DISC e-Science and Future Technology Conference
Sheffield

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National e-Science Centre
& e-Science Institute

www.nesc.ac.uk
16th May 2006
Take Home Message

- **UK e-Science**
  - Has worked well with industry
  - Has delivered innovation and scientific results
  - Has e-Infrastructure & support in place
  - Has a thriving community

- **UK e-Science is ready for more**
  - New, intellectually challenging projects
  - Collaboration will make this possible

- Collaboration is a Key Issue
Overview

- Brief History
  - Investment, Engagement & Community
- Present
  - Activities & Technologies
- Future
  - People
  - Behaviour
  - Commitment
What is e-Science?

- Goal: to enable better research in all disciplines
- Method: Develop collaboration supported by advanced distributed computation
  - to generate, curate and analyse data
    - From experiments, observations and simulations
    - Quality management, preservation and reliable evidence
  - to develop and explore models and simulations
    - Computation and data at all scales
    - Trustworthy, economic, timely and relevant results
  - to enable dynamic distributed collaboration
    - Facilitating collaboration with information and resource sharing
    - Security, trust, reliability, accountability, manageability and agility
A Grid Computing Timeline

I-Way: SuperComputing ’95

US Grid Forum forms at SC ’98

European & AP Grid Forums

Grid Forums merge, form GGF

“Anatomy” paper

“Physiology” paper

OGSA-WG formed

OGSA v1.0

1995 ’96 ’97 ’98 ’99 2000 ’01 ’02 ’03 ’04 ’05 2006

• DARPA funds Globus Toolkit & Legion
• EU funds UNICORE project
• US DoE pioneers grids for scientific research
• NSF funds National Technology Grid
• NASA starts Information Power Grid

• UK e-Science program starts

Source: Hiro Kishimoto GGF17 Keynote May 2006

Today:
• Grid solutions are common for HPC
• Grid-based business solutions are becoming common
• Required technologies & standards are evolving

Japan government funds:
• Business Grid project
• NAREGI project
Commitment to e-Infrastructure

- A shared resource
  - That enables science, research, engineering, medicine, industry, ...
  - It will improve UK / European / ... productivity
    - Lisbon Accord 2000
  - Commitment by UK government
    - Sections 2.23-2.25
  - Always there
    - c.f. telephones, transport, power

Science & innovation investment framework
2004 - 2014

July 2004

Gordon Brown
Chancellor of the Exchequer

Charles Clarke
Secretary of State for Education and Skills

Patricia Hewitt
Secretary of State for Trade and Industry
UK e-Science Budget (2001-2006)

Total: £213M + £100M via JISC

EPSRC Breakdown

- Applied (£35M) 45%
- Core (£31.2M) 40%
- HPC (£11.5M) 15%

+ Industrial Contributions £25M

Source: Science Budget 2003/4 – 2005/6, DTI(OST)

Slide from Steve Newhouse
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Help for your e-Science
The e-Science On The Map Today

- National Centre for e-Social Science
- Digital Curation Centre
- NERC e-Science Centre
- OMII-UK
- EGEE-II
- NGS Support Centre
- National Institute for Environmental e-Science
- Funded centres
- National Grid Service

Globus Apache Project & CDIG
A partnership between projects:

- myGrid at Manchester (Carole Goble - Chair)
- OGSA-DAI at Edinburgh (Malcolm Atkinson)
- OMII at Southampton (Dave De Roure)

Started January 2006

- Manchester – Expanded Engineering activity
- Southampton – Expanded Community activity
- Edinburgh – Continuation of OGSA-DAI team
Objectives of OMII-UK

- To distribute a sustained, well-engineered, interoperable, documented and supported set of easily-used integrated middleware services, components and tools
- To engage proactively with user communities in defining and developing this distribution
- To maintain a leading international role in advanced e-Infrastructure middleware provision
OMII-UK Activities

- User engagement
  - Forming partnerships with targeted user communities
- Sourcing
  - Working with UK and international service developers and middleware providers
- Software Engineering
  - Quality-assured software engineering, coordinated across OMII-UK partners and the managed programme
- Grid engagement
  - Tracking and engagement with the standards processes
- Sustainable business
  - Attracting partnerships and new investors
OMII-UK & National Grid Service: Life Sciences Gateway

Talk to us about other ‘gateways’
- Computational Chemistry
- Engineering
- Image Analysis
- …
Composable Services

- Job Submission & Monitoring service (GridSAM)
- Workflow services (Taverna, BPEL)
- Data Access & Integration service (OGSA-DAI)
- UDDI Registry service (Grimoires)
- Reliable messaging: WS-R & WS-RM (FIRMS)
- Notification using WS-Eventing (FINS)
- Scripting Environments:
  - Matlab & Jyton (GeodiseLab)
  - PERL (WSRF::Lite)
The National Grid Service

Core sites
White Rose (Leeds)
Manchester
Oxford
CCLRC

Partner sites
Bristol
Cardiff
Lancaster

Access to HPC facilities
HPCx
CSAR

Capacity
300 + CPUs
30+ Tera Bytes

Specialist facilities
Cardiff 4x16 proc SGI
Bristol: Intel
Lancaster SUN Cluster

Services:
Job submission (GT2)
Storage service (SRB)
Oracle Service
OGSA-DAI
A Knowledge Transfer Network project funded by the DTI Technology Programme aimed at transferring knowledge about Grid Computing Technologies to Public and Private Sectors in the UK.

