



Enabling Grids for E-sciencE

gLite Application Developers Course

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Application development for the EGEE grid

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What is a grid application?

Software that interacts with grid services to achieve requirements that are specific to a particular VO or user.



Goals of this session

- This talk maps the landscape a high-level view of application development in Grids
- Practicals will explore specific features in that landscape

Contents



- What are grids for??
- Types of Grid applications
- Challenges to researchers who write applications
- More about gLite Services
- Overview of the rest of the afternoon



What are grids for?

Collaborative "virtual computing"

Improvised cooperation

People with shared goals

Sharing data, computers, software Enabled by Grids:

National, regional, International: EGEE grid

Email File exch

File exchange ssh access to run programs Enabled by networks:

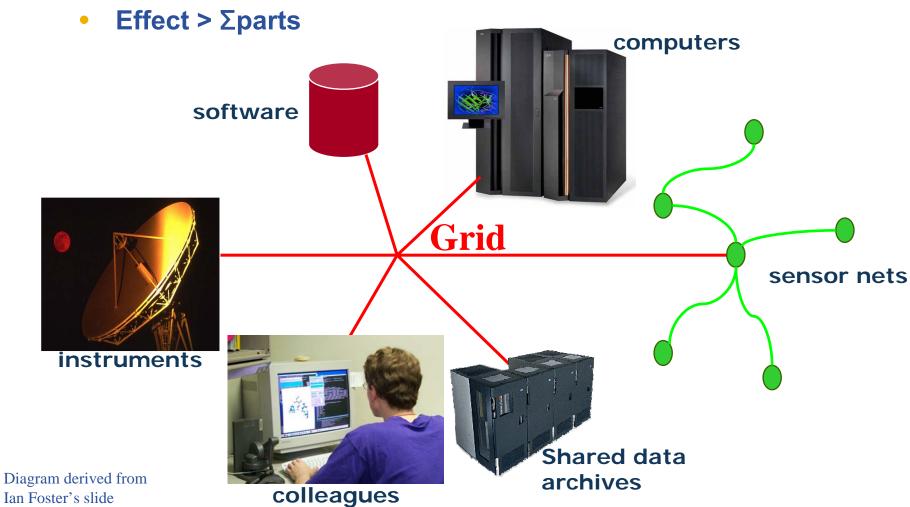
national, regional and International: GEANT



CGC Grids: a foundation for e-Research

Enabling Grids for E-sciencE

- **Enabling a whole-system approach**
- A challenge to the imagination





"Effect > Σparts"

- Flexible orchestration of resources available to a Virtual Organisation (VO)
 - Across administrative domains
 - Abstractions hide detail of individual resources
 - Conform to Grid's procedures to gain benefit
 - Decoupled provision of resources and their use
 - Additional benefits from
 - Operations services (people and software)
 - Engagement in diverse e-research communities
- Increased utilisation of resources
 - Within a VO
 - Between VOs EGEE, ...
 - Each VO can benefit from
 - Heterogeneity
 - Scale



The vital layer



Where computer science meets the application communities!

VO-specific developments built on higher-level tools and core services

Makes Grid services useable by non-specialists

Grids provide the compute and data storage resources

Production grids provide these core services.



Types of grid applications



Types of grid applications

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1. Simple jobs – submitted to WMS to run in batch mode

2. Job invokes grid services

- To read & write files on SE
- Monitoring
- For outbound connectivity (interactive jobs)
- To manage metadata
- •

3. Complex jobs

- An environment controls multiple jobs on users' behalf
 - High-level services
 - Portals with workflow e.g. P-GRADE
 - Software written for the VO (or by the user)
 - •



Invocation of applications

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From the UI

- Command Line Interfaces / Scripts
- APIs
- Higher level tools

From desktop Windows applications

- Use Grids without awareness of them!
- But gLite not (yet) supporting Windows

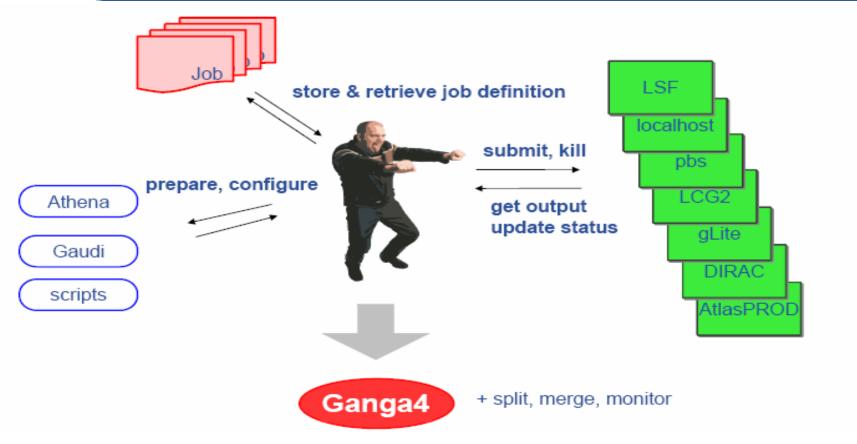
From portals

- For recurring tasks: "core grid services" as well as application layer
- Accessible from any browser
- Tailored to applications
- In EGEE: P-GRADE and GENIUS



