

VAMDC and the GRID

[GRID enabled web services]

Authors:

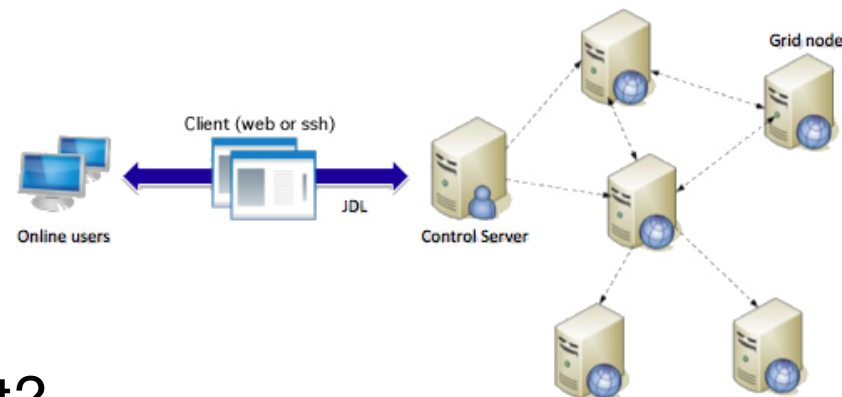
- Juan González
- Claudio Mendoza
- Luis Nuñez



- Introduction
- XSTAR on the GRID
 - ✓ What is it? Where to get it? How is it used today?
 - ✓ How to port it to the GRID
 - ✓ How to use it
- XSTAR web service
 - ✓ Soaplab2
 - ✓ Web client
 - ✓ Taverna workflows
- Next steps
 - ✓ GRID enabled web services
 - ✓ How to accomplish the task (Dirac, Ganga, Genius, etc)

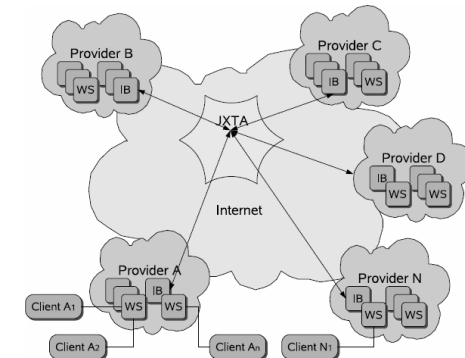
- What is GRID computing?

“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.”

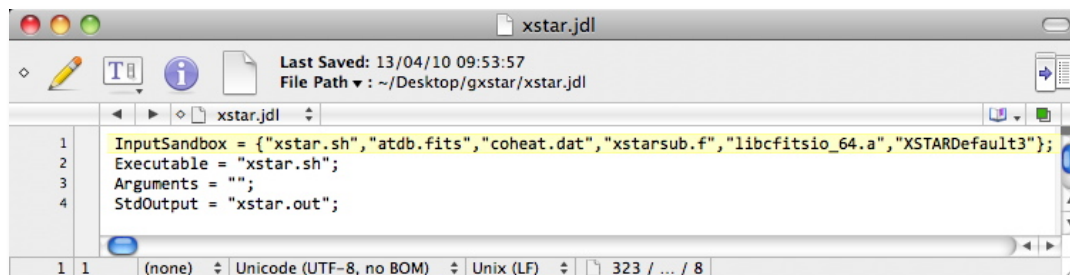


- Why should we embrace it?
 - ✓ Accomplish great-challenge tasks
 - ✓ Massive computer power
 - ✓ Massive storage capacity

