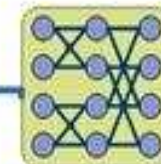




What the University of Westminster Gained from Being an NGS Partner Site

Gabor Terstyanszky & Stephen Winter
Centre for Parallel Computing
University of Westminster

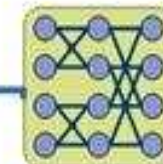
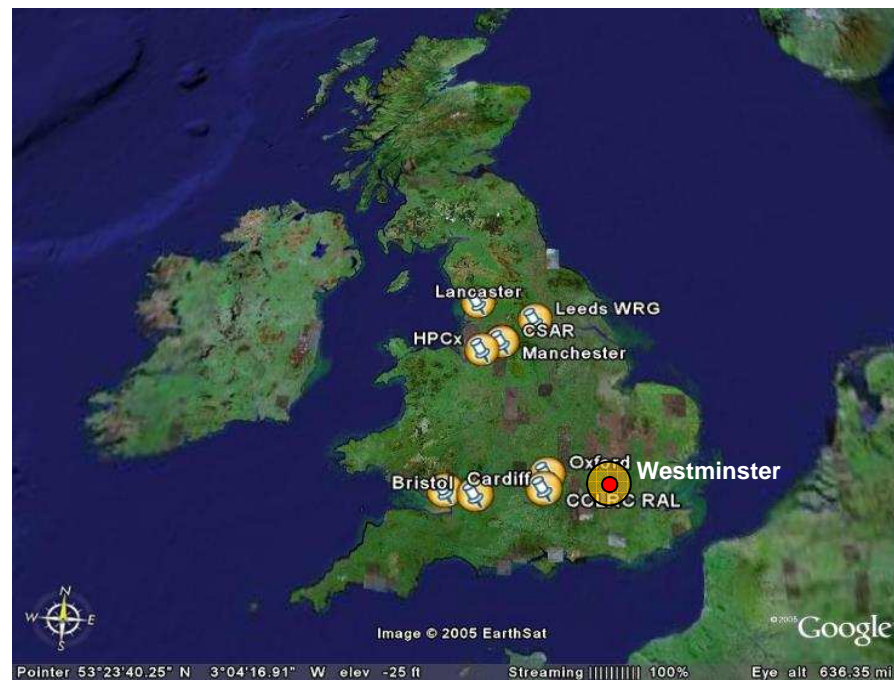




NGS and Westminster

University of Westminster joined NGS as a Partner site in February 2007. Since that time we have obtained expertise in:

- infrastructure management
- production-level service provisioning
- application and user support



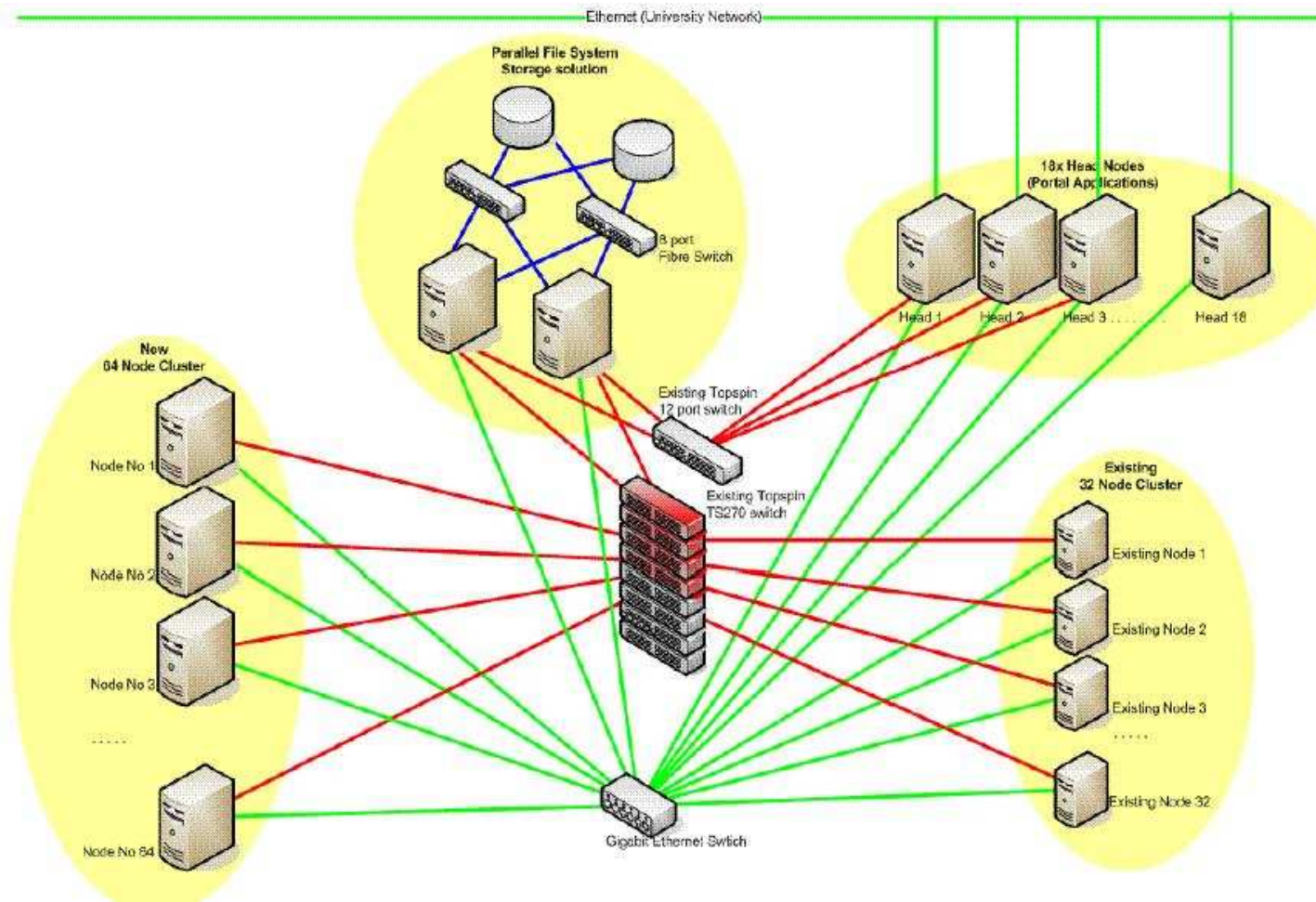


Infrastructure offered by Westminster

Tristan cluster/services	Carmen cluster/services
32 nodes with Intel Xeon / 512MB (Sun Cluster)	64 nodes with 256 AMD Opteron Rev F cores, 4GB (IBM Cluster) + 18 head nodes
SLES9 x86	SLES10 (SP1) x86_64
Infiniband (Topspin drivers)	Infiniband (OFED drivers)
70GB NFS - IPoIB	11TB RAID5 GPFS – RDMA
No virtualisation	Xen virtualisation
Condor	Torque + Maui
Vdt 1.2	Vdt 1.8.1
GT4	GT4



