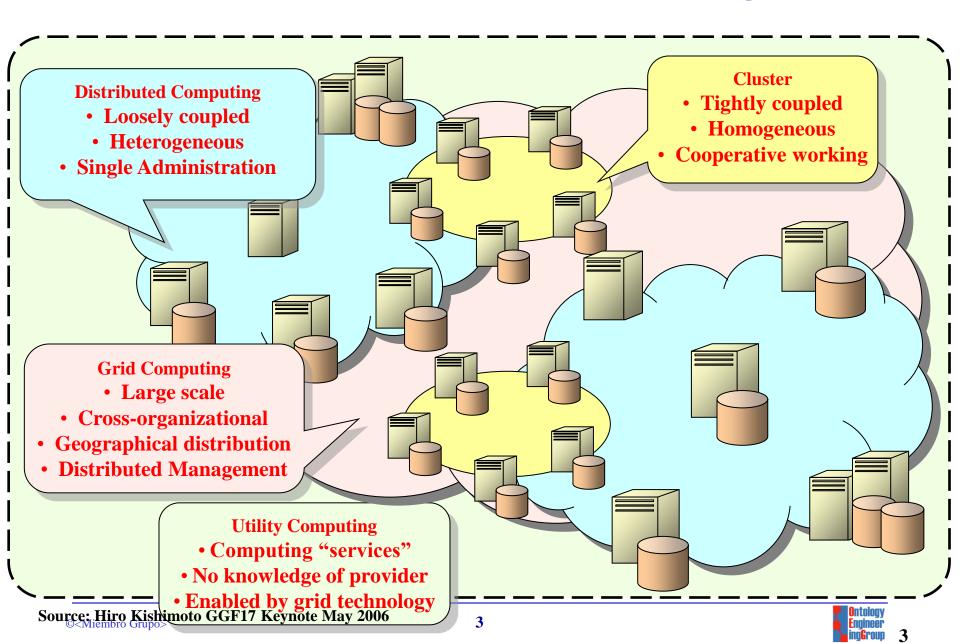
International Summer School on Grid Computing 2008

Carlos Buil Aranda

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- Grid important technologies
 - Security
 - Computational Resources & Job management
 - HTP (High Throughput Computing)
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 - Condor
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 - gLite
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- Interfaces to Grid middleware
 - SAGA
 - Services and Workflows

Introduction - Grid & Related Paradigms



Introduction – The Grid

- What does the Grid provide?
 - Combine different and heterogeneous systems
 - Heterogeneity of data, systems, instruments, research processes, etc.
 - Grids provide virtual communities (virtual homogeneity)
 - Component for e-Infrastructure
- Why use/build Grids?
 - New Research: enabling new ways of doing research in many disciplines
 - Economic reasons
 - Computer science reasons (distributed systems problems)

Introduction - eScience

- What is e-Science?
 - E-Science is the application of the Grid infrastructure in order to obtain a better, faster or new research result in ALL research disciplines
- What is e-Infrastructure?
 - "e-Infrastructure is the term used for the distributed computing infrastructure that provides shared access to large data collections, advanced ICT tools for data analysis, large-scale computing resources and high performance visualisation"
 - Not only Grids but also networks, data centre and specially enabling collaboration techniques.
- Collaboration

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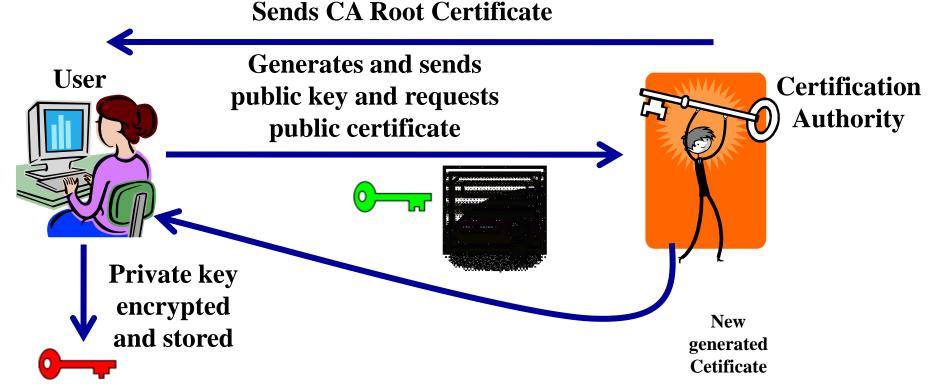
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Grid Security

