

### 2nd EUDAT User Forum

#### Data staging to HPC

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SuperComputing, Application and Innovation – CINECA, Italy

2nd EUDAT User Forum, London – 11, 12 March 2013







## Agenda

#### **Topic**

**Data Staging to HPC** - Conveners: P.Coveney, G. Fiameni

09:30 Introducing Data Staging in EUDAT, plus DEMO - G.Fiameni, S. Zesada

10:00 Euro-VO HPC data needs - Sebastien Derriere

10:15 **EISCAT HPC data needs** - *Ingemar Häggström* 

10:30 Mapper HPC data needs - Derek Groen

11:40 Open discussion





## Preliminary services

 Data Staging to facilitate communities to stage stored data onto external computational facilities, such as HPC resources



 Safe Replication to enable communities easily create replicas of their scientific datasets in multiple data centres for improving data curation and accessibility

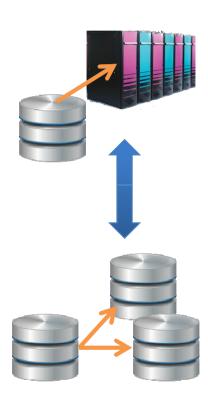






## Preliminary services

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## Building Blocks of the CDI



#### **EUDAT Access Interface**

Integrated APIs and harmonized access to EUDAT facilities

#### **Metadata Catalog**

Aggregated EUDAT metadata domain. Data inventory



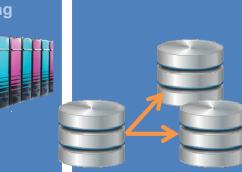
**Simple Store** 

Researcher data

store (simple

#### **Data Staging**

Dynamic replication to HPC workspace for processing



#### Safe Replication

Data curation and access optimization



#### AAI

Network of trust among authentication and authorization actors



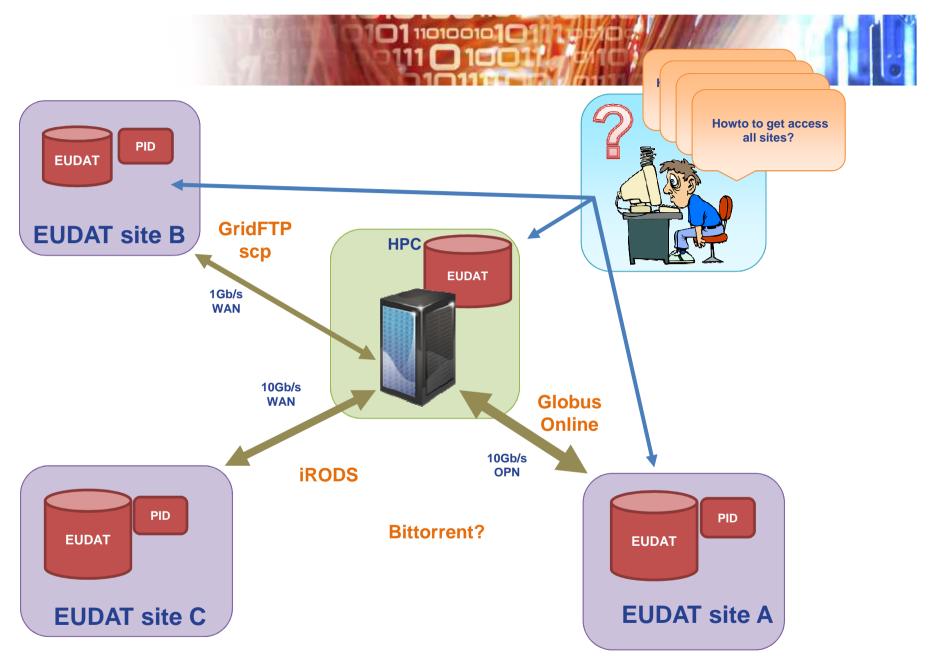




## Driving principles

- Work close to scientific communities
- Leverage on existing technologies, experiences, knowledge
- Short term, very frequent, delivers
- Services are meant for the production
- Collaboration with other activities, projects, einfrastructures is fundamental (i.e. PRACE, EGI)
- Focus on "Low-hanging fruits" Easy things come first









### Goals

- Allow communities move easily large amounts of data between EUDAT storage resources and workspace areas on HPC systems to be further processed
- Offer reliable, efficient, easy-to-use tools to manage data transfers
- Provide the means to re-ingest computational results back into the EUDAT infrastructure
- Permit integration with existing infrastructure (i.e. PRACE), data services

