IDGF
International Desktop Grid Federation

Running applications on Desktop Grids from the WS P-GRADE portal

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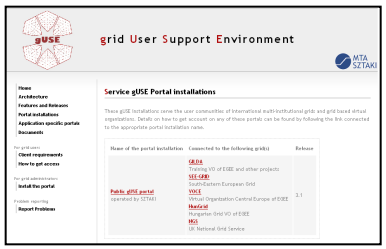
Family of P-GRADE Portal products

- P-GRADE portal
  - Creating (basic) workflows and parameter sweeps for clusters, service grids, desktop grids
  - *www.portal.p-grade.hu*
- P-GRADE/GEMLCA portal (University of Westminster)
  - To wrap legacy applications into Grid Services
  - To add legacy code services to P-GRADE Portal workflows
  - *http://www.cpc.wmin.ac.uk/cpcsite/gemlca*
- WS-PGRADE
  - Creating complex workflow and parameter sweeps for clusters, service grids, desktop grids, databases
  - Creating complex applications using embedded workflows, legacy codes and community components from workflow repository
  - *www.wspgrade.hu*

References and WS-PGRADE/gUSE installations

- WS-PGRADE Portal service is available for
  - GILDA - Training VO of EGEE and other projects
  - SEE-GRID - South-Eastern European Grid
  - VOCE - Virtual Organization Central Europe of EGEE
  - HunGrid - Hungarian Grid VO of EGEE
  - NGS - UK National Grid Service
  - Desktop Grids: SZTAKI DG, UoW Local DG
- Users and projects using WS-PGRADE/gUSE
  - EDGeS project (Enabling Desktop Grids for e-Science)
    - Integrating EGEE with BOINC and XtremWeb technologies
    - User interfaces and tools
  - ProSim project
    - In silico simulation of intermolecular recognition
    - JISC ENGAGE program
  - EPSRC Cloud Pilot
    - Using AutoDock on institutional PCs extended with Cloud workers
  - CancerGrid project
    - Predicting various properties of molecules to find anti-cancer leads
    - Creating science gateway for chemists



WS-PGRADE in a nutshell

- **General purpose, workflow-oriented portal.** Supports the development and execution of workflow-based applications
- Based on **GridSphere (latest version on Liferay)**

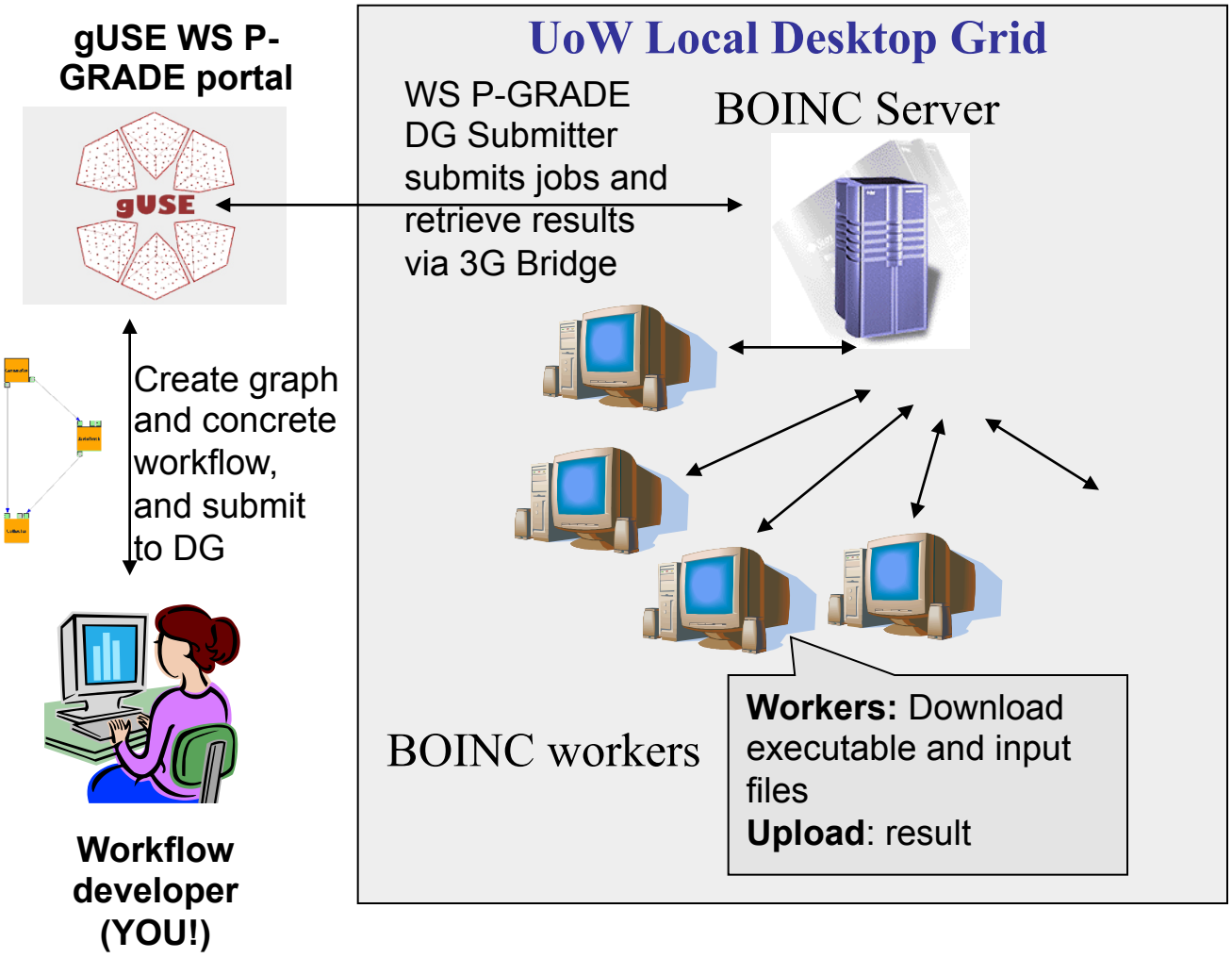
Service	EGEE grids (LCG2,GLite)		Globus grids (GT2,GT4)		Desktop grids	clusters
Job execution	✓	✓	✓	✓		
File storage	✓	✓	✓	✓		
Certificate management	✓	✓	✓	✓	✓	✓
Information system	✓	✓	✓	✓		
Brokering	✓	✓	✓	✓		
Job monitoring	✓	✓	✓	✓		
Workflow & job visualization	✓	✓	✓	✓		

