P-GRADE portal family

Peter Kacsuk
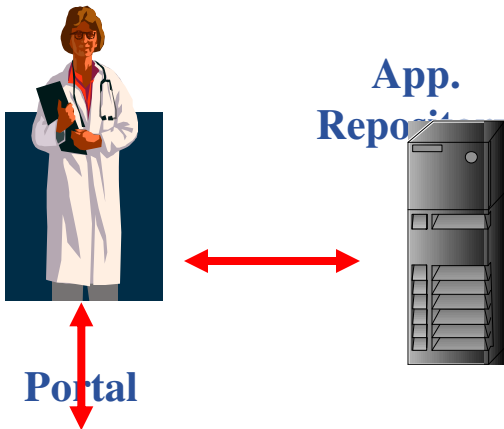**MTA SZTAKI**
kacsuk@sztaki.hu
www.lpds.sztaki.hu/pgrade

5th EGEE User Forum
Uppsala, 12-15 April 2010
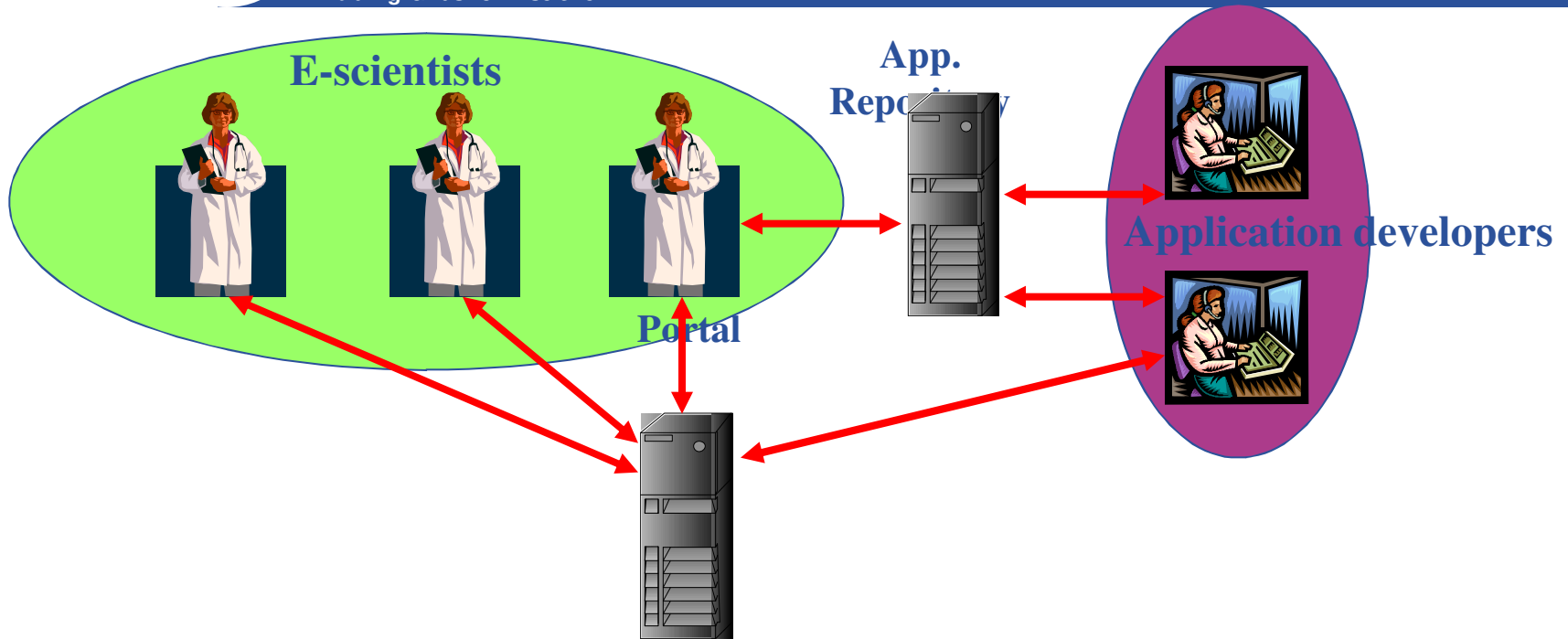
www.eu-egee.org

Using a portal to parameterize and run these applications

by transparently accessing a large set of various IT resources from the e-science infrastructure

App. Repository

Access to a large set of ready-to-run scientific applications (services)

Portal

Supercomputer based SGs (DEISA)

Cluster based service grids (SGs) (EGEE, OSG, etc.)

Desktop grids (DGs) (BOINC, Condor, etc.)

