## GridPP Infrastructure and Approaches

T. Whyntie\*

\* Queen Mary University of London

**SKA/GridPP F2F, University of Manchester** 

Wednesday, 2<sup>nd</sup> November 2016





## **Outline of the talk**

- GridPP: an introduction:
  - GridPP and the Worldwide LHC Computing Grid (WLCG); But what is a Grid? When is a Grid useful? Can I use the Grid?
- Engaging with the Grid:
  - Infrastructure for non-LHC VOs; documentation; advances approaches for large VOs.
- Selected case studies:
  - GEANT4 simulation campaigns; GalDyn (Galaxy Dynamics); the Large Synoptic Survey Telescope.
- Summary and conclusions.





## **GridPP: an introduction**

GridPP and the Worldwide LHC Computing Grid (WLCG); But what is a Grid? When is a Grid useful? Can I use the Grid?

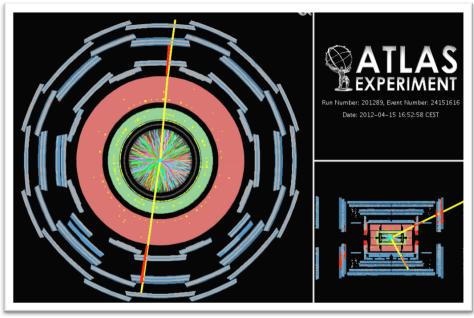




## **GridPP and the WLCG**

- The Worldwide LHC Computing Grid (WLCG) was developed to meet the challenges presented by data from CERN's Large Hadron Collider (LHC):
  - 40 million particle collisions per second;
  - 150 million channels in ATLAS/CMS detectors;
  - At least 15 PB of data per year;
  - Expect a few per million of e.g. Higgs events.
- GridPP (the UK Grid for Particle Physics) represents the UK's contribution:
  - A collaboration of 20 institutions, 100+ people;
  - 101k logical CPU cores, 37 PB storage;
  - Accounts for ~11% of WLCG resources.





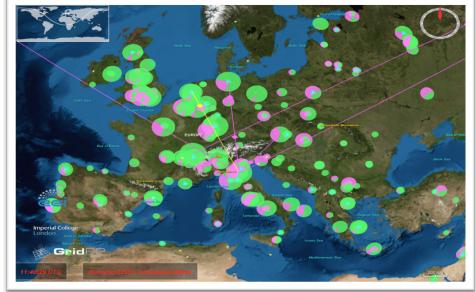




### **But what is a Grid?**

- 'Grid' computing key concepts:
  - All processing power and storage always on, always available, whenever it is needed;
  - The end user doesn't know or care about where or how (c.f. electricity grid) thanks to middleware technologies.
- The WLCG itself is distributed computing/High Throughput Computing (HTC) on a huge scale:
  - As of August 2013, 152 sites in 36 countries, 365k logical CPUs, 210 PB storage;
  - By number of cores (not a fair measure), it would rank 3<sup>rd</sup> in the current top-10 super computers worldwide;
  - As acknowledged by CERN DG, crucial in the discovery of the Higgs boson in July 2012.

