Overview of White Rose Grid Operations

Content

- The beginning
- Organisation
- Services
- Activities
- Looking into the future

The beginning

- 1997: White Rose University Consortium established
  - a strategic partnership between Yorkshire's leading research Universities of Leeds, Sheffield and York
- 2000: the VCs decided to combine computing resources using emerging Grid technologies
  - White Rose Grid launched in 2002
  - Strategic partnership with Esteem Systems
- 2003: the White Rose Grid e-Science Centre formally established

NeSC Glasgow
NeSC Edinburgh
NEeSC Newcastle
BeSC Belfast
Lancaster
White Rose Grid - York
White Rose Grid - Leeds
White Rose Grid - Sheffield
ESNW Manchester
CLRCeSC Daresbury
Leicester
Birmingham
CeSC Cambridge
Oxford
Reading
Grid Support
Centre (RAL)
LeSC London
WeSC Cardiff
UCL
Bristol
SeSC Southampton

UK e-Science Centres

Our Objectives

- to facilitate and strengthen e-Science research across the three Universities

- to enlarge the consortium by including new communities e.g. geography, biology at Leeds

- to collaborate with other UK e-Science Centres and Grids in the UK and beyond

- to offer focus for a variety of e-Science activities in the region

WRG setup

- Purposely acquired and later enhanced - with over £5m investment – 5 nodes

- Heterogeneous grid: clusters of Sun shared-memory systems, and Intel Xeon and AMD Opteron processor based Beowulf type clusters

- Needed to balance local ownership with a Grid sharing capability

- Our distinct approach is to offer both:
  - local HPC services (75% resources)
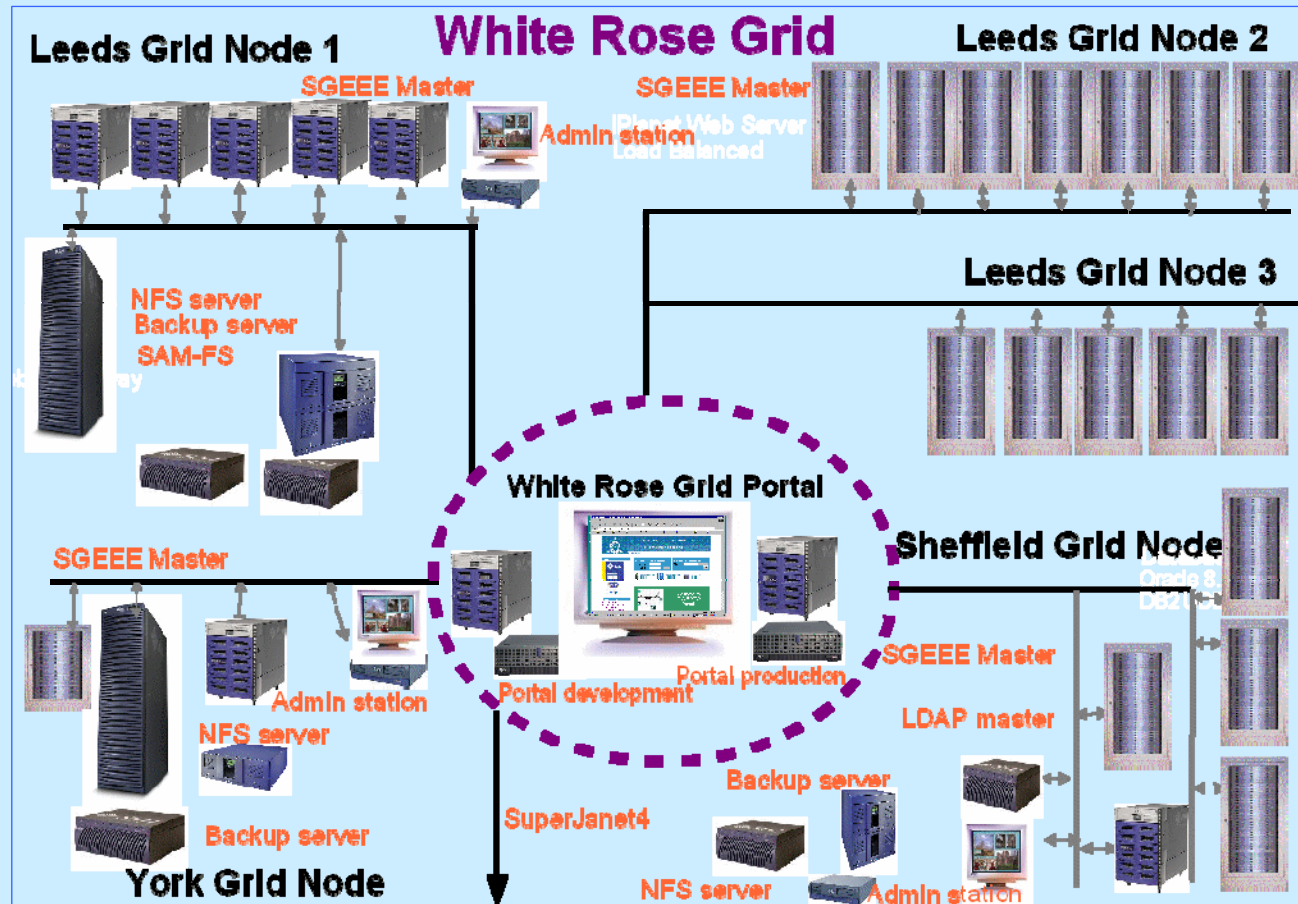 - the grid infrastructure (25% resources)

