Project objectives

Creation of a dynamic database of materials properties that ...

1. Uses grid computing to compute properties not yet in the database

2. Exploits emerging XML technologies within the data flow from the user interface through to the database

3. Uses modern portal technologies (JSR-168, etc)

Data generation

Ab initio electronic structure computation of materials properties

- ▸ Large resource requirements
- ▸ Computation time in terms of hours
- ▸ Our codes generate XML output files

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We use the Chemical Markup Language

▸ Our simulation codes write CML

▸ Our Golem toolkit is used to read CML files in a generic way

▸ We are exploiting the use of XML dictionaries, eg to drive the portal interface seen by the user

▸ CML2SQL parser developed for archiving material properties into the database

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Workflow is managed by Pipeline Pilot

‣ Pipeline Pilot provides a web service interface that is used by the portal to manage the whole simulation process

‣ Service-oriented interactions between components of the MaterialsGrid infrastructure

‣ The workflow automates the complete process without any additional user interaction
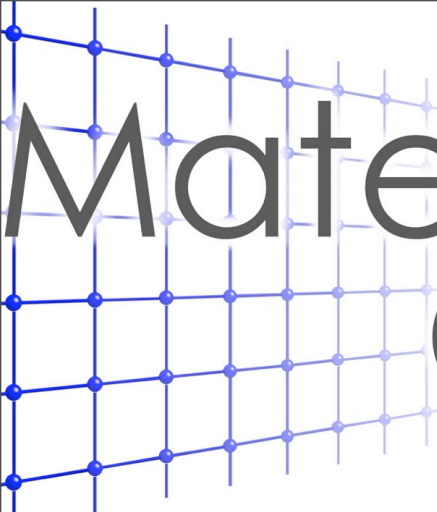
Grid methods

Grid jobs are handled by standard Grid middleware plus ...

- ‣ Job submission and management handled by the eMinerals RMCS tool

- ‣ Data staging is handled using a Webdav approach

Demonstration

Materials Grid
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We will now show:

‣ Job creation from the portal

‣ Monitoring of job and other services

‣ Accessing data in the database

Finally ...

- ▸ Visit us on the NIEeS stand (#14)

- ▸ Partners are Cambridge, STFC, Frankfurt, Accelrys, IBM

- ▸ Thanks also to members of the eMinerals project and NIEeS

Buzzword Bingo
Did you spot them all?

▸ Ajax

▸ Portals / portlets / JSR168

▸ XML

▸ Web Services / SOAP

▸ Grid

▸ Ontologies

▸ Workflow

▸ ...