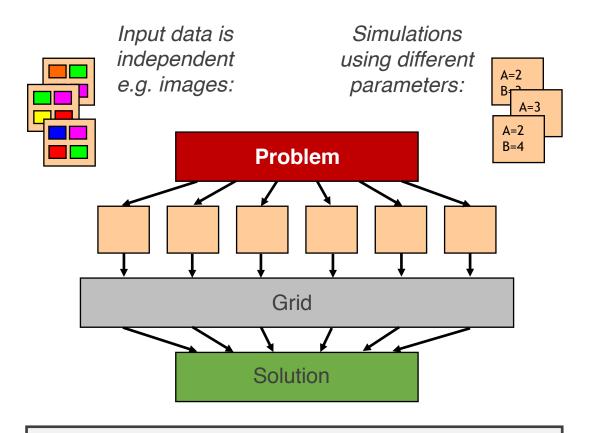








## When is a Grid useful?

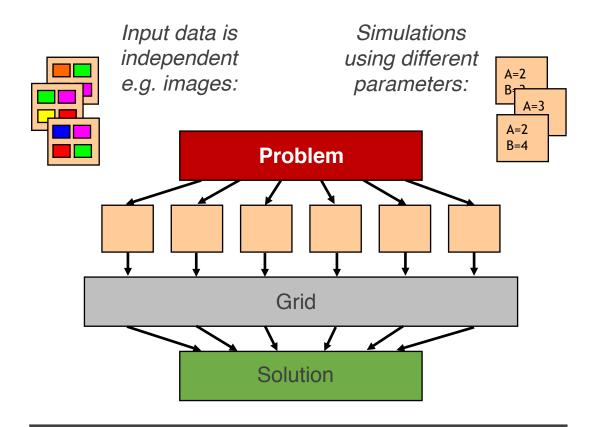


**Problems that are highly parallelizable** 

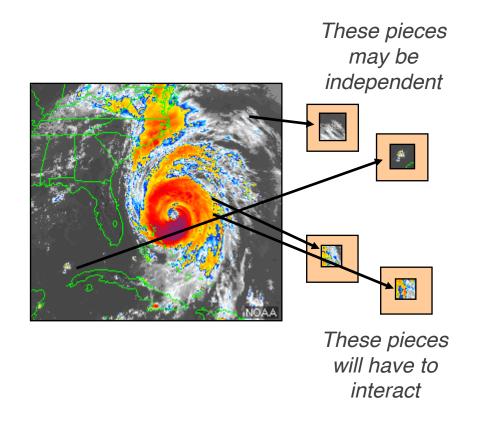




## When is a Grid useful?



**Problems that are highly parallelizable** 

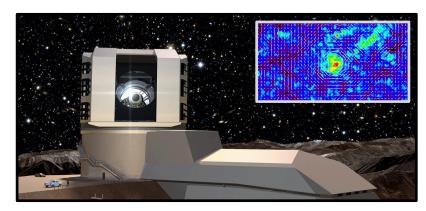


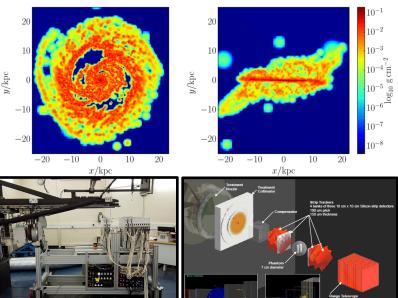
Not so good for closely coupled problems



## Can I use the Grid?

- Yes! GridPP offers up to 10% of its resources to non-LHC Virtual Organisations (VOs):
  - *VO community of users grouped by e.g. experiment;*
  - All users need a Grid certificate (X509);
  - Problem: smaller groups tend to lack the resources needed to develop the infrastructure required to engage with the Grid, e.g. Uis, middleware framework.
- GridPP's New User Engagement Programme:
  - Provide infrastructure, tools and documentation for engaging with GridPP resources;
  - Present a standardised approach for small VOs.
- Key components:
  - A multi-VO job and data management system (DIRAC), use of a software distribution system (CVMFS), and standard User Interface (Ganga, CernVM) for small/non-LHC user communities;
- Results many non-LHC/non-HEP user communities now using GridPP resources.









## **Engaging with the Grid**

Infrastructure for non-LHC VOs; documentation; advanced approaches for larger VOs.





## Infrastructure for non-LHC VOs

Software deployment

Job and data management

**User Interface** 





CernVM-FS

**DIRAC** 

Ganga, CernVM





#### **Distributed Infrastructure with Remote Agent Control**

A software framework for distributed computing with grid resources.

See <a href="http://diracgrid.org/">http://diracgrid.org/</a>

**CernVM-FS** 

**DIRAC** 

Ganga, CernVM

# OVERVIEW

#### **CernVM File System**

A network file system for delivering experiment software in a scalable, fast, reliable way via http.

Distributed Infrastructure with Remote Agent Control

A software framework for distributed computing with grid resources.

See the website <u>here</u>.

DIRAC

See <a href="http://diracgrid.org/">http://diracgrid.org/</a>

Ganga, CernVM

CernVM-FS



# OVERVIEW

#### **CernVM File System**

A network file system for delivering experiment software in a scalable, fast, reliable way via http.

See the website <u>here</u>.

## Distributed Infrastructure with Remote Agent Control

A software framework for distributed computing with grid resources.

See <a href="http://diracgrid.org/">http://diracgrid.org/</a>

CernVM-FS

DIRAC

Supported by Imperial College London, Uni. Birmingham: http://ganga.readthedocs.io

Ganga, CernVM

http://cernvm.cern.ch/

#### Ganga and the GridPP CernVM

Ganga is a Python-based interface for distributed computing.
The CernVM is a baseline Virtual Software Appliance developed for the participants of CERN LHC experiments with built-in CVMFS access.





OVERVIEW

RAL hosts a CernVM-FS Stratum 0 for non-LHC VO software repositories. The GridPP DIRAC instance is hosted and supported by Imperial College London.

See the website <u>here</u>.

