VAMDC and the GRID
[GRID enabled web services]

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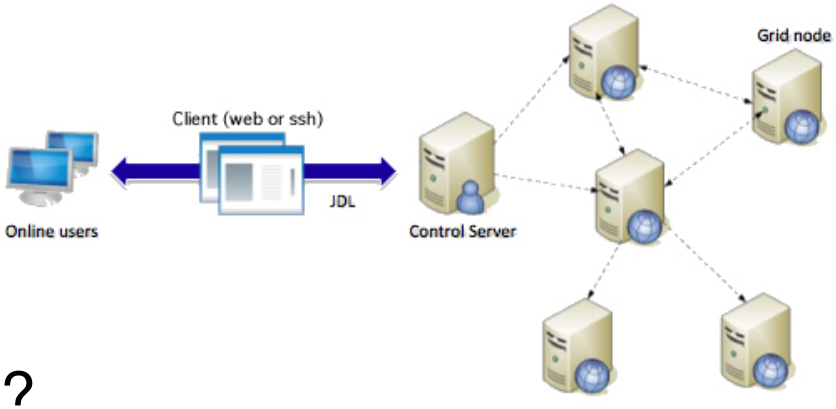
Introduction

- What is GRID computing?

  "Grids are a form of distributed computing whereby a 'super virtual computer' is composed of many networked loosely coupled computers acting in concert to perform very large tasks."

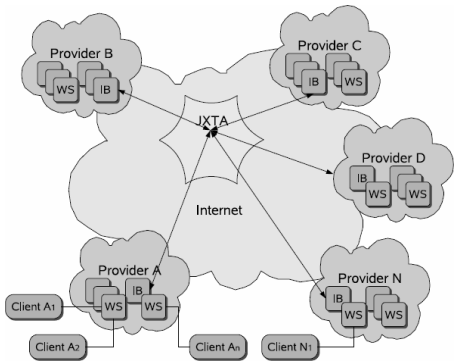


- Why should we embrace it?
  - ✓ Accomplish great-challenge tasks
  - ✓ Massive computer power
  - ✓ Massive storage capacity

Introduction

- Data producer perspective
  - ✓ Large storage capabilities
  - ✓ Data publication and dissemination
  - ✓ A long-term access to published data (data preservation)

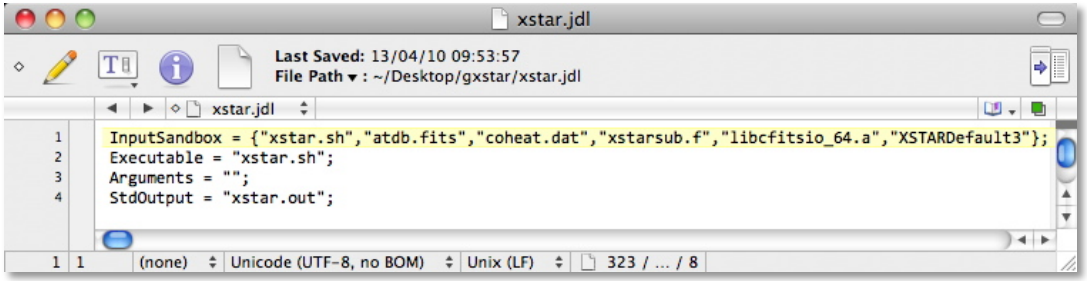
- Data consumer perspective
  - ✓ High-speed data connection
  - ✓ Wide range of data access clients
  - ✓ HPC resources for data manipulation, analysis, and curation
  - ✓ Job's distribution and parallelization