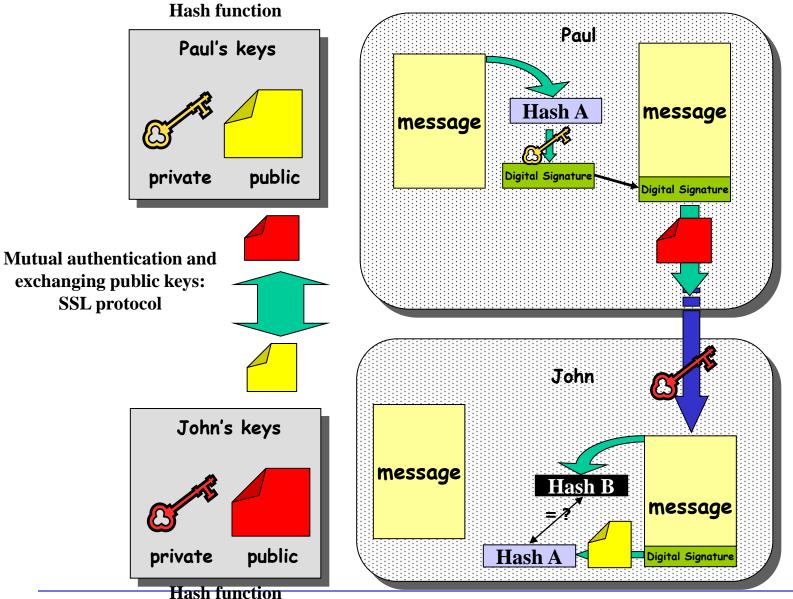
- Different clusters access to other clusters information
- Why should the OEG cluster trust the cluster UPC in Barcelona? Who do I know they are who they say they are?
 - Sensitive information must be protected
 - The cluster resources must be protected
- Communication happens through internet
 - Internet is not the most secure channel
- Two levels of security
 - Network level security (Authentication)
 - VO level security (Authorization)

Grid Security Infrastructure (GSI)

- Security at network level: Public Key Infrastructure (PKI)
- Based on pair of keys: Public and Private keys



PKI in action – the big picture



Grid Security

- VO Security
 - To what resources can user X access?
 - Authorization problem
 - Keeping a database on every site
 - Keeping a list centrally
- Delegation of access rights
 - Proxy certificates

Distributed Systems Principles

P.H. Enslow, "What is a Distributed Data Processing System?" Computer, January 1978

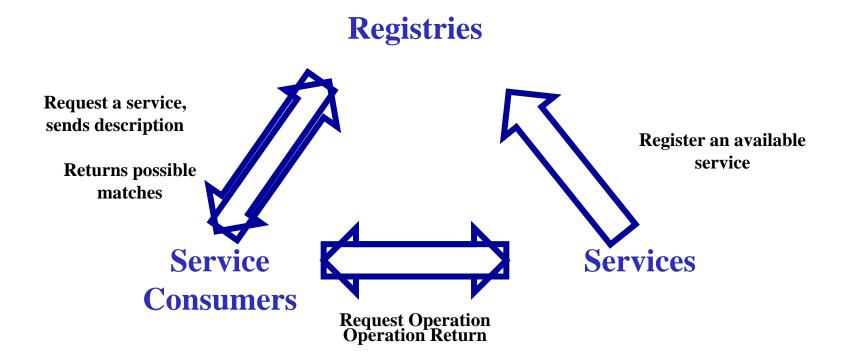
- High Availability and Reliability
- High System Performance
- Ease of Modular and Incremental Growth
- Automatic Load and Resource Sharing
- Good Response to Temporary Overloads
- Easy Expansion in Capacity and/or Function

Distributed Systems Principles (problems)

Distributed systems problems

- Lack of Knowledge
 - Due to technical reasons (latency, failures, tec.), human reasons (incomplete knowledge, lack of understanding, poor models)
- Heterogeneity
 - Hardware heterogeneity (computer architectures, storage systems, input instruments), OS heterogeneity, different implementations systems
- Latency
 - It always be there (and probably it will get worse due to geographic scale, system complexity, processing time)
- Unreliability
 - Failures can happen (Network outages, Power outages, software errors, etc.)
- Autonomy & Change
 - Changes on local systems, services

Distributed Systems Principles (Service Oriented Architecture)



Computational Resources & Job management

- Multiprocessor systems
 - Shared memory
 - Distributed memory
 - Distributed shared memory
- Usage
 - submission of jobs by the users
 - Processing of these jobs
 - High amount of jobs, resources are not so large
- Ways for managing submission of jobs is required
 - Time sharing
 - Space sharing



Job submission

- High heterogeneity of computational resources:
 - Different types of machines, OS, requirements for submission, memory, cores, duration of the tasks, etc.
- Abstraction is needed for submitting jobs
 - JSDL: Job Submission Description Language
 - OGF standard
 - Every system has its own submission language

• JSDL

- XML based
- Defines the job requirements (type of processor, OS, memory, etc.) and parameters (inputs, outputs, etc.)
- It is not possible to submit jobs directly to resources

JSDL Example

```
<jsdl:JobDefinition xmlns="http://www.example.org/"
  xmlns:jsdl="http://schemas.ggf.org/jsdl/2005/11/jsdl"
  xmlns:jsdl-posix="http://schemas.ggf.org/jsdl/2005/11/jsdl-posix"
  xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
 <jsdl:JobDescription>
  <isdl:JobIdentification>
   <jsdl:JobName>Simple Application GW Template vs JSDL</jsdl:JobName>
   <jsdl:Description> This is a simple example to describe the main
       differences between GW Template and the JSDL schema.
   </jsdl:Description>
  </jsdl:JobIdentification>
  <jsdl:Application>
   <jsdl:ApplicationName>ls</jsdl:ApplicationName>
   <jsdl-posix:POSIXApplication>
    <jsdl-posix:Executable>/bin/ls</jsdl-posix:Executable>
    <jsdl-posix:Argument>-la file.txt</jsdl-posix:Argument>
    <jsdl-posix:Environment name="LD_LIBRARY_PATH">/usr/local/lib</jsdl-posix:Environment>
    <jsdl-posix:Input>/dev/null</jsdl-posix:Input>
    <jsdl-posix:Output>stdout.${JOB ID}</jsdl-posix:Output>
    <jsdl-posix:Error>stderr.${JOB_ID}</jsdl-posix:Error>
   </isdl-posix:POSIXApplication>
  </jsdl:Application>
  <jsdl:Resources>
   <jsdl:CandidateHost>
    <jsdl:HostName>*.dacya.ucm.es</jsdl:HostName>
   </jsdl:CandidateHost>
   <isdl:CPUArchitecture>
    <jsdl:CPUArchitectureName>x86 32</jsdl:CPUArchitectureName>
   </jsdl:CPUArchitecture>
  </jsdl:Resources>
```

