

Computing and Data Handling

### **ARC Tutorial**

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## What is Grid?

- Relatively new term definition is fuzzy.
  - Many users, many definitions
  - Common misunderstandings
  - Standardization just http://www.globalgridforum.org/.
- Old idea
  - Uniform and safe access to geographically remote and inhomogeneous computing resources.
  - Dynamic pool of users and resources.
  - Distributed management.
  - Resources belonging to different institutions are linked into system.
  - Collaboration and social networking are as important as technology
- Grid environment is usually formed a layer over operating system installed on participating resources and other services.
  - Term used "middleware".
- I. Foster and C. Kesselmann, <u>The Grid: Blueprint for a New Computing</u> <u>Infrastructure.</u> Morgan Kaufman Publishers, 1998



- Physical location of computing and data resources not important.
- Unification is important
  - Usernames and passwords are not used
  - Unification of resources: virtualization or unified interfaces.
    - A lot of unsolved problems.
    - Standardization just started.
    - Maybe virtual computers can help.
    - What should adapt, user's application or Grid environment?



### **Common misunderstandings**

- Grid increases resources
  - One computing resource won't be able to compute more if put on a Grid.
  - But resources can be used more effectively.
- Grid is black box and everything inside it happens automatically.
  - So far in future plans only
  - In reality users still have to learn about peculiarities of implementation. Possibility to monitor job becomes very important.



- Should users' applications be adapted to be able to execute in a Grid environment?
  - 1) No changes. Grid is like big cluster and Grid middleware takes care of transferring job and date to execution location.
  - 2) Application is installed on resources in advance or on demand and is contacted through Grid interface. Usually this approach is problematic if application is interactive.
  - 3) Application is modified so it can take advantage of Grid. That is a proper approach if Grid provides own OS-like interface. Especially useful for applications which are able to divide tasks into loosely coupled sub-tasks.



### **Middleware - Legion**

Number of base Grid implementations is not high. Most others are built on top of them.

- Legion Worldwide Virtual Computer http://legion.virginia.edu
  - An example of middleware which creates own operating system.
  - For user whole system looks like one computer
    - Everything is an object computing resource, application, device.
    - For new kind of resources new classes are created.
    - It defines interfaces and functionality But not implementations. Only basic objects are implemented.
    - Users can create own classes and even own implementations of existing classes.
  - Commercial.



- UNICORE "Uniform Interface to Computing Resources" http://www.unicore.org
  - Hides differences of computing resources behind unified interfaces.
  - Easy to use because it has own graphical user interface for job creation and control.
    - Job is abstract and complex. Job can depend on each other.
    - For every important application new user interface being developed.
    - There is an interface for legacy jobs. But specialized interface are preferred
  - Recently became Open Source.



- Globus Toolkit<sup>™</sup> "fundamental technologies needed to build computational grids" - http://www.globus.org.
  - Initially set of services and libraries.
  - Now significant part is standards and interface definitions based on "Web Service Resource Framework" (WSRF) http://www.globus.org/wsrf/.
  - Not a single system
    - Services can be used separately.
    - Own services may be created.
  - There are many Grid projects which produce middleware based on Globus Toolkit<sup>™</sup>.
  - Open Source.



If number of users grows high (10<sup>3</sup>,10<sup>6</sup>,...). And number of resources too (10,100,...). And all handled under different policies. It becomes difficult to manage and synchronize usernames and passwords everywhere and foe everyone. Another method is needed:

- Secure and reliable identification of user authentication
- Control over users' possibilities authorization



## **Grid users - authentication**

- Many Grid projects use Public Key Infrastructure (PKI) for authentication of all participating objects. Usually X.509.
  - Key private big enough set of random bits (usually from 1024 to 4096 bits).
  - Certificate public key bound to private through special algorithm with attributes describing participant attached and digitally signed by private key of higher level participant.
  - Non-symmetric encryption modification of information through encryption algorithm (cypher). Algorithm uses one the keys. For extracting initial information another key from the pair must be used.



- request based on it.Request is sent to CA.
- CA uses own methods to check authenticity of the user.
- All Grid participants trust CA and it's methods of checking users.