Local clusters

Supercomputers

Clouds

Grid systems
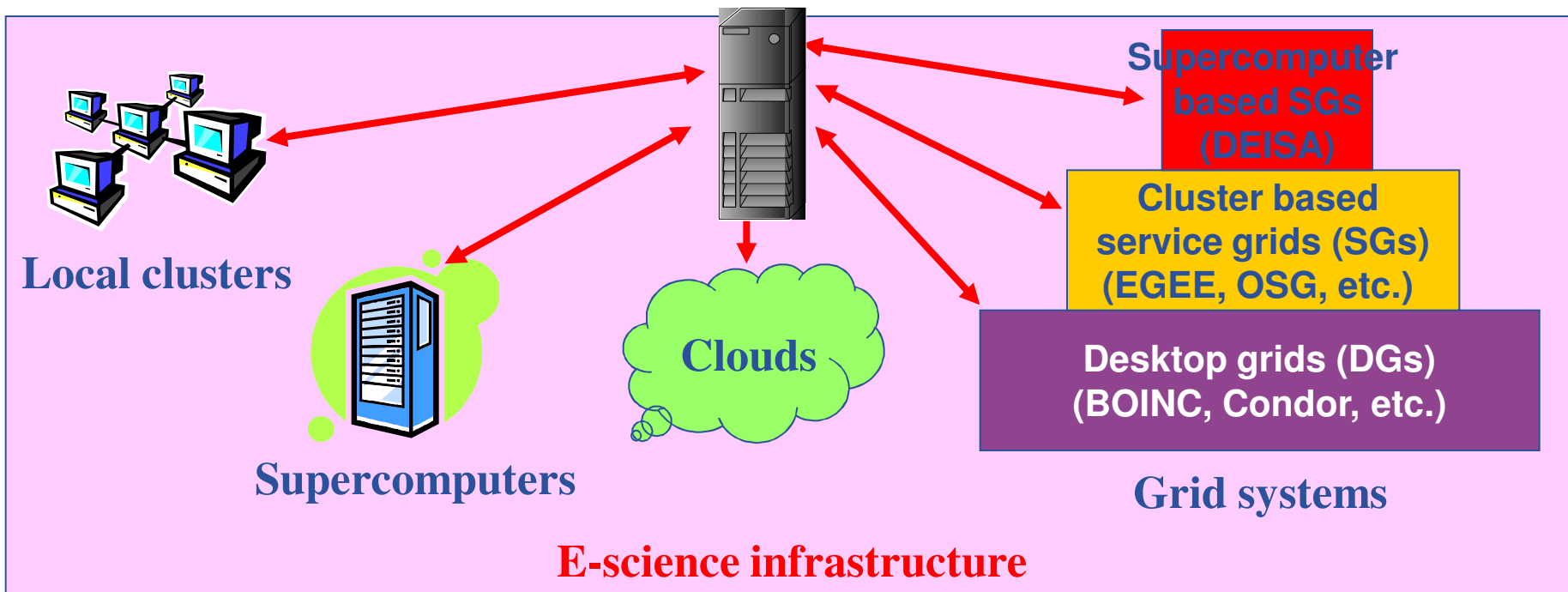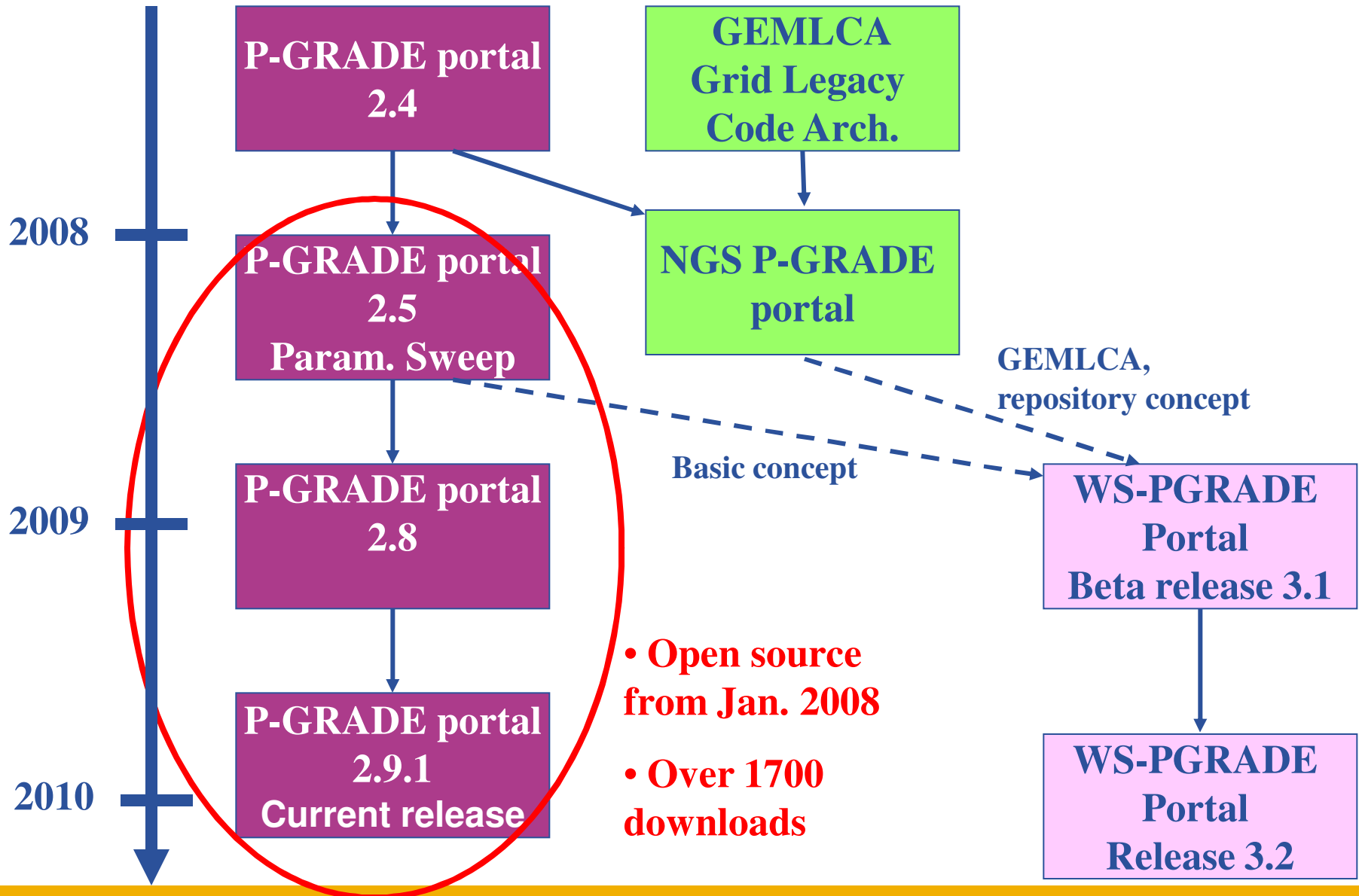
E-science infrastructure

Application Developers

• Develop e-science applications via the **portal** in collaboration with e-scientists

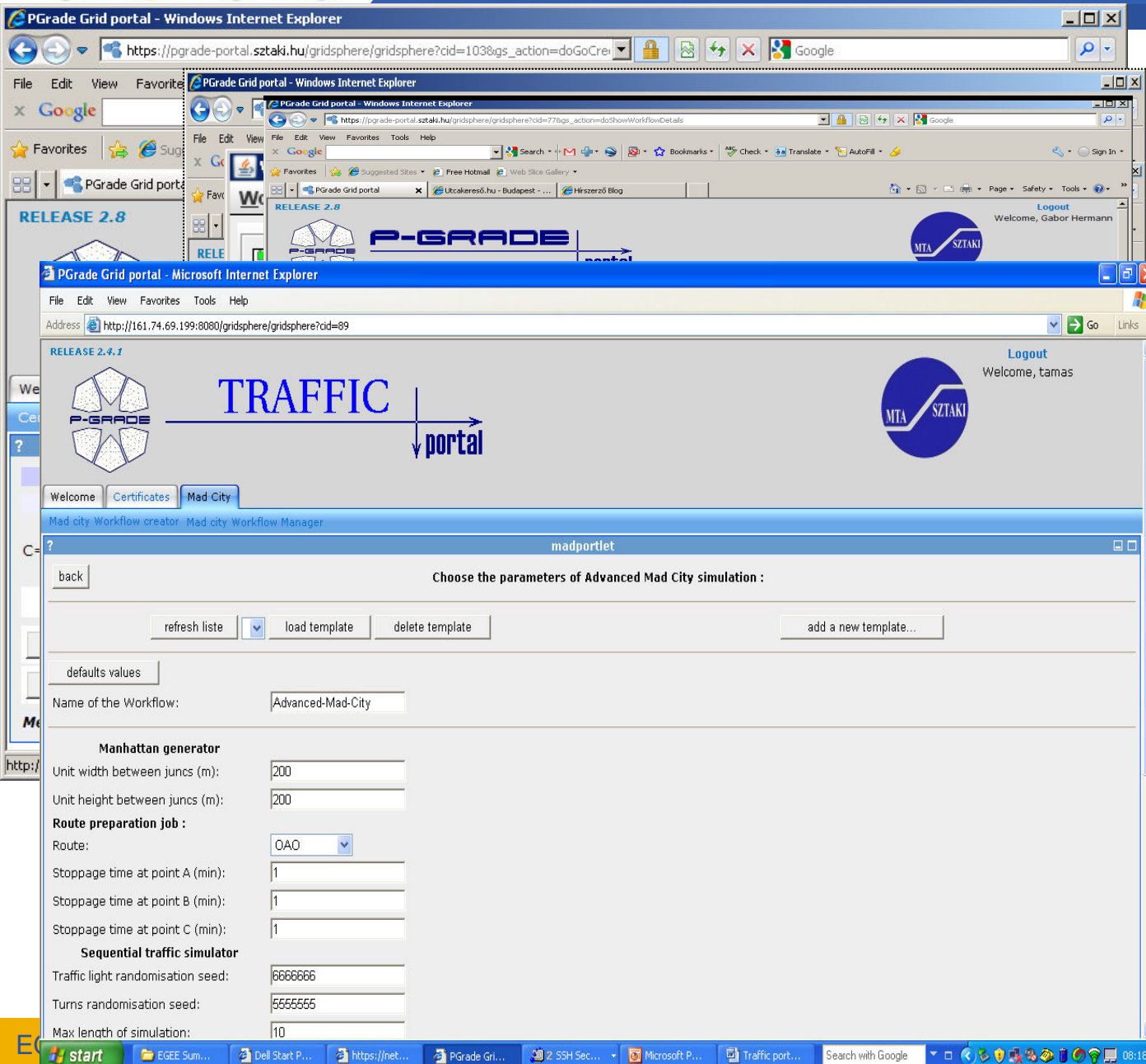• Publish the completed applications for end-users via an **application repository**