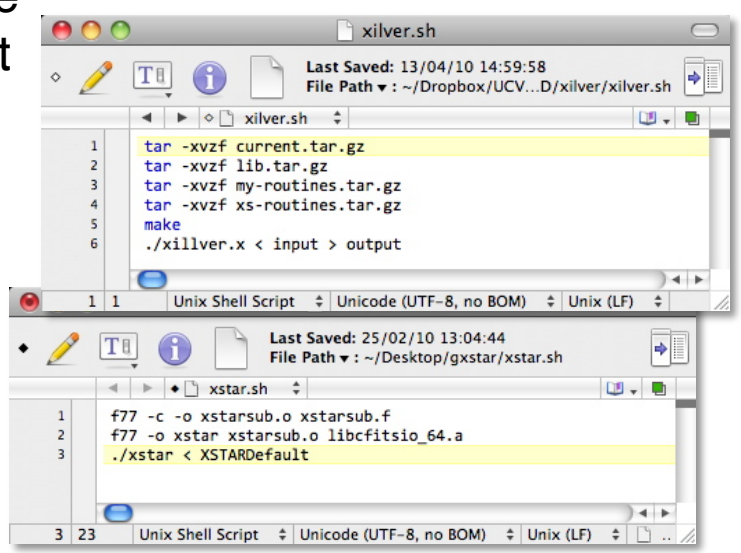


XSTAR on the GRID

- What is it? Where to get it? How is it used today?
  - ✓ Physical conditions and emission spectra of photoionized gases
  - ✓ Available on the web
  - ✓ Invoked as any standard shell application

- How to port it to the GRID
  - ✓ Modifications in the source need to be made
  - ✓ External file and/or library should be present
  - ✓ Scripting is helpful for flexibility





XSTAR on the GRID

- How to use it
  - ✓ Get the appropriate GRID account and certificate
  - ✓ Prepared an input and a JDL files
  - ✓ Through a web interface on top of GENIUS

```
-bash-3.00$ glite-wms-job-submit -d juang -o xstarjob xstar.jdl

Connecting to the service https://grid007.cecalc.ula.ve:7443/glite_wms_wmproxy_server


====================== glite-wms-job-submit Success ======================

The job has been successfully submitted to the WMProxy
Your job identifier is:

https://grid007.cecalc.ula.ve:9000/dPYjQBWgmKW_j_8PxTAGnQ

The job identifier has been saved in the following file:
/home/juang/xstar/xstarjob

==========================================================================


-bash-3.00$ vi xstarjob
-bash-3.00$ glite-job-status -i xstarjob


*************************************************************
BOOKKEEPING INFORMATION:

Status info for the Job : https://grid007.cecalc.ula.ve:9000/dPYjQBWgmKW_j_8PxTAGnQ
Current Status:     Ready
Status Reason:      unavailable
Destination:        grid001.cecalc.ula.ve:2119/jobmanager-lcgpbs-ula
Submitted:          Tue Apr 13 19:12:55 2010 VET
*************************************************************
```

```
*************************************************************
BOOKKEEPING INFORMATION:

Status info for the Job : https://grid007.cecalc.ula.ve:9000/dPYjQBWgmKW_j_8PxTAGnQ
Current Status:     Running
Status Reason:      Job successfully submitted to Globus
Destination:        grid001.cecalc.ula.ve:2119/jobmanager-lcgpbs-ula
Submitted:          Tue Apr 13 19:12:55 2010 VET
*************************************************************
```

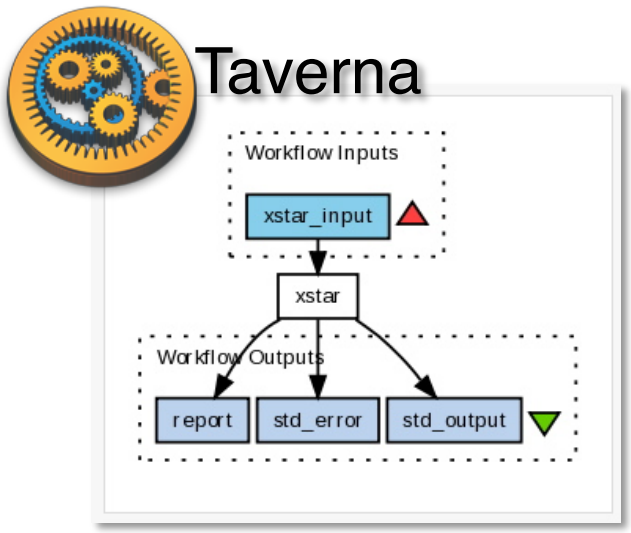
```
*************************************************************
BOOKKEEPING INFORMATION:

Status info for the Job : https://grid007.cecalc.ula.ve:9000/dPYjQBWgmKW_j_8PxTAGnQ
Current Status:     Done (Success)
Logged Reason(s):
    -
    - Job terminated successfully
Exit code:          0
Status Reason:      Job terminated successfully
Destination:        grid001.cecalc.ula.ve:2119/jobmanager-lcgpbs-ula
Submitted:          Tue Apr 13 19:12:55 2010 VET
*************************************************************
```