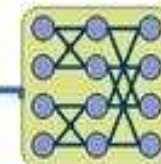
Carmen and Tristan clusters





Services provided by Westminster

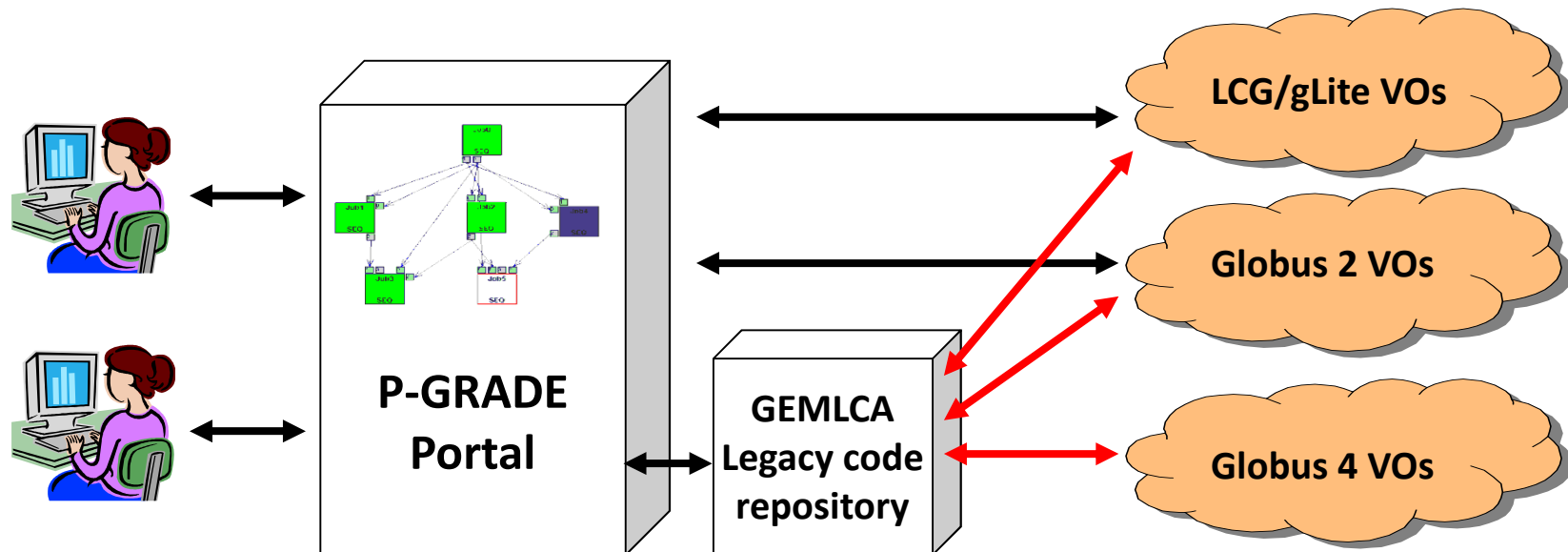
Previous Tristan cluster/services	Current Carmen cluster/services
Portal - NGS P-GRADE portal v2.3	Portal - NGS P-GRADE portal v2.4.1
Legacy code support - GEMLCA 2.3	Legacy code support – GEMLCA 3.2
Workflow editing and execution support	Workflow editing and execution support
	Workflow interoperability (Kepler, P-GRADE, Taverna and Triana WE's)
	Data transfer support (GridFTP, OGSA-DAI, SRB and SRM)
	Access to multiple Grids (gLite-based and GT2/GT4-based)





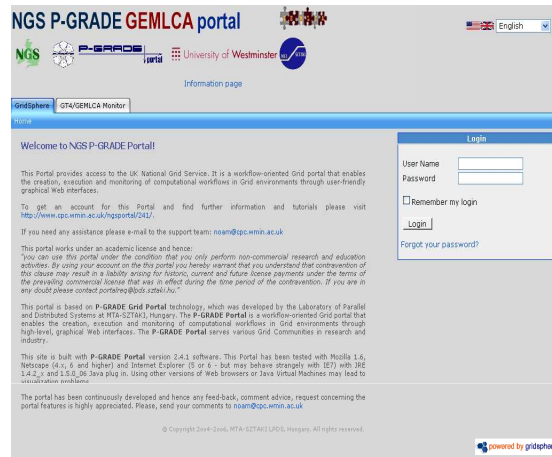
Services: NGS P-GRADE Portal

- General-purpose, workflow-oriented computational Grid portal
- Enables running legacy code applications on the Grid
- Provides access to multiple Grids



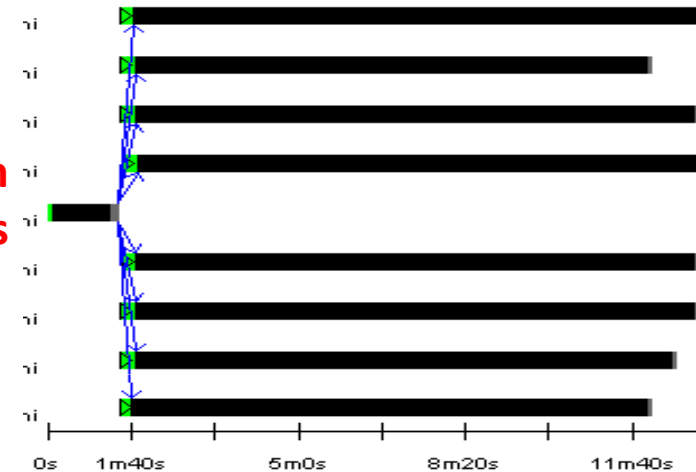


Services: NGS P-GRADE Portal

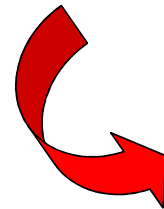


Log in to portal

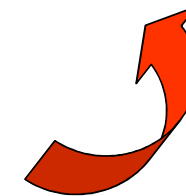
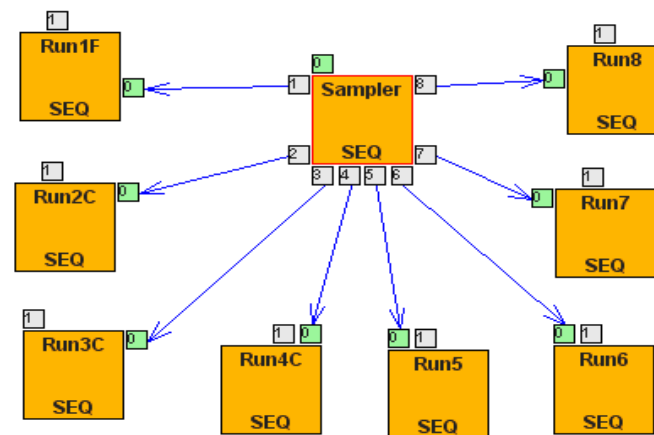
Visualise execution and download results