#### Staging of data









Safe replication of data





### Challenges

- Many technologies are available outside
- Communities prefer to extend their existing solutions rather than acquiring new ones
- Computational infrastructures already have their own data services which EUDAT should comply with
- Transferring large amount of data across the public network is not a trivial task
- Limited effort to be allocated on developing new software





## Who might benefit from it?

- The Data Staging service is aimed at researchers, who:
  - need access to both large-scale data storage and high-performance computing systems;
  - wish to move data easily between the EUDAT data stores and remote HPC facilities such as those provided by the PRACE distributed infrastructure.



# 

#### How it works

#### Server side

 the data staging functionality is realized by extending the iRODS system with a GridFTP interface using the Griffin technology so as to permit the transfer of data through a reliable, highperformance protocol



#### Client side

 any existing client, supporting the GridFTP protocol can be employed – globus-url-copy, Globus On Line, UberFTP, gTransfer, etc.



 Among available clients, EUDAT recommends the XSEDE-EUDAT File Manager which supports a range of transfer protocols (i.e. GridFTP, FTP, native iRODS, etc.) and provides an intuitive and friendly interface



 Users need a personal certificate (X.509) to fully exploit the service





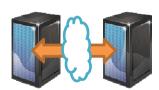


#### Different flavors of the same service

 Local data staging: staging of data among the resources of the same site using low level tools



 Remote data staging: staging of data using remote data services (e.g. external GridFTP service). Many more implications and constraints!

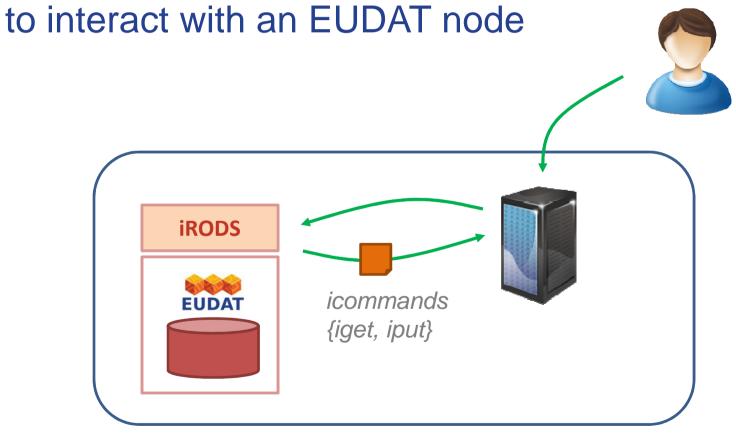






## Local data staging

• iRODS icommands provide a low level interface

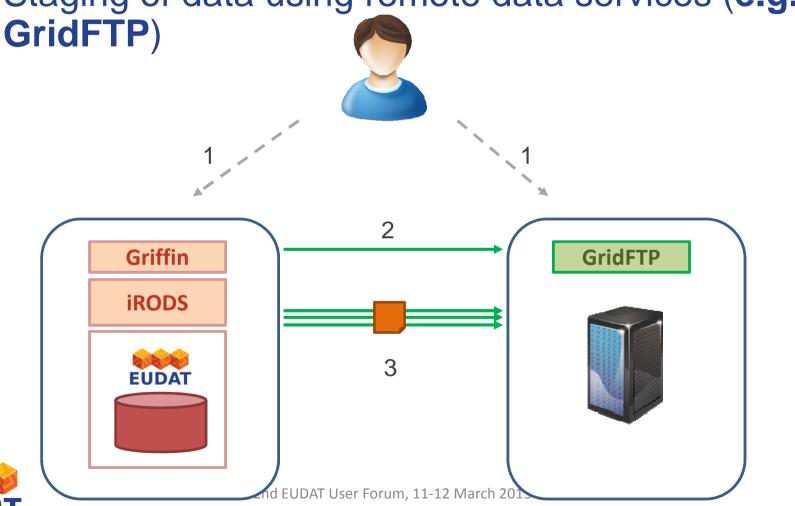






## Remote data staging

• Staging of data using remote data services (e.g.