XSTAR web service

- Soaplab2
  - ✓ Generate and deploy Web Services on top of existing command-line analysis programs
  - ✓ Encapsulate with Perl wrappers
  - ✓ Spinet web client (demo)

- Taverna workflows
  - ✓ Tool for designing and executing workflows
  - ✓ Integration with Soaplab2 web services
  - ✓ Integration with GRID infrastructure
  - ✓ Expansion through plugin development
  - ✓ Integration with myExperiment



XSTAR web service

- Demo (try it at: http://caoba.ivic.ve:8180/soaplab2-axis/)

IVIC - Soaplab Web Services

[Soaplab version: 2.2.0, build: vie abr 2 13:12:05 VET 2010]

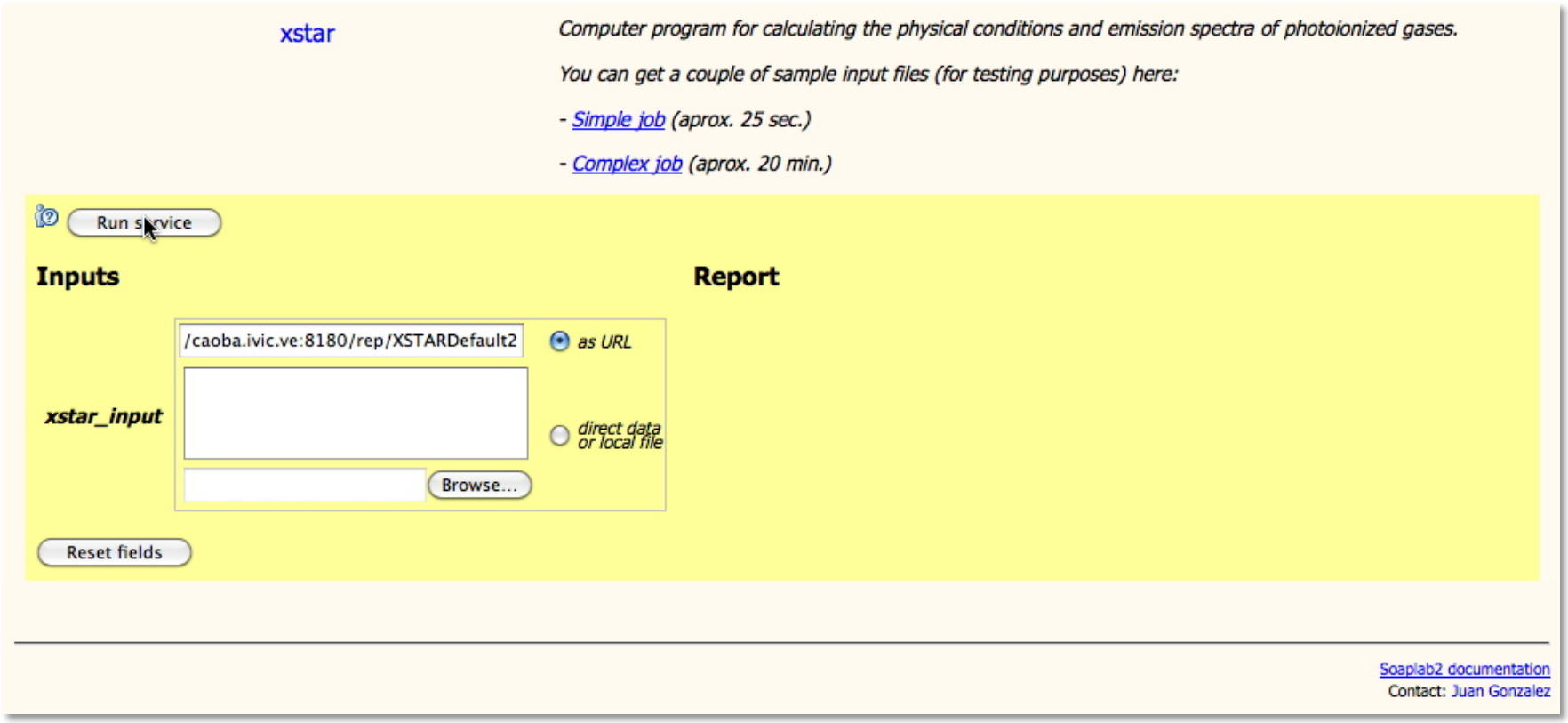
List of WSDL files for programmatic access