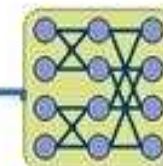
Create workflow



Map workflow to resources



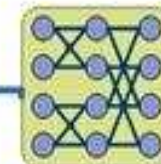
Execute workflow





Technical experience gained

- Deploying and managing resources and services on clusters
- Interfacing with gLite and GT2/GT4 clusters
- Creating and managing Virtual Organisation
- Learning how to use virtualisation technology in e-infrastructure
- Providing automated mapping of NGS users to GT4 grid-mapfile
- Mapping cluster accounts to users' e-mail addresses



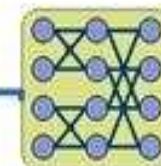
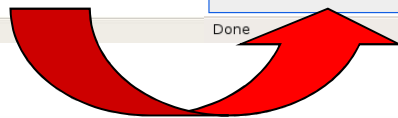


WS-PGRADE Science Gateway

Set input parameters
Upload input files
Select execution sites

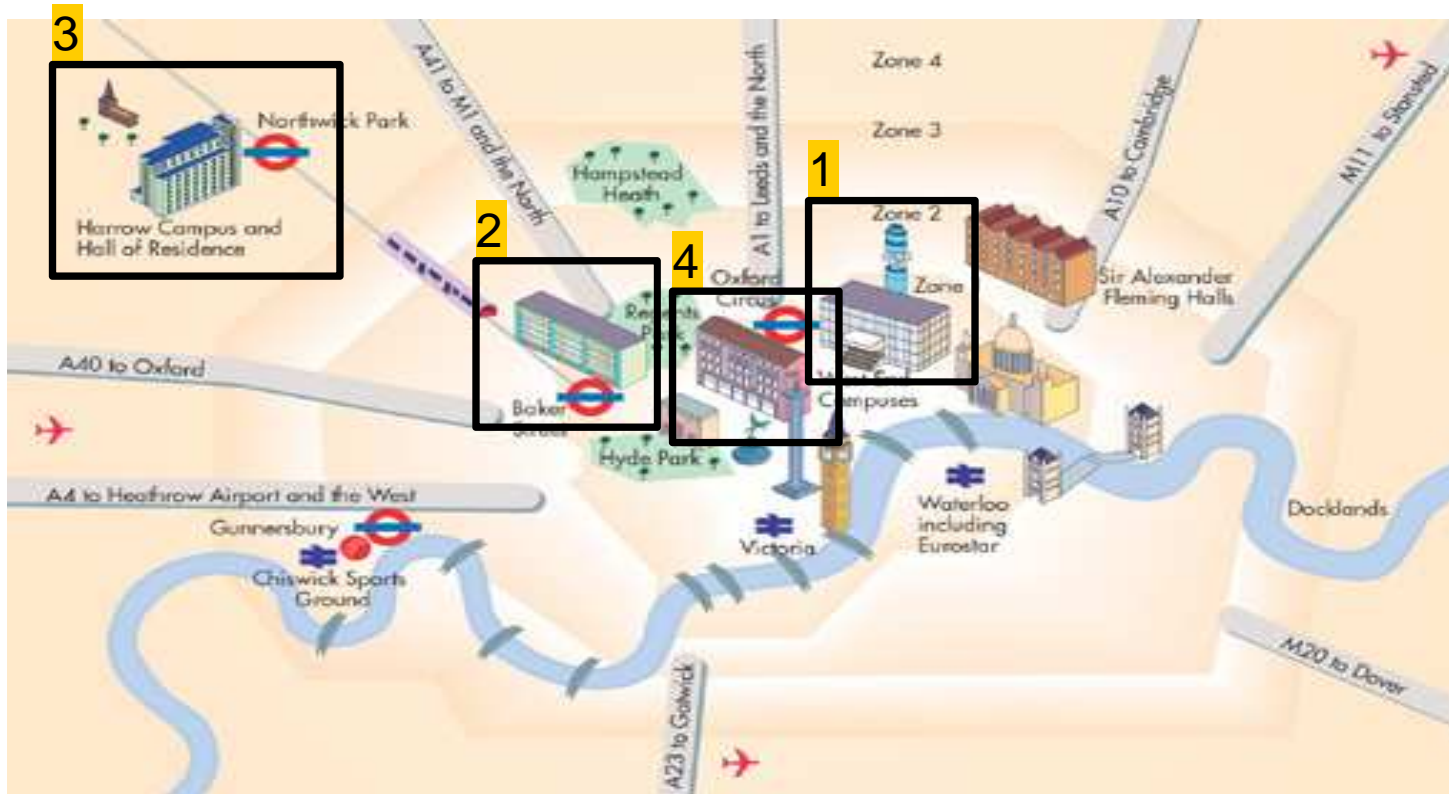
Follow execution progress
Typical execution time: 24 hours

Status	Instances
init	66
running	1
done	2
error	0
sum:	69

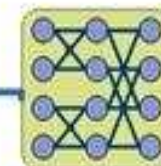




Westminster Local Desktop Grid



Cavendish Campus	550 nodes
Marylebone Campus	550 nodes
Harrow Campus	250 nodes
Regent Campus	400 nodes