End-users (e-scientists)

• Specify the problem/application needs

• Execute the published applications via the **portal** with custom input parameters by creating application instances

Enabling Grids for E-sciencE

- **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*

2008

2009

2010

P-GRADE portal 2.4

P-GRADE portal 2.5 Param. Sweep

P-GRADE portal 2.8

P-GRADE portal 2.9.1 Current release

GEMLCA Grid Legacy Code Arch.

NGS P-GRADE portal

GEMLCA, repository concept

Basic concept

WS-PGRADE Portal Beta release 3.1

WS-PGRADE Portal Release 3.2

• **Open source from Jan. 2008**

• **Over 1700 downloads**
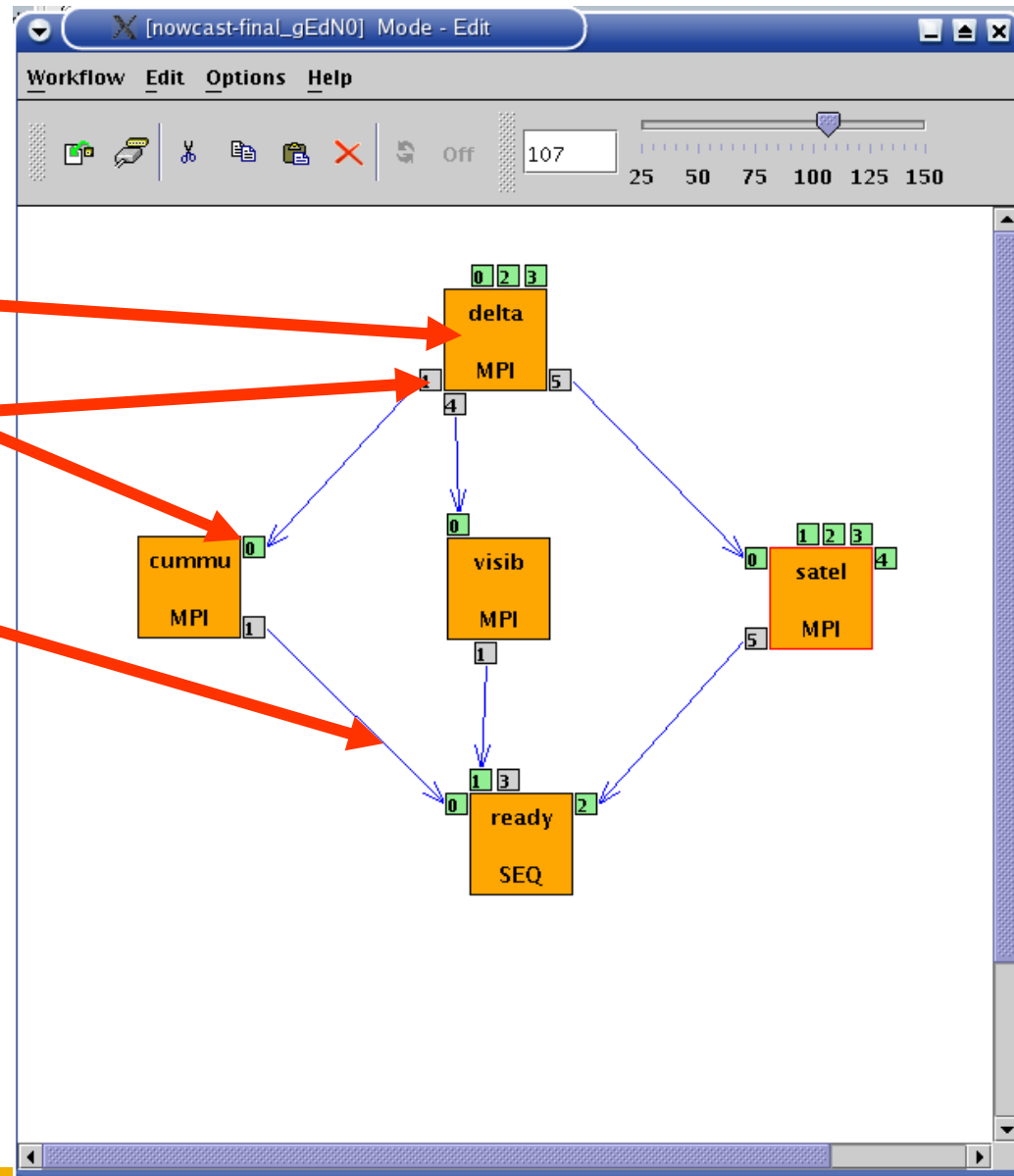
Certificate and proxy management

