The Application Hosting Environment

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AHE Motivation

- Problems for individual users installing/compiling/optimizing application
- Complexities of using computational infrastructures
  - Job workflows, from staging data to launching jobs
- Security can be complicated
  - Applying for certificates
  - Generating MyProxy
- A solution is needed to simplify usage for scientific end users → allow clinical scientists to run simulations at the click of a button.

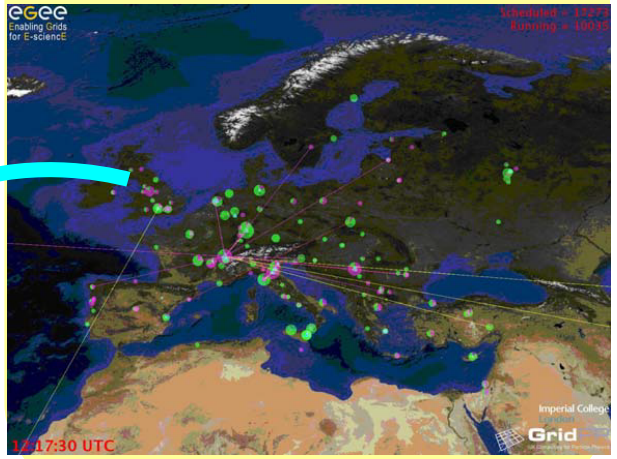
- **Application Hosting Environment**
  - Simplifying Access to the Grid
  - Community Model.
- **Simplifies security**
  - End-User avoids grid security and MyProxy configuration and generation.
- **Simplifies application setup**
  - End-User does not have to compile, optimise, install and configure applications.
- **Simplifies basic workflow**
  - AHE stages the data, runs and polls the job and fetches the results automatically
- **Simplifies compute access through RESTful web-services**
  - Provides a RESTful interface
  - Clients and services access infrastructure and apps with ‘Software as a Service’