Execution & Job management

- Initiating/submitting, monitoring and managing jobs
 - Translate job to the target system language, submit the job, get the job status, cache the job if something goes wrong, etc.
- Handling and organizing all the job data
 - Manage the job data (internal directories, intermediate data used by the jobs, etc.). All these data is preserved/organized after the successful job completion.
- Coordinating and scheduling jobs
 - Coordinate workflow resources, manage the initiation of the workflow execution, monitor the workflow, etc.

High Throughput Computing

- Provide to the users a high amount of computational resources
 - Goal: be able to maintain a high number of processes running with high performance and reliability
 - Reliability is a key question in these systems
- High amount of resources
- High availability of these resources
 - The greater the degree of replication of resources, the better the ability of the system to maintain high reliability and performance
- Principal unity of control
 - One unit that leads the goal of all resources working together
- Transparency for the user
 - Remember VOs?
- Component autonomy
 - The resources are independent of allowing or not the use of their capabilities



Distributed Data Management

- Data characteristics
 - Distributed, produced in large quantities, etc.
 - Where the data is used?
 - Scientific applications consume large amounts of data
 - Problems
 - Storage is not a problem anymore
 - Computing power is still a problem
 - But not a big deal, we still produce large amounts of data but storage systems and processing systems are growing
 - New problem: the power needed to analyse/use the data

Principles of Distributed Data Management (I)

- Data Processing, data access, data replication
- Data processing
 - Co-scheduling: moving computation to data
 - Desirable for large amounts of data
 - Problems
 - assure required data near execution host is online
 - second code near data without long wait time
 - Clean up after execution or failure
 - Evtl. licence availability
 - ~70% of all failures in distributed systems are due to failure to properly manage data
 - Complexities
 - some data can not be distributed
 - metadata stores use to be central (information about the execution of a process, for example)

Principles of Distributed Data Management (II)

Remote Data Access

- Streaming
 - Direct access to the information: it is processed when it is accessed/created
- Caching
 - Use local data caches
- Difficulties
 - Data validity

Replication

- Keeping replicas of data in many places in a Grid
 - It is possible to keep data close to the computation system allowing to:
 - Improving throughput and efficiency
 - Reducing latency
 - Both problems previously stated (see previous slide)
- Replica problems
 - Consistency of replicas
 - Locating the replicas
 - Where do I store replicas? Country problems, legal issues
 - Semantically equivalent but not identical replicas



Principles of Distributed Data Management (III)

- Space Management
 - assure that target has enough space
 - output can be written
- File Transfer
 - Grid ftp
 - Reliable GridFTP
 - System's own implementations
- Trust
 - Site policies: Do not trust the users
 - Who can access what information
 - VO policies: Do not trust the sites
 - Accessing sensitive data
 - Managing user and group at VO level
 - An agreement must be achieved

Distributed File Management

- Distributed File Systems
 - Wide Area File Access
 - Storage Resource Manager SRM interface to File Storage
 - Exists OGF Standard
 - Difficulties
 - Scaling issues (servers, clients, updates), secutiry
- Managed Storage Systems
 - Stores data in the order of Petabytes
 - Total-throughput scales with the size of the installation
 - Supports several hundreds to thousands of clients
 - Adding / removing storage nodes w/o system interruption

Others

Google File System

- MapReduce parallel data programming model
 - Allows for automatic parallelization of data intensive tasks
 - Generate intermediate key/value pairs for a regular key/value
 - Reduce(merge) all generated ones back together
- GoggleFS filesystem Open Hadoop implementation

Hadoop

- NOT for Wide Area yet
- Built with reliability in mind for commodity hardware
- Optimized for streaming access, not generic posix
- Built in java for large files
- Write once read many patterns best
- Very new, changing fast
- Watch out for scaling