Grid and Grid resource management

Graphical editor to define workflows and parametric studies

Accessing resources in multiple VOs

Built-in workflow manager and execution visualization

GUI is customizable to certain applications
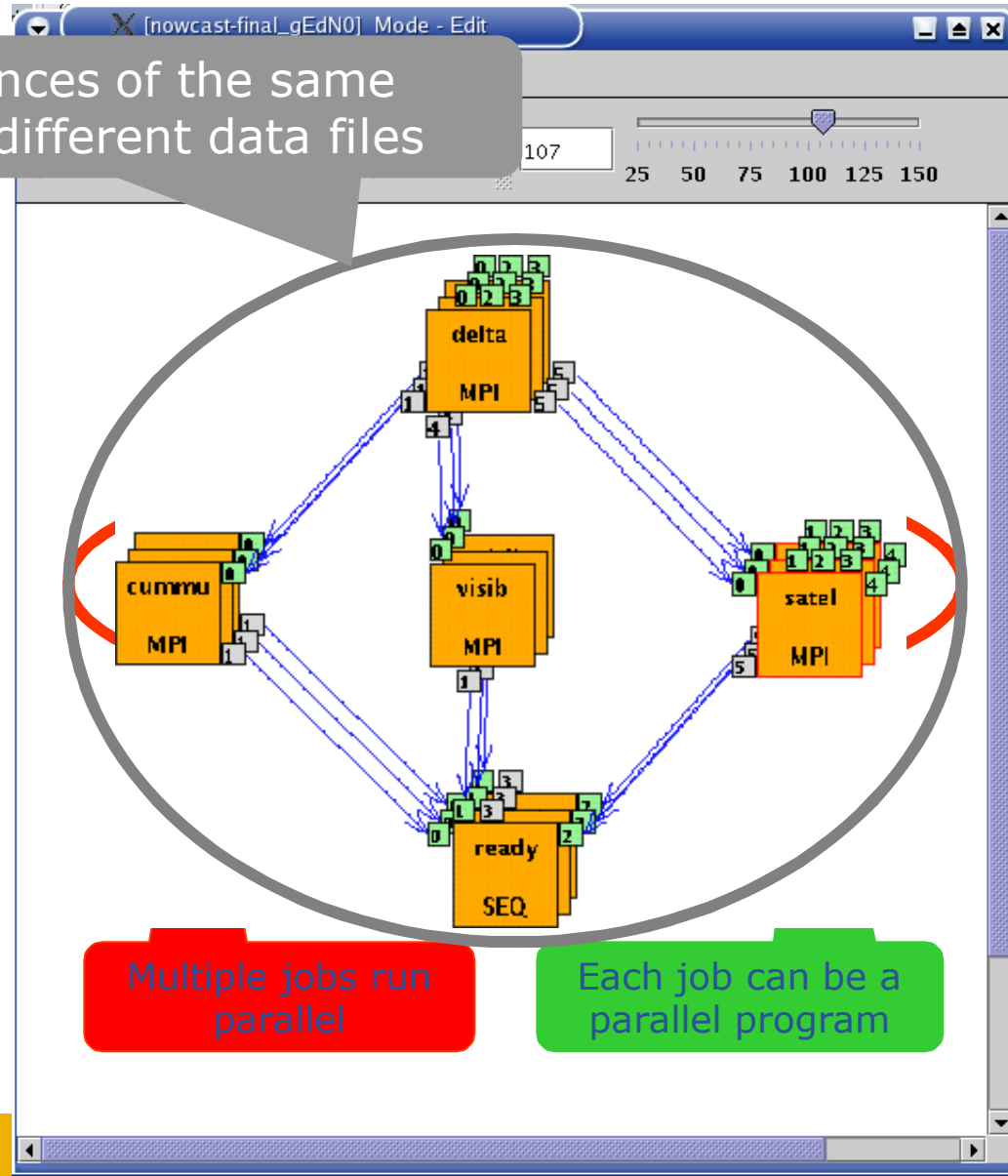
6

- A directed acyclic graph where
  - Nodes represent **jobs** (batch programs to be executed on a computing element)
  - **Ports** represent input/output files the jobs expect/produce
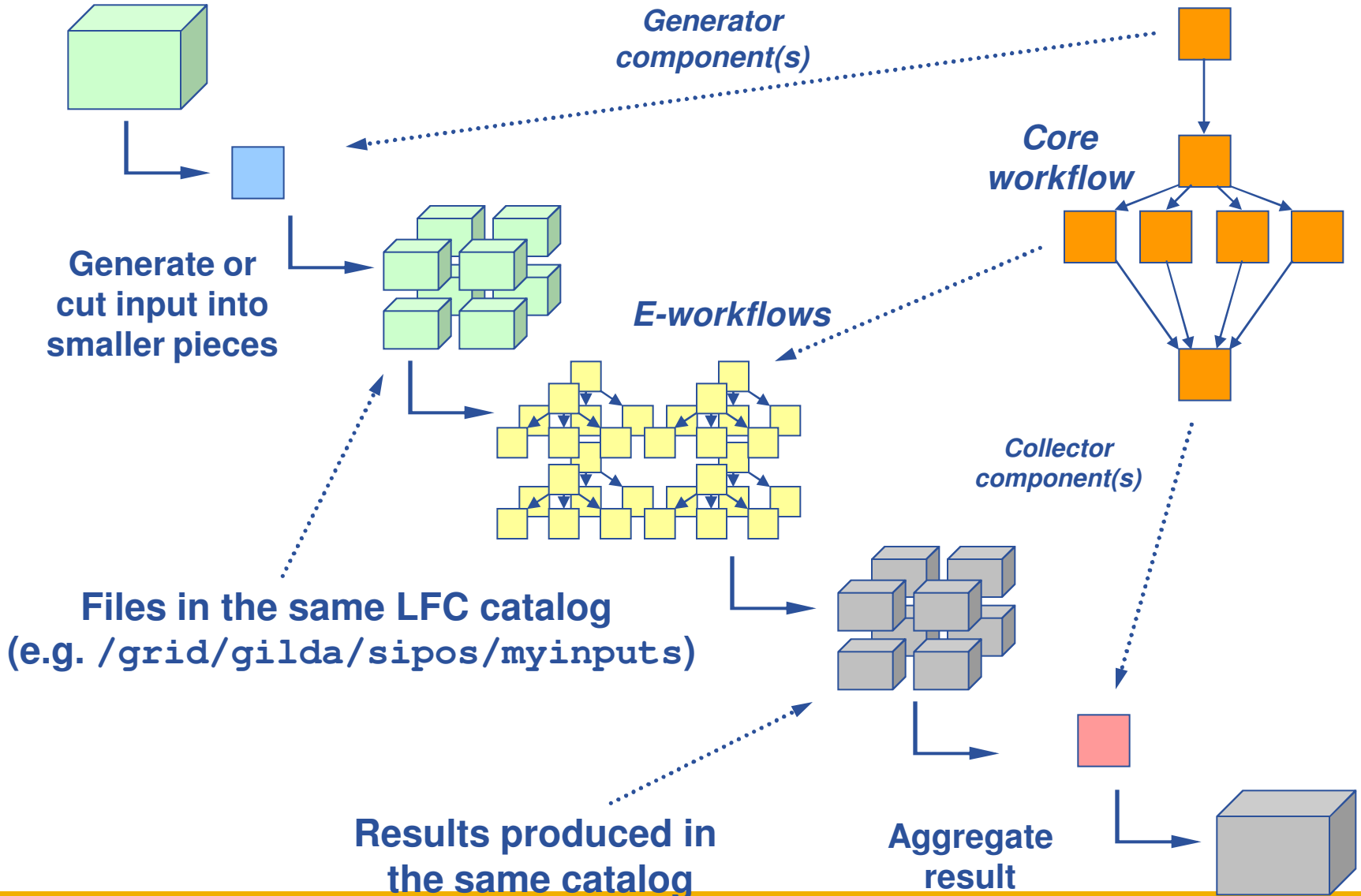 - **Arcs** represent file transfer operations and job dependencies

