



University of
Westminster
and
University of
Portsmouth,
private
desktop grids
in academy
environments

University of Westminster and University of Portsmouth, private desktop grids in academy environments

Title

Dario Ferrer

Overview

Server Side

Clientside

Private DG

User
Interfaces

Apps

End

FST Faculty of Science and Technology
School of Electronics and Computer Science
University of Westminster

25 September 2013





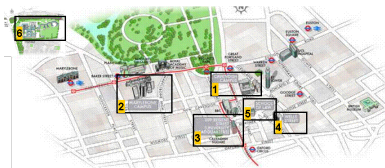
Overview



UoW and University of Portsmouth Desktop Grids

The Local Desktop Grids connect laboratory PCs of the universities into their respective BOINC based Desktop Grid infrastructures

It includes over 3000 registered machines over all the campuses.





Server Side

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and
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private
desktop grids
in academy
environments

Debian packages

We use .deb packages compiled by SZTAKI optimized for local Desktop grids.

```
deb http://www.desktopgrid.hu/debian/ squeeze szdg
```

The 3G-Bridge middleware run as BOINC daemons:

```
DAEMON pid status lockfile disabled commandline
1 23477 running locked no feeder -d 3
2 23479 running locked no transitioner -d 3
3 23481 running locked no file_deleter -d 3
4 23483 running locked no 3g-bridge
5 23487 running locked no wssubmitter
6 23504 running locked no wsmonitor
7 23508 running locked no validator_autodock -app autodock_vina
...
```

Title

Overview

Server Side

Clientside

Private DG

User
Interfaces

Apps

End



3G-Bridge

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private
desktop grids
in academy
environments

3G-Bridge

We use a special submitting interface called 3G-Bridge.
This middleware was been developed by SZTAKI (Hungary)
within the EDGES and EDGI European projects.

The bridge is able to connect lots of different grid technologies.
It has interface for EGI (Globus & gLite) infrastructure,
interface for cloud submission, interface portal based
submission, etc



Title
Overview
Server Side
Clientside
Private DG
User
Interfaces
Apps
End



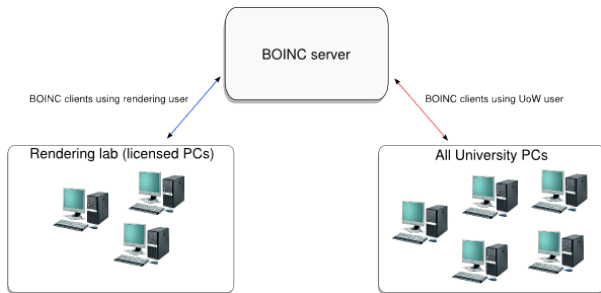
Server Side

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Users

We use "BOINC users" to distribute different applications to specific labs, specially for licensed apps.

Ex: Those licensed Desktops able to run a particular rendering app are registered in the project as user "render".



Title

Overview

Server Side

Clientside

Private DG

User Interfaces

Apps

End



Boinc Clients

University of Westminster and University of Portsmouth, private desktop grids in academy environments

Title

Overview

Server Side

Clientside

Private DG

User Interfaces

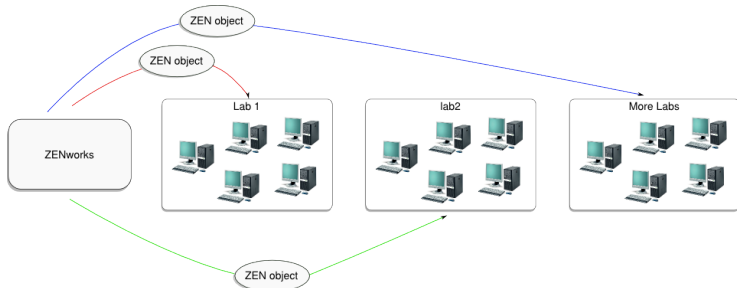
Apps

End

ZENworks

Every single desktop at the Universities is managed using ZENworks or similar automatic software deploy systems.

BOINC clients are preconfigured in a so called "ZEN object". We customize the version and parameters of the BOINC client depending on the lab it's going to be installed. All the rest is done automatically.





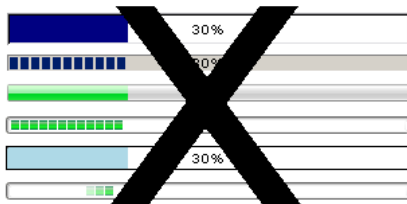
Credits, Statistics

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desktop grids
in academy
environments

No Credits

As our desktop grids are formed only by the University computers, we do not grant credits.

We also do not spend effort in decorating the apps with progress bars, we neither take care about large input/output sizes.





Green IT

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desktop grids
in academy
environments

As the majority of PC labs are used by students, the policy is to completely switch off BOINC during class time.

We also have environmental policies and scripts that switch off the machines if there are no BOINC jobs running.



Title

Overview

Server Side

Clientside

Private DG

User
Interfaces

Apps

End



WS-PGRADE portal

University of Westminster and University of Portsmouth, private desktop grids in academy environments

Title

Overview

Server Side

Clientside

Private DG

User Interfaces

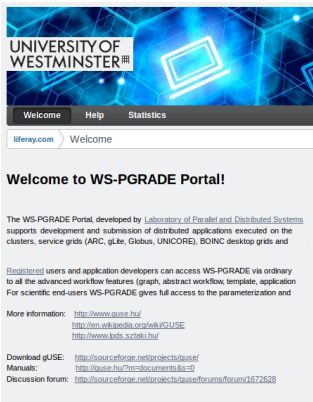
Apps

End

Is a web portal capable of submitting jobs in BOINC and many other grids.

