate.
- where appropriate, this should change

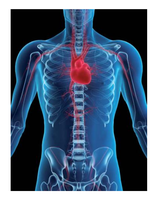
Internationally

- MAPPER partners have significant experience with the **trans-Atlantic grid** and HPC
- Collaborate with the US **TeraGrid** to integrate infrastructures across the globe.

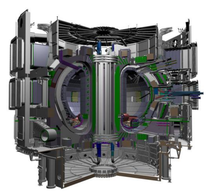
Applications



computational biology



virtual physiological human



fusion

hydrology

nano material science

Networking

- Create and maintain a stable management of the project
- Realize strong internal and external communication
  - Perform targeted **dissemination** actions
- Development of plans for **sustainability** of MAPPER
- Perform foresight study addressing policy makers

Development

In complementing twin tracks:

- Developments in the deep track will feed into the already usable fast track
- the **fast track**
  - will start working on application deployment **as early as possible**
  - manually adapts, integrates and deploys a minimal set of infrastructure components to enable multiscale applications
- the **deep track**
  - will work on higher level services and full integration
  - realises the full and integrated MAPPER infrastructure, enabling the coupling of multiscale components