- Semantics of the workflow:
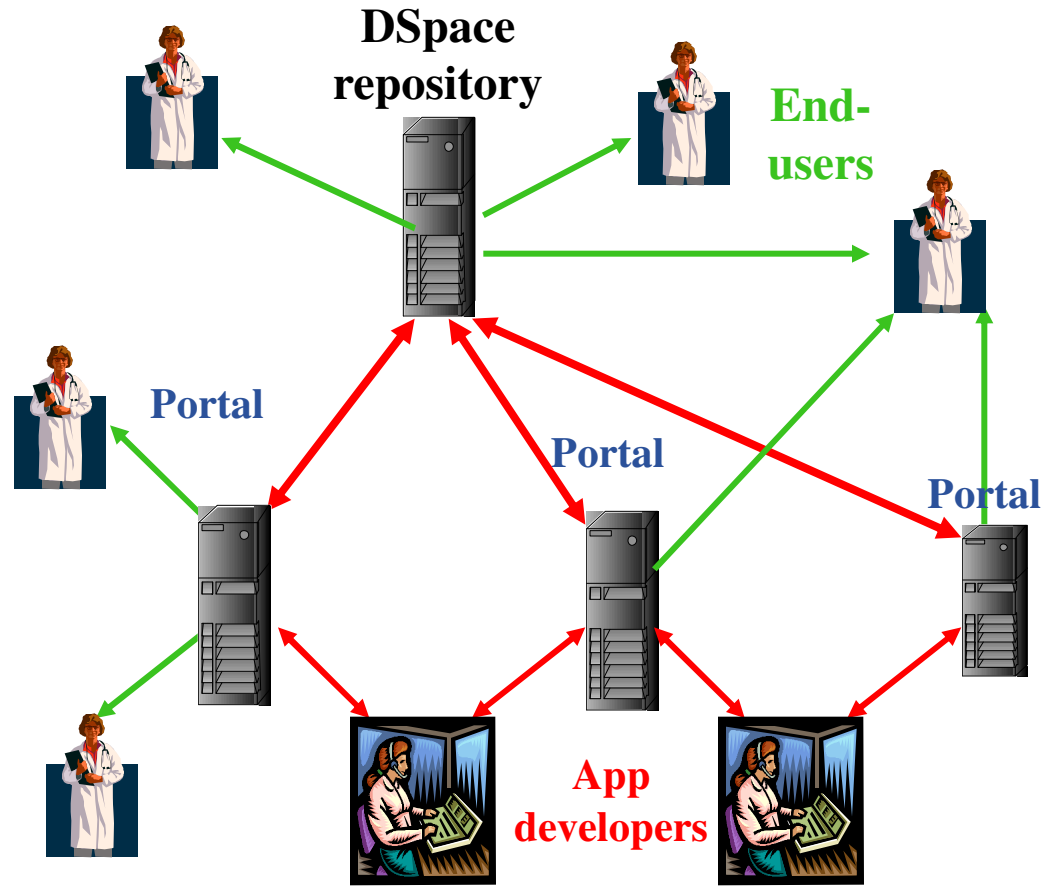 - A job can be executed if all of its input files are available

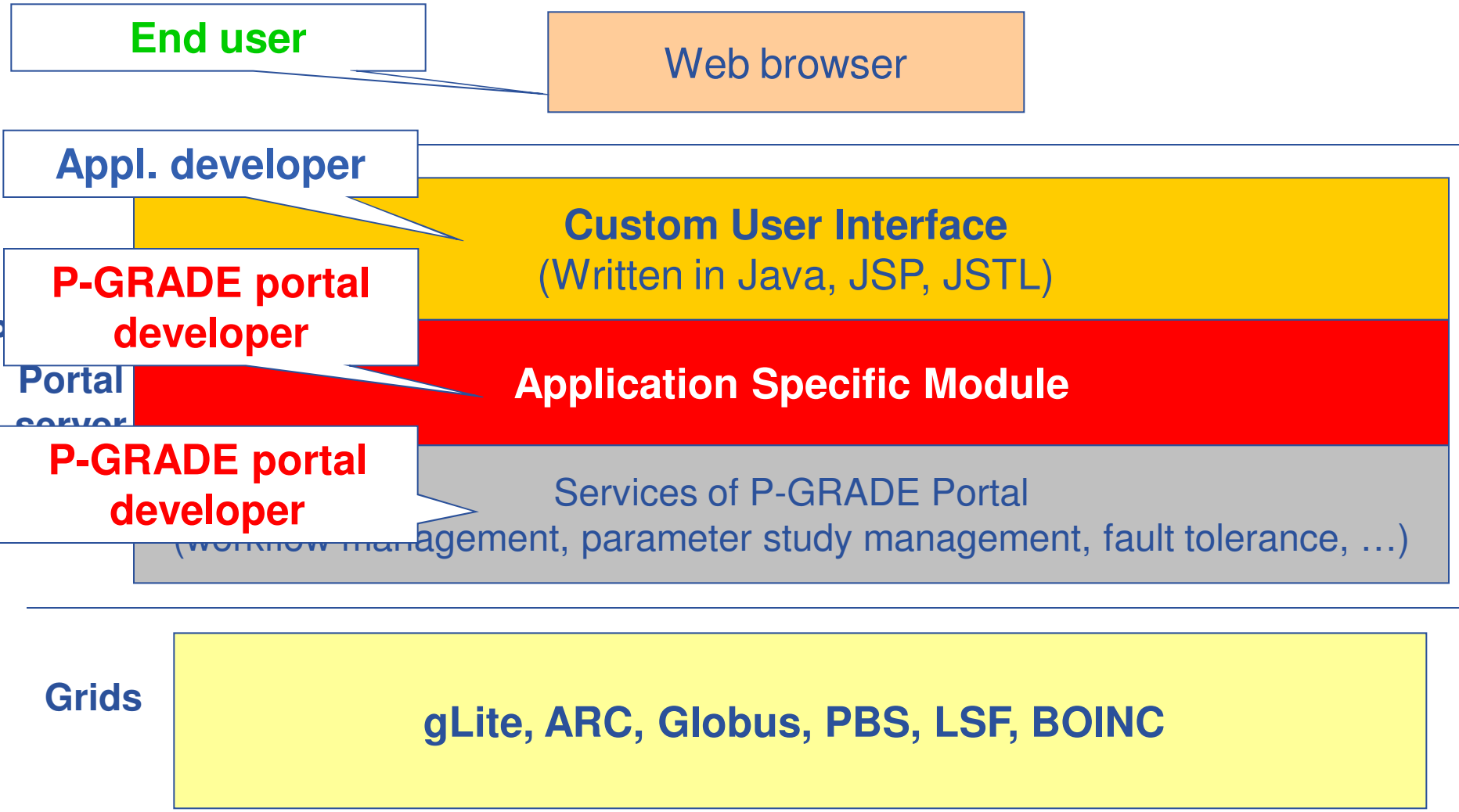Multiple instances of the same workflow with different data files

– **Parallel execution inside a workflow node**

– **Parallel execution among workflow nodes**

– **Parameter study execution of the workflow**

Multiple jobs run parallel

Each job can be a parallel program

Generator component(s)

Core workflow

Generate or cut input into smaller pieces

E-workflows

Collector component(s)