Requirements mapping							
	Griffin	UNICORE	FTS	Globus	Parrot	iRODS +	gTransfer
		FTP		Online		iCommands	
			-		Functional		
Capability to stage entire directory	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Stage large data sets without big performance penalty	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Search mechanism	N.A.	N.A.	N.A.	Yes	N.A.	Yes	No
Multi-point transfers (i.e. from many sources to one destination)	N.A.	N.A.	No	No	N.A.	No	Yes
API	Yes	No	No	Yes (beta)	No	Yes (Jargon, PyRords)	No
Automatic deletion of staged data sets	No	Unknown	No	No	Unknown	Yes	No
Compatibility with GridFTP (to permit interaction with PRACE)		Yes	Yes	Yes	Yes	No	Yes
Support for X.509 credentials	Yes	Yes	Yes	Yes	Yes	Yes	Yes
				No	n-functional		
Ease of use	N.A.	Good	N.A.	Very good	Medium	Medium	Medium
Support for third-party ransfers	Yes	Yes	Yes	Yes	No	Yes	Yes
Possibility to tune network parameters	Manual	No	Manual	Automatic	Manual	No	Semi-automatic
Compatibility with iRODS	Yes	No	Through Griffin	Through Griffin	Through Griffin	Yes	Through Griffin
Transfer restart/resume	Yes (only for third-party)	No	Unknown	Yes	No	No	Yes (only for third-party)
Ability in managing many transfers simultaneously	No	No	Yes	Yes	No	No	No



## Some examples





### iRODS icommands

- Low level command-line tools to manage data which are stored onto iRODS resources
- Reliable and programmatic
- Provide high performance
- Easy to setup and portable on many systems

prompt\$ iget -N 4 /home/irods/data/archive /shared/data/userprace/tmp
prompt\$ iput -N 4 /shared/data/userprace/tmp /home/irods/data/archive





## **Griffin (GridFTP interface)**

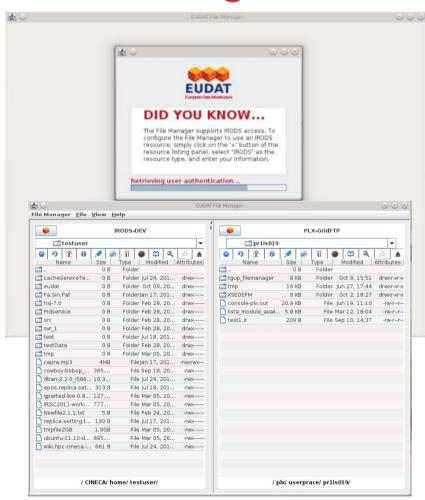
- GridFTP server, entirely written in JAVA, being able to access iRODS resources as well as plain file systems
- Supports most of GridFTP features, including multiple streams, tcp-buffer size tuning and files pipelining
- Unfortunately multiple-stripe is not supported
- Several tests were performed at CINECA and SARA where large data sets, of the order of hundreds of GBs, have been transferred back and forth the two sites with success





## XSEDE/EUDAT File Manager

- Client interface
- Developed within the XSEDE (Extreme Science and Engineering Discovery Environment) project
- Provides users with an easy-touse, drag-and-drop interface for managing data transfers over GridFTP/iRODS servers.
- Heavily tested within EUDAT in collaboration with Texas
   Advanced Computing Center







## **Data Staging Script**

- A simple python modular staging script to help communities integrate the data staging service within their exiting solutions
- Based on Globus Online API and iRODS rule mechanism for data selectio

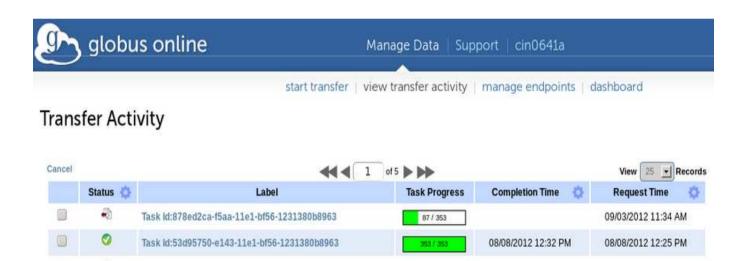
prompt\$ ./datastager.py -p /home/irods/data/archive -y 2004 -n MN
-s AQU -c BHE -u cin0641a --ss ingv --ds GSI-PLX -dd
/shared/data/userprace/tmp





### Globus Online

 Globus Online functionalities were evaluated with success and the Griffin component extended in order to support it



