

# **NW-GRID and NGS - working together -**

*<http://www.nw-grid.ac.uk>*

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# NW-GRID Partners and Aims



## NW-GRID Partners and Resource Providers

- Daresbury Laboratory: CSED, e-science centre, STFC Innovations Ltd.
- Lancaster University: management school, physics, e-science and computer science
- University of Liverpool: physics and computer services
- University of Manchester: computing services
- Proudman Oceanographic Laboratory, Liverpool
- University of Central Lancashire (provisional)
- Huddersfield University (in discussion)

## Aims

- ✓ Establish, for the region, a world-class activity in the deployment and exploitation of Grid middleware
- ✓ realise the capabilities of the Grid in leading edge academic, industrial and business computing applications
- ✓ Leverage 100 posts plus £15M of additional investment
- “Successful outcome” – independent project reviews early 2010

# NW-GRID Vision



Technology "tuned to the needs of practicing scientists".

Work with other Grid consortia: NGS, WRG, NorthGrid

Applications and industry

*Pharma, meds, bio, social, env, CCPs*

*Portals, client toolkits, active overlays*

User interfaces

Sensor networks and experimental facilities

Advanced Network technology

Desktop pools: Condor etc.

Mid range: NW-GRID and local clusters

Top end: HPCx and CSAR



# Main NW-GRID Resources



## Daresbury

- \* 96 node Streamline-Sun cluster with 2.4GHz twin dual core Opterons
- \* IBM BlueGene/P with 4096 processors
- \* 32 node Streamline cluster with twin quad core Harpertown, Nehalem and nVidia GPU
- IBM Power7, 4x 32-way nodes
- Condor pools

## Manchester

- \* 44 node IBM cluster with dual twin core Opterons
- \* 25 node Streamline-Sun cluster with 2.4GHz twin dual core Opterons
- \* SGI Prism visualisation engine with 8x Itaniums and 4x ATIFireGL X3 graphics pipes

## Lancaster

- \* 48 node Streamline-Sun cluster with 2.6GHz twin dual core Opterons
- 124 node Streamline-Sun cluster with 2.6GHz twin dual core Opterons (local HPCF)
- \* 67 node Streamline-Sun cluster with 2.3GHz twin quad core Opterons
- \* 12TB Streamline-Sun data Grid
- Viglen system currently being installed

## Liverpool

- \* 104 node Streamline-Sun cluster with 2.2GHz twin dual core and 2.3GHz twin quad core Opterons
- \* 96 node POL IBM cluster with twin Xeons
- 960 node Dell cluster with Pentium IV (local Physics)
- \* 108 node Streamline-Sun cluster with 2.4GHz twin dual core and 2.3GHz twin quad-core Opterons and InfiniPath
- Condor pools

# 2006 Hardware



# Grid Compatibility



## Middleware and standards

- Globus pre-web services v4.2.1 - predominant access layer for users
- Condor v7.2.1 and Condor-G
- Middleware compatibility with NGS, including additional VOMS, LCAS, LCMAPS (and MEG for STFC users)
- Monitored as part of conformance testing

## Client software designed to enhance usability

- GROWL and GROWL Scripts – now part of G-R-Toolkit
- RMCS (Remote MyCondor Submit) – Grid and Condor resource broker, now part of G-R-Toolkit
- AgentX
- CCP1 GUI etc.
- Sakai Portal and NGS Portal (Virtual Research Environment)

Daresbury, Liverpool and Lancaster NGS affiliates. Manchester hosts an NGS node. Partners work alongside NorthGrid too (for GridPP).

# Example: GROWL and the CCP1 GUI



The screenshot displays the GROWL and YTKMolView software interface. The main window, YTKMolView, shows a 3D molecular model of a molecule with a color gradient from red to blue. The interface includes several control panels:

- GROWL Panel (Top Left):** Contains fields for Title (methanol), Task (Energy), Charge (0), and Spin (1). It also has a Basis Selector with Default Basis (sto3g) and Current Basis Assignment table.
- Coloured Isosurface Panel (Bottom Left):** Allows editing of colors (oDo), contour height (0.01), and color field (potential). It includes a color mapping section with Lo (-50) and Hi (50) values, and an opacity slider (0.8).
- Molecule view Panel (Bottom Center):** Contains checkboxes for Wireframe, Spheres, Sticks, and Labels, along with a Sphere Scale slider (0.7) and a Label Size slider (0.19).