Files in the same LFC catalog (e.g. /grid/gilda/sipos/myinputs)

Results produced in the same catalog

Aggregate result

- **Goal:** to make available workflow applications for the whole P-GRADE portal user community

- **Solution:** Integrating P-GRADE portal with DSpace repository

- **Functions:**
  - **App developers** can publish their ready-to-use and half-made applications in the repository
  - **End-users** can download, parameterize and execute the applications stored in the repository

DSpace repository

End-users

Portal

Portal

Portal

App developers

- **Advantage:**
  - Appl. developers can collaborate with appl. developers and with end-users
  - Members of a portal user community can share their WFs
  - Different portal user communities can share their WFs

End user

Web browser

Appl. developer

Custom User Interface
(Written in Java, JSP, JSTL)

P-GRADE portal developer

Application Specific Module

P-GRADE portal developer

Services of P-GRADE Portal
(workflow management, parameter study management, fault tolerance, …)

Portal server

Grids

gLite, ARC, Globus, PBS, LSF, BOINC

- **Extends P-GRADE portal with**
  - GEMLCA legacy code architecture and repository
  - SRB file management
  - OGSA-DAI database access
  - WF level interoperation of grid data resources
  - Workflow interoperability support
- **All these features are provided as production service for the UK NGS:**
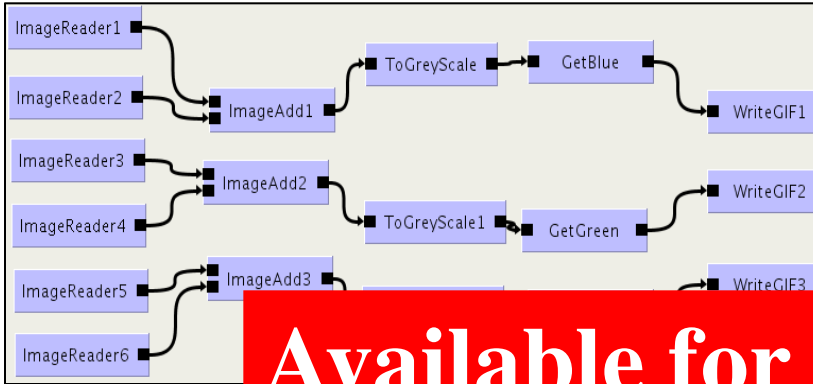 - *http://www.cpc.wmin.ac.uk/cpcsite/gemlca*
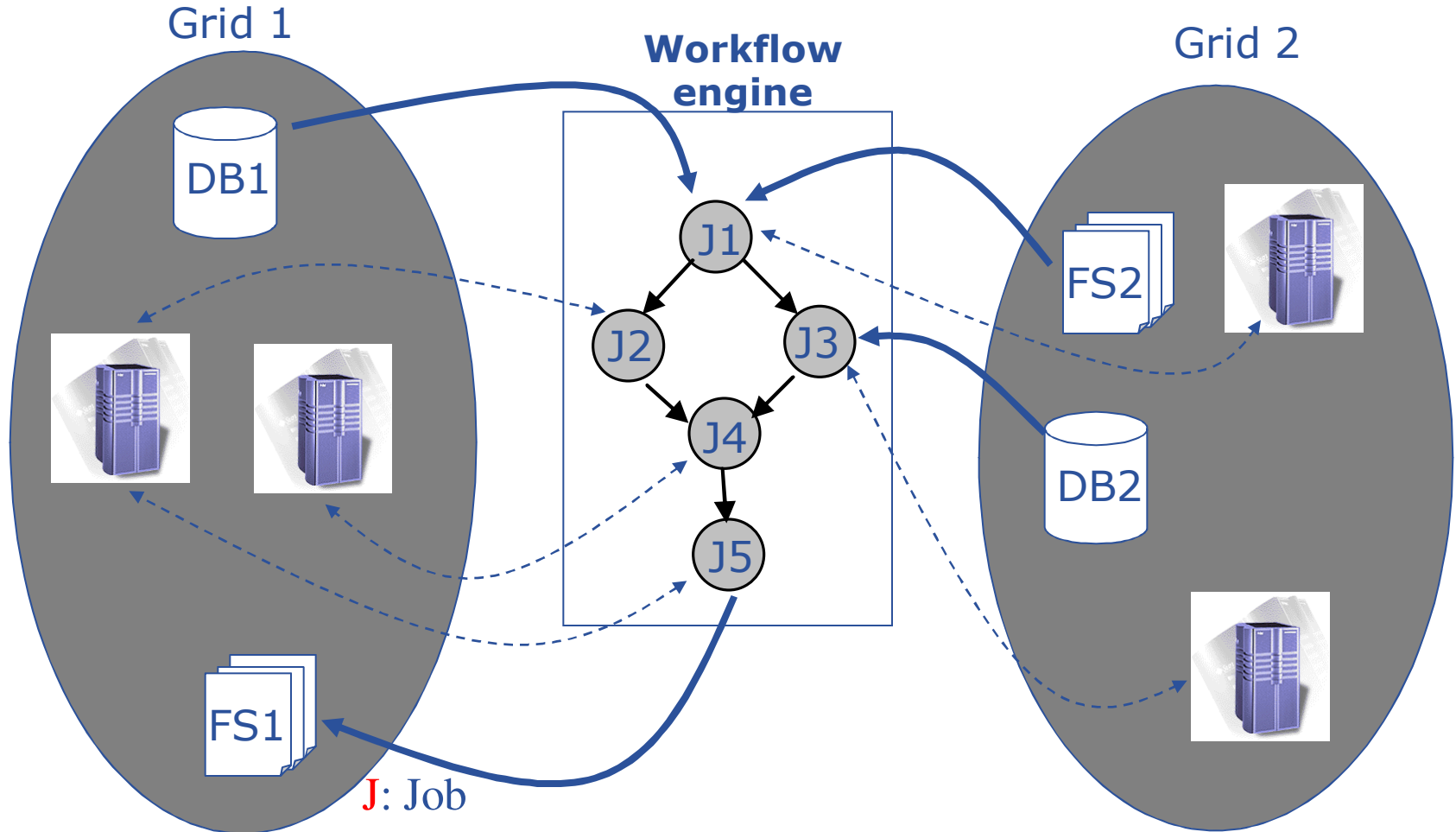
J: Job

