Building e-Infrastructure services & meeting diverse demands

David Wallom
UK NGS & University of Oxford

NGS

Overview

- Mission, goals and where we sit in national/international infrastructure
- Services and resource providers from within the UK research community
- Supporting user communities across the spectrum

NGS Mission and Goal

To enable coherent electronic access for all UK researchers to all computational and data based resources and facilities required to carry out their research, independent of resource or researcher location.

Goal:

- To enable a production quality e-infrastructure
- To deliver core services and support
- Integrate with international infrastructures following user community demand

UK e -Infrastructure

Users get common access, tools, information, nationally supported services, through NGS

ScotGRID

ULGrid

Regional and Campus grids

HPCx + HECtoR

HEIs

GridPP UK Computing for Particle Physics

eMinerals

BRIDGES

Community Grids

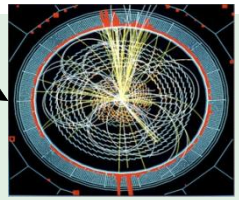
NGS

ja.net

VISTA

ALMA

diamond



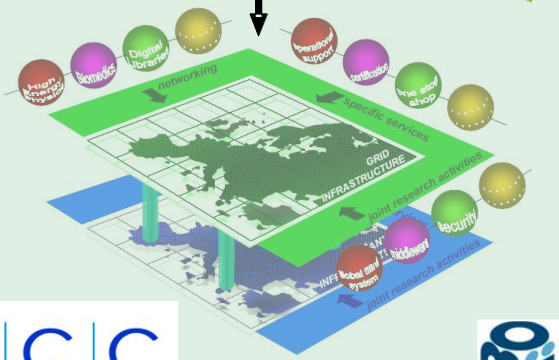
LHC

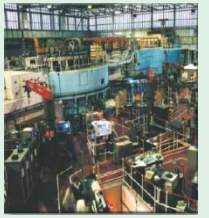
Integrated internationally

EMBL-EBI European Bioinfo

JISC

VRE, VLE, IE





ISIS TS2

EDINA®

MIMAS

BRITISH LIBRARY

DCC

open middleware infrastructure institute

Organisational Membership

- Personnel
  - Appointment of an institutional Campus Champion
    - Liaison between university/research organisation and NGS
  - Nomination of a senior institutional staff member for the NGS Collaboration Board
- Resource Exchanging
  - Regularly tested installation of NGS defined interfaces as described in the NGS Site Level Services Document
  - Partner
    - Supporting access by a significant body of NGS users
    - Publish a service level description (SLD) detailing the services offered
  - Affiliate
    - Maintains control over permitted users

NGS NGS Member Institutions, 2010

The University of Edinburgh
Manchester 1824
Imperial College London
University of Oxford
Royal Holloway University of London
BeSC Belfast e-Science Centre
University of Bristol
Science & Technology Facilities Council Rutherford Appleton Laboratory
University of Westminster
Brunel University West London
University of Southampton
Cardiff University
University of Glasgow
The University of Reading
Lancaster University
Keele University
Durham University
University of Birmingham
The University Of Sheffield
University of Liverpool
Queen Mary University of London
The University of York
wellcome trust sanger institute

Connecting Infrastructure Connecting Research

What does the NGS offer users?

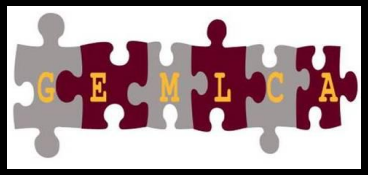
- Compute services
  - Access to more and different resources
  - Different ways of running jobs e.g. multi site MPI
  - Supporting ALL current available middlewares
- Data services
  - Access to data storage
  - Support and advice
  - New ways of accessing data (Including remote relational DB, Metadata Catalogues etc)
- Access Services
  - User facing services providing exemplar instances for methods to use available resources, developing new and innovative methodologies, e.g. Drop and Compute, Uniform Execution Environment
- Central Support services
  - Individual services needed to support user access, control and management

NGS

Specialist services

Westminster

- Operates and supports P-GRADE portal and GEMLCA legacy application support services



Belfast e-Science Centre

- Web Service Hosting Container Service
  - Web service containers into which projects or VOs can deploy their own Web or Grid services, using automatic deployment technology