AHE – Bridging the Gap

UCL

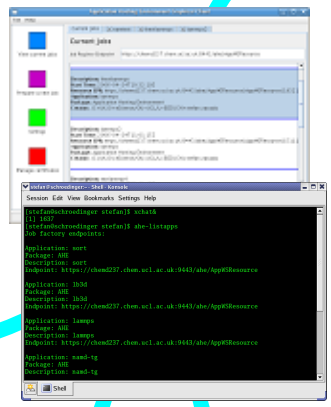
Local resources

EGI/PL-Grid



QCG Computing

GridSAM

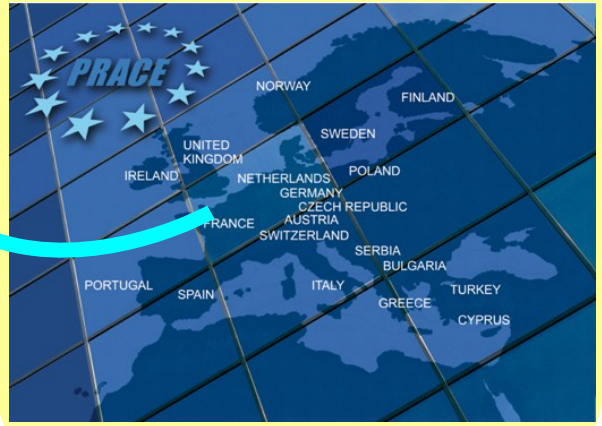


XSEDE

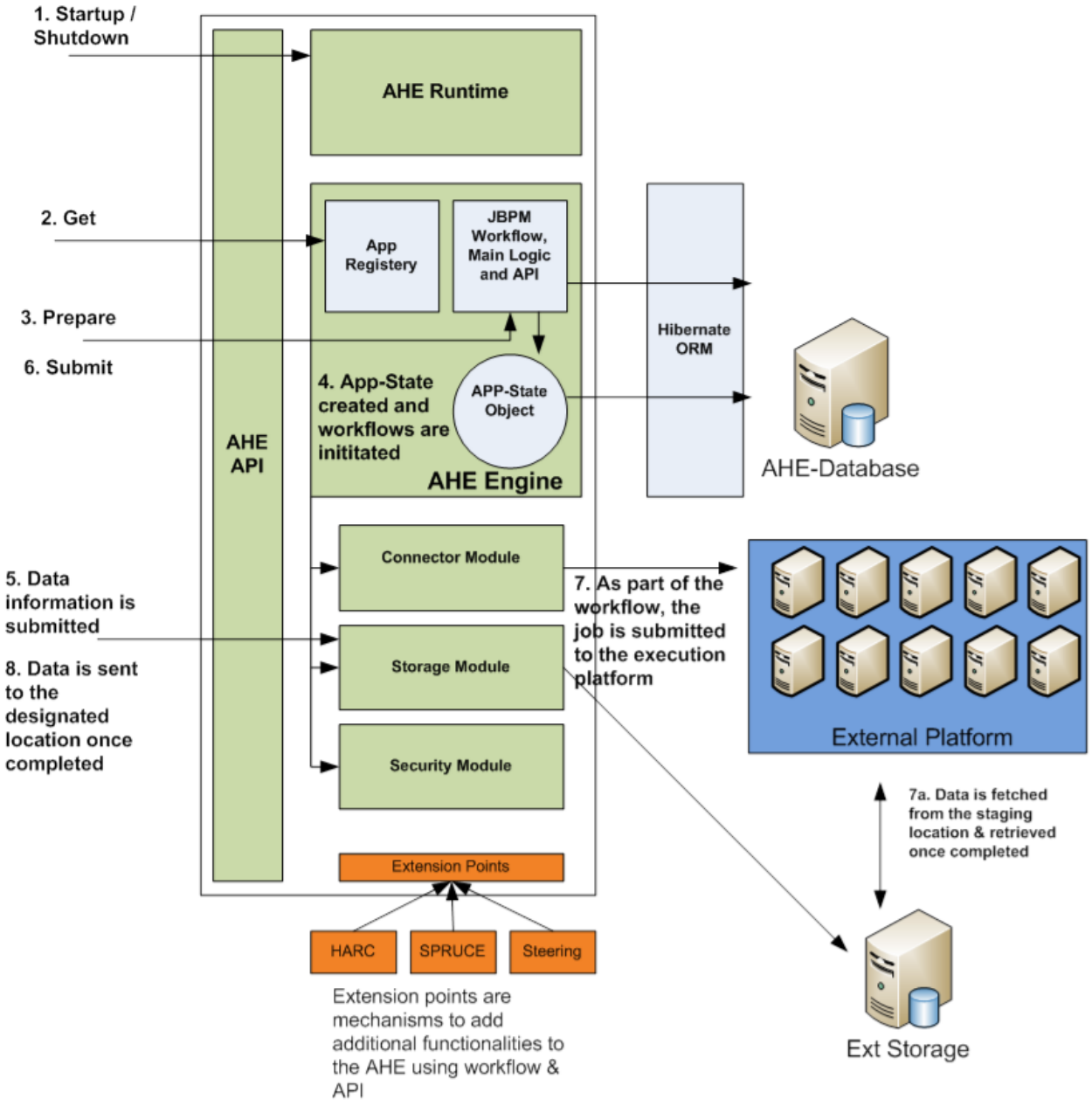
Globus

UNICORE

PRACE

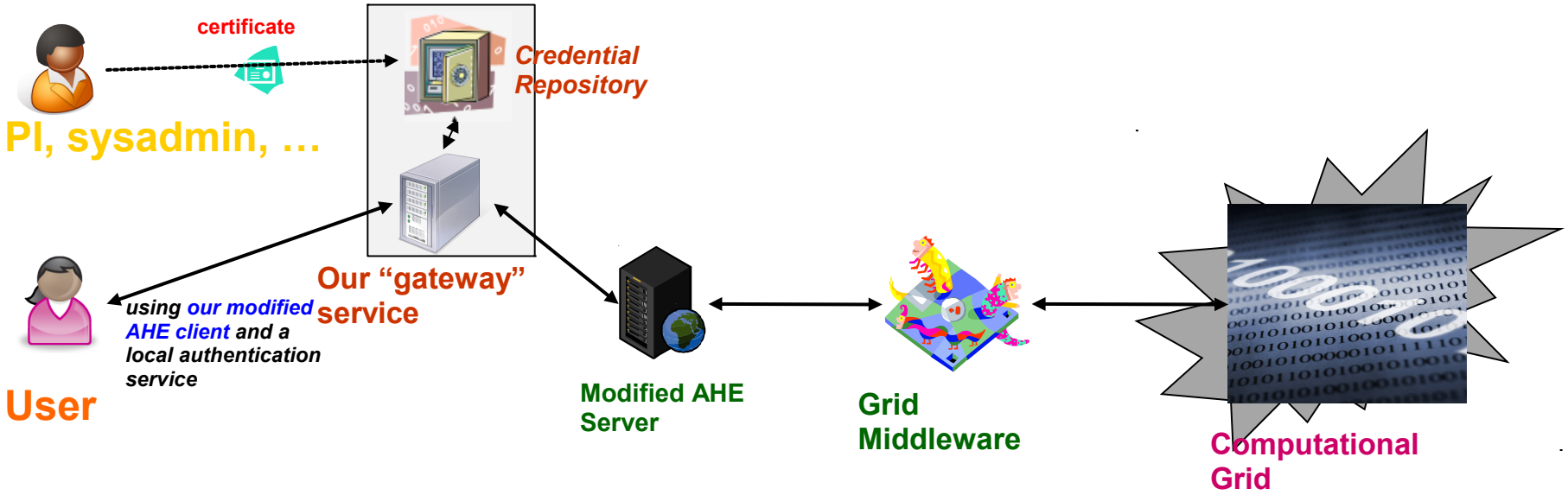


How AHE Works



Authentication via local credentials

Audited Credential Delegation



- A designated individual puts a *single* certificate into a credential repository controlled by our new "gateway" service.
- User uses a *local authentication service* to authenticate to our service.
- Our gateway service provides a session key (*not shown*) to *our modified AHE client* and *our modified AHE Server* to enable the *AHE client* to authenticate to the *AHE Server*.
- Our gateway service obtains a *proxy* certificate from its credential repository as necessary and gives it to *our modified AHE Server* to interact with the grid.
- User now has no certificate interaction.
- Private key of the certificate is never exposed to the user.