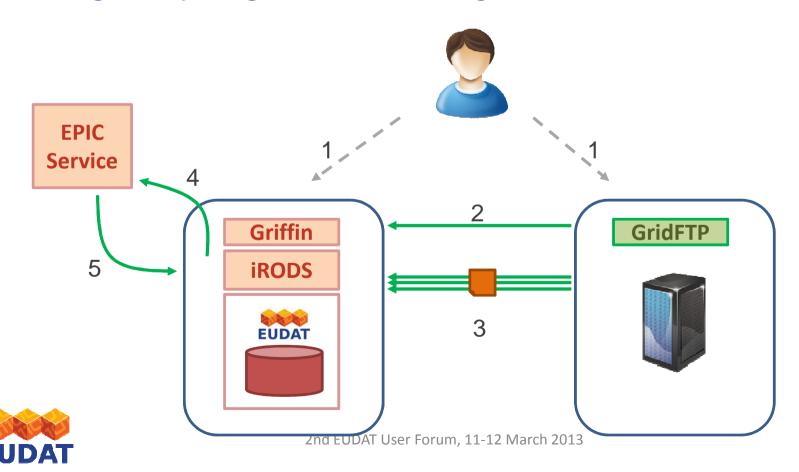






### PIDs to staged data sets

 Data ingested back onto EUDAT resources are regularly registered through PID





#### Conclusions

- Data staging building blocks are right now available!
- Some extensions could be needed to better fit with the upcoming Authentication/Authorization
   Infrastructure
- XSEDE/EUDAT File Manager valuable interface to move data across different infrastructures (EUDAT, PRACE, XSEDE)
- Other transfer protocols, such HTTP or WebDav, are under investigation





### Keep involved...

- Visit: http://www.eudat.eu/data-staging
- Email: <u>eudat-datastaging@postit.csc.fi</u>
- Periodic news:
   http://www.eudat.eu/newspublications





#### **Useful links**

- XSEDE-EUDAT File Manager
  - github.com/TACC/filemanager/tree/eudat
- gTransfer
  - github.com/fr4nk5ch31n3r/gtransfer
- iRODS
  - www.irods.org
- GridFTP
  - www.globus.org/toolkit/data/gridftp
- Globus OnLine
  - www.globusonline.org
- Griffin
  - https://projects.arcs.org.au/trac/griffin





## Any question?





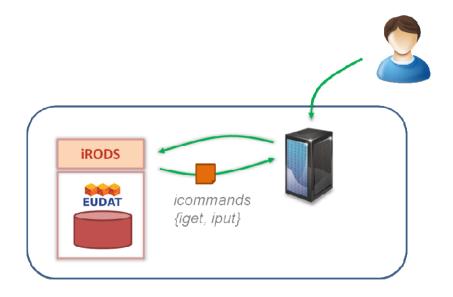
## Final Wrap-up





#### **Demonstration**

- Staging of data within the same site (CSC) through the VPH web portal
- Stefan Zasada (VPH@UCL)





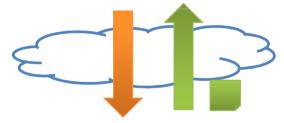
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Data staging Session Wrap-up

 Data Staging to facilitate communities to stage stored data onto external computational facilities, such as HPC resources









Safe replication of data





#### Overall comments

- Authentication/Authorization/Accounting
  - Access to data replicas
  - Use of certificate
  - Harmonization of existing solutions/systems!
- Checksum of transferred data
  - Protocol specific
- SRM (Storage Resource Manager) interface
- How to get new communities onboard?





### **EURO-VO**

- Astronomical data collected worldwide
- Heterogeneous, large data sets
- Metadata in XML (OAI-PMH)
- Using iRODS for managing data
- Many similarities with EUDAT
  - Simple store
  - Meta-data
  - Data Staging
- Move computation to data





### EISCAT\_3D

- Data from radar
  - atmospheric studies of the Fenno-Scandinavian Arctic
- Moving from 2D to 3D images
- Need of computational power
  - Targeting:100000 Pflops!
- Evolution roadmap
  - EISCAT 2D 60TBs
  - EISCAT 3D 1<sup>st</sup> Phase (2018) 1PB
  - EISCAT 3D 2<sup>nd</sup> Phase (2023) 10 PB (EUDAT?)





## Mapper

- Multi-scale models
  - Different communities being involved
- Distributed simulations
  - HPC, HTC resources
- GridFTP for data staging
- Efficiently organize data between resources
- Performance is a key
  - Small data sets but transferred frequently
- Data service for long term preservation and analysis