Oxford e-Research Centre

- OMII-UK GridSAM
  - OGF HPC-Basic Profile compliant Job submission
  - Promoting interoperability with international grids
- Eucalyptus Cloud system
  - Exposing AWS compatible interfaces and functionality to NGS users

Edinburgh

- Eucalyptus Cloud system

STFC Rutherford Appleton Laboratory

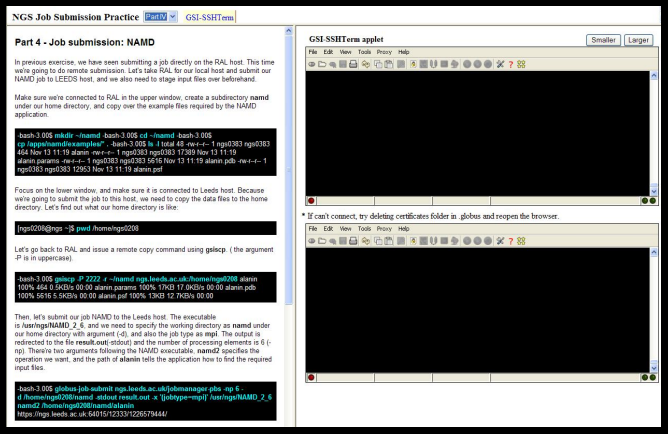
- Visualisation using specialised cluster from within the STFC e-Science Viz group

NGS Support and Training

National helpdesk
Campus Champion

NGS Road Shows

Local & national training events



Online tutorials
and practicals

Connecting Infrastructure Connecting Research

NGS Outreach

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Collaborations

GridPP
UK Computing for Particle Physics

UKIF
UK & Ireland Federation

omii-uk
Software Solutions for e-Research

EGI

eGee
Enabling Grids for E-sciencE

TeraGrid

LONI

SAGA

Open Science Grid

KiSTi

OpenGridForum
OPEN FORUM | OPEN STANDARDS

IGTF
International Grid Trust Federation

arcs
Australian Research Collaboration Service

DataMINX

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NGS

Events

NGS UF/IF, road shows

IEEE Celebrating 125 Years of Engineering the Future

18th - 21st September East Midlands Conference Centre UK e-Science ALL HANDS MEETING 2006

GridPP UK Computing for Particle Physics

SC2004 SC08 AUSTIN,TX SC06 POWERFUL BEYOND IMAGINATION SC07 SC05

eGee Enabling Grids for E-sciencE

EGEE'08 Conference 22-26 September 2008 Harbiye Askeri Museum, Istanbul - Turkey

CONDOR

globusWORLD™

- Community Conferences
  - CCPb, Bioinformatics,

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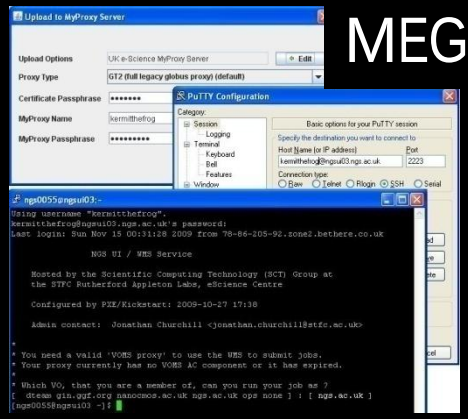
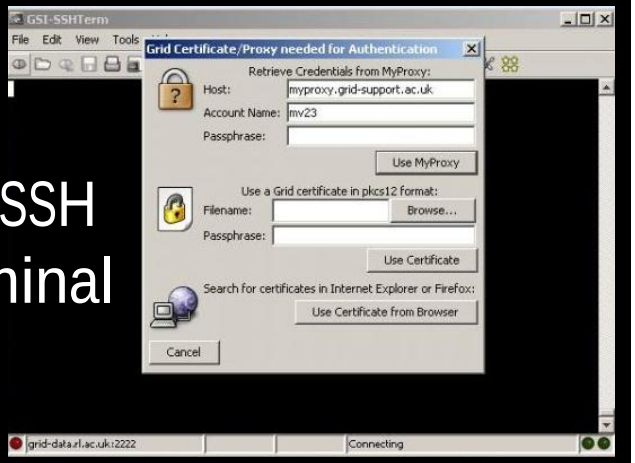
User access