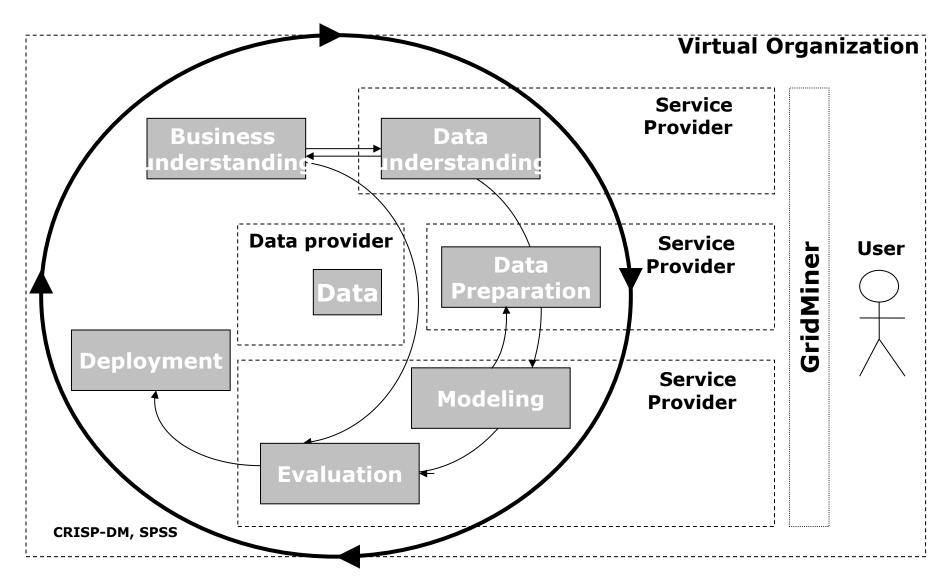
Distributed Data Mining

- Large amounts of distributed data
- It is possible to extract useful information from the data generated
- Possibility of distributing data mining processes
 - Adaptation of data mining processes to a distributed environment

ADMIRE

- Advanced Data Mining and Integration research for Europe
- Accelerate access to and increase the benefits from data exploitation;
- Deliver consistent and easy to use technology for extracting information and knowledge;
- Cope with complexity, distribution, change and heterogeneity of services, data, and processes, through abstract view of data mining and integration; and
- Provide power to users and developers of data mining and integration processes.

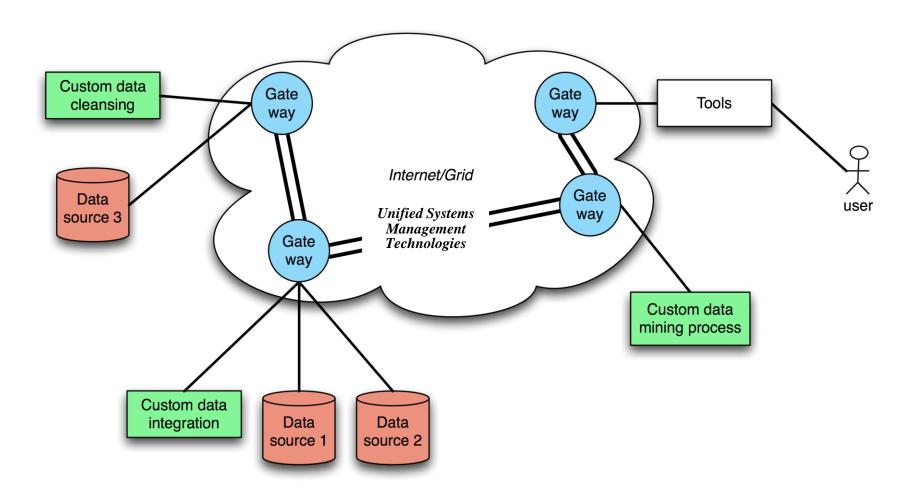
GridMiner Data Mining Model



Slide by Peter Brezany – ISSGC08 Balatonfüred, Hungary

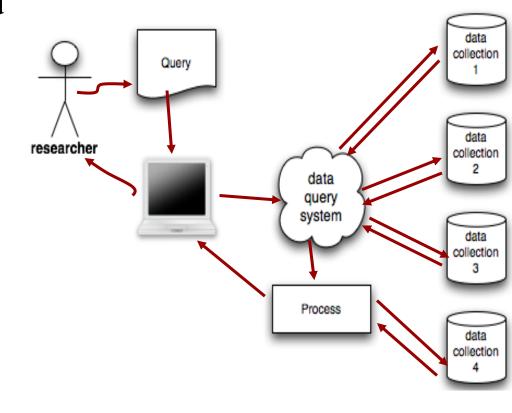
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ADMIRE's High-Level Architecture



Data Access and Integration

- Gather data from different and distributed sources
- Scientists/researchers make queries to different data sources
- DAI system distributes the queries
- DAI system integrates and process the results to form the requested data
- The data is processed as the user demanded

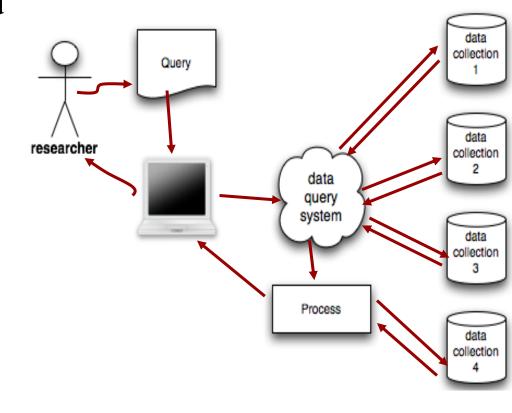




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Data Access and Integration

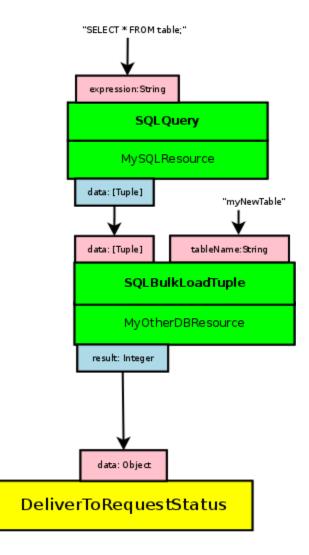
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- DAI system distributes the queries
- DAI system integrates and process the results to form the requested data
- The data is processed as the user demanded