- 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

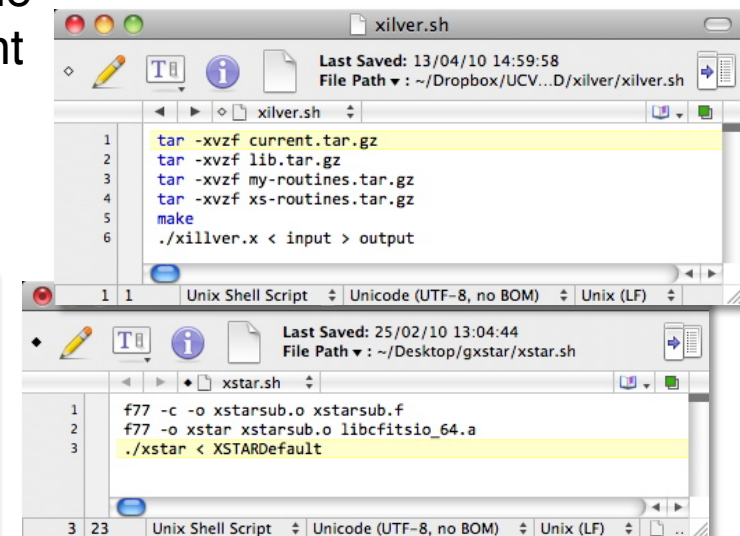


- What is it? Where to get it? How is it used today?
 - ✓ Physical conditions and emission spectra of photoionized gases
 - ✓ Available on the web
 - ✓ Invoked as any standard shell application
- How to port it to the GRID
 - ✓ Modifications in the source need to be made
 - ✓ External file and/or library should be present
 - ✓ Scripting is helpful for flexibility



```

1 InputSandbox = {"xstar.sh", "atdb.fits", "coheat.dat", "xstarsub.f", "libcfitsio_64.a", "XSTARDefault3"};
2 Executable = "xstar.sh";
3 Arguments = "";
4 StdOutput = "xstar.out";
  
```



```

xilver.sh
1 tar -xvzf current.tar.gz
2 tar -xvzf lib.tar.gz
3 tar -xvzf my-routines.tar.gz
4 tar -xvzf xs-routines.tar.gz
5 make
6 ./xilver.x < input > output

xstar.sh
1 f77 -c -o xstarsub.o xstarsub.f
2 f77 -o xstar xstarsub.o libcfitsio_64.a
3 ./xstar < XSTARDefault
  