Example of higher-level tools -1: GANGA

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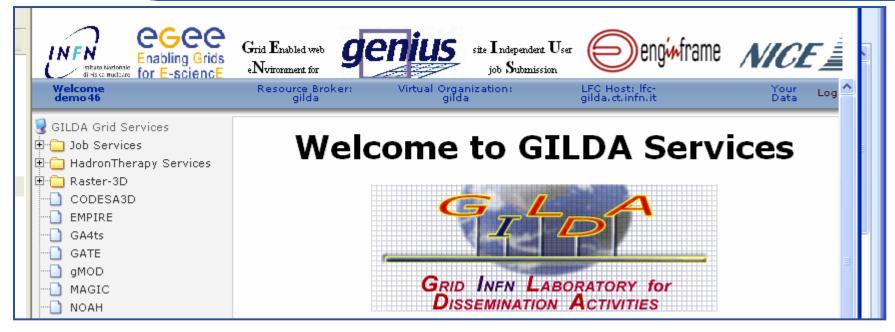


- •Ganga is a lightweight user tool ganga.web.cern.ch/
- But also: Ganga is a developer framework



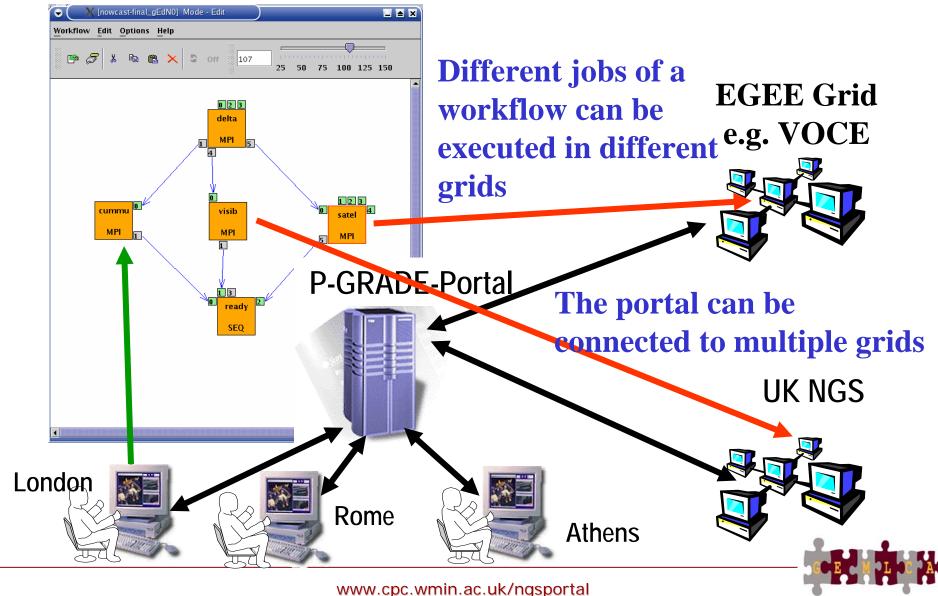
GENIUS

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- For many application communities
 - Interface can be tailored for specific requirements
- For demonstration purposes
 - https://glite-demo.ct.infn.it/
 - Available for anyone to use
 - https://glite-tutor.ct.infn.it/
 - Fuller functionality for users who have stored long-lived proxy in MyProxy server

Multi-Grid P-GRADE Portal





Characteristics of VOs

• What is being shared?

- resources of storage and/or compute cycles
- software and/or data

Developers and users

- Some VOs have distinct groups of developers and users...
 - Biomedical applications used by clinicians,....
- Some don't
 - Physics application developers who share data but write own analyses
- Effect: need to
 - hide complexity from the 1st type of VOs.... E.g. AA
 - expose functionality to 2nd type of VOs



- I need resources for my research
 - I need richer functionality
 - MPI, parametric sweeps,...
 - Data and compute services together...
- I provide an application for (y)our research
 - How!?
 - Pre-install executables ?
 - Hosting environment?
 - Share data
 - Use it via portal?
- We provide applications for (y)our research
 - Also need:
 - Coordination of development
 - Standards
 - •

ngineering challenges increasing



Challenges to researchers who write grid applications



Challenges

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- Research software is often
 - Created for one user : the developer
 - Familiarity makes it useable
 - Short-term goals:
 Used until papers
 are written and
 then discarded

- Grid applications are often used
 - by a VO
 - Without support from developer
 - In new contexts and workflows

- Grid application developers are
 - In a research environment
 - Yet their s/w must have:
 - Stability
 - Documentation
 - Useability
 - Extendability
 - i.e. Production quality

Need expertise in:

- software engineering
- application domain
- grid computing/



Consequences

- Team work!
- Engaged in world-wide initiatives reuse don't make your own!
 Cross disciplines for solutions.
- From research to production software: ~5 times the effort.
 - "80% of the time for last 10% of the functionality & reliability"
- Standardisation is key
 - For re-use, for dynamic configuration of services,...
 - Both for middleware and domain specific (e.g. GEON)
- Need development process discipline!!
 - Discipline = formal, staged, deliberate process
 - Waterfall? Rapid prototyping?
 - Need a deliberate approach: requirements engineering, design, implementation, validation, deployment
 - Need formalising, need deliberation because aiming for
 - Production quality, through teamwork, with distinct user community

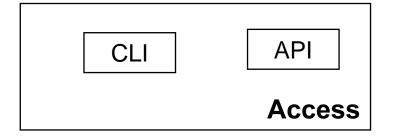


More about gLite services



gLite Grid Middleware Services

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Authorization
Auditing
Authentication
Security Services

Information & Application
Monitoring Monitoring

Information &
Monitoring Services

Package Job Metadata File & Replica Accounting Provenance Manager Catalog Catalog Storage Workload Data Computing Connectivity Element Movement Management Element **Workload Mgmt Services Data Management**



More about gLite services

Enabling Grids for E-science

- During this afternoon focus is on:
 - New functionality in gLite 3.0 Workload Management
 - Integrating workload and data management
 - Accessing data on SEs
 - Can have massive files, too big to copy
 - How to access these?
 - Management of metadata
 - May have many thousands of files
 - Need to access and re-use based on characteristics... more than by their logical file names.
 - Monitoring of applications
 - May be running many long jobs
 - What's happening?!



Workload Management System

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- Helps the user accessing computing resources
 - resource brokering
 - management of input and output
 - management of complex workflows
- Support for MPI job even if the file system is not shared between CE and Worker Nodes (WN) – easy JDL extensions
- Web Service interface via WMProxy



WMProxy

 WMProxy is a SOAP Web service providing access to the Workload Management System (WMS)

Client

Job characteristics specified via JDL

jobRegister

create id

 map to local user and create job dir

register to L&B

return id to user

input files transfer

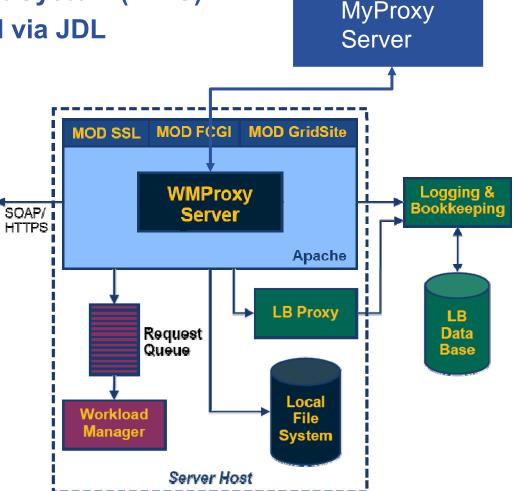
jobStart

register sub-jobs to L&B

 map to local user and create sub-job dir's

unpack sub-job files

deliver jobs to WM

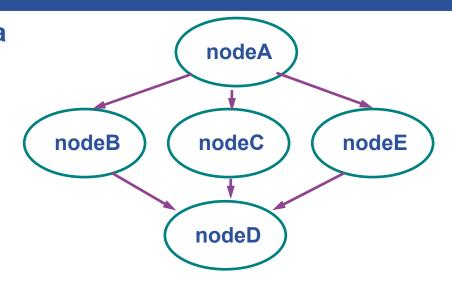




Complex Workflows

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- Direct Acyclic Graph (DAG) is a set of jobs where the input, output, or execution of one or more jobs depends on one or more other jobs
- A Collection is a group of jobs with no dependencies
 - basically a collection of JDL's



- A Parametric job is a job having one or more attributes in the JDL that vary their values according to parameters
- Using compound jobs it is possible to have one shot submission of a (possibly very large, up to thousands) group of jobs
 - Submission time reduction
 - Single call to WMProxy server
 - Single Authentication and Authorization process
 - Sharing of files between jobs
 - Availability of both a single Job Id to manage the group as a whole and an Id for each single job in the group



WMProxy: users' view

- glite-wms-job-submit will supercede glite-job-submit
- Its support for compound jobs will simplify application software
 - WMProxy manages sub-jobs
 - Shared Input and Output "sandboxes"
- MUST establish MyProxy delegation before this can be used!
- (Today we are not using WMProxy)



Overview of practicals



Overview of the practicals

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- Previous gLite tutorial introduced basic services.
- Today: building more complex applications
 - Use of script to submit multiple jobs
 - Coordinating Workload Management with Data Management
 - Parallelism using MPI
 - Within a CE not across domains
 - Use of GFAL functions to access files on SEs
- Use of AMGA: metadata service
- Use of R-GMA: monitoring service



Acknowledgements

- GILDA team for GILDA and associated Wiki etc.
- Many discussions with EGEE colleagues, in particular
 - Emidio Giorgio, University of Catania and INFN, Italy
 - Richard Hopkins & Guy Warner, TOE, Scotland
 - Gergely Sipos, SZTAKI, Hungary