CernVM-FS

**DIRAC** 

See <a href="https://dirac.gridpp.ac.uk/">https://dirac.gridpp.ac.uk/</a>

Supported by Imperial College London, Uni. Birmingham: <a href="http://ganga.readthedocs.io">http://ganga.readthedocs.io</a>

Ganga, CernVM

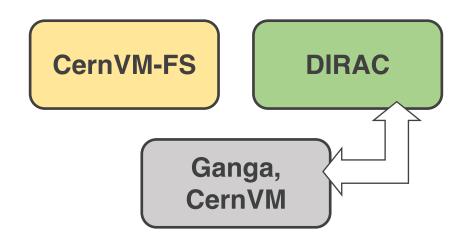
http://cernvm.cern.ch/

#### Ganga and the GridPP CernVM

Ganga is available to anyone with CVMFS access via a grid-enabled cluster or a GridPP CernVM. GridPP offers a contextualised CernVM suitable for new users if cluster access cannot be arranged.







Ganga is a Python-based interface for distributed computing with local, batch, or grid running.

Ganga can be configured to use the GridPP DIRAC system as a backend.

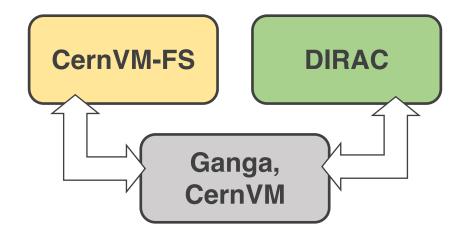
Switching from local to batch to grid is trivial thanks to CVMFS, making local testing before Grid running easy.



Users can build their software (executables and libraries) on their local SL6 cluster or GridPP CernVM ready for deployment to the grid.

Users can upload their software to their own CernVM-FS repository from using the gsi\* tools in the repository /cvmfs/grid.cern.ch

Custom CernVM-FS repository software can be accessed from CVMFS-enabled cluster or a contextualised GridPP CernVM.



Ganga is a Python-based interface for distributed computing with local, batch, or grid running.

Ganga can be configured to use the GridPP DIRAC system as a backend.

Switching from local to batch to grid is trivial thanks to CVMFS, making local testing before Grid running easy.

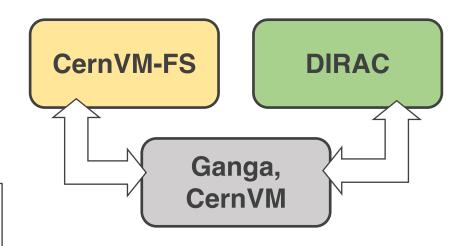




Users can build their software (executables and libraries) on their local SL6 cluster or GridPP CernVM ready for deployment to the grid.

Users can upload their software to their own CernVM-FS repository from using the gsi\* tools in the repository /cvmfs/grid.cern.ch

Custom CernVM-FS repository software can be accessed from CVMFS-enabled cluster or a contextualised GridPP CernVM.



Ganga is a Python-based interface for distributed computing with local, batch, or grid running.

Ganga can be configured to use the GridPP DIRAC system as a backend.

Switching from local to batch to grid is trivial thanks to CVMFS, making local testing before Grid running easy.

18

Combined with Ganga, this gives the user the ability to run local/batch jobs immediately (e.g. for testing) – without needing a grid certificate.

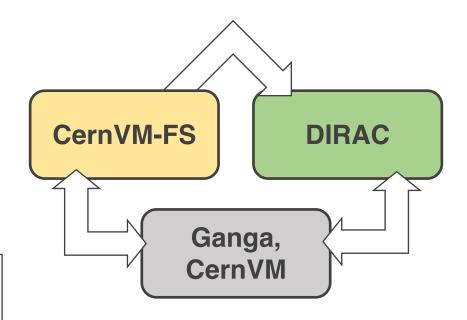
DIRAC, Ganga and experiment software can be deployed via CernVM-FS for local running.



Users can build their software (executables and libraries) on their local SL6 cluster or GridPP CernVM ready for deployment to the grid.

Users can upload their software to their own CernVM-FS repository from using the gsi\* tools in the repository /cvmfs/grid.cern.ch

Custom CernVM-FS repository software can be accessed from CVMFS-enabled cluster or a contextualised GridPP CernVM. User software in (custom) CernVM-FS repositories can used by Grid jobs managed by the GridPP DIRAC system (i.e. sites with CVMFS access).



Ganga is a Python-based interface for distributed computing with local, batch, or grid running.

Ganga can be configured to use the GridPP DIRAC system as a backend.