The Windows taskbar at the bottom shows the Start button, several application icons, and the system clock displaying 08:04.

(from Jens Thomas)

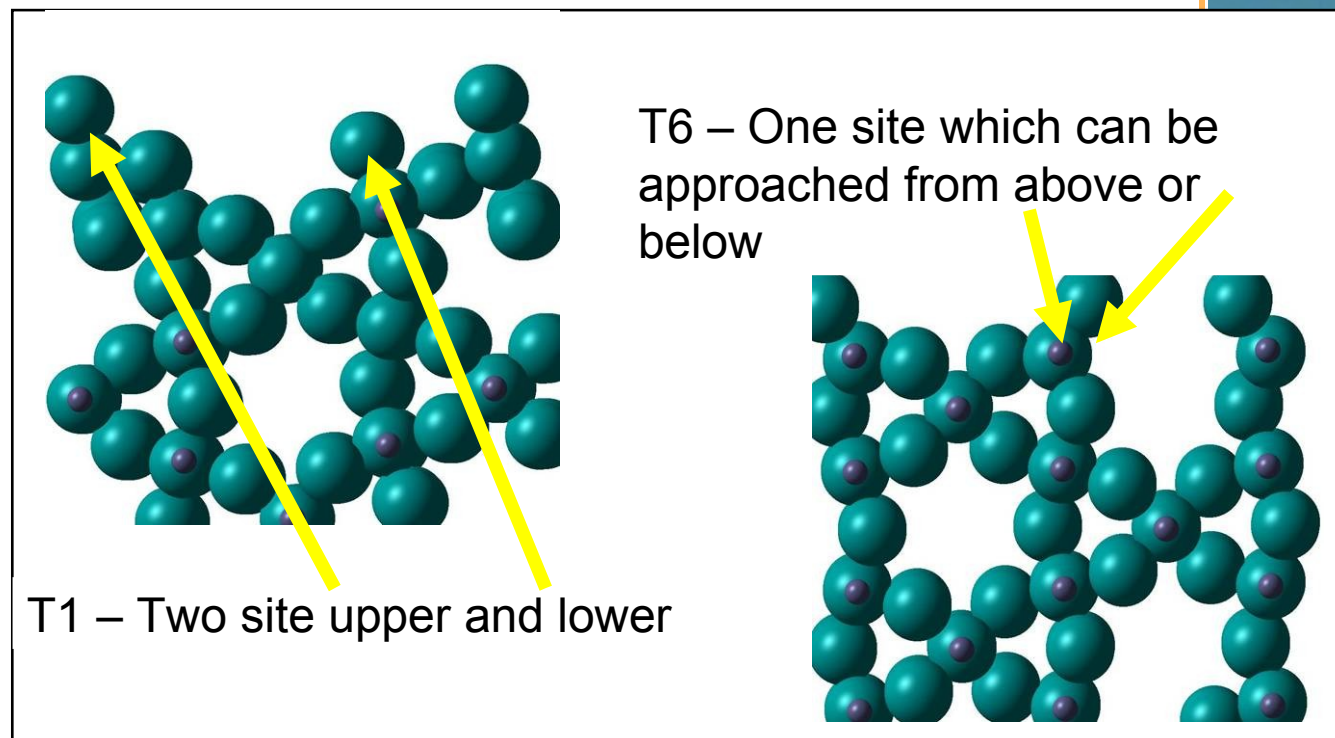
# Example: CCP3 - Aluminium Fluorides



High surface area Aluminium Fluorides (HS- $\text{AlF}_3$ ) have great industrial potential as a strong Lewis acid catalysts used in the large scale production of chlorofluorocarbons and hydrofluorocarbons for a wide range of applications including aerosol propellants, refrigerants and solvents.