### **Grid users - authentication**

#### • Proxy

- Globus uses additional pair of certificate and key created automatically.
- They are not protected by password.
- Protected only by means of operating system.
- Have short validity period usually 12 hours since creation.
- Single log in concept user has to enter password only once.





### **Grid users - authorization**

- It would be quite problematic for owners of resources to decide for every Grid user what he/she is allowed to do on their resources.
- Users are gathered into groups called Virtual Organizations (VO).
- Inside VO roles/capabilities are managed by VO administrators.
- Resources trust VOs and set restrictions per VO.
- Resources can also be part of VO and delegate decisions to VO administrators.
- Globus uses simple text list of users for authorization.
  - There are applications which can manage those files dynamically.
  - But there are more flexible solutions being developed and deployed.



### NorduGrid

- NorduGrid is a research collaboration established by universities in Denmark, Estonia, Finland, Norway and Sweden
  - Focuses on providing production-capable Grid-like middleware for academic researchers
  - Currently supports one of the largest Grid production systems
    - 10 countries, 40+ sites,
       ~4000 CPUs, ~30 TB storage





#### ARC

- ARC (Advanced Resource Connector) is Grid middleware developed by NorduGrid project.
  - It consists of set of services and user interface utilities
  - Based on Globus Toolkit<sup>™</sup>
- Basic requirements during development
  - Simple
  - Stable
  - Non-intrusive



 User creates job's description and pass to client application









• Job is directed to cluster





Data is gathered to job Job is directed to cluster management system Information system Dataindet Client Information about cluster and jobs being processed ARC Crid-manager FID Data Server Cridk John Physics Juster

#### www.nordugrid.org







## **ARC – job description -xRSL**

#### ARC accepts jobs written in xRSL (Resource Specification Language).

&(attribute=value)(attribute=value)...

Mostly used attributes are

- executable main executable
- *arguments* executable's arguments
- cputime how much time job needs
- *memory* how much memory job can take
- jobname job's name
- *runtimeenvironement* application/runtime environment (RE) required by job
- stdin, stdout, stderr UNIX standard streams' redirection to files
- *inputfiles* list of input files
- outputfiles list of output files

Every file is described by 2 elements

- name of job during job's execution
- source/destination



## **ARC – environment preparation**

#### This step is already performed

- Installation of User Interface
  - Standalone User Interface is available at http://ftp.nordugrid.org/download/ - releases - standalone.
  - Unpack it
  - *\$ tar -zxvf nordugrid-standalone-0.5.24-1.i386.tgz*
  - Initialize it
  - \$ cd nordugrid-standalone-0.5.24
    \$ source setup.sh
    \$ cd ..

Working environment is ready. But user must be identified.



## ARC - Obtain certificate

#### This step is already performed

- User needs certificate which identifies his/her authenticity Usually users are supposed to contain a CA of own country.
  - Create certificate request
  - \$ grid-cert-request -int
  - Answer question:
    - password
    - organization
    - name
  - New directory .globus will be created in your home directory. It will contains private key protected by password and certificate request . globus/usercert\_request.pem .
  - Sent certificate request to your CA with your personal data included.
  - Obtained response store in *globus/usercert.pem*. That can take few days.



### **ARC - Become a member**

#### This step is already performed

- User must be allowed to use resources
  - Simplest way is to join some VO
  - Contact your VO's administrator
  - NorduGrid Guest VO can be used for testings.
    - Almost everyone is allowed
    - Only very limited amount of resources accept members of that VO.



## ARC - at beginning of work

#### Start your work from setting up an environment

\$ cd nordugrid-standalone-0.5.24
\$ source setup.sh
\$ cd ..

• Create proxy certificate and key

*\$ grid-proxy-init* 

• If your jobs require more that 12 hours to finish

*\$ grid-proxy-init -valid 24:00* 

• There few prepared jobs in a directory *examples* 

*\$ cd examples* 



• Simplest job

\$ cat hello.rsl & (executable="/bin/echo") (arguments="Hello Grid") (stdout="out.txt")

- No own executable. Using */bin/echo*, available inmost UNIX-like operating systems.
- No input and output data. Standard output is redirected to a file *out.txt* and automatically appended to the list of output data.
- Submit job

```
$ ngsub -f hello.rsl
Job submitted with jobid
gsiftp://farm.hep.lu.se:2811/jobs/162941110665573478034132
```

- This can take some time because client must contact all resources and find suitable one.
- Message from command contains identifier of a job.