25%

75%
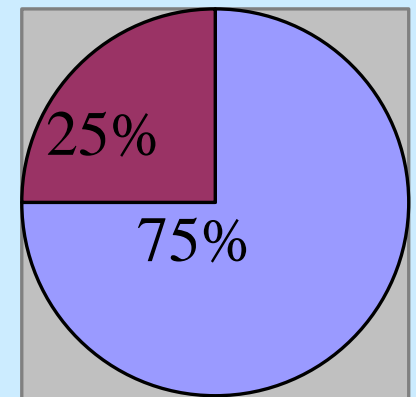
WRG resource allocation

WRG resources: nodes

General Purpose HPC node

General Compute node plus bioinformatics and biomedical appl.

CFD node

Engineering Application node

Core node services

- **Computation**
  - HPC delivered via traditional means
  - Innovative Grid computing
- **Data (& metadata) storage management**
  - Storage Resource Broker
- **Software environment & applications**
  - Queuing and resource scheduling system: Sun Grid Engine Enterprise Edition
  - Compilers: PGI, Sun, and Intel for C, C++, Fortran & Java
  - Libraries & tools: OpenMP, MPI, HPC Cluster Tools, NAG Fortran Library, Sun Forte Developer
  - Scientific visualisation: IRIS Explorer, IBM Explorer, IGNUplot
  - Application packages: Fluent, Ansys, Abaqus, Matlab, DIRAC,DL_POLY, NW Chem, Dalton
- **User management & support**
  - e.g. operating UK CA, WRG CA
- **Training (e.g. courses, seminars, workshops –e.g. on e-Infrastructure, conferences)**

Grid technologies

- Supported on the WRG:
  - Authentication using PKI X.509 and UK e-Science Certification; accepts WRG CA certificates
  - Certificate management- MyProxy
  - Job submission/batch service (Globus Toolkit 2.4.3: Sun Grid Engine) – Globus Toolkit 4 recently deployed on the new Leeds Grid Node 3
  - Information service – MDS
  - Grid monitoring- Ganglia, GITS, Inca
  - Data access/integration services (GridFTP, SRB)
  - Accounting (via Sun Grid Engine Enterprise Edition)
  - WRG portals
    - the e-Social scientists portal based on the EASE web application technology
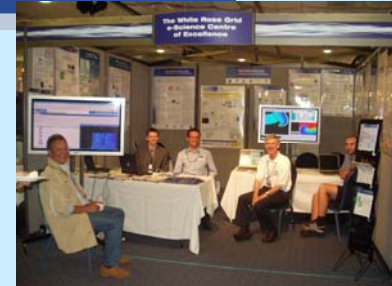   - Other, e.g. the DAME portal utilising the Struts framework