OGSA-DAI

OGSA-DAI is

- An extensible framework that allows to
- Access, integrate, transform and deliver
- Distributed and heterogeneous sources of dat
- OGSA-DAI key elements are
 - Resources (Data request execution resource,
 - Activities (=operations or named unit of func
 - Activity connectors for connecting inputs and
 - Workflows (=composition of activities)
 - Pipeline workflow (A set of chained activities data flowing between the activities)
 - Sequence workflow
 - Parallel workflow



Desktop Grids

- Resource Donors and Users
 - if U ~ D => generic Grid model
 - if U >> D => service Grid model
 - if U << D => desktop Grid model
- Generic Grids
 - Anyone can donate resources, heterogeneity, run own applications
- Service Grids
 - Push Model
 - Guaranteed service
 - Many users: anyone can use the assigned resources for running their own applications

Desktop Grids (II)

- Desktop Grid model
- Dynamic resource donation
 - Based on desktop computers
 - More donors of resources than consumers
 - Not guaranteed service
 - Pull model
 - Not large number of grid applications
- BOINC (Berkeley Open Infrastructure for Network Computing)
 - A donor (participant) can define the distribution of idle CPU time for different projects



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Grid Middleware

- Middleware between the computational resources and the users (computer scientists, researchers)
- The middleware interacts with both
 - User requirements
 - Available resources
- Provides
 - Security infrastructure, job management, data management, job monitoring
- Different implementations for different Grid systems
 - Supercomputers, large clusters, high amount of personal computers,

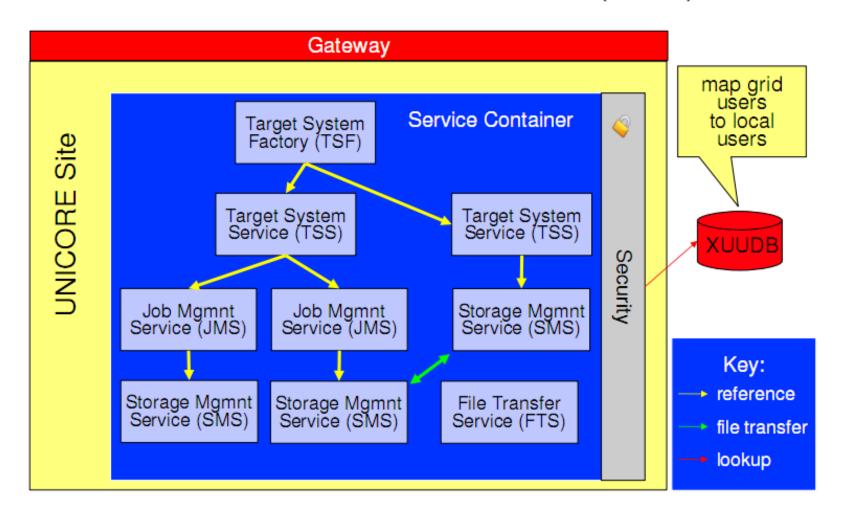
UNICORE

- Uniform Interface to Computing Resources
- UNICORE is a Grid middleware that provides seamless, secure, and intuitive access to distributed Grid resources
 - Grid resources: supercomputers or clusters systems
- Submitting a job
 - Client establishes a SSL connection with the UNICORE gateway
 - XUUDB checks the user
 - UNICOREX send the job to TSI
- TSI (Target System Interface)
 - Executes the job



UNICORE (II)

UNICORE Atomic Services (UAS)



System 1 Submit job file

```
Executable: "/bin/date",
  Arguments: ["-v", "-d"],
  Environment: ["SHELL=/bin/bash", "JAVA_OPTS=-v"],
  Imports: [
    { File: myfile, To: uspaceFile },
  ],
  Exports: [
   { File: uspaceOutFile, To: "localName" },
    { File: otherUspaceOutFile, To: "otherLocalName"},
  ],
  Stage in: [
             From: "RBYTEIO: http://localhost: 8080/XNJS/etcetc",
             To: "uspaceFileName"
  ],
   Stage out: [
             From: stdout,
             To: "RBYTEIO: http://someserver/someresource"
  1,
  Resources: {
    Memory: 128000000,
    CPUs: 32.
    Nodes: 4.
    Runtime: 3600
User name: fred,
User email: fred@fred.invalid
Name: my test job,
Description: a sample job,
```

Condor

- Grid middleware for HTC systems
- Installed in a large number of computer
- Key concepts:
 - Matchmaker
 - Get an agreement between users of resources and providers of resources (machines)
 - Machine requirements: only jobs from OEG computers, only work from 6pm to 4am
 - Users requirements: to be executed only on Linux machines, dual core processor
 - ClassAd file represents the state of jobs and machines
 - Submitting a job
 - Selecting the job universe (vanilla, Java, standard, MPI, etc.)
 - Using a job description file, possibility of monitoring jobs
 - Job dependencies (DAGMan)
- High importance to the system reliability
 - Job checkpoints, parameter sweep management (clusters and processes)