Direct access

MEG



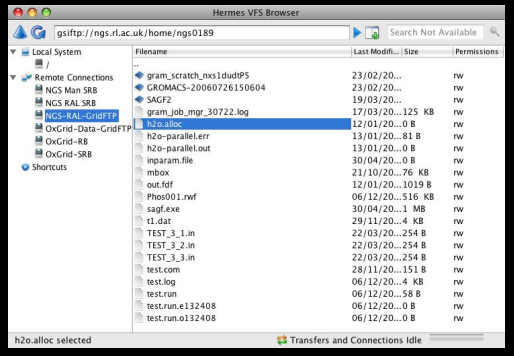
GSI-SSH terminal



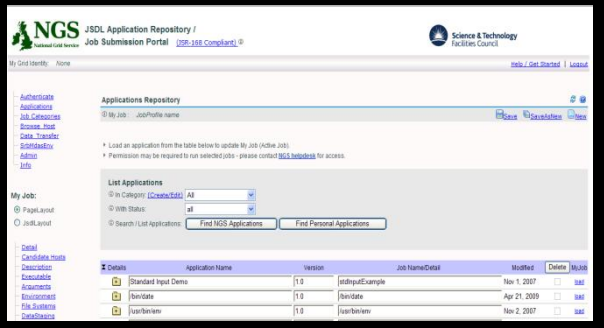
SARoNGS

WMS

Application Hosting Environment (AHE)



HERMES Data Access



NGS Portal/ Applications Repository

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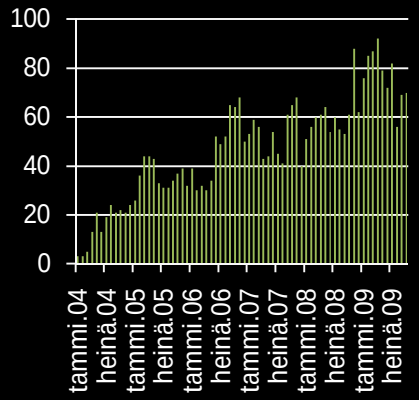
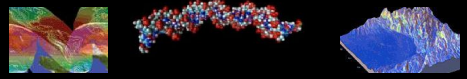
NGS