THE WHITE ROSE GRID
e-Science Centre of Excellence
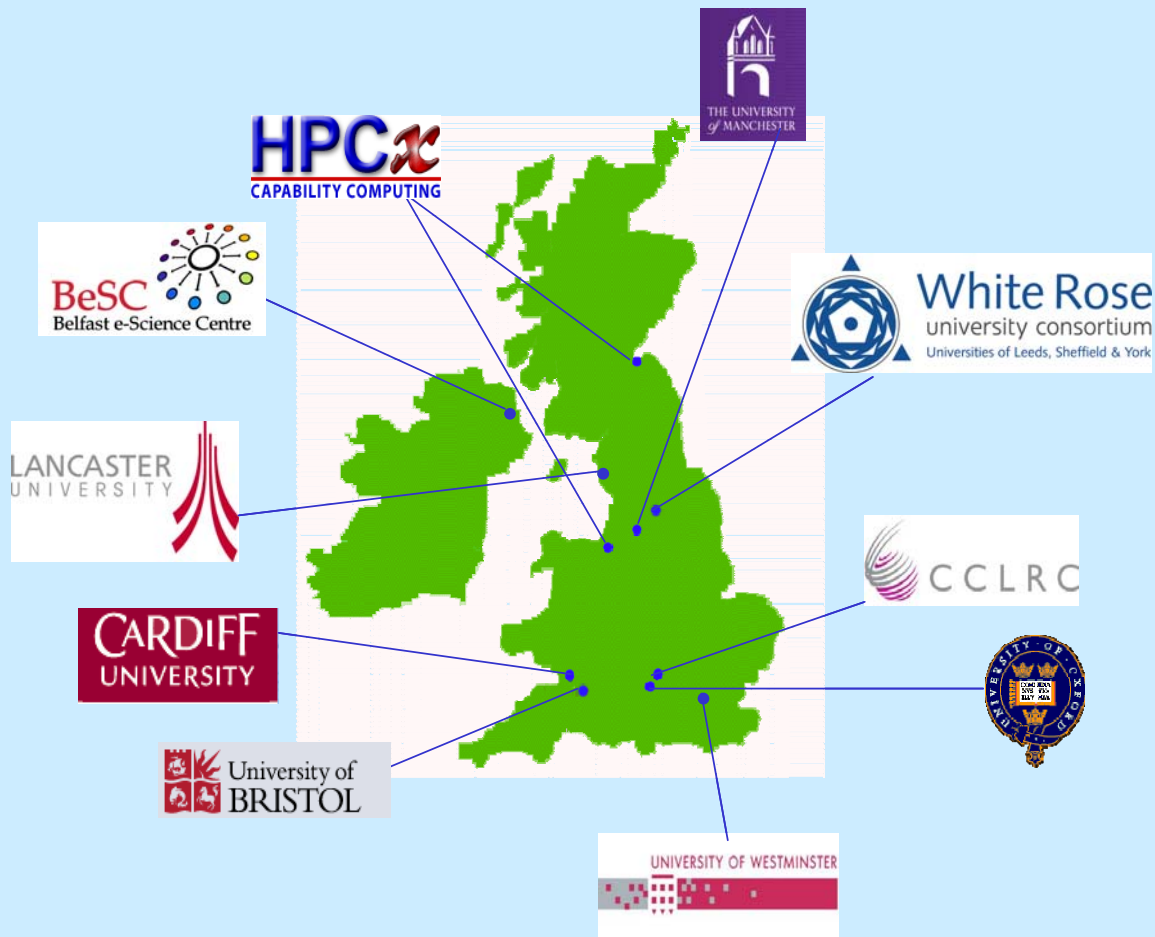
Our strengths are:

- **Successful support of production grids**
  - WRG, NGS core node, Tier-2 node of GridPP
- **Professional user support and grid training**
  - HPC (e.g. use of MPI)
  - Grid Computing (e.g. Java CoG kit, Globus Toolkit)
- **Successful engagement with a broad application user community within the White Rose Universities**
  - huge amounts of scientific research: e-Science projects, more traditional projects requiring HPC resources;
  - common conferences and workshops, user group meetings, seminars e.g. GT4
- **Productive engagement with international grid activities**
  - WUN data grid
  - Chinese grid community through CROWN project
- **Outreach and dissemination**
  - Provided training in the technology to companies and with them assessed potential demand for grid facilities; WRG conference, web site , working closely with IT partners (e.g. Esteem, Sun, IBM)
- **Proven ability to collaborate effectively at every level**
  - user, technical and scientific level

Examples of e-Science projects at WRG

- **Grid system engineering and system security**
  - e-Demand, IBHIS (Integration Broker for Heterogeneous Information Sources) => the Systems Engineering component of EPSRC/BAE-Systems project aiming to advance Network-Enabled Capability.
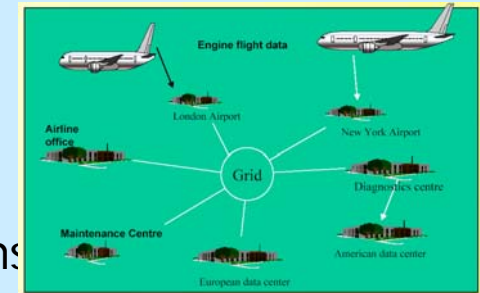
- **Distributed diagnostics & engine health monitoring**
  - Distributed Aircraft Maintenance Environment (DAME) led by York
  - Business Resource Optimisation for Aftermarket and Design on Engineering Networks led (BROADEN) by Rolls-Royce
  - ESRC funded HYDRA and HYDRA2 => MoSeS (Modelling and Simulation for e-social Science)
- **Distributed Collaborative Visualisation Services**
  - e-Viz (An Advanced Env. to Enable Visual Supercomputing), Integrative Biology, VOTech –towards the European Virtual Observatory; VizNET
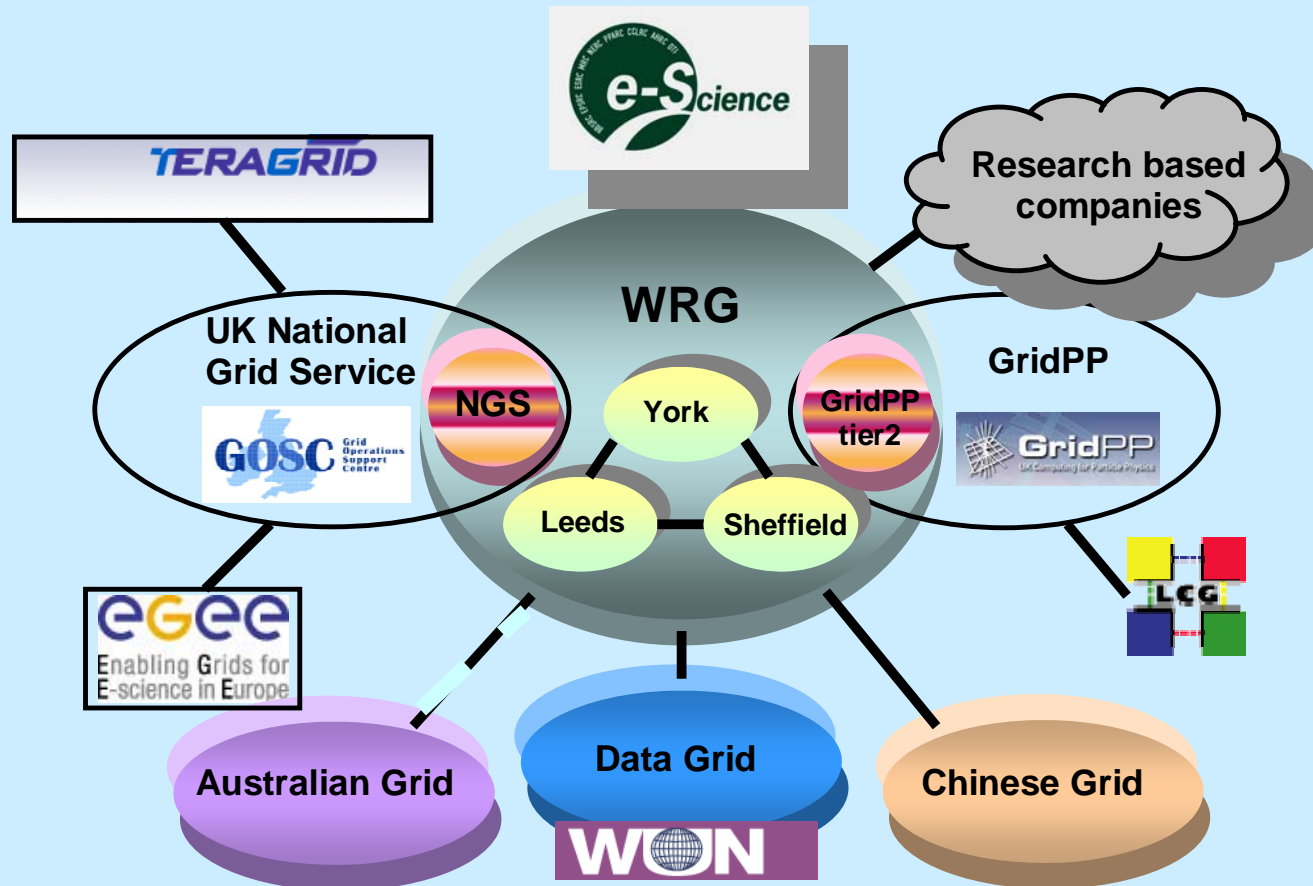
DAME Grid Services Distribution