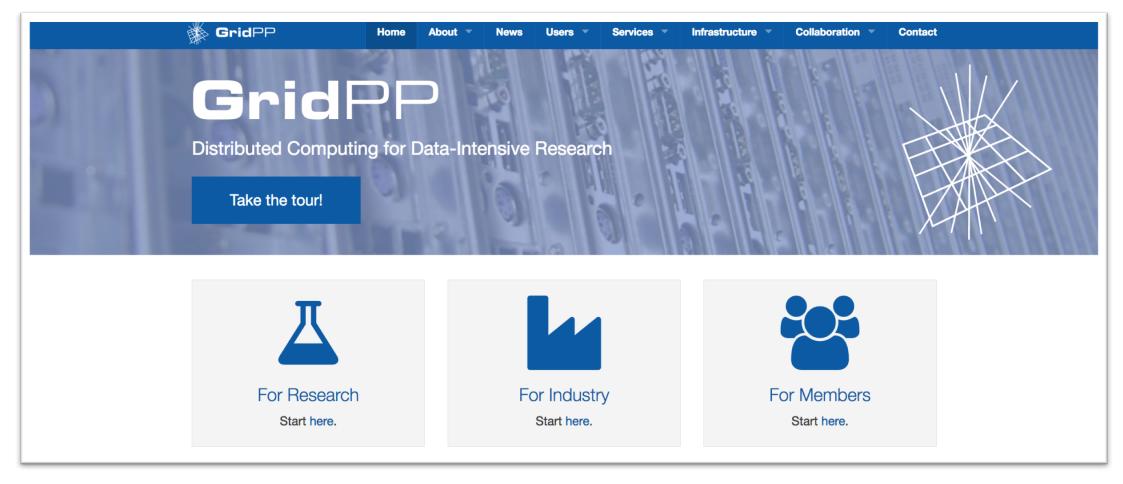
Switching from local to batch to grid is trivial thanks to CVMFS, making local testing before Grid running easy.

Combined with Ganga, this gives the user the ability to run local/batch jobs immediately (e.g. for testing) – without needing a grid certificate.

DIRAC, Ganga and experiment software can be deployed via CernVM-FS for local running.



## **Documentation**



#### http://www.gridpp.ac.uk



## **Documentation**

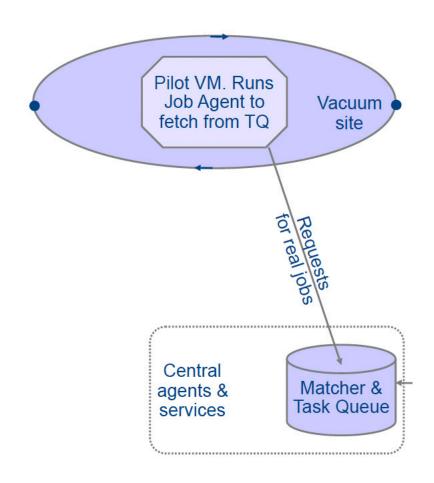


#### http://www.gridpp.ac.uk/userguide



## Advanced approaches for larger VOs

- GridPP DIRAC is optimised for multiple, smaller VOs with HTC in mind;
- Larger VOs (i.e. those with resources for development work) could take advantage of additional DIRAC functionality:
  - e.g. LHCb DIRAC.
- Some possibilities:
  - Rather than jobs, create custom Virtual Machines/clusters on the fly – the VAC model;
  - Integration with HPC systems;
  - Dedicated storage areas and functionality.
- See Andrew McNab's talk...







## Selected case studies

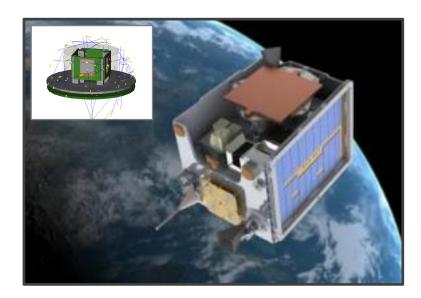
GEANT4 simulations; GalDyn (Galaxy Dynamics); LSST.