www.ngs.ac.uk

>1000 cpu, ~500 db
~200 MyProxy users

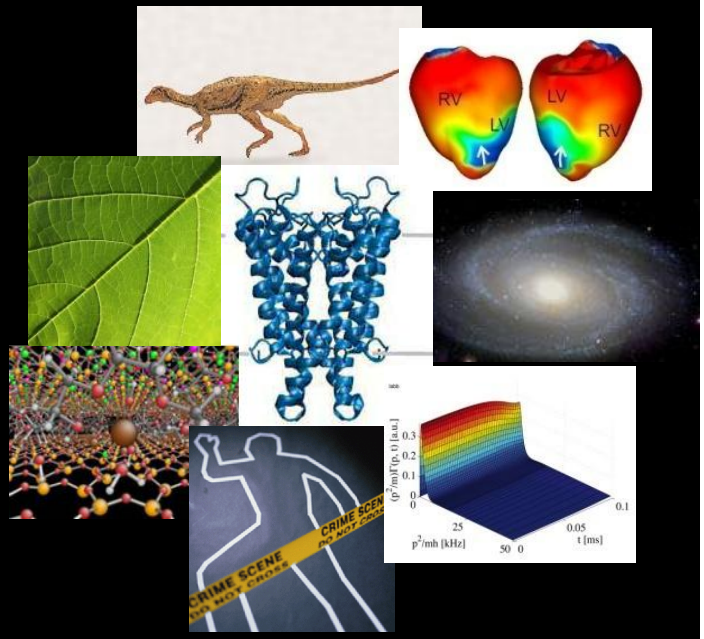


> 75 applications

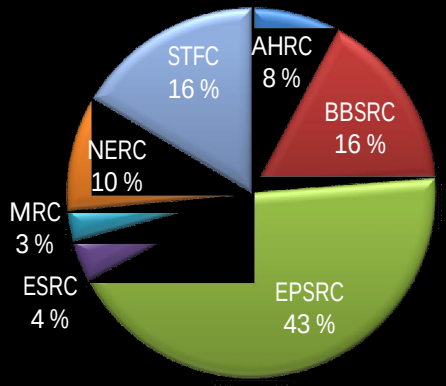


25 member institutes
33 heterogeneous resources
15,000 processing cores

Diverse User Community



Funding Source



2nd largest e-Science CA
- 22,121 certificates issued
- 4,911 active currently

In the last 12 months
- 4,629,127 CPU hrs used
- 888,862 jobs ran

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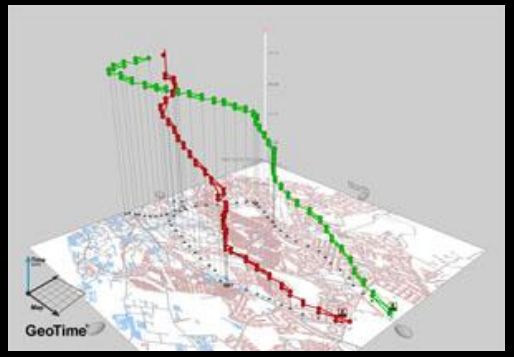
Security

Predicting Crime
Nick Malleston, Leeds University

- burglary rates
- agent-based predictive models
- vary environmental factors, predicts burglar's behaviour



adapted Java program to run across Grid

NGS speeds things up
- 2.5 years of results in under a week

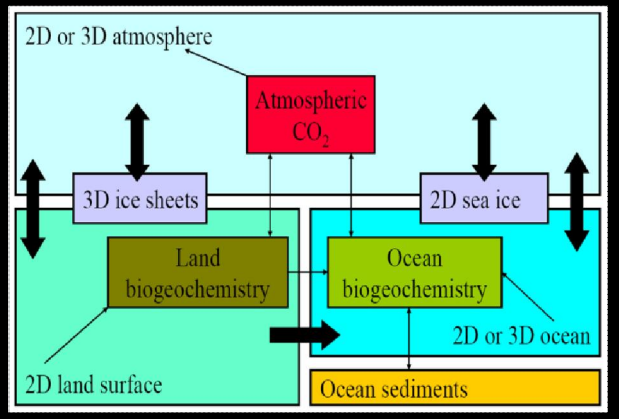
NGS

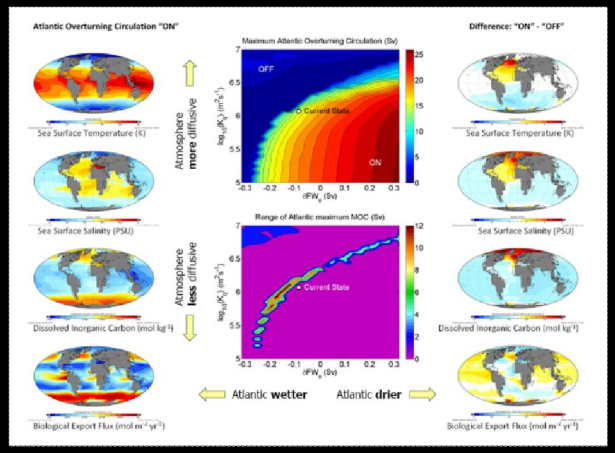
Environment

Oceans and Climate

Andrew Price, GENIE project, Southampton

- thermohaline circulation in oceans
- integrates component earth models
- future climate prediction





- 5 yrs computations in 3 months
- integrates NGS, National HPC and institutional computation
- NGS hosts database
- users share simulations, metadata