FS: File storage system, e.g. SRB or SRM
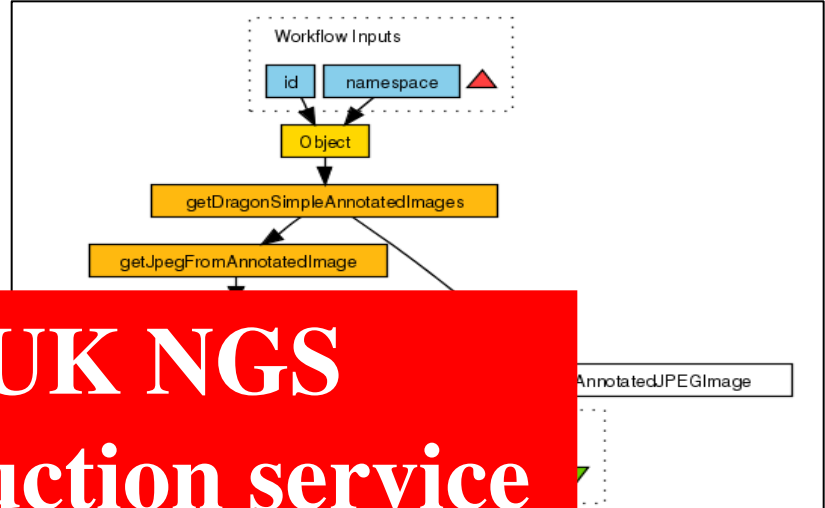
DB: Database management system (based on OGSA-DAI)
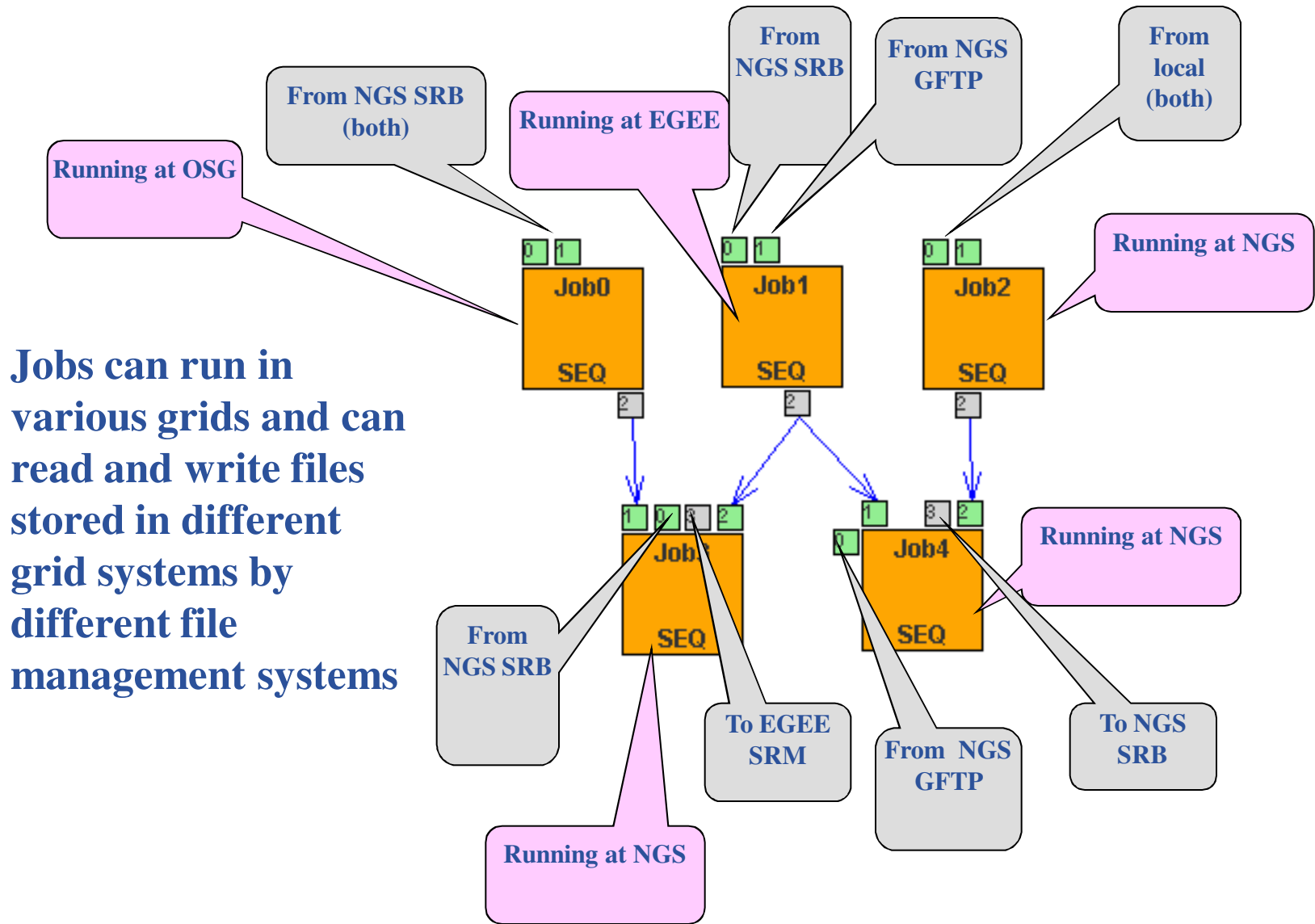
Jobs can run in various grids and can read and write files stored in different grid systems by different file management systems
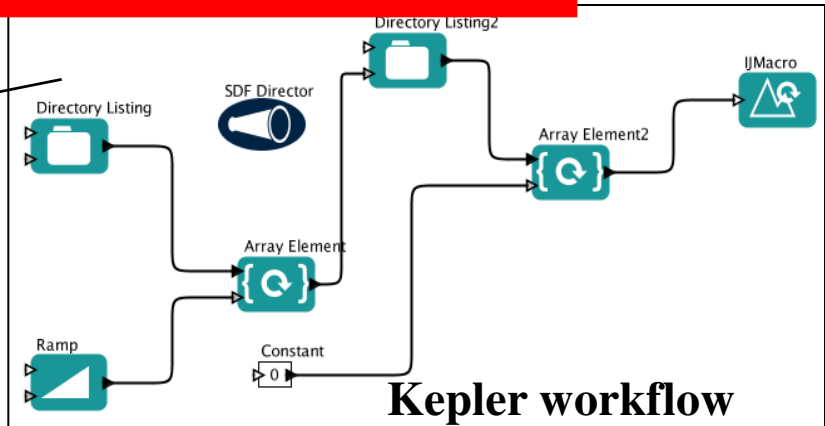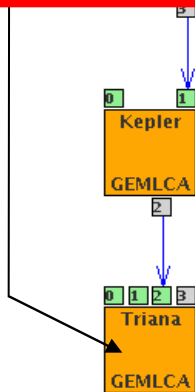
Triana workflow

