e-infrastructure

CAPACITIES

EGI-EUDAT-PRACE Pilot 4
MAPPER Use Case

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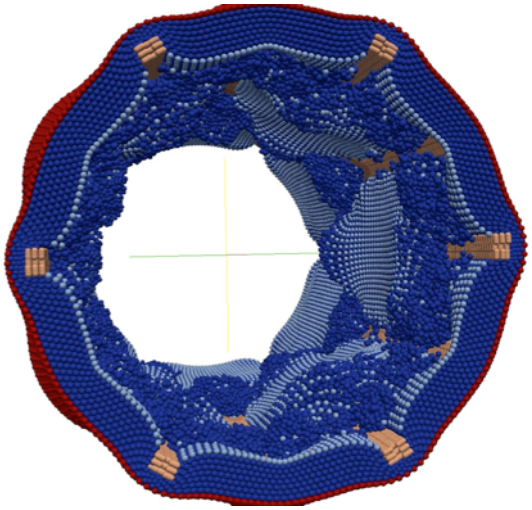
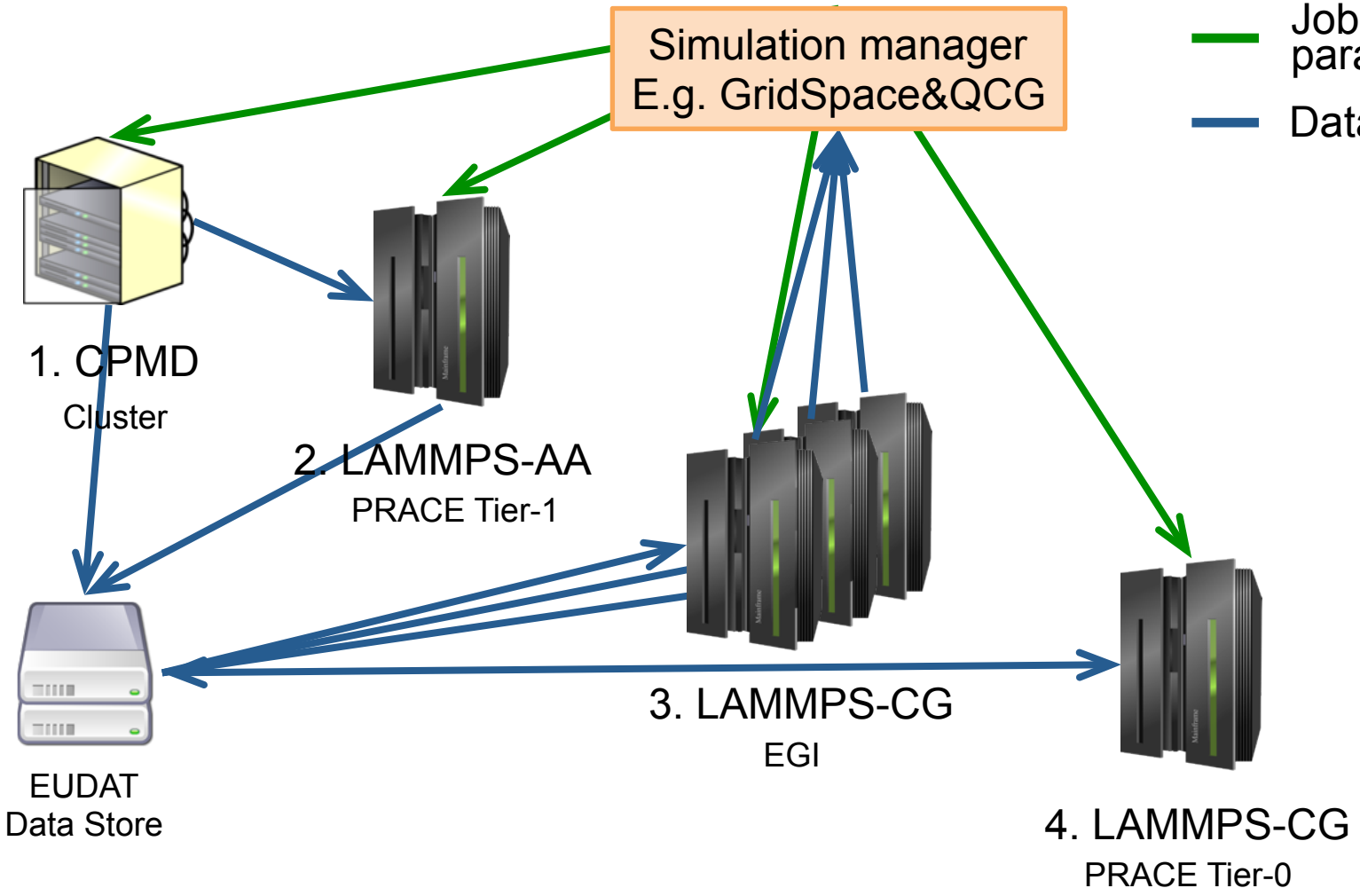
MAPPER & Multiscale Systems



- The world is multiscale
  - Scale of biomedical applications:
    - Temporal scale $O(10^{15})$
    - Spatial scale $O(10^{9})$
- MAPPER objectives:
  - Develop models for multiscale computing
  - Work and develop services supporting novel computational paradigms
  - Enable multiscale computing on European e-Infrastructures

Nanomaterials use case



Use case description

1. CPMD - quantum mechanical simulation for calculating potentials for clay and polymer molecules
2. LAMMPS-AA - atomistic MD simulation to determine accurate microscopic system properties
3. LAMMPS-CG - iterative coarse-grained simulations intend to find the right potential for the coarse-grained system
4. LAMMPS-CG - large-scale coarse-grained simulation to model the final system and obtain important macroscopic properties

Use case requirements

- List of services I can access and use
  - Services that are available and functional
  - Services that will not be down for a maintenance before the end of my simulation
- Properties of compute and storage services
  - Quota, capacity, performance
- Network performance between sites/ resources providing the above services

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