eGee

Supporting Diverse Local Virtual Organisations

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e-infrastructure

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    - Issues and Experiences
    - Outcomes

- **Lessons Learned**

Enabling Grids for E-sciencE

- **Local Device Modelling group**
  - Approx 10 Users in UK based in Glasgow and Manchester
  - 1 Month Usage Trial
  - Originally used to direct batch submission
  - Usage: Python Code, 7 day, serial array jobs
- **Issues**
  - Initial access to the system
    - It was felt this was overly complicated.
  - Job Submission
    - Various methods; command line, Ganga, proxy lifetime issues.
  - Job Monitoring
    - Disparity between command line and Ganga.
  - Reliability
    - Perception that there has a high failure rate.

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Enabling Grids for E-sciencE

- **Outcomes**
  - Initial access to the system
    - Streamlined local documentation for access.
  - Job Submission
    - Creation of gqsub, a qsub like interface to gLite middleware
      - *See poster contribution titled 'Data awareness in gqsub'.*
  - Job Monitoring
    - The usage of gqsub re-introduced consistency with command line tools.
  - Reliability
    - The perception of unreliable system was unfounded. It seemed to stem from past experiences with early gLite components such as the RB.
    - Update of procedures surrounding middleware upgrade notifications.

- **Local Photonics group**
  - 3 local users and potential UK users in London, Southampton and some in France. Now installed in Greece.
  - Usage: Licensed software by Lumerical Inc, MPI

- **Issues**
  - License Management
    - Always a sticking point for Grid, EGEE and gLite.
  - Integration for use with gLite middleware
    - In order to support licences management at the batch level custom job parameters need to be able to passed from JDL.
  - MPI specification
    - MPI version available but not all PBS/Torque node specifications available.
  - Small VO
    - Lack of resources, limited site licenses, potential external users.
      - *SL4/5 & UI install a stumbling block.*

Enabling Grids for E-sciencE

- **Outcomes**
  - License Management
    - Licences dealt with via consumable resources in the scheduler and the batch system.
  - Integration for use with gLite middleware
    - Passing custom job parameters with JDL, in this case a software license tag, was made possible with the introduction of CREAM.
  - MPI specification
    - MPI works but still additional development required. Using custom job parameters with JDL allowed specification of whole nodes and processes per node (:ppn).
  - Small VO
    - Creation of an off-the-self optics UI Virtual Box image.
      - *Copy your certificate and submit the test job.*

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JDL

Submission of a licensed Lumerical job

JDL

cerequirements =
" GlueHostApplicationSoftwareRunTimeEnvironment==\"FDTD\"";

Requirements= other.
GlueHostApplicationSoftwareRunTimeEnvironment=="FDTD";

or

In [pbs/lsf]_local_submit_attributes.sh

```
if [ "$GlueHostApplicationSoftwareRunTimeEnvironment" ==
"FDTD" ]; then
echo "#PBS -l software=FDTD"
fi
```

WMS

In /opt/glite/etc/glite_wms.conf

CeForwardParameters =
"GlueHostApplicationSoftwareRunTimeEnvironment"};

CREAM CE (via BLAH)

FDTD LICENSE MANAGER

PBS Batch System

Resource_List.software = FDTD

PBS/MAUI manages licenses through specification of:
NODECFG[GLOBAL] GRES=FDTD:10

Enabling Grids for E-sciencE

- **Local Solid State Physics group**
  - 2 local users
  - New to batch/grid submission
  - Usage: User code and CASTEP

- **Issues**
  - MPI Integration
    - MPI versions from EGEE not suitable in all cases.
  - MPI Specification
    - MPI over many nodes expected but again propagation of generic parameters from JDL not possible.
  - Small VO
    - Lack of resources, limited experience.

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- **Outcomes**
  - MPI Integration
    - Rebuild of OPENMPI for F90 and Torque Support.
  - MPI Specification
    - 'cerequirements' JDL attribute for CREAM coupled with pbs_local_submit_attribute.sh functionality allowed specification on :ppn and wholenodes.

  - Small VO
    - Customised user scripts as a precursor to gqsub usage.

Enabling Grids for E-sciencE

- **'We just want direct submission to the batch system'**
  - Custom tools can provide the interface users desire
  - They should be shielded from needless complexity

- **As you would expect small VOs require more help**
  - NA4 and SA1 co-location at Glasgow has helped a great deal.
    - Allowing middleware customisation to fit with user needs.

- **Computing Element**
  - Fundamental to support the needs of the smaller VO
    - CREAM has made this possible.