Partnership between Intellect, the UK Hi-Tech Trade Association; National e-Science Centre, a world leader in Grid Computing research; and CNR Ltd, a consultancy focused on SME organisations and business intermediaries.

Substantial number of industrial, business and academic partners

Website
Background Information
Industry News/Events
User Case Studies

Events programme
Technical Overviews
Multiple vendor perspectives
User Case Studies

Sector Agenda
Healthcare; Government; Telecoms; Services; etc..

User Community
Network with peers
Find useful contacts
Contribute experience

www.gridcomputingnow.org
Collaboration is the key to e-Science
Integrative Biology

Tackling two Grand Challenge research questions:

• What causes heart disease?
• How does a cancer form and grow?

Together these diseases cause 61% of all UK deaths

Will build a powerful, fault-tolerant Grid infrastructure for biomedical science

Enabling biomedical researchers to use distributed resources such as high-performance computers, databases and visualisation tools to develop complex models of how these killer diseases develop.
Optimal Parallel Codes

Graz
Sheffield CVC
Utrecht
Tulane
Auckland
Oxford Heart
UCSD
......
Cancer Modelling

Basic Models
Visualization: Meshalzyer (Unstructured Grids)
New projects in e-Science
CARMEN
Code Analysis, Repository and Modelling for e-Neuroscience
Understanding the brain may be the greatest informatics challenge of the 21st century

Worldwide >100,000 neuroscientists (~ 5,000 in UK) are generating vast amounts of data

Principal experimental data formats:

- molecular (genomic/proteomic)
- neurophysiological (time-series electrical measures of activity)
- anatomical (spatial)
- behavioural

Neuroinformatics concerns how these data are handled and integrated, including the application of computational modelling
Understanding the brain may be the greatest informatics challenge of the 21st century

- determining ion channel contribution to the timing of action potentials
- resolving the ‘neural code’ from the timing of action potential activity
- examining integration within networks of differing dimensions
CARMEN Consortium

Leadership & Infrastructure

Colin Ingram

Paul Watson

Leslie Smith

Jim Austin
CARMEN Consortium

International Partners

Ad Aertsen
(Freiburg)
Neural network modelling and large-scale simulations

George Gerstein
(Pennsylvania)
Analysis of spike pattern trains

Sten Grillner
(Karolinska Institute)
Chairman of the OECD, International Neuroinformatics Coordinating Facility

Shiro Usui
(RIKEN Brain Science Institute)
Lead for the Japan Node of the International Neuroinformatics Coordinating Facility

Daniel Gardner
(Cornell)
Lead for the US NIH, Neuroscience Information Framework and Brain ML
CARMEN Consortium

Commercial Partners

AstraZeneca
- applications in the pharmaceutical sector

NeuroServe
- interfacing of data acquisition software

Neuralynx
- application of infrastructure

Microsoft
- commercialisation of tools

CYBULA
- high performance pattern recognition systems
Meeting the Design Challenges of Nano-CMOS Electronics

Asen Asenov
Department of Electronics and Electrical Engineering
University of Glasgow

Richard Sinnott
National e-Science Centre
University of Glasgow

Stephen Pickles
e-Science North West
University of Manchester

16th March 2006
University Partners

Advanced Processor Technologies Group (APTGUM)
Device Modelling Group (DMGUG)
Electronic Systems Design Group (ESDGUS)
Intelligent Systems Group (ISGUY)
National e-Science Centre (NeSCG)
Microsystems Technology Group (MSTGUG)
Mixed-Mode Design Group in IMNS (MMDGUE)
National e-Science Centre (NeSCE)
e-Science NorthWest Centre (eSNW)
The Challenge

International Technology Roadmap for Semiconductors

<table>
<thead>
<tr>
<th>Year</th>
<th>2005</th>
<th>2010</th>
<th>2015</th>
<th>2020</th>
</tr>
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<tbody>
<tr>
<td>MPU Half Pitch (nm)</td>
<td>90</td>
<td>45</td>
<td>25</td>
<td>14</td>
</tr>
<tr>
<td>MPU Gate Length (nm)</td>
<td>32</td>
<td>18</td>
<td>10</td>
<td>6</td>
</tr>
</tbody>
</table>

Device diversification

90nm: HP, LOP, LSTP
45nm: UTB SOI
32nm: Double gate

2005 edition Toshiba 04
Industrial Partners

Global EDS vendor and world TCAD leader
600 licences of grid implementation, model implementation

UK fabless design company and world microprocessor leader
Core IP, simulation tools, staff time

UK fabless design company and world mixed mode leader
Additional PhD studentship for mixed mode design

Global semiconductor player with strong UK presence
Access to technology, device data, processing

Global semiconductor player with strong UK presence
Access to technology, device data, processing

Global semiconductor player with UK presence
CASE studentship, interconnects

Trade association of the microelectronics industry in the UK
Recruiting new industrial partners and dissemination
Collaboration

- Essential to assemble experts
  - Multi-discipline, Multi-organisation, Multi-national
- Hard to achieve
  - Instinctive competition
  - Trust slow to build
  - Communication is difficult
- Requirements
  - Leadership
  - Investment
  - New culture
  - Technology
Collaboration

- **Essential to assemble experts**
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- **Requirements**
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  - Investment
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Address these issues

Focus here
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