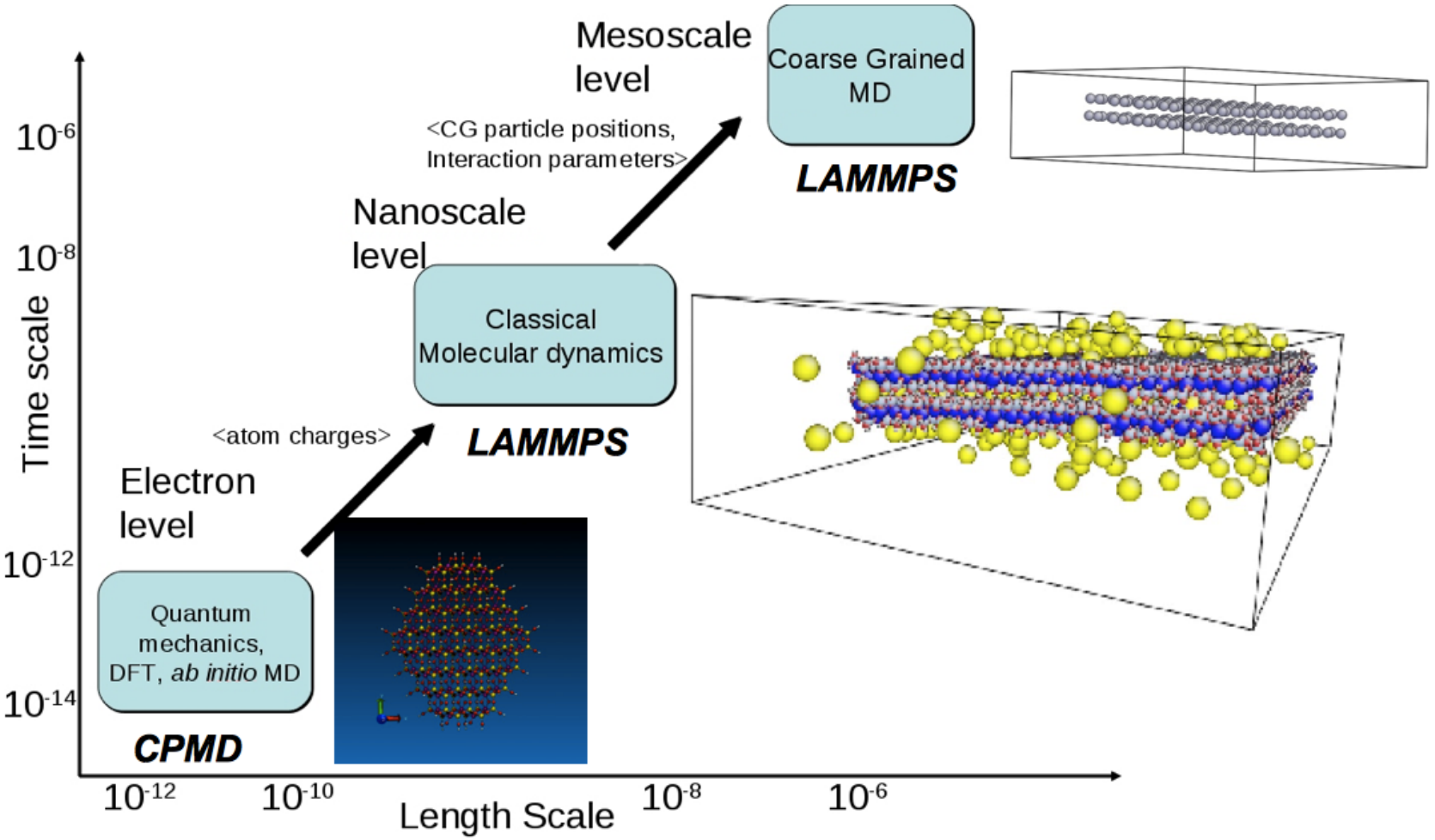
AHE & ACD Usability Study

- Usability: we have completed a comprehensive usability study that involved:
  - Comparing AHE+ACD (GUI), AHE (GUI) and UNICORE GUI, AHE command line and Globus TK command line
  - 40 users from different UCL departments (Physics, Computer Science, Medical school, Business School, Chemistry, Cancer Institute, Law School)
  - Task: run a simulation on Grid (NGS) using the above middlewares and use credentials given to them (username/password, X509 Certificate)
  - Result: AHE+ACD scored best in respect of:
    - Time needed to run the task
    - Ease of Configuring the tool
    - Ease of running the whole task.

S. J. Zasada, A. N. Haidar, and P. V. Coveney, “On the Usability of Grid Middleware and Security Mechanisms”. *Phil. Trans. R. Soc. A* , 2011, 369 (1949) 3413-3428; doi:10.1098/rsta.2011.0131