System 2 Submit job file

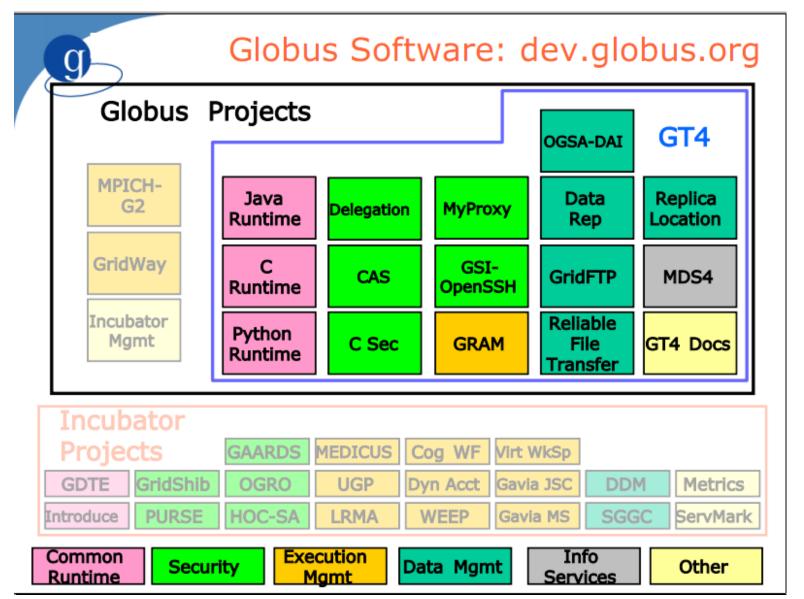
```
Universe = vanilla
Executable = my_job
Log = my_job.log
InitialDir = run_$(Process)
ShouldTransferFiles = IF_NEEDED
Transfer_input_files = dataset$(Process),
common.data
Requirements = Memory >= 256 && Disk > 10000
Rank = (KFLOPS*10000) + Memory
Queue 600
```

Globus

- Globus is a Grid middleware that provides means for building collaborative and distributed applications
 - It is a middleware that solves the problem of heterogeneity between user applications and computing resources
- Core runtime
- Security (Authentication and authorization)
 - GSI (Grid Security Infrastructure), X509 standard, VOMS (Virtual Organization Membership Service)
- Execution management
 - Supports the GRAM interface (Grid Resource Allocation and Management)
 - It provides a single protocol for communicating with different batch/cluster job schedulers.
- Data management
 - GridFTP (XIO), RFT, Replica Location Service, OGSA-DAI
- Monitoring
 - Monitoring and Discovery System (MDS4): information providers, collective services, clients



GLOBUS (II)



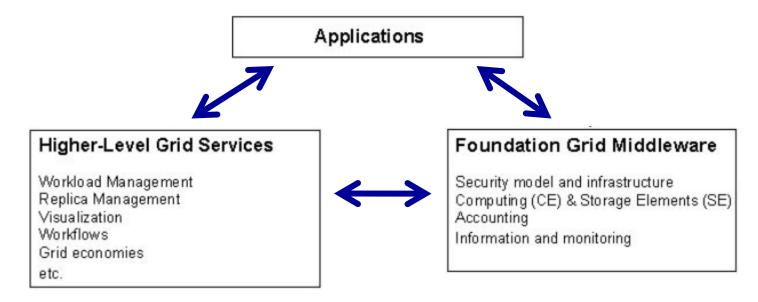


System 3 Submit job file

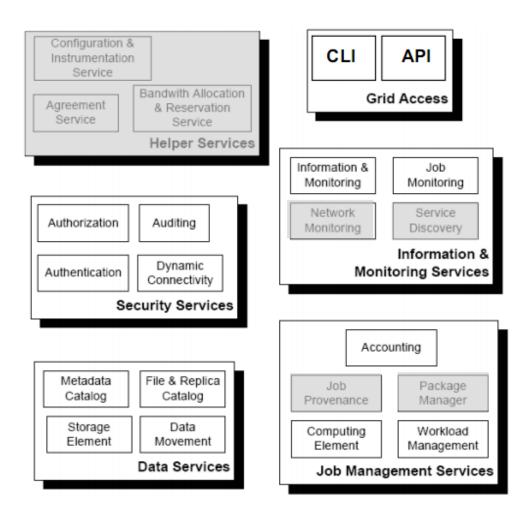
```
<job>
  <executable>${GLOBUS_USER_HOME}/genr</executable>
  <argument>5</argument>
  <argument>4</argument>
  <stdout>${GLOBUS_USER_HOME}/genr.out.${GLOBUS_USER_NAME}</stdout>
  <fileStageIn>
    <transfer>
      <sourceUrl>gsiftp://tc02.nesc.ed.ac.uk:2812/tmp/my_genr/sourceUrl>
      <destinationUrl>file:///${GLOBUS USER HOME}/genr</destinationUrl>
    </transfer>
  </fileStageIn>
  <fileStageOut>
    <transfer>
      <sourceUrl>file:///${GLOBUS USER HOME}/genr.out.${GLOBUS USER NAME}</sourceUrl>
      <destinationUrl>gsiftp://tc02.nesc.ed.ac.uk:2812/tmp/</destinationUrl>
    </transfer>
  </fileStageOut>
  <fileCleanUp>
    <deletion>
      <file>file:///${GLOBUS_USER_HOME}/genr</file>
    </deletion>
    <deletion>
      <file>file:///${GLOBUS USER HOME}/genr.out.${GLOBUS USER NAME}</file>
    </deletion>
  </fileCleanUp>
</job>
```

gLite

- Is a Grid middleware powering the EGEE infrastructure
 - EGEE is the largest interdisciplinary Grid infrastructure in the world
 - Provides the necessary components to process the users jobs (security, workflow management, metadata management, etc.
 - Middleware Structure:



gLite Services Decomposition

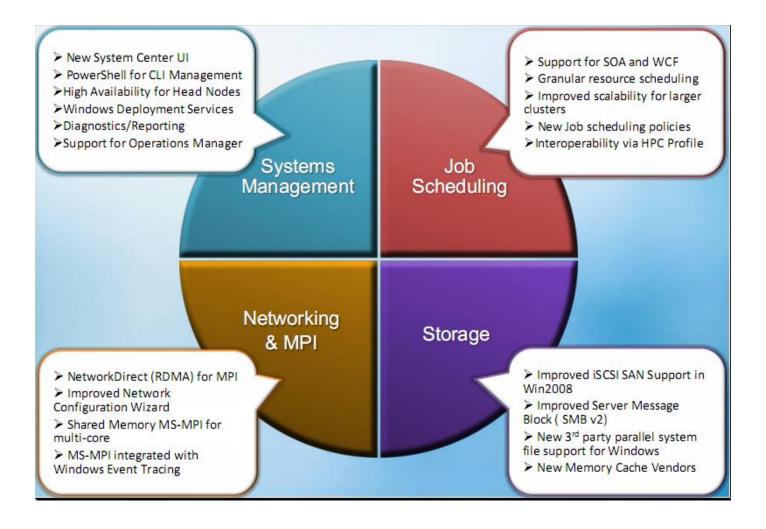




System 4 Submit job file

```
Type = "Job";
JobType = "Normal";
Executable = "startGen4.sh";
Environment = {"CLASSPATH=./gfal.jar:./gint.jar","
       LD_LIBRARY_PATH=.: $LD_LIBRARY_PATH",
       "LCG_GFAL_VO=gilda","LCG_RFIO_TYPE=dpm"};
Arguments = " 0 0 10 4 10000 aliserv6.ct.infn.it
       lfn:/grid/gilda/valeria/2000pillar.dat/gilda/issgc07/";
StdOutput = "sample.out";
StdError = "sample.err";
InputSandbox = { "startGen4.sh", "gint.jar", "gfal.jar",
       "libGFalFile.so" };
OutputSandbox = { "sample.err", "sample.out", "sample.log" };
Requirements = Member("GLITE-3_0_0"
       ,other.GlueHostApplicationSoftwareRunTimeEnvironment);
```

MS-HPC



MS-HPC (II)

- "Engagement with standards"
 - High heterogeneity of computer systems (different types of computers with different types of OS)
 - Use of standards for achieving interoperability
 - File sharing
 - SUA (Subsytem for Unix-based Applications)
 - SCOM (Systems Centre Operations management)
 - Monitoring
 - MS-HPC support standard specifications
 - Basic Execution Service (BES), JSDL, etc.



System 5 Submit job file

```
<jsdl: JobDefinition>
    <jsdl:JobDescription>
            <jsdl:JobIdentification>
             </jsdl:JobIdentification>
            <jsdl: Application>
                <jsdl-hpcp:HPCProfileApplication name="HostDate" >
                    <jsdl-hpcp:Executable>C:\GridSchool\sfk\scan.bat
                       </i></isdl-hpcp:Executable>
                    <jsdl-hpcp: Input></jsdl-hpcp: Input>
                    <jsdl-hpcp:Output>output.txt</jsdl-hpcp:Output>
                </jsdl-hpcp: HPCProfileApplication>
            </jsdl:Application>
        <jsdl:Resources>
            <jsdl:ExclusiveExecution>false</jsdl:ExclusiveExecution>
            <jsdl: TotalCPUCount/>
        </isdl:Resources>
        <jsdl: DataStaging>
        </jsdl: DataStaging>
    </jsdl:JobDescription>
</jsdl:JobDefinition>
```

Submission script

#!/usr/bin/env perl

```
open(SUBMIT, ">submit-big");
print SUBMIT "Universe = java\n";
print SUBMIT "Executable = sfkscanner.jar\n";
print SUBMIT "jar files = sfkscanner.jar,issgc sfk nesc.jar\n";
print SUBMIT "Log
                       = explorer.log\n'';
print SUBMIT "Output = explorer.\$(PROCESS).output\n";
print SUBMIT "Error = explorer.\$(PROCESS).error\n";
print SUBMIT "transfer input files = BoxData.txt,PillarsData2.txt.en\n";
print SUBMIT "should transfer files = YES\n";
print SUBMIT "when to transfer output = ON EXIT\n";
print SUBMIT "\n";
#my $y;
for (\$x = -15; \$x < -11.12; \$x += 0.1)
  for (\$v = 9861.9; \$v < 9862.49; \$v += 0.1)
#
     my $xx = $x + 10; #-15.0
#
     mv \$vv = \$v + 10; #9861.9
    mv \$zz = \$z; #-11.12
    mv $ff = $f; #9862.49
    print SUBMIT "Arguments = uk.ac.nesc.toe.sfk.radar.Scanner ";
    print SUBMIT "$x $y -11.12 9862.49 0.001\n";
    print SUBMIT "Queue\n";
    print SUBMIT "\n";
close(SUBMIT);
exit 0:
```