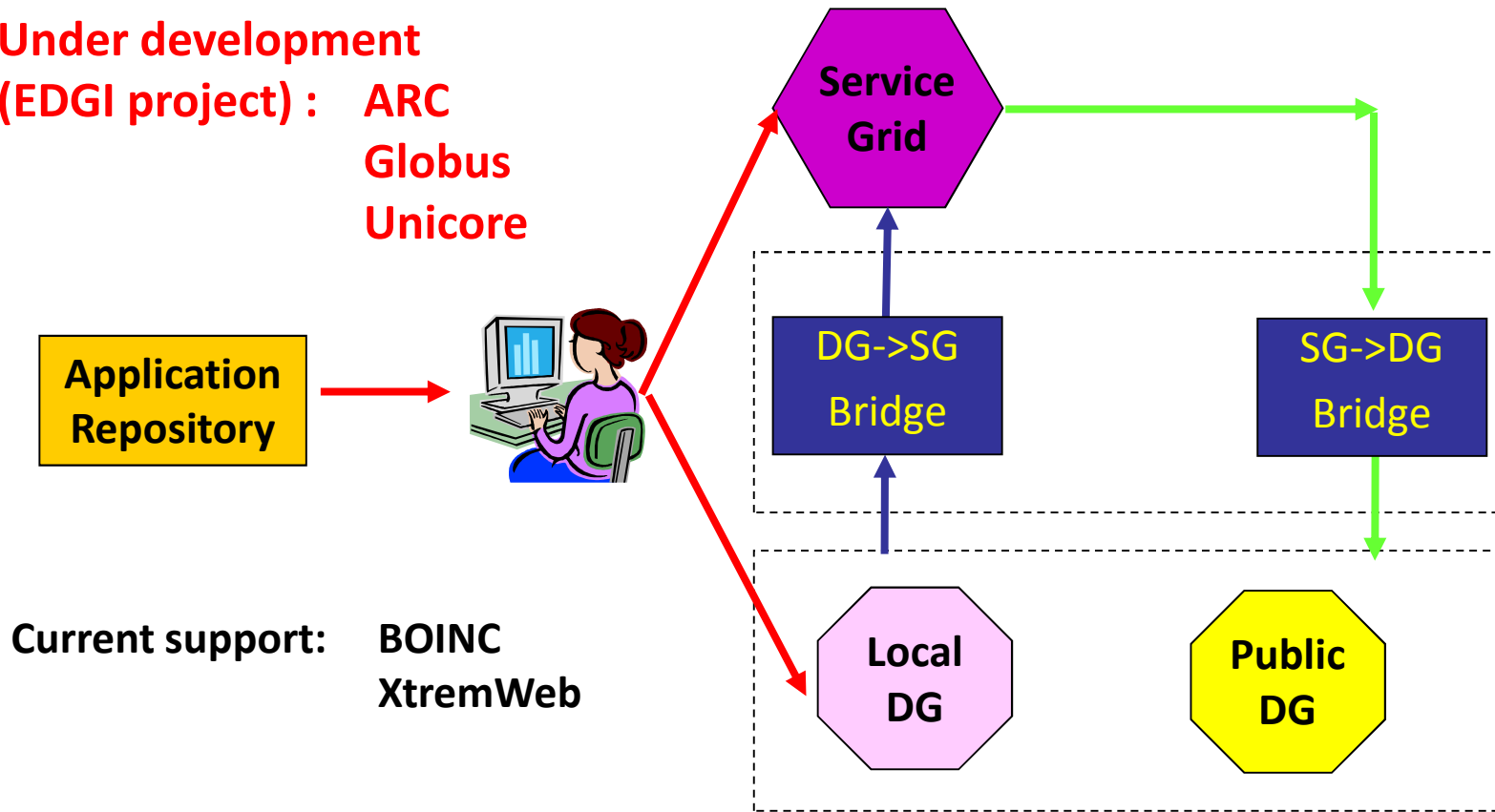




Desktop & Service Grid Interoperability

Current support: gLite

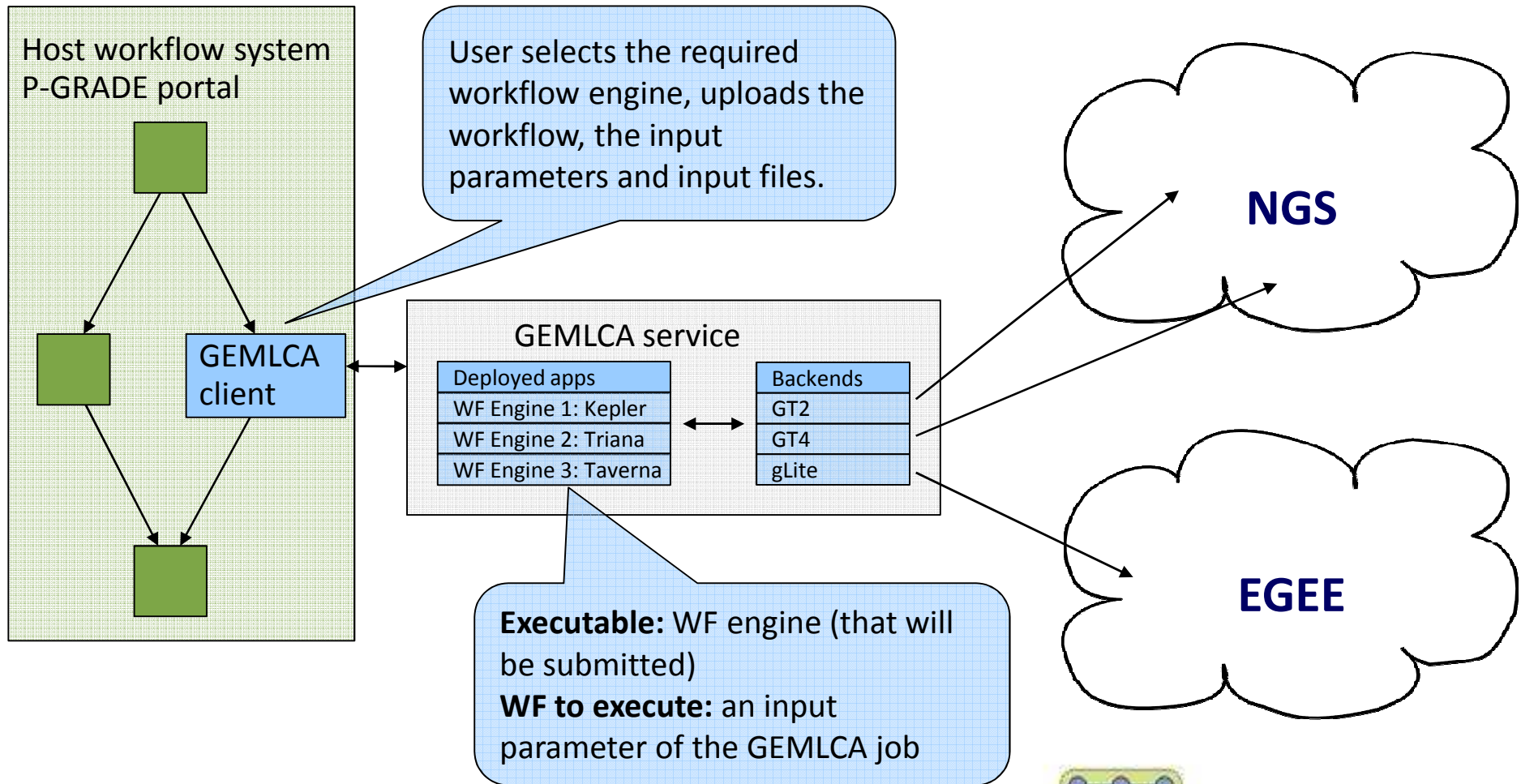
Under development
(EDGI project): ARC
Globus
Unicore