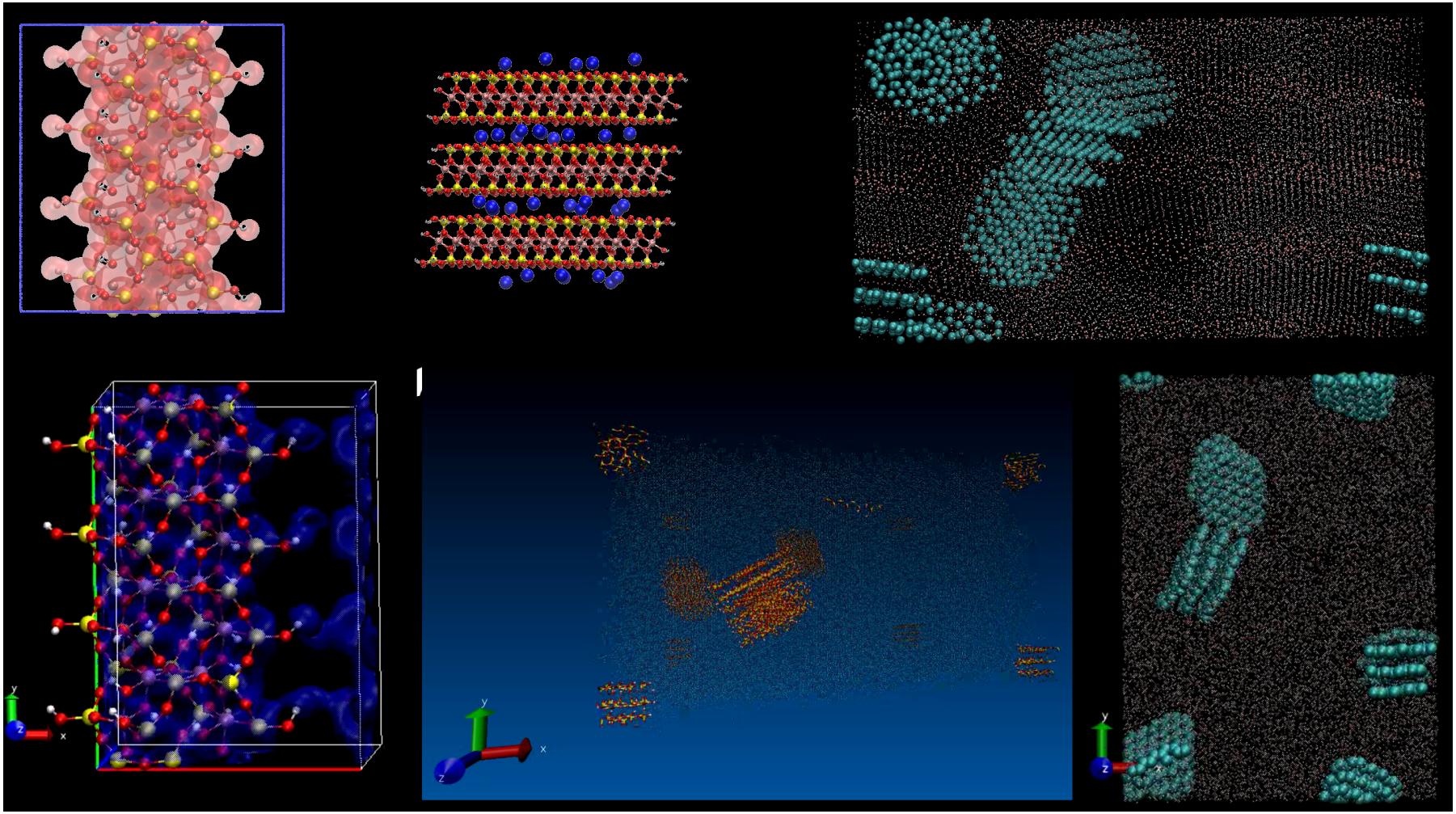
AHE Use case: Nanocomposites

Scale Separation Map

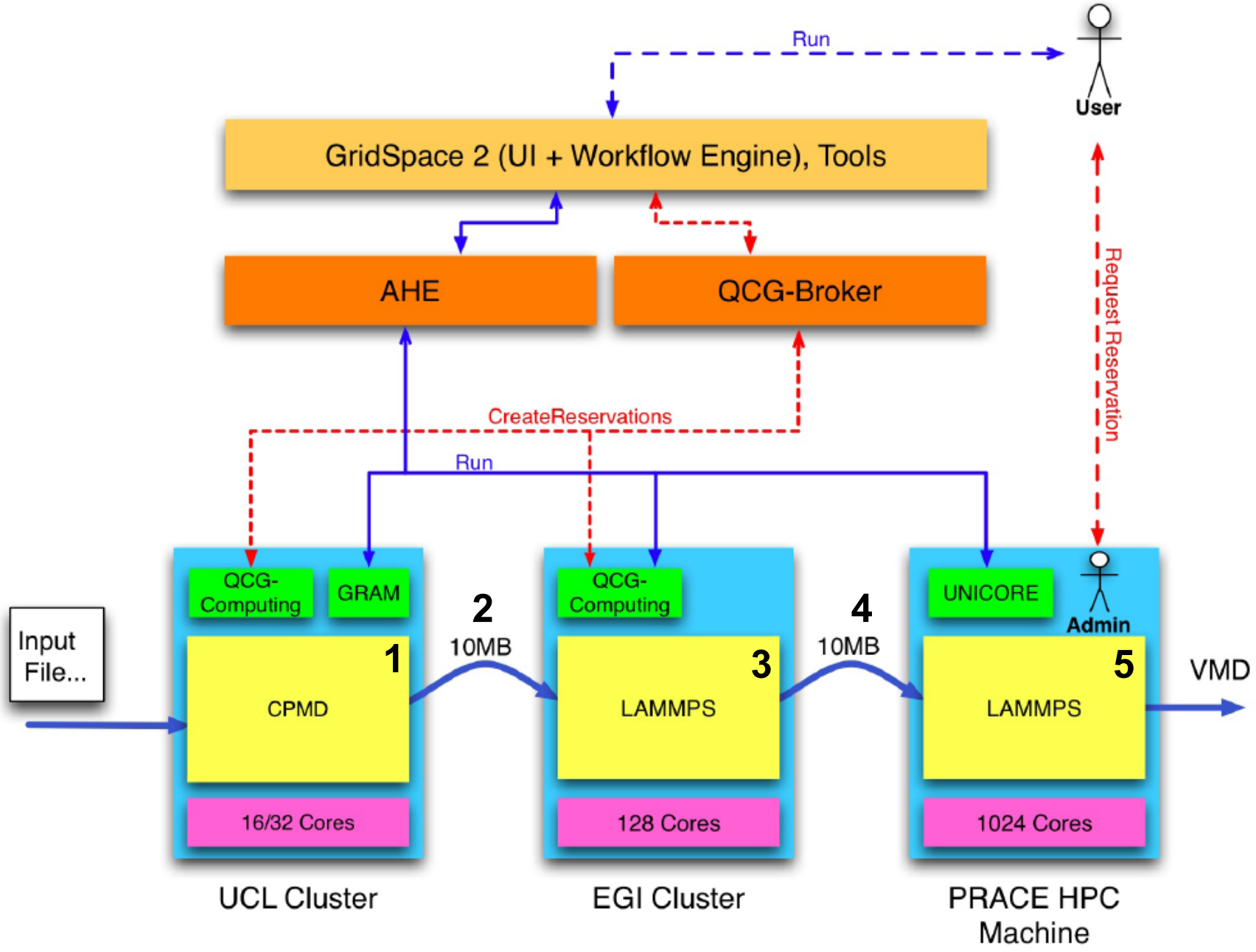


AHE Use case: Nanocomposites

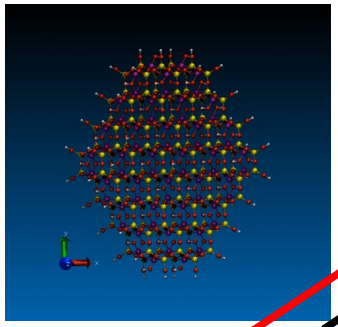
Quantum Mechanics | **Atomistic** | **Coarse-grained**



AHE Use case: Nanocomposites year 1



AHE Use case: Nanocomposites now

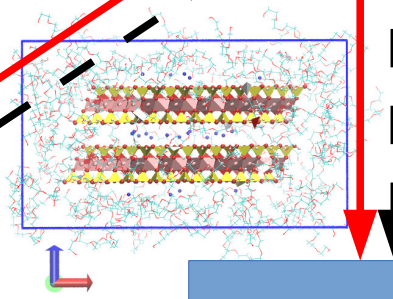


Coordinating software (GridSpace, AHE, QCG)

LAMMPS-CG

PRACE site (Tier-0)

4



CPMD

1 *Local cluster*

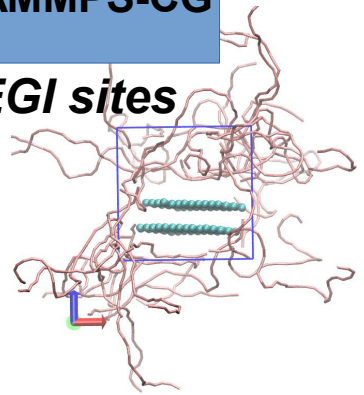
LAMMPS-AA

2 *PRACE site (Tier-1)*

L L L LAMMPS-CG

3

EGI sites



(EUDAT) distributed data store

Short & long-term data storage needed. Data size can grow to more than 10TB.

Summary

- AHE provides a single user interface to local, grid and supercomputing resources.
- AHE middleware allows federated access to different other middlewares – Globus, Unicore, QCG, RealityGrid etc.
- The client is easily installed by users, and requires no intervention by system/network administrators.
- By calling the command line clients from scripts, users can build complex scientific workflows.
- User federation of resources allows us to make efficient use of our allocations, and investigate problems that would take too long on a single grid

Thank you