## **ARC - Hello Grid**

• Job's state can be monitored using *ngstat* command

\$ ngstat gsiftp://farm.hep.lu.se:2811/jobs/162941110665573478034132
Job gsiftp://farm.hep.lu.se:2811/jobs/162941110665573478034132
Status: FINISHED

- Most possible results
  - ACCEPTED job is accepted and waiting
  - PREPARING job's input data is being processed
  - INLRMS job is being executed
  - FINISHING output data is being processed
  - FINISHED job is finished
- While job is being run You can look at it's standard output with

\$ <u>ngcat</u> gsiftp://farm.hep.lu.se:2811/jobs/162941110665573478034132 Hello Grid

• After job finished all results can be obtained by command

\$ <u>ngget</u> gsiftp://farm.hep.lu.se:2811/jobs/162941110665573478034132 ngget: downloading files to /home/user/examples/162941110665573478034132 ngget: download successful - deleting job from gatekeeper.



## **ARC – Hello Grid - Enhancements**

- Try to enhance this example
  - Try to use command ngsub -d 1 -f hello.rsl. This should show resource ngsub ngsub is talking to and how it choses one.
  - Add (jobname="Test") to job's description (hello2.rsl) and try to use this name instead of job's identifier.
  - Add (gmlog="log") to job's description (hello3.rsl) and look what new appears in job's results.
  - Try commands mentioned before with -h argument.



## **ARC – useful job - GAMESS**

#### Let's try job with some sense.

- GAMESS The General Atomic and Molecular Electronic Structure System quantum chemistry application.
   Path to executable is defined thorough
- RSL gamess.rls

Path to executable is defined thorough variable provided by RE

&(executable="\$GAMESS\_LOCATION/rungms") (arguments=gamess.inp)

(stdout="stdout")(stderr="stderr")(gmlog="gmlog")

(inputfiles=("gamess.inp" ""))

(runtimeenvironment="APPL/CHEM/GAMESS")

(cputime="1h")

(jobname="GAMESS")

transferred to session directory from user's computer

Input file without source will be

Job requires application/RE GAMESS

- Input file gamess.inp consists of GAMESS command which form standard test task.
   Let's request 1 hour of CPU. That is too much but in this way we are on a safe side
- This a testing job. Hence all we need are standard streams. Make sure generated files do not contain any messages about processing errors.



# **ARC – Sophisticated job**

Lets try a job with input and output data, own executable. And it also requires preinstalled application - Executable file - Bash script povray.sh #! /bin/sh \_\_\_\_ Runs main application with defined arguments povray +H600 +W800 +omonolith.png monolith.pov Executable to be run. It will be delivered to session - RSL - povray.rsl directory from user's computer &(executable=runpov.sh) -- Job requires runtime environment POVRAY (runtimeenvironment=POVRAY) (inputfiles= Input file will be delivered into session ("monolith.pov" directory from defined source URL "http://www.nordugrid.org/tutorial/dapsys\_tutorial/povraydemo/monolith.pov") ("front.png" "http://www.nordugrid.org/tutorial/dapsys\_tutorial/povraydemo/front.png")) (outputfiles=("monolith.png" "")) (stdout=out.txt)(stderr=err.txt) Output file will be stored on a cluster in session directory (gmlog=logs) (cputime=1h) (jobname=povray)



## **ARC – Grid Monitor**

- Whole system and every job can be monitor using Web interface. http://www.nordugrid.org/monitor/
- Main window shows a list of all computing resources and their usage.
- Find yourself
  - Use gridcert-info -subject, to find out your name
  - Choose *p* to get list of all users
  - Find your name in that list
  - New window will show list of available resources and your jobs

Try it. Almost every element can be clicked.



### **ARC – Sophisticated job**

After job finished obtain results

ngget povray Result is made of 3 files out.txt - output stream err.txt - errors' stream monolith.png - generated picture

This example was derived from one by Leif Nixon which also shows how to split task into multiple jobs by rendering image in slices. http://www.nsc.liu.se/~nixon/ng-povray/