Current support: BOINC
XtremWeb



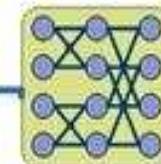
Workflow Interoperability





Service Provisioning experience gained

- Deploying and managing a general-purpose, workflow-oriented computational Grid portal
- Supporting running legacy code applications on the Grid
- Providing access to multiple Grids including desktop and service Grids
- Offering coarse-grained workflow interoperability solutions
- Providing access to different databases and file systems

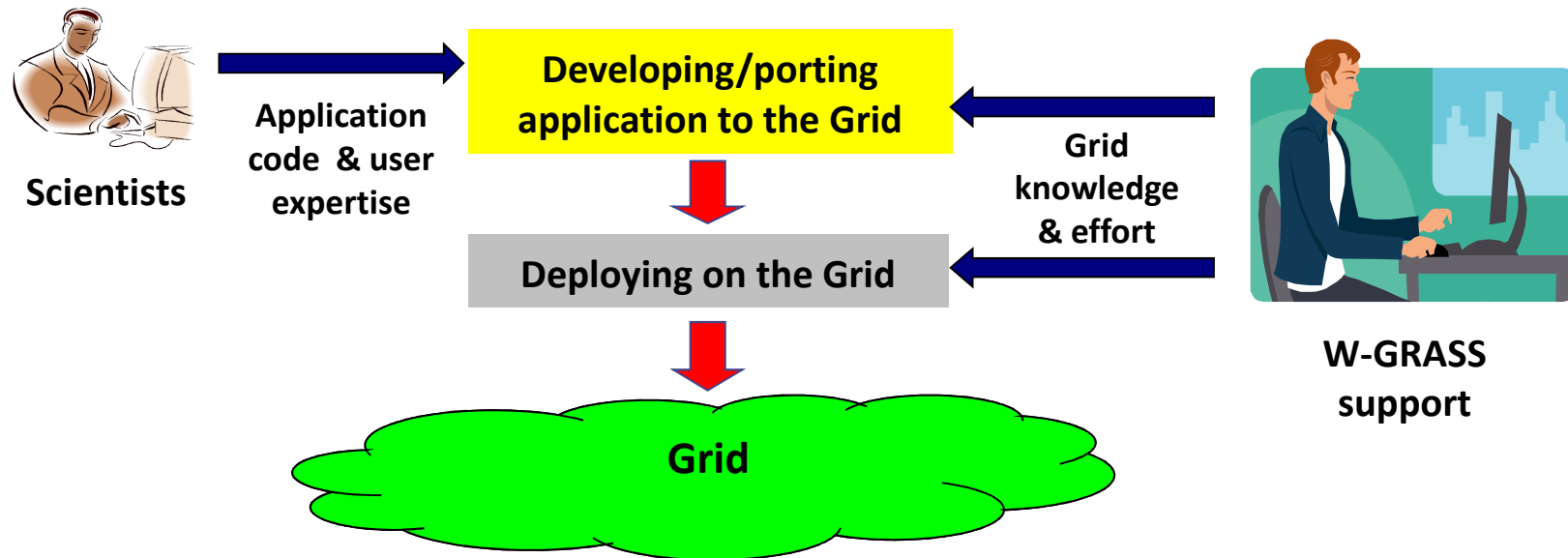




Application and User Support

W-GRASS: Westminster GRid Application Support Service

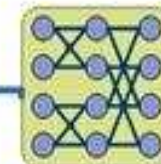
- Migrating existing applications to the Grid
- Developing new applications for the Grid
- Deploying desktop Grids





W-GRASS: Applications ported

	Desktop Grid	Service Grid
Astrophysics	1	2
Bio-science	4	8
Engineering	1	2
Multimedia	1	2
Physics	2	2





Some Applications supported by W-GRASS

Astrophysics:

- **VisIVO** - Visualisation Interface to the Virtual Observatory

Bio-science:

- **CHARMM** - Macromolecular simulation for energy minimisation
- **Patient Readmission**
 - NHS hospital patient readmission rate analysis using R
- **ProSim** - AutoDock & GROMACS to model docking
- **RNAP** - Simulating ribonucleic acid polymerases (RNAP)

Engineering:

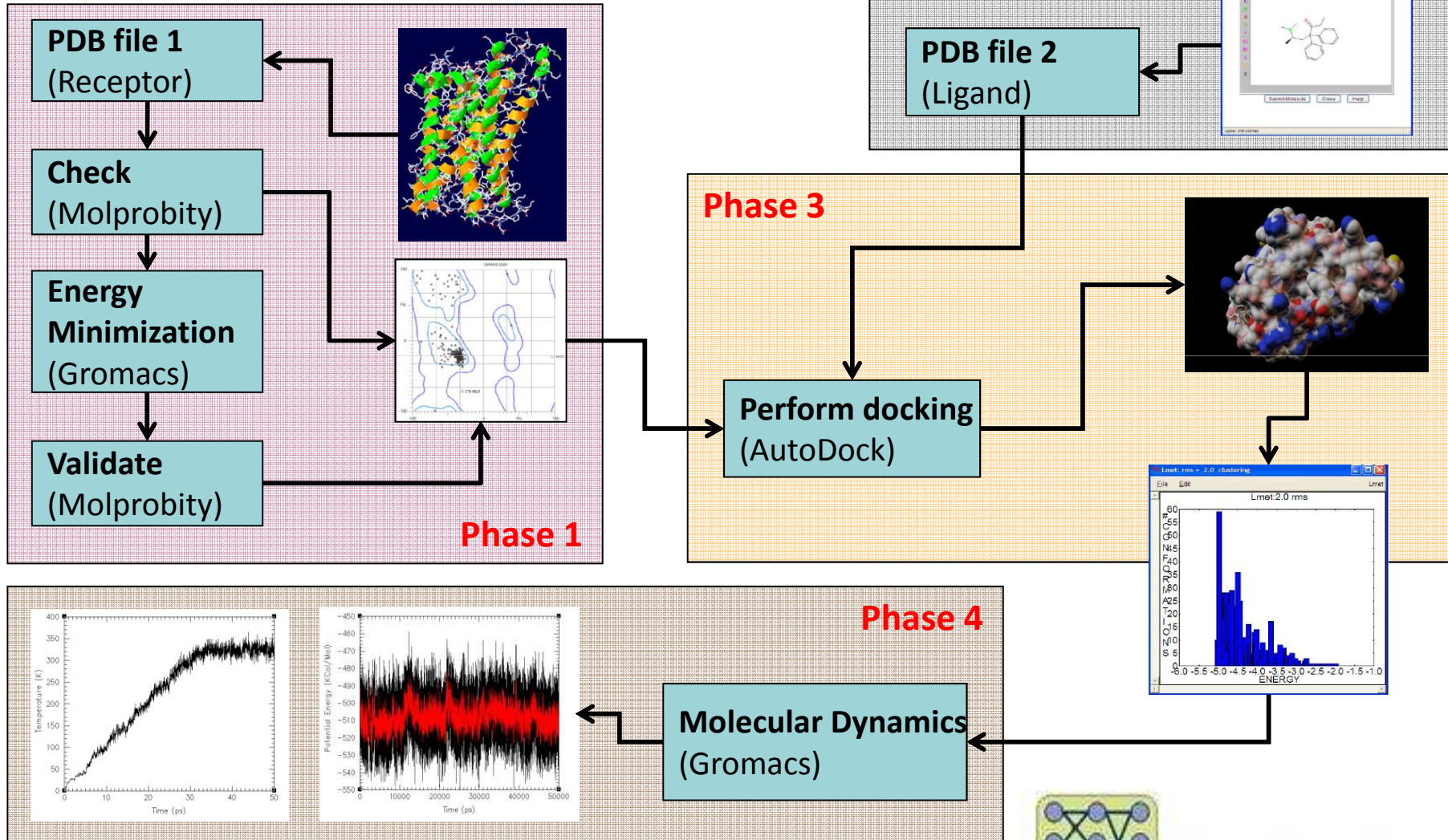
- **DSP** - Optimal periodic non-uniform sampling sequence calculation
- **MadCity** - Urban road traffic simulation

Multi-media:

- **Rendering** - Animation & image rendering using Blender
- **Video Streaming**
 - On-line access to arts film archive