```

• 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 WMPProxy
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
*****
```

- Soaplab2

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

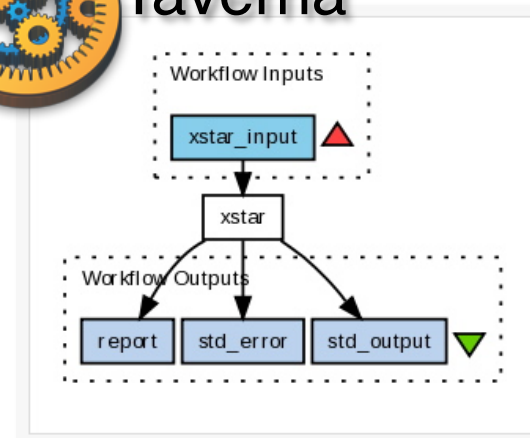


- Taverna workflows

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



Taverna



- 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	<p>Computer program for calculating the physical conditions and emission spectra of photoionized gases.</p> <p>You can get a couple of sample input files (for testing purposes) here:</p> <ul style="list-style-type: none"> - Simple job (aprox. 25 sec.) - Complex job (aprox. 20 min.)

[Soaplab2 documentation](#)
Contact: Juan Gonzalez

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

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.)

Run service

Inputs

/caoba.ivic.ve:8180/rep/XSTARDefault2

☒ as URL
 ☐ direct data or local file

xstar_input

Browse...

Reset fields

Report

[Soaplab2 documentation](#)
 Contact: Juan Gonzalez

VAMDC Annual Meeting
Open University (OU), Milton Keynes, April 19th – 23rd, 2010

Speaker: Juan González

9

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

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.)

Run service

RUNNING (i)

Status updated every seconds

Result Size Type

 **report** 290 text

Inputs

☒ as URL

☐ direct data or local file

xstar_input

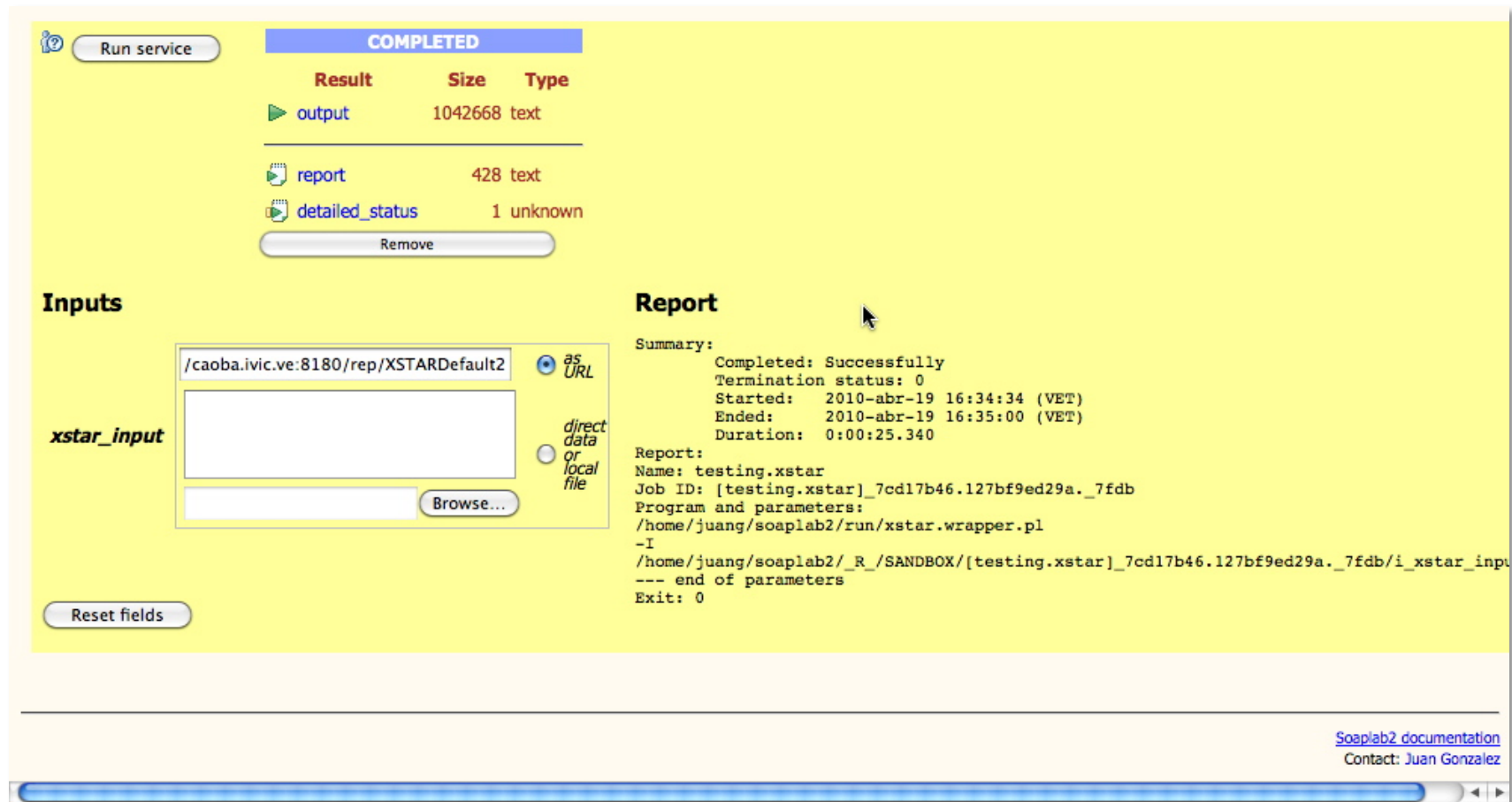
```

top - 16:52:49 up 25 days, 23:46, 2 users, load average: 0.08, 0.02, 0.01
Tasks: 105 total, 2 running, 103 sleeping, 0 stopped, 0 zombie
Cpu(s): 24.7%us, 0.4%sy, 0.0%hi, 74.9%id, 0.0%wa, 0.0%hi, 0.0%si, 0.0%st
Mem: 8200316k total, 4328320k used, 3871996k free, 192572k buffers
Swap: 3903784k total, 0k used, 3903784k free, 3620508k cached