Has been developed by the SZTAKI, Hungary in collaboration with many partners under the umbrella of a number of European projects such as EDGI, SCI-BUS, SHIWA ...

It does communicate with desktop grids using the 3G-Bridge



The screenshot shows the homepage of the WS-PGRADE Portal. At the top, there is a blue header with the University of Westminster logo and a navigation menu with 'Welcome', 'Help', and 'Statistics'. Below the header is a search bar with 'liferay.com' and 'Welcome' entered. The main content area features a large heading 'Welcome to WS-PGRADE Portal!' followed by a paragraph describing the portal's purpose and supported systems. It also includes links for 'Registered users', 'More information', 'Download gUSE', 'Manuals', and 'Discussion forum'.

UNIVERSITY OF WESTMINSTER

Welcome Help Statistics

liferay.com Welcome

Welcome to WS-PGRADE Portal!

The WS-PGRADE Portal, developed by [Laboratory of Parallel and Distributed Systems](#) supports development and submission of distributed applications executed on the clusters, service grids (ARC, gLite, Globus, UNICORE), BOINC desktop grids and

[Registered](#) users and application developers can access WS-PGRADE via ordinary to all the advanced workflow features (graph, abstract workflow, template, application) For scientific end-users WS-PGRADE gives full access to the parameterization and

More information: <http://www.guse.hu/>
<http://en.wikipedia.org/wiki/GUSE>
<http://www.lads.sztaki.hu/>

Download gUSE: <http://sourceforge.net/projects/guse/>
Manuals: <http://guse.hu/?m=documento&g=0>
Discussion forum: <http://sourceforge.net/projects/guse/forums/forum/1672620>



WS-PGRADE Specific Portlets

University of Westminster and University of Portsmouth, private desktop grids in academy environments

Title

Overview

Server Side

Clientside

Private DG

User Interfaces

Apps

End

Most of users are students who submit through app oriented specific GUIs.

They are extremely easy to use, such as upload input → download screening of a library output.

Users are mainly video production students and bio-computing PhDs

The screenshot shows the 'AutoDock Vina - Virtual screening of a library of ligands' page. It includes a navigation menu with options like Release, Workflow, Storage, Settings, Information, Statistics, Publications, Help, End User, Security, Docking toolbar, and Mental Ray. Below the menu, there are tabs for 'Mental Ray' and 'AutoDock Vina'. The main content area contains a form for configuring the virtual screening process, with fields for 'Number of parallel jobs', 'Number of processors', 'Task name', and 'Task type'. A table at the bottom lists 'Task Name', 'Task Name', and 'Actions'.

The screenshot shows the 'Mental Ray Rendering Portlet' page. It features the same navigation menu as the previous screenshot. Below the menu, there are tabs for 'Mental Ray' and 'AutoDock Vina'. The main content area displays a 'Welcome to Mental Ray Task Control' message, followed by a brief description of the software and a 'Create new task' button. The 'Autodesk Maya' logo is visible in the bottom right corner.



WS-client command line tool

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private
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in academy
environments

wsclient is a command line tool.

Some WminDG users prefer this method to submit their jobs, this way they can also integrate it with their own scripts.

UoW developed its own scripts based on this tool and they have been used by some scientists.

```
COMMAND="wsclient --mode=add --endpoint=${WSSUBMITTER_URL}"
for i in ${INPUT_LOGICAL_NAMES}
do
    FILE_NAME="${i}_${EXP_NUMBER}_${WU_NUMBER}"
    ln -s 'pwd'/$1

    ${DIRECTORY_TO_BASE_URL}/${APPLICATION_NAME}_${EXP_NUMBER}/${FILE_NAME}
    URL="${BASE_URL}/${APPLICATION_NAME}_${EXP_NUMBER}/${FILE_NAME}"

    COMMAND="${COMMAND} --in=${i}=${URL}"
done
```

...

Title

Overview

Server Side

Clientside

Private DG

User
Interfaces

Apps

End



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and
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private
desktop grids
in academy
environments

Mentalray

Used in teaching to render student projects

Specific testbed of 40 PCs fully licensed for the AutoDesk
package

Custom user interface in the WS-PGRADE portal

Browse and upload the project zip file



Title

Overview

Server Side

Clientside

Private DG

User
Interfaces

Apps

End



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University of
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and
University of
Portsmouth,
private
desktop grids
in academy
environments

Title

Overview

Server Side

Clientside

Private DG

User
Interfaces

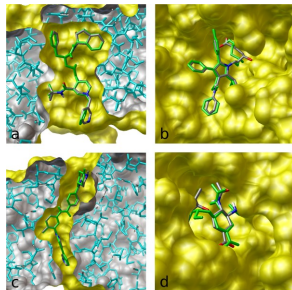
Apps

End

AutoDock Vina

Outputs possible ligands of a
family 38 mannosidase.

Approximately 180.000 small
molecules have been docked
consuming one computer year
of processing within a couple of
weeks.





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desktop grids
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Title

Overview

Server Side

Clientside

Private DG

User
Interfaces

Apps

End

```
exit(0);
```