We have used the CCP3 application CRYSTAL to predict the surface structure of  $\beta\text{-AlF}_3$ .

Three different Lewis acid sites have been identified and quantified via studies of  $\text{NH}_3$  adsorption using NW-GRID resources.



This represents the first atomic scale model of possible active sites present on the surface of amorphous high surface area  $\text{AlF}_3$ .

(from Christine Bailey et al., J. Phys. Conf. Series 2008 )

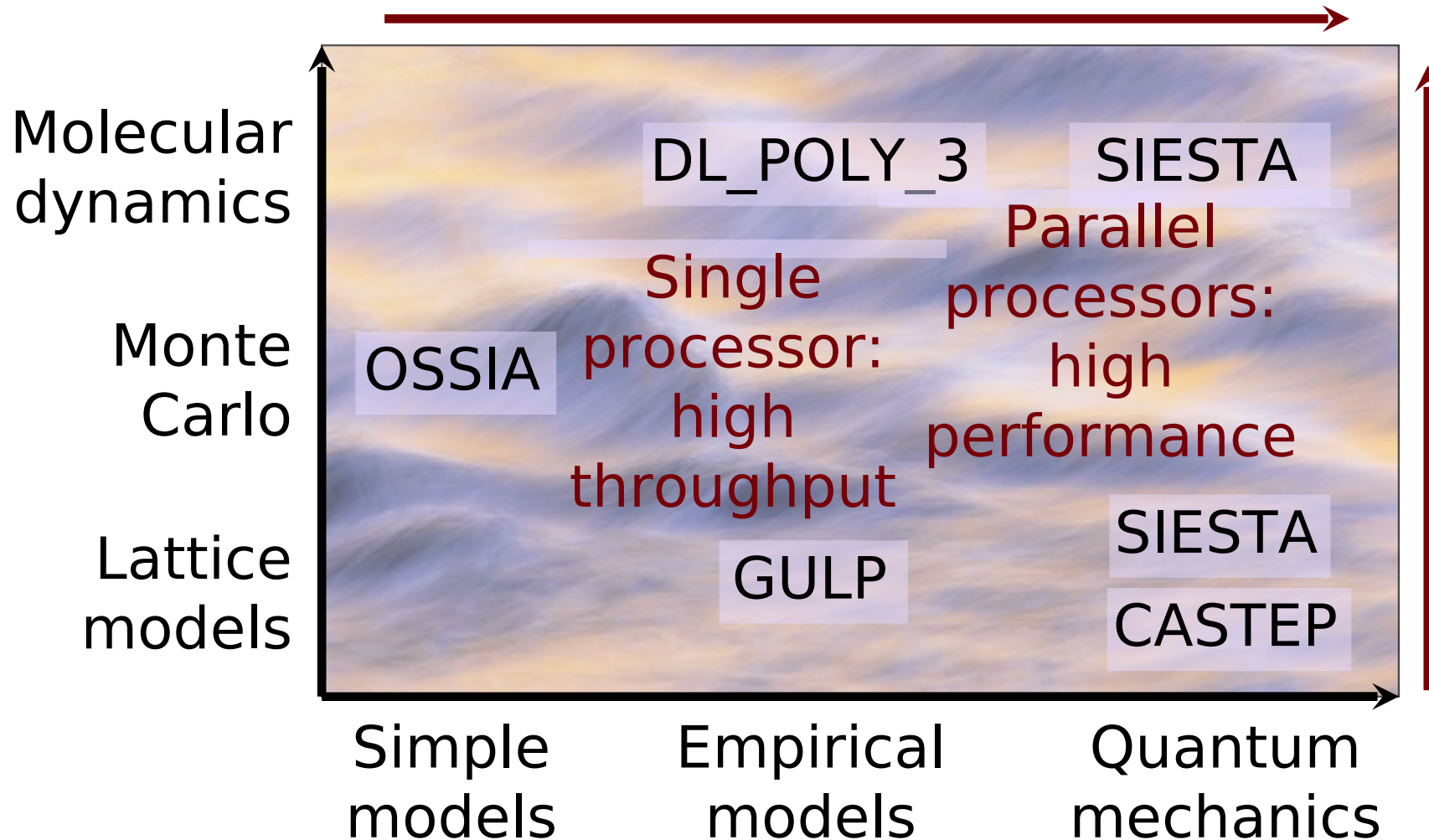
# Example: CCP5 and e-Minerals



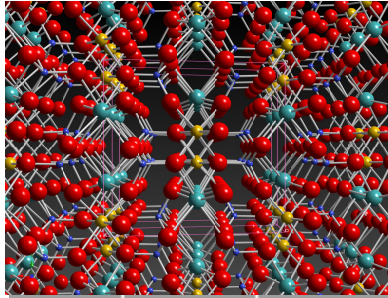
(from Martin Dove et al.)

A range of methods and applications was used to study minerals and capture of environmental pollutants.

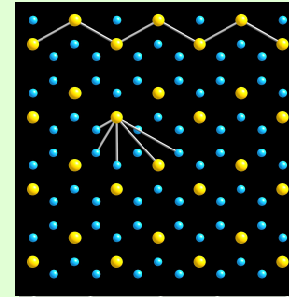
Computational demands



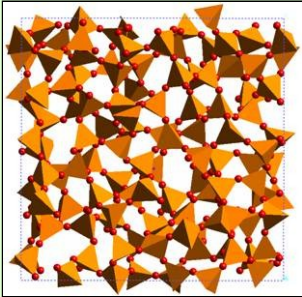
# E-Minerals Case Studies



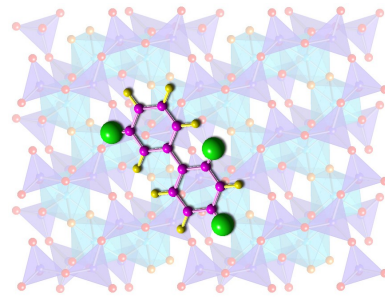
Compression of the mineral diopside using CASTEP