  PID USER      PR  NI  VIRT  RES  SHR  S  %CPU  %MEM    TIME+  COMMAND
 26097 tomcat55  20   0  287m  72m 1416  R   99   0.9   0:02.96 xstar
   6899 root        20   0  93708 7436 4540  S    1   0.1  18:07.27 Xorg
 18200 tomcat55  20   0  538m 196m 9336  S    1   2.4  67:05.38 jsvc
   6913 gdm         20   0  167m  33m 9084  S    0   0.4   6:25.28 gdmgreeter

```

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



The screenshot displays the XSTAR web service interface. At the top left, there is a "Run service" button. The main area is titled "COMPLETED" and shows a table of results:

Result	Size	Type
output	1042668	text
report	428	text
detailed_status	1	unknown

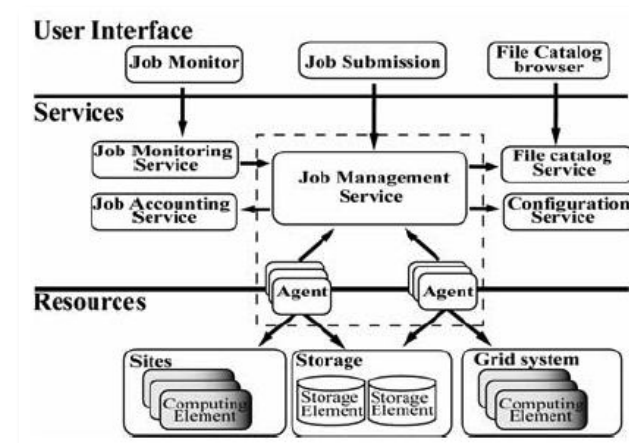
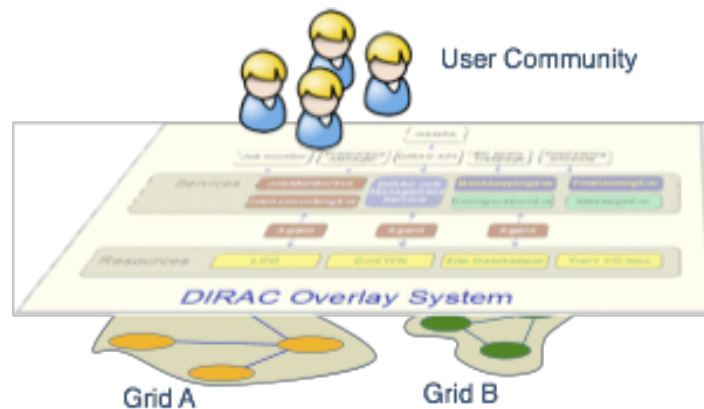
Below the table is a "Remove" button. The "Inputs" section on the left shows a text box with the URL "/caoba.ivic.ve:8180/rep/XSTARDefault2" and a "Browse..." button. The "Report" section on the right contains the following text:

Summary:
 Completed: Successfully
 Termination status: 0
 Started: 2010-abr-19 16:34:34 (VET)
 Ended: 2010-abr-19 16:35:00 (VET)
 Duration: 0:00:25.340

Report:
 Name: testing.xstar
 Job ID: [testing.xstar]_7cd17b46.127bf9ed29a._7fdb
 Program and parameters:
 /home/juang/soaplab2/run/xstar.wrapper.pl
 -I
 /home/juang/soaplab2/_R/SANDBOX/[testing.xstar]_7cd17b46.127bf9ed29a._7fdb/i_xstar_inpu
 --- end of parameters
 Exit: 0

At the bottom right, there is a link to "Soaplab2 documentation" and contact information for Juan Gonzalez.

- GRID enabled web services



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

Thank you!