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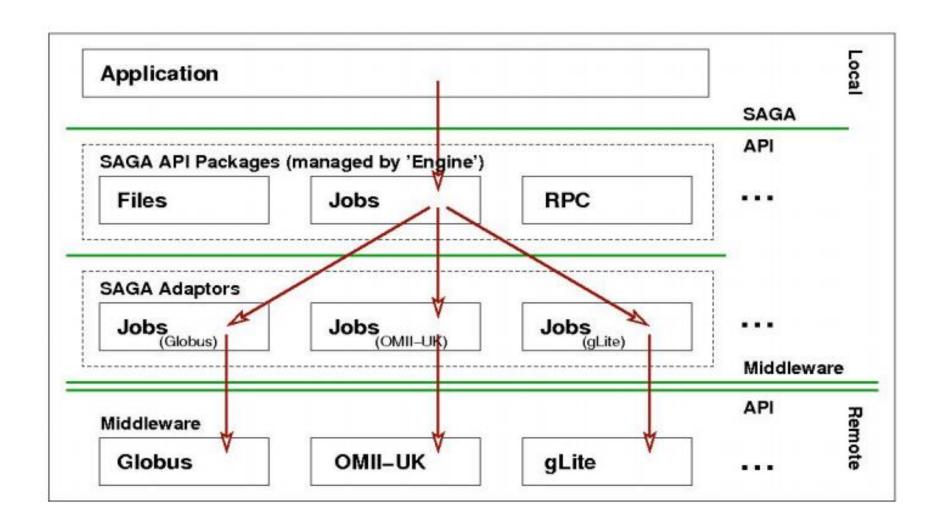


SAGA

- Simple API for Grid Applications (SAGA)
 - SAGA is a simple API (as it sounds)
 - SAGA is an emerging standard
- What is the Grid (brief reminder)
 - Dynamic
 - Heterogeneous
 - Complex
- What SAGA provides?
 - A high level abstraction hiding middleware details
 - Details of distribution are hidden
 - Simple API to access the existing Grid middleware
 - Is a client side software



SAGA Architecture



SAGA Example

```
void copy_file(std::string source_url,
std::string target_url)
{
  try {
    saga::file f(source_url);
    f.copy(target_url);
  }
  catch (saga::exception const &e) {
    std::cerr << e.what() << std::endl;
  }
}</pre>
```

```
int copy file (char const* source, char const* target)
globus_url_t
                        source_url;
globus io handle t
                           dest io handle;
globus ftp_client_operationattr_t source_ftp_attr;
globus result t
                         result:
globus gass transfer requestattr t source gass attr;
globus gass copy attr t
                             source gass copy attr;
globus_gass_copy_handle_t gass_copy_handle;
globus gass copy handleattr t gass copy handleattr;
globus_ftp_client_handleattr_t ftp_handleattr;
globus io attr_t
                          io_attr;
int
                    output file = -1;
if (globus_url_parse (source_URL, &source_url) !=
GLOBUS SUCCESS
 printf ("can not parse source URL\"%s\"\n",
source URL);
 return (-1);
```

Workflow Principles

Scientific workflows

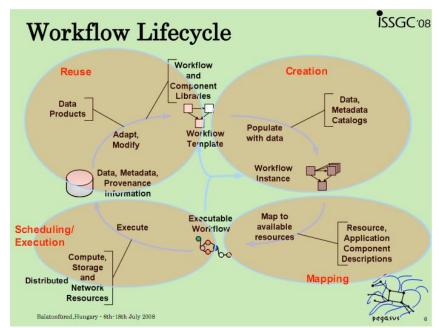
- Allow to compose applications from other execution units/programs
- Provide automation for the applications
- Types of workflow applications
 - provide a service to a community
 - supporting community based analysis
 - process large amounts of shared data on shared resources

Critical issues

- Find the right components
- set the right parameters
- find the right data
- connect appropriate pieces together

Workflow lifecycle

- Creation
- Mapping
- Planning/execution
- Reuse





Workflow principles (lifecycle I)

Creation

- Find the right components
- set the right parameters
- find the right data
- connect appropriate pieces together

Mapping

- Map tasks to available resources
- Where to run the computation units?
- What data do I have to access?

Workflow principles (lifecycle II)

Scheduling/execution

- Consists in the execution of the planned workflows in other systems
 - Workflow systems send tasks to systems like Condor or Globus (depending on what specific functionality want to use)

Reuse

- how to find what is already there?
- how to determine the quality of what is already there?
- how to invoke an existing workflow?
- how to share a workflow with a colleague?
- how to share a workflow with a competitor?

Conclusions (I)

- Grid is about collaboration and sharing resources
 - Computational resources (large amount of computers, large systems)
 - Data resources
- New ways for doing research in many and different areas
 - High use of computing resources
 - Data intensive applications
 - Distributed applications
 - Grid creates virtual homogeneity of resources (virtualization)
 - E-Science, e-Infrastructure, grid security
- Virtual homogeneity
 - Standards



Conclusions (II)

- Systems provide similar functionalities but:
 - UNICORE focused in large scale systems (high computing power)
 - Condor focused in high amount of jobs and computers
 - Globus focused in high amount of computers
 - gLite high amount of computers/large infrastructure
- Same as data management in Grids:
 - Every problem (high rate of data generation, high amounts of data, high distribution of data) has its own solution
- Workflow systems allow to compose and submit complex jobs

Distributed Reasoning

- Distribution of data/ontologies
 - Where are the classes/properties/relations
 - Where are the instances
 - How to access them
 - Availability of the resources
- Distribution of processes
 - What processes can I distribute?
 - Where do I send these processes?
 - Reliability of the system
 - Gather and join the results
 - Possible use of workflow systems/scripts?