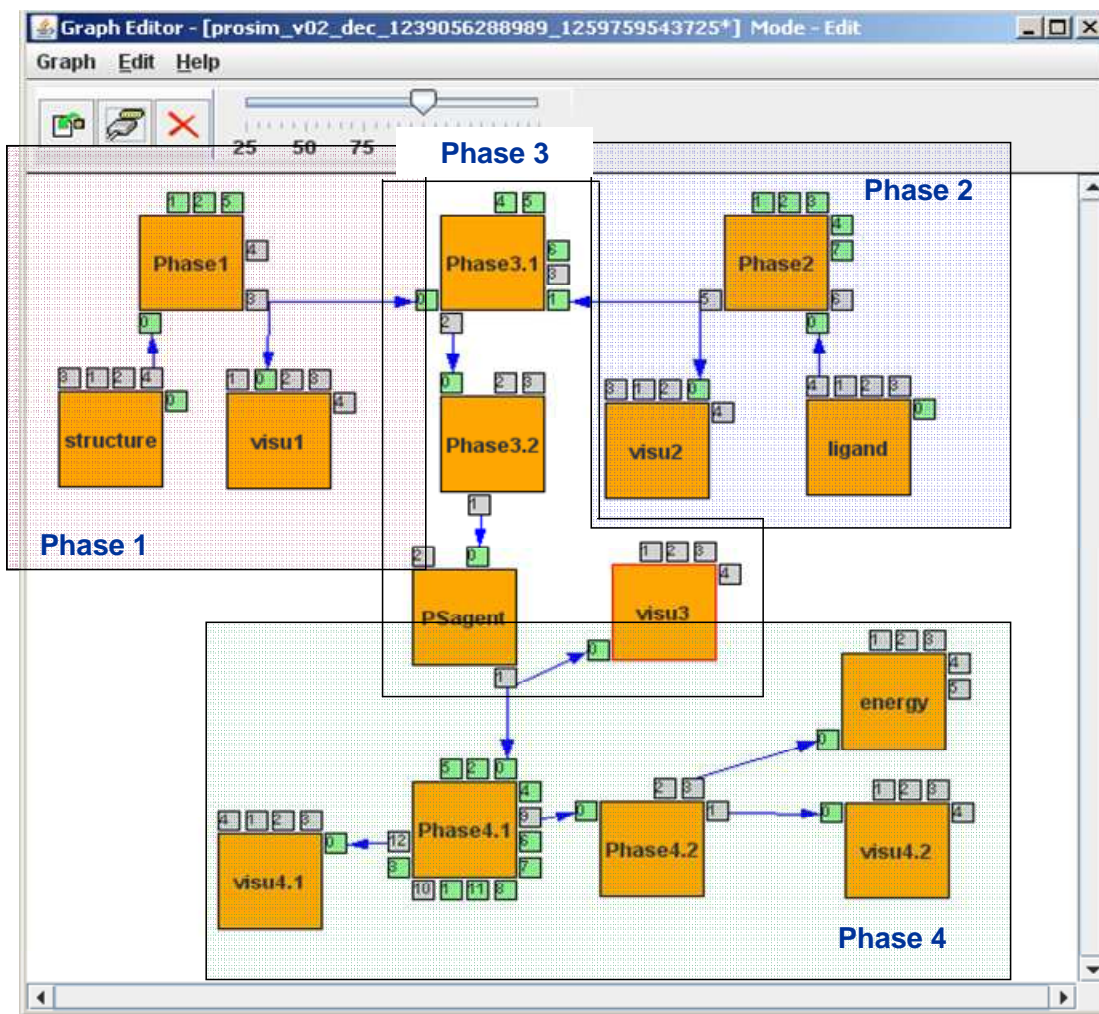


The ProSim User Scenario





The ProSim Workflow in WS-PGRADE



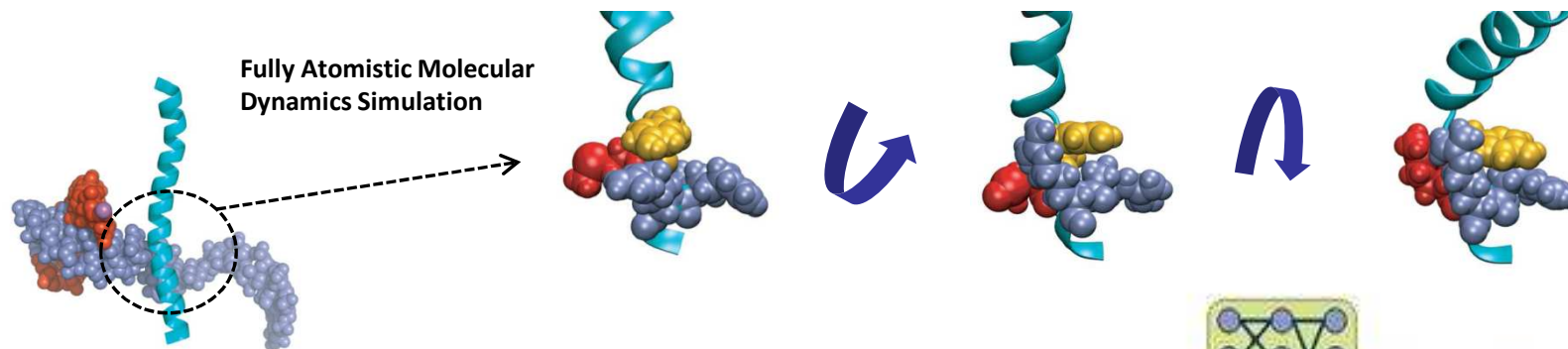
- Combination of GEMLCA and standard g-USE (ie. Globus) jobs
- Executed on 5 different sites of the UK NGS
- Parameter sweeps in phases 3 (via a script) and 4 (via WS-PGRADE parameter sweep)



RNAP: Ribonucleic Acid Polymerases Simulation

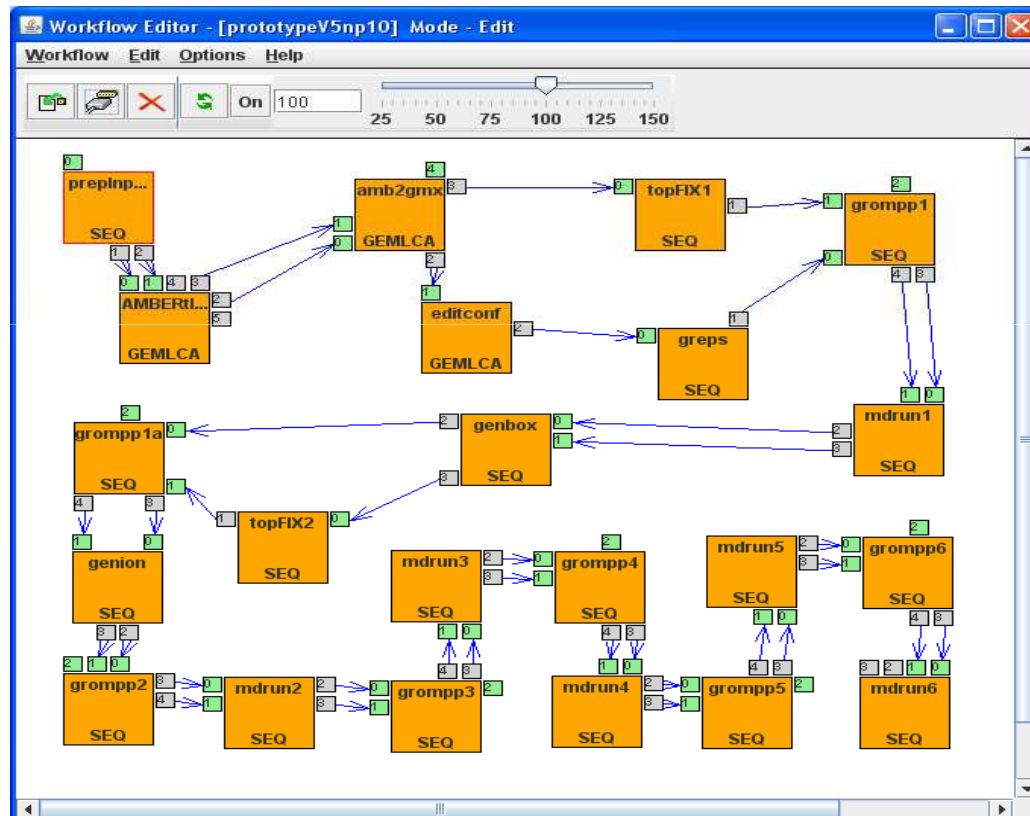
Motivation and challenges:

- Conventional *in-vitro* experiments are slow and expensive. Prefer to model RNAP structure using molecular dynamics packages, but on conventional systems, *in-silico* experiments are laborious.
- MD is compute resource hungry, and also error prone - available packages may not produce accurate binding solutions, requiring multiple parameter sweeps.
- Ideal test case.





RNAP: Simulation Workflow



- GEMLCA and g-USE jobs
- Several NGS sites
- Includes parameter sweeps



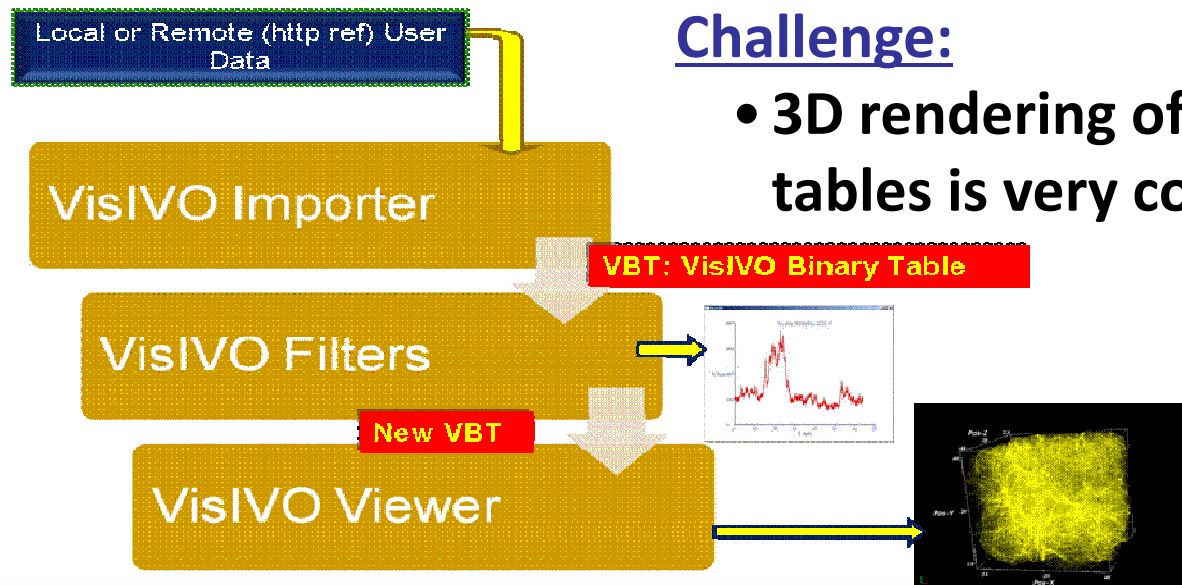
VisIVO: Visualization Interface to the Virtual Observatory