WS-PGRADE + gUSE = ✓

P-GRADE = ✓

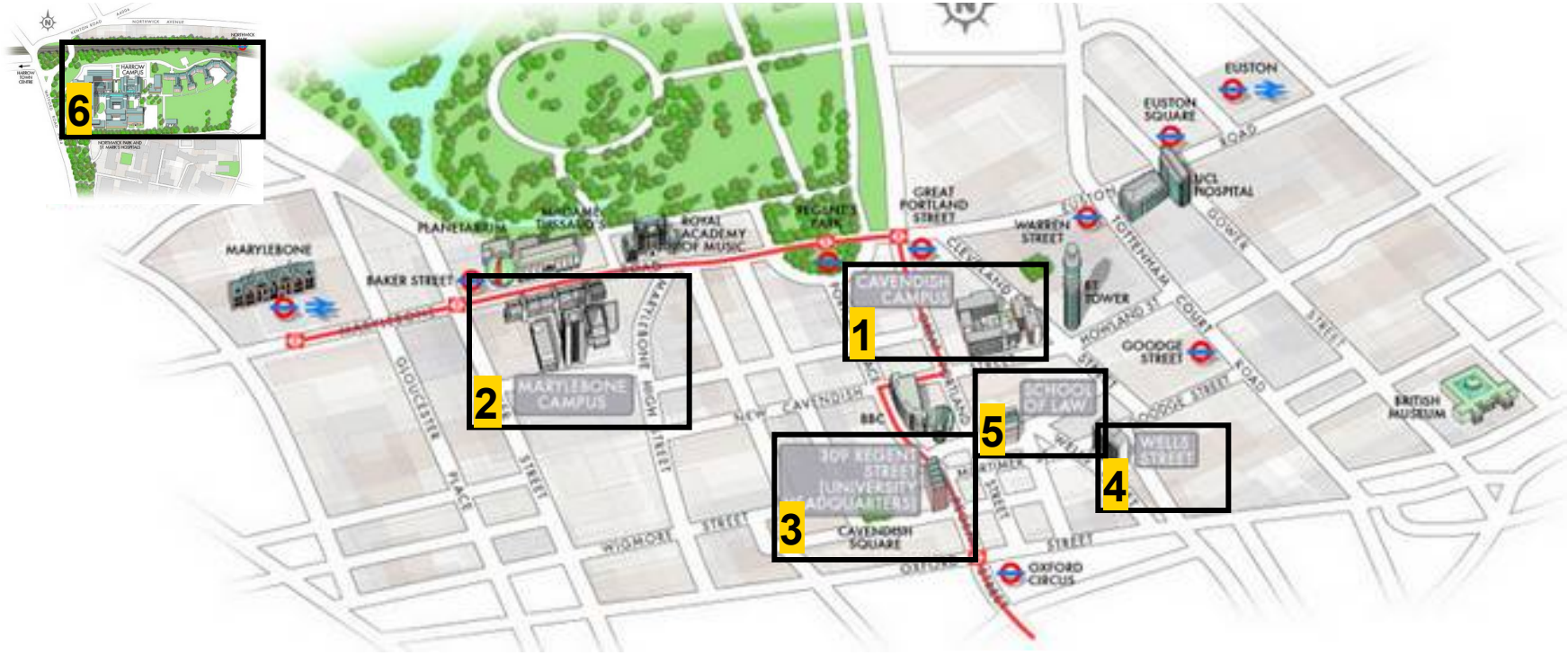
Solves service Grid/desktop Grid/cluster interoperability problems at workflow level