Category	Service name	Description
Testing		
	alloutputtypes_plugin	*Showing how a plugin can create all kinds of outputs*
	binaries	*Dealing with binary data*
	files	*Copying and merging files to standard output*
	inputtypes	*Testing various types of inputs*
	lists	*How to use lists*
	medlinesrs	*Get MEDLINE citation (in XML)*
	sleep	*Just sleep for a while*
	streams	*Filtering stdin into stdout and stderr streams*
	xstar	*Computer program for calculating the physical conditions and emission spectra of photoionized gases.*
		You can get a couple of sample input files (for testing purposes) here:
		- Simple job (aprox. 25 sec.)
		- Complex job (aprox. 20 min.)

Soaplab2 documentation
Contact: Juan Gonzalez

XSTAR web service

- Demo (try it at: http://caoba.ivic.ve:8180/soaplab2-axis/)



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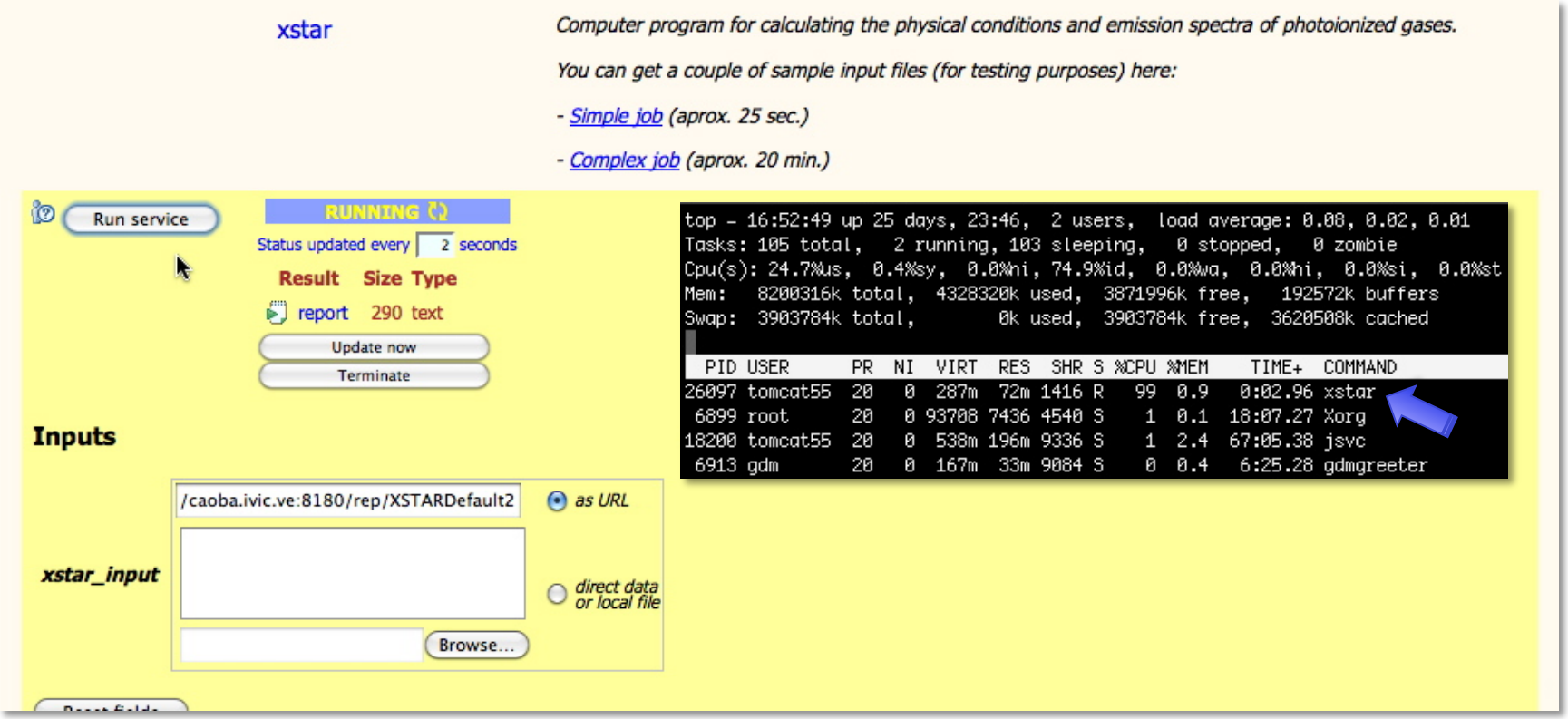