Taverna workflow

P-GRADE workflow hosting the other workflows

Available for UK NGS users as production service
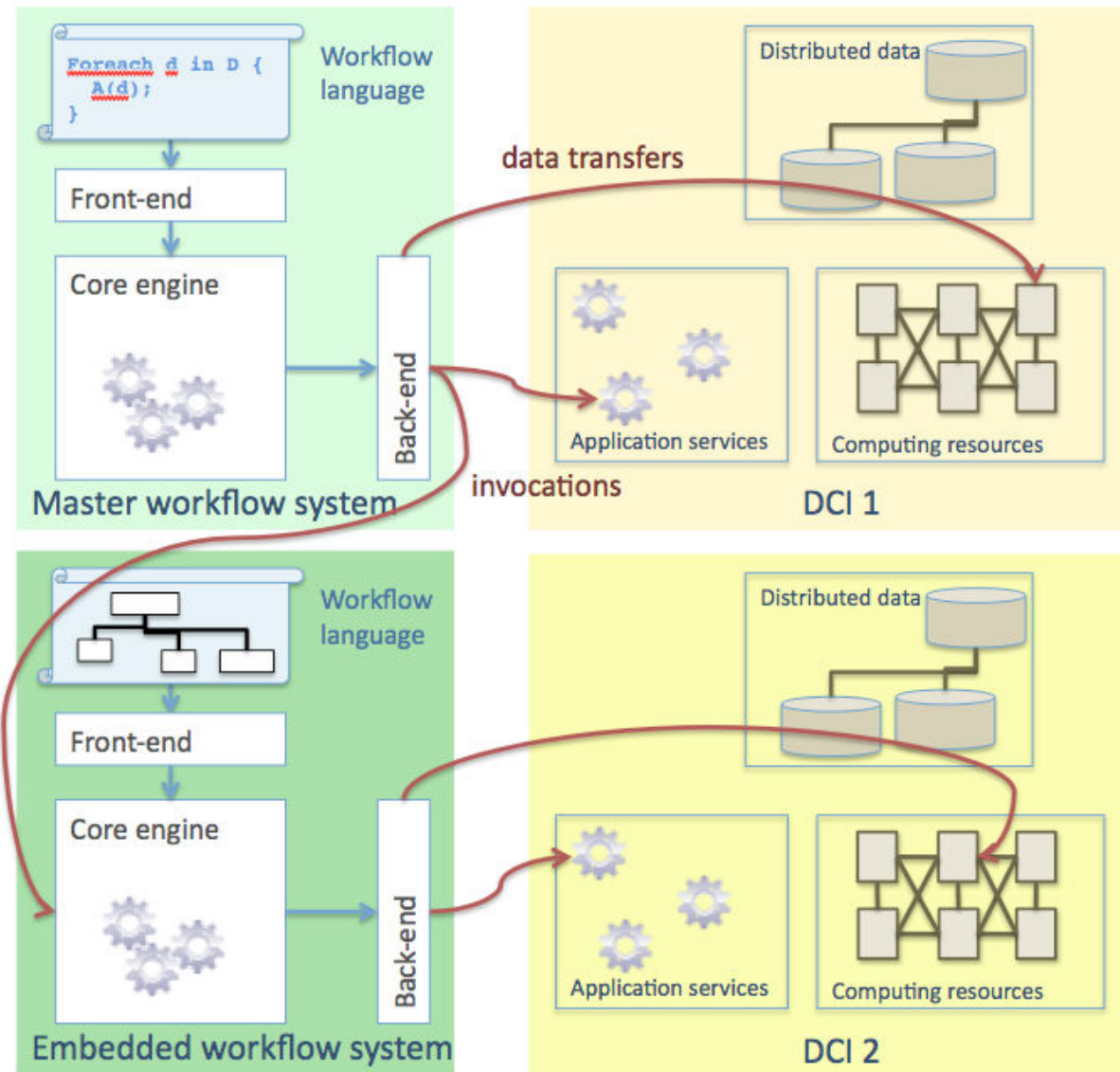
Kepler workflow

Enabling Grids for E-sciencE

• Will further develop the idea of the NGS P-GRADE portal for the following WF systems:

- • P-GRADE
- • ASKALON
- • Triana
- • Pegasus
- • MOTEUR
- • Kepler

Workflows repository
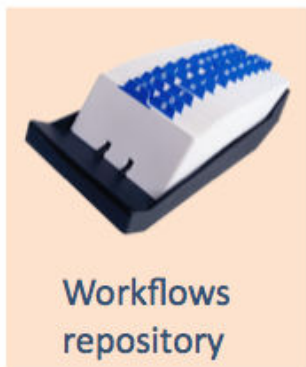
• Will create SHIWA science gateway based on P-GRADE

• Will create SHIWA WF repository

Enabling Grids for E-sciencE

- **Motivations: To overcome (most of) the limitations of P-GRADE portal:**
  - To provide better modularity → to replace any service
  - To improve scalability → to millions of jobs
  - To enable advanced dataflow patterns
  - To separate Application Developer view from Application User view
- **WS-PGRADE (Web Services Parallel Grid Runtime and Developer Environment)**

  and

  gUSE (Grid User Support Environment) architecture
- **Detailed presentation by Gergely Sipos in Section Workflow management at Thursday 9:40, room IX:**
  - Services for advanced workflow programming on gLite with WS-PGRADE portal

PUCOWO

www.portal.p-grade.hu/pucowo

1st P-GRADE Portal User COmmunity WOrkshop

**Zurich, Switzerland
June 10-11, 2010**

•Free event!

•Register now!

•WS-PGRADE tutorial

- Home
- Program
- Tutorial
- Program committee
- Organizing committee
- Call for presentations
- Important dates
- Contact

Home

In the last two years P-GRADE portal became popular and many Grids and VOs selected it as their science ga their user communities (see http://portal.p-grade.hu/?m=installations&s=0). Due to the increased inte number of user communities, the developers would like to provide stronger support and faster respons requirements of the user communities. In order to achieve this goal we organize the 1st P-GRADE Po COmmunity WOrkshop. The major goal is to share experience of using P-GRADE Portal among the vari communities and portal developers. The program is discussion-oriented. Every presentation will be followed by minutes discussion time in order to give opportunity for the users to express their P-GRADE experience developers to better understand the problems.

The presentations and discussions will be organized in the following sessions:

1. P-GRADE portal installation, administration and maintenance This session is for system admins who manage P-GRADE portal installations. Here we would like to discuss problems they encountered and improvements they recommend.

2. Applications developed by P-GRADE portal This session is for application developers who develop appli the portal. Here we would like to discuss what they like and what they do not like or miss in the portal.

3. End-user experience with P-GRADE portal Representatives of end-user communities are welcome to sh experience wit the portal.

4. Further development of P-GRADE portal Portal developers will present future plans on the further develo the portal. User communities are welcome to give presentation on their additional needs to improve the

A half-day WS-PGRADE portal tutorial will be also part of the program. WS-PGRADE is the second generation portal that will be presented and demonstrated during the tutorial. Two application-specific portals developed the generic purpose WS-PGRADE portal will also be presented: ProSim portal for protein folding simula CancerGrid portal for drug design.

The whole event is **free of charge**. We would like to share experience with the P-GRADE portal user community i improve the portal for their sake and not to make profit from this event.

Enabling Grids for E-sciencE

- **P-GRADE Portal remains supported**
  - Features can serve most grid scenarios
  - Open source project on Sourceforge
- **It will be further developed in the framework of several FP7 EU infrastructure projects:**
  - SHIWA:
    - To support workflow interoperability
    - To connect to workflow repository
  - EDGI:
    - To support SG/DG/cloud mixed usage
    - To connect to application repository
- **It is also further developed as part of national grid projects:**
  - Swiss Grid project
  - Malaysian Grid project
- **The P-GRADE portal community is ready to support any new requirements from any user community**

Thank you

www.portal.p-grade.hu
http://www.cpc.wmin.ac.uk/cpcsite/gemlca
www.wspgrade.hu

www.eu-egee.org