York

Data Mining Services

AURA-G
GT3 Service
Zmod data
search facility

DAME GUI
GT3 Service
Browser based GUI
to DAME services

AURA-G Database

Zmod Viewer
GT3 Service
Browser based data
viewer for zmod files

DataStore-G
GT3 Service
Simulates arrival &
storage of QUOTE
data

Collaboration tools
GT3 Service
Toolset for multiuser
collaboration

Sheffield

Modeling & Decision Support

EngineModel-G
GT3 Service
BD25 Engine
model wrapped
as Grid Service

CBRAnalysis-G
GT3 Service
CBR advisor

SDM Database

DAME   workbench

WRG
GT3/2

WRG
GT3/2

WRG
GT3/2

WRG
GT3/2

Oxford

Engine Data Store

Engine Data Database

Leeds

Grid Middleware Services

**DAME WRG
Sign-on Portal**

Workflow
Browser based
workflow tool.
Compliant with
Resource Broker

XTO-G
GT3 Service
XTO plug-ins via a Grid
Service

Security
GT3 Security
Service
Proxy-
Management

DataVisualiser
GT3 Service
Jchart Viewer for
viewing XTO output

Resource Broker
GT2 Service
Schedule workflow
tasks on WRG
resource

Conclusions

- Secured UK e-Science Core Programme funding for our Centre for the next two years
- Continuously enhancing WRG facilities and expanding the portfolio of e-Science projects
- More information at the WRG web site at `http://www.wrgrid.org.uk/`

THE WHITE ROSE GRID
e-Science Centre of Excellence

Thank you for your attention

Our organisational structure

White Rose University Consortium Board

3 VCs, 3 PVCs, CEO

Dr Julian White

Senior academic representatives from the three Universities (Leeds – P Jimack, York -J Austin, Sheffield –P Fleming); Director and Coordinator of e-Science Centre (J Xu,J Schmdt), Manager; Esteem Manag Director.

White Rose Grid Executive Board

White Rose Grid Staff

Architecture Group	**Technical Team**	**User Management**	**Training & Education**	**Business Outreach**

Partnership with Computing Services

Leeds Computing Service Computer Science	**Sheffield** Computing Service	**York** Computer Science