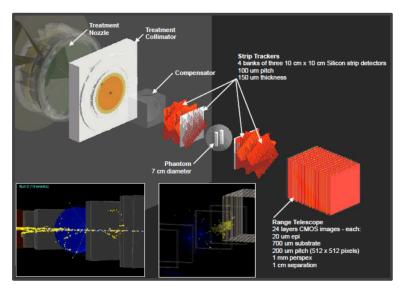


## **GEANT4** simulation campaigns

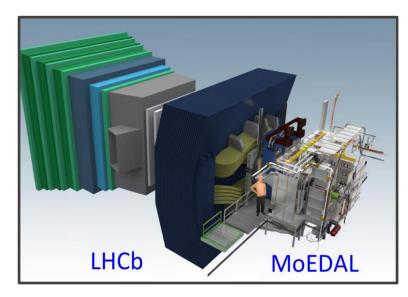
The Grid is ideal for running large-scale simulation campaigns over a large parameter space, e.g. GEANT4 particle transport simulations requiring millions of individual (independent) events. Some examples:



**LUCID**: estimation of data rates in Low Earth Orbit (LEO).



**PRaVDA**: optimisation of new proton therapy systems.



**MoEDAL**: detector acceptances for magnetic monopole searches.

In each case, GridPP DIRAC was used to manage thousands of jobs and data from millions of events across multiple Grid sites, and users reported reductions in running times of **months/weeks** to a **few days**.



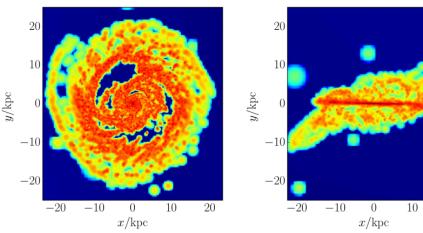
## GalDyn – Galaxy Dynamics (UCLan)

- Galactic Dynamics group at UCLan have been simulating orbits of galactic matter:
  - Focus on particles within galaxies (stars, dark matter, etc.) with thousands of parameters to vary so highly parallelisable.
- Use of GridPP infrastructure:
  - Supported by Lancaster and Liverpool Tier-2s;
  - Software and workflows tested with a CernVM;
  - Jobs run via GridPP DIRAC on NorthGrid VO.

#### • Impact:

- Thousands more parameters new studies;
- 'We can run our code on the Grid and are looking to move into production for our final results. It's nice to know the facility is there and quick to get setup."







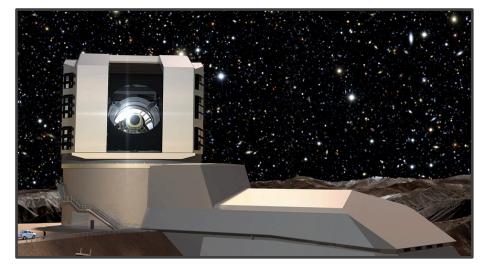


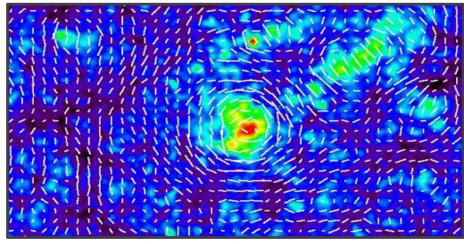
## The Large Synoptic Survey Telescope

- Manchester LSST researchers have been using the Grid to study cosmic shear:
  - Pilot exercise: use im3shape software to analyse O(100k) Dark Energy Survey images.
- Use of GridPP infrastructure:
  - Software tested on local (Manc.) Grid cluster;
  - Analysis jobs managed with Ganga, locally to begin with before switching to GridPP DIRAC;
  - Data managed with the DIRAC File Catalog.

#### • Impact:

- Results 'significantly faster', no longer relying on highly-contested HPC resources;
- GridPP/LSST collaboration continuing.









## Summary and conclusions

- The Worldwide LHC Computing Grid (WLCG) offers substantial computing resources for HTC using the 'Grid' concept:
  - Computing and data always there, where and how we do not care;
  - Crucial to the success of the Large Hadron Collider's physics programme.
- GridPP represents UK's contribution to the WLCG (~11%):
  - 20 institutes, 100+ people, 101k logical CPU cores, 37 PB storage;
  - Commitment to make 10% of resources available to non-LHC users.
- We can offer infrastructure, tools and documentation for new users:
  - GridPP DIRAC for job/data management, Ganga for UI, CVMFS for software;
  - Potential to collaborate to develop solutions for larger communities (later talk);
  - Case studies: <a href="https://www.gridpp.ac.uk/users/case-studies/">https://www.gridpp.ac.uk/users/case-studies/</a>

Huge thanks to the GridPP Collaboration, particularly Imperial College London GridPP DIRAC team (<u>GitHub</u>) and Imperial College London/Birmingham Ganga team (<u>GitHub</u>).





## Thanks for listening! Any questions?

T. Whyntie\*, †

\* Queen Mary University of London

**SKA/GridPP F2F, University of Manchester** 

Wednesday, 2<sup>nd</sup> November 2016