The tutorial scenario



The University of Westminster Local DG

- Over 1500 Windows PCs from 6 different campuses



1.	New Cavendish Street	576 nodes
2.	Marylebone Campus	559 nodes
3.	Regent Street	395 nodes
4.	Wells Street	31 nodes
5.	Little Tichfield Street	66 nodes
6.	Harrow Campus	254 nodes

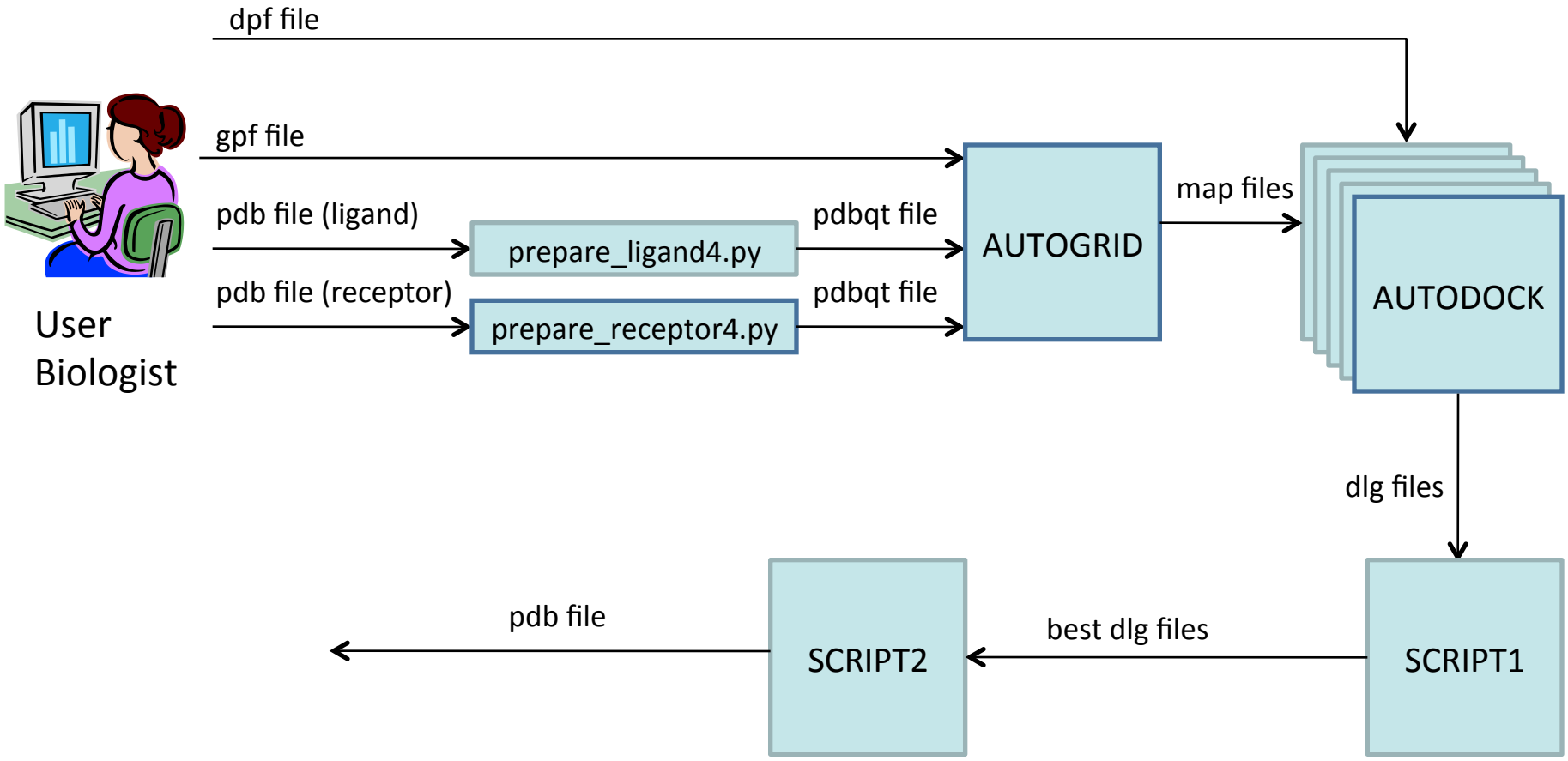
Lifecycle of a node:

1. PCs basically used by students/staff
2. If unused, switch to Desktop Grid mode
3. No more work from DG server -> shutdown (green solution)

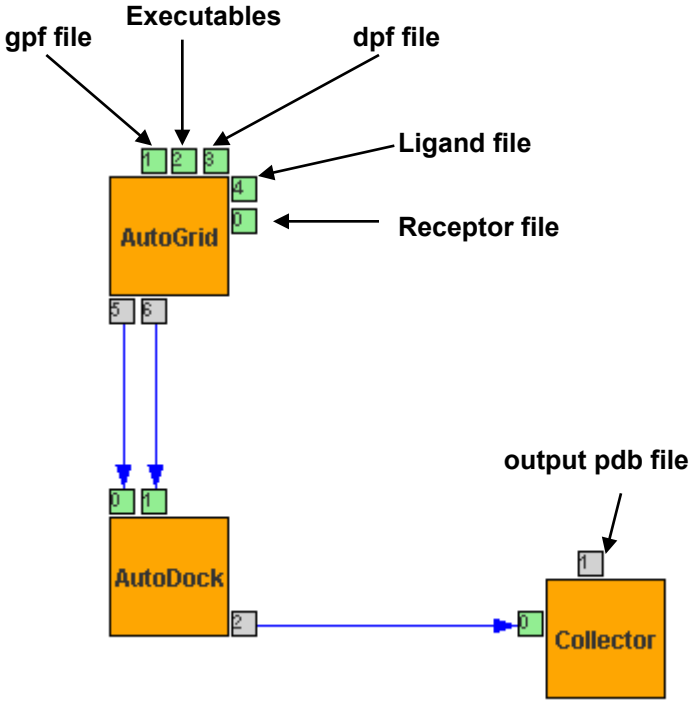
e-infrastructure

The Application
AutoDock molecular docking

AutoDock is a suite of automated docking tools designed to predict how small molecules, such as substrates or drug candidates, bind to a receptor of known 3D structure.

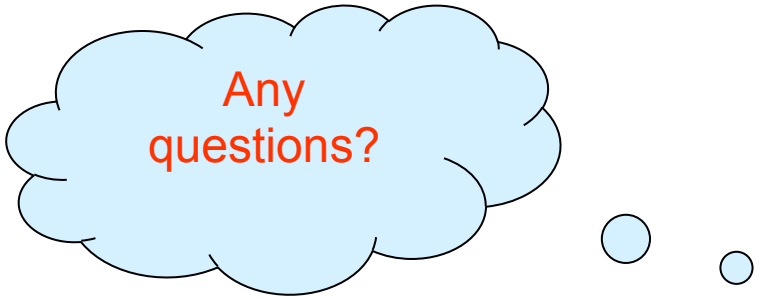


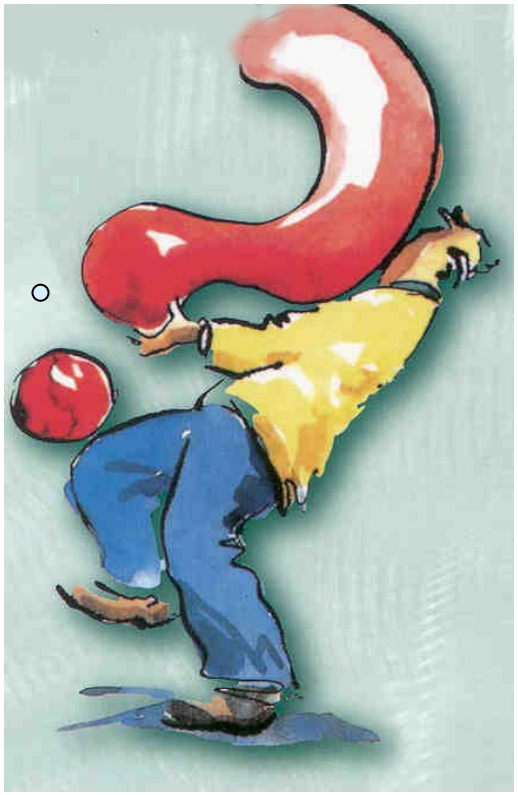
The workflow you will create



1. The AutoGrid job runs the AutoGrid application and creates specified numbered of AutoDock jobs.
2. The AutoDock jobs are running on the Desktop Grid. As output they provide dlg files.
3. The Collector job collects the dlg files. Takes the best results and concatenates them into a pdb file.

Thank you for your attention …





Please contact us if you need support in porting your application!

Email: kisst@wmin.ac.uk

Join the International Desktop Grid Federation:

http://desktopgridfederation.eu