Cation ordering in layer silicates using OSSIA

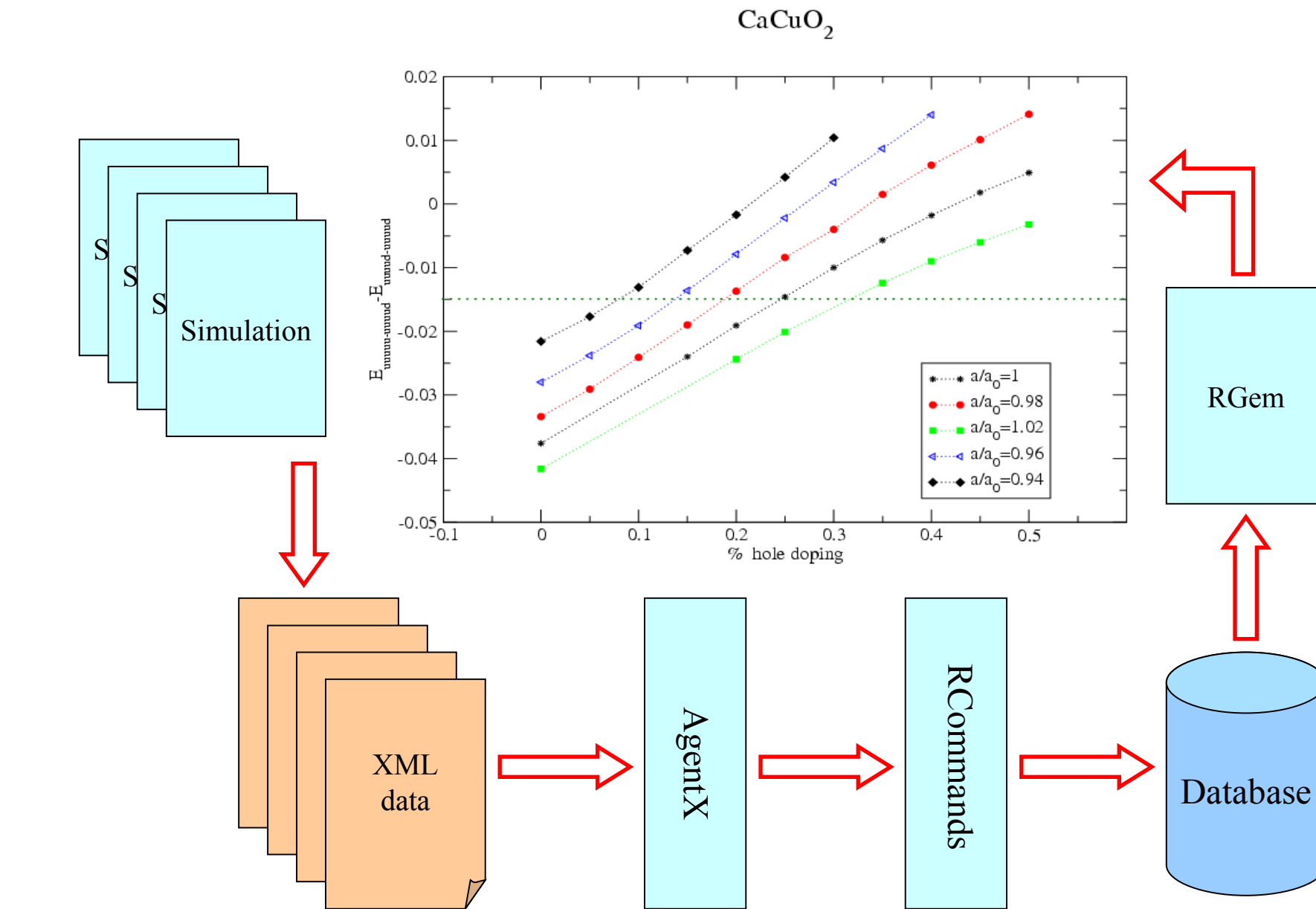


Compressibility anomaly in amorphous silica using DL\_POLY 3



Adsorption of molecules on mineral surfaces using SIESTA

# CCP9 – Properties of new Materials



(from Rik Tyer)

# Access to NW-GRID



## Academic access

- For DSIC staff by contacting Rob Allan, your Campus Champion - [robert.allan@stfc.ac.uk](mailto:robert.allan@stfc.ac.uk) 01925 603207. For others see the NW-GRID Web site: <http://www.nw-grid.ac.uk/Access>

## Commercial Grid computing packages

- Purchase computer cycles by the hour. This allows you cost effective access to capacity scale computing – “Infrastructure as a Service”
- Solution based Grid Computing to answer scientific problems using NW-GRID and pre-installed applications – “Software as a Service”
- Project based work, extending features or parallelising existing code to make best use of cluster or Grid computing – make best use of regional expertise to answer your research questions

Commercial access to NW-GRID can be obtained through DAComS by visiting the Web site <http://www.nw-grid.ac.uk/Access>

For further information on commervial services contact Michael Gleaves - [michael.gleaves@stfc.ac.uk](mailto:michael.gleaves@stfc.ac.uk) 01925 603710

# Support and Future Roles



- Helpdesk via RT ticket system [nw-grid-daresbury@request.dl.ac.uk](mailto:nw-grid-daresbury@request.dl.ac.uk)
- Popular software can be installed for shared use – please ask
- Sakai Web portal for collaboration and information – NGS portal for job submission and data management
- GROWL scripts and other user interfaces
- Resources to support various needs – from HPC clusters to Condor pools for parameter sweeps
- A vision of a federated Grid system, NW-GRID → NGS → EGI → ...
- Messages and user guides on Web site: <http://www.nw-grid.ac.uk/Daresbury>
- Support and information about novel systems via EPSRC's Distributed Computing Programme: <http://www.cse.scitech.ac.uk/disco>
- Applications developed by the CCPs, Collaborative Computational Projects, see <http://www.ccp.ac.uk>

Thanks to the NGS team for coming to the Daresbury Science and Innovation Campus and for their ongoing support.