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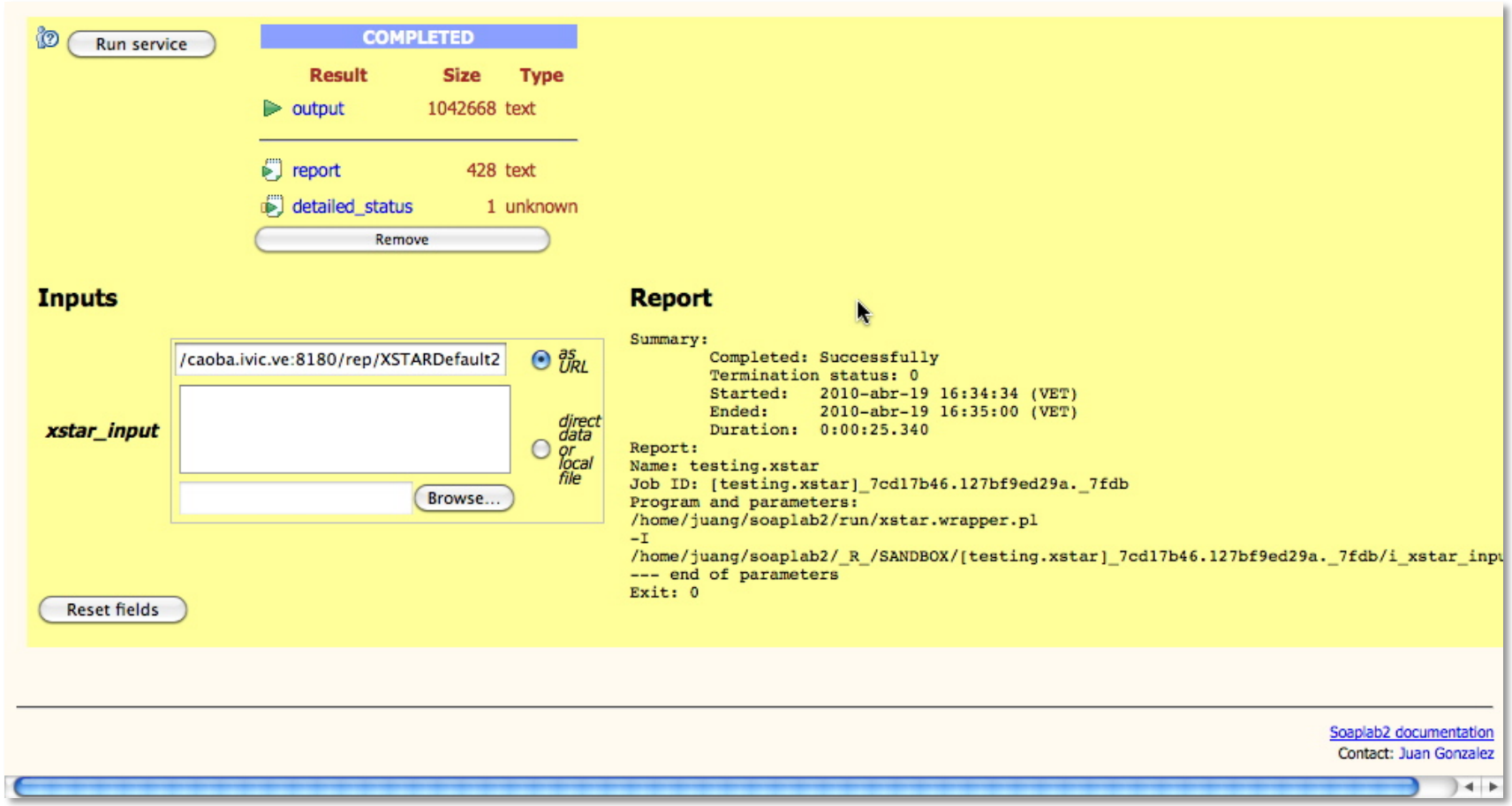
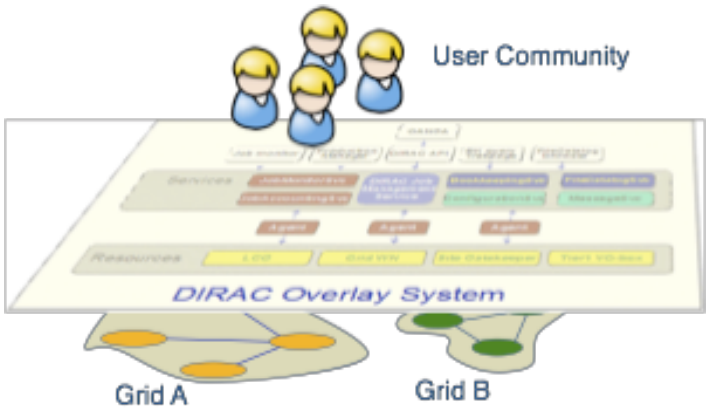
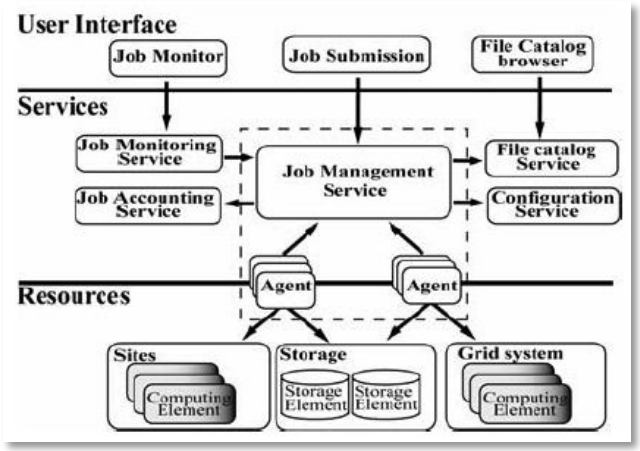


Next steps

- GRID enabled web services





- How to accomplish the task
  - ✓ Dirac
  - ✓ Ganga
  - ✓ Genius, etc.

Thank you!