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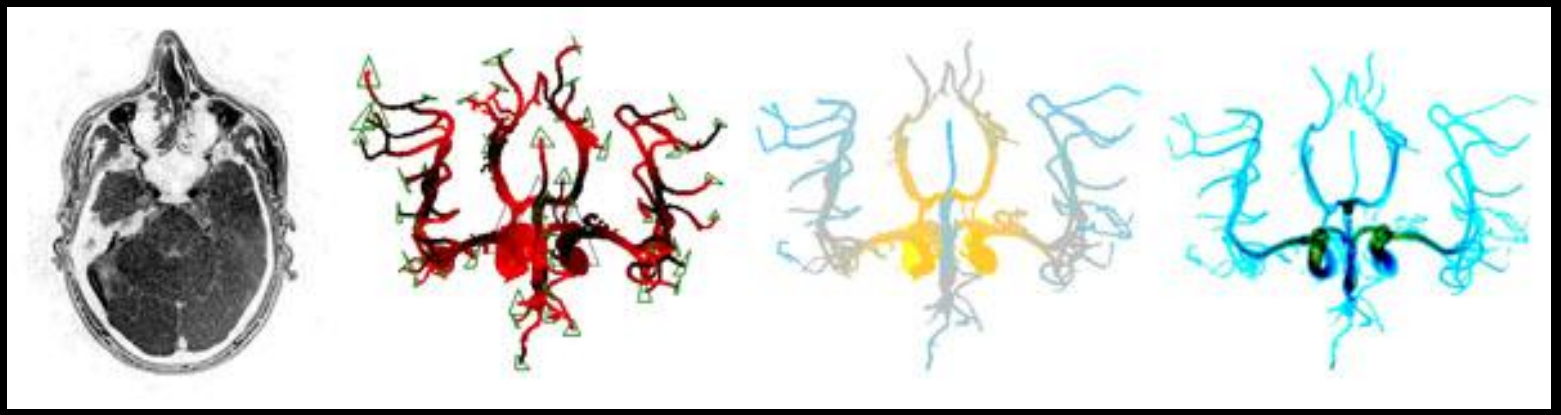
Health

Cerebral blood flow

GENIUS project

- processes 2D MRI images, recreates 3D vasculature map
- visualise and steer the model in real time
- advanced resource reservation
- utilize international federated grid of supercomputers



http://wiki.realitygrid.org/wiki/GENIUS

NGS

Astrophysics

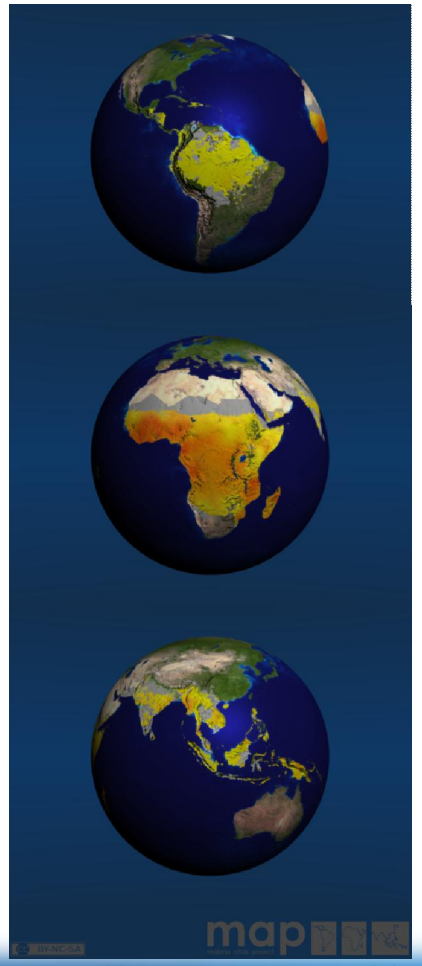
Distributed Astronomy Databases on the NGS

- *Helen Xiang and Professor Robert Nicol at the University of Portsmouth*
- *Linking multiple data sources, private and public*
- *Utilising open, standard interfaces*
- *Simple retrieval of the data using one command.*

Institutional User communities

- Malaria Mapping (HTC, large data)
- Phylogenetic Analysis of DNA (large data)
- Analysis of Clinical ECG data (real-time processing)
- Biochemistry (linked HPC & HTC)
- Astronomy (national data access)
- Chemistry (Specialist software)
- Satellite image analysis (HPC & special software)
- Heart modelling (National, regional and institutional HPC access)

- Supporting direct campus to national resourcs integration.



http://www.maps.ox.ac.uk/

NGS

Conclusions

- NGS is here to support university research computing services support their research communities by making connection of ITS enabled resources easier
- Connectivity using standard interfaces to include UK national data sources including EDINA, MIMAS, NADS as well as experimental facilities such DIAMOND, e-Merlin, ISIS and JET
- The NGS supports UK participation in all ESFRI projects for connectivity of e-infrastructure
- We must remember the importance of all users

NGS

Thank you & questions

david.wallom@oerc.ox.ac.uk

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