Motivation:

- Enable e-scientists to create customized views of 3D renderings from astrophysical data tables and support high-performance, multidimensional visualization

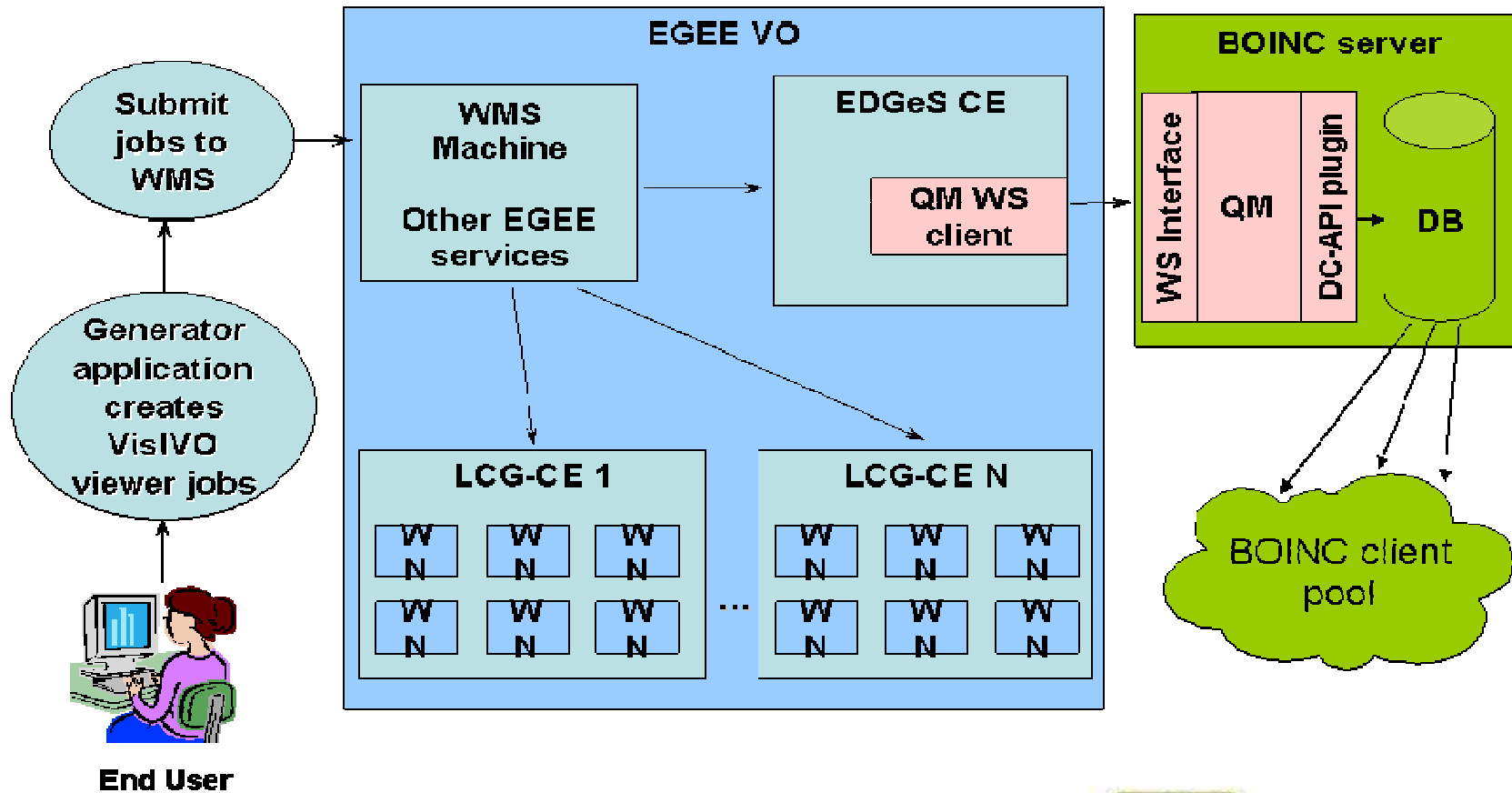
Challenge:

- 3D rendering of extremely large data tables is very compute intensive





VisIVO: Implementation





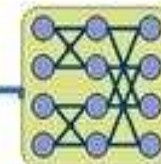
3D Model Rendering Portal

The screenshot shows the 'Rende Rendering' portal interface. At the top, it says 'RELEASE 2.5' and 'P-GRADE'. The main navigation includes 'New rendering job', 'Manage rendering jobs', and 'Help'. A 'portal' logo is also visible. The 'New rendering job' form contains fields for 'Name' (knight), 'Type' (Blender), 'Start frame' (1), 'End frame' (100), and 'Step size' (1). A 'Next' button is at the bottom of the form. A callout bubble points to the 'Create' button, stating 'Workflow created by pressing this button'. Below the form, a 'File Upload' dialog is open, showing a file list in the 'EGEE 07 demo' directory. The file list includes 'knight.blend', 'knight-Fast.blend', 'long.blend', 'longer.blend', 'lostride.blend', and 'SZTAKI_tamas_charmm_NGS_12[1].tar'. A callout bubble points to the 'knight.blend' file, stating 'Select Blender input file'. A curved arrow points from the 'Next' button to the 'File Upload' dialog. Another callout bubble points to the 'Name' field, stating 'Give unique name, define frames to be rendered'.



Application Support experience gained

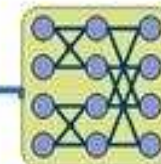
- Running application support for e-scientists who have only basic IT knowledge
- Learning how to identify and approach prospective user communities
- Developing a methodology to migrate applications to desktop and service Grid
- Working together with e-scientists, and citizens, to migrate and run their applications on the Grid





Some Lessons Learnt

- Developing rapport with users in any domain, including science, takes time and patience
- Keep within your respective domains of expertise and avoid straying
 - Invest in developing cross-domain collaboration
- Graphical workflow is universal abstraction
 - Can capture user workflow
 - Maps readily into grid workflow
- Keep the GUI simple





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Any questions?

