



Requirements for Multiscale Simulations



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MAPPER project

Mapper Project

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What is MAPPER?



- **M**ultiscale **A**PPlications on **E**uropean e-inf**R**astructures (FP-7 EU Project)
- **G**oal: Deploy a computational science environment for distributed **m**ultiscale computing on and across European e-infrastructures: **E**GI & **P**RACE
- Driven by five big user communities: **V**PH, **c**omputational **b**iology, **f**usion, **h**ydrology, **n**ano-material science
- + external groups: astronomy, metallurgy, etc.

Multiscale applications



- Holistic simulation of multiscale phenomena in a single code is often impossible, thus **coupling** of **many** single scale **modules (applications)** in efficient way is needed
- The elementary codes may have different **heterogeneous resource requirements**
- Usually at least one module **requires** specific HPC resources, libraries, etc.
- In case of **tightly-coupled multiscale** applications a **resource co-allocation** is needed

 (QCG middleware – part of **UMD** now, provides Advance Reservation capabilities for MAPPER)

What is the strength of Mapper?



- Gathers many applications/communities from various domains under one umbrella
- Addresses both **loosely** and **tightly coupled multi-scale** approaches
- Provides support for **highly parallel jobs**
- Thanks to **QCG** middleware integrates **heterogeneous production resources/e-infrastructures** (PRACE/EGI/campus resources) in solving large-scale multiscale problems across Europe



MAPPER requirements



- Access to **EGI/PRACE** and **EUDAT, GEANT** resources and services (**QCG-Broker**)
 - Unified (computing and data movement) interfaces
 - Advance Reservation (**QCG-Computing**)
 - Co-allocation of resources (**QCG-Broker**)
- Easy deployment of applications and data sharing – directories for groups of users
- Integrated Authentication/Accounting/Monitoring/User support systems (**QCG-Accounting**)





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