



**All Hands Meeting: April 21, 2014**

# **VO Status & Workflow Options**

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***A Quick Update on  
SURAGRID Resources ...***



## Available Compute Elements

| OSG Sitename      | Available Job Slots |
|-------------------|---------------------|
| TTU-ANTAEUS       | 456                 |
| TAMU_BRAZOS       | 512                 |
| TAMU_Calclab      | 892                 |
| GridUNESP_CENTRAL | 2048                |
| SWT2_CPB          | 2500                |
| UTA_SWT2          | 1164                |
| BNL-ATLAS         | 887                 |
| LUCILLE           | 954                 |
| NUMEP-OSG         | 240                 |
| SPRACE            | 203                 |
| FLTECH            | 152                 |

Source: OSG BDII via <http://www.math.tamu.edu/osg/sgstatus.php>



## Compute Element Resource Status from Contributing Members

04/18/2014 12:19:53 CDT

refresh 10 minutes

| <b>Resource Group</b> | <b>Globus Resource</b>                                 | <b>Free Slots</b> | <b>Max Jobs</b> | <b>Walltime (minutes)</b> | <b>Sched Factor</b> |
|-----------------------|--|-------------------|-----------------|---------------------------|---------------------|
| TTU-ANTAEUS           | antaeus.hpcc.ttu.edu:2119/jobmanager-sge-grid-serial   | 456               | 456             | 9999999                   | 100                 |
| TAMU_Calclab          | calclab-ce.math.tamu.edu:2119/jobmanager-slurm-night   | 1526              | 1526            | 720                       | 200                 |
| TAMU_Calclab          | calclab-ce.math.tamu.edu:2119/jobmanager-slurm-weekend | 0                 | 1526            | 4320                      | 50                  |
| TAMU_BRAZOS           | hurr.tamu.edu:2119/jobmanager-pbs-grid                 | 164               | 512             | 4320                      | 104.453125          |

Sched Factor = experimental scheduling weight

Source: <http://www.math.tamu.edu/osg/sgstatus1.php>



**Resources: *the more the merrier!***



**Spin up help desk as needed  
to assist with OSG stack installation.**





***Q: Why Workflows?***



Ten years ago most computational scientists accessed HPC/HTC via some high level language.  
C/C++/FORTRAN, even Java.

... and a batch scheduler.



That's not necessarily the case today.

W M S

As a Virtual Organization, one of the tools we can provide to SURAGRID users is a Workflow Management Service, and we don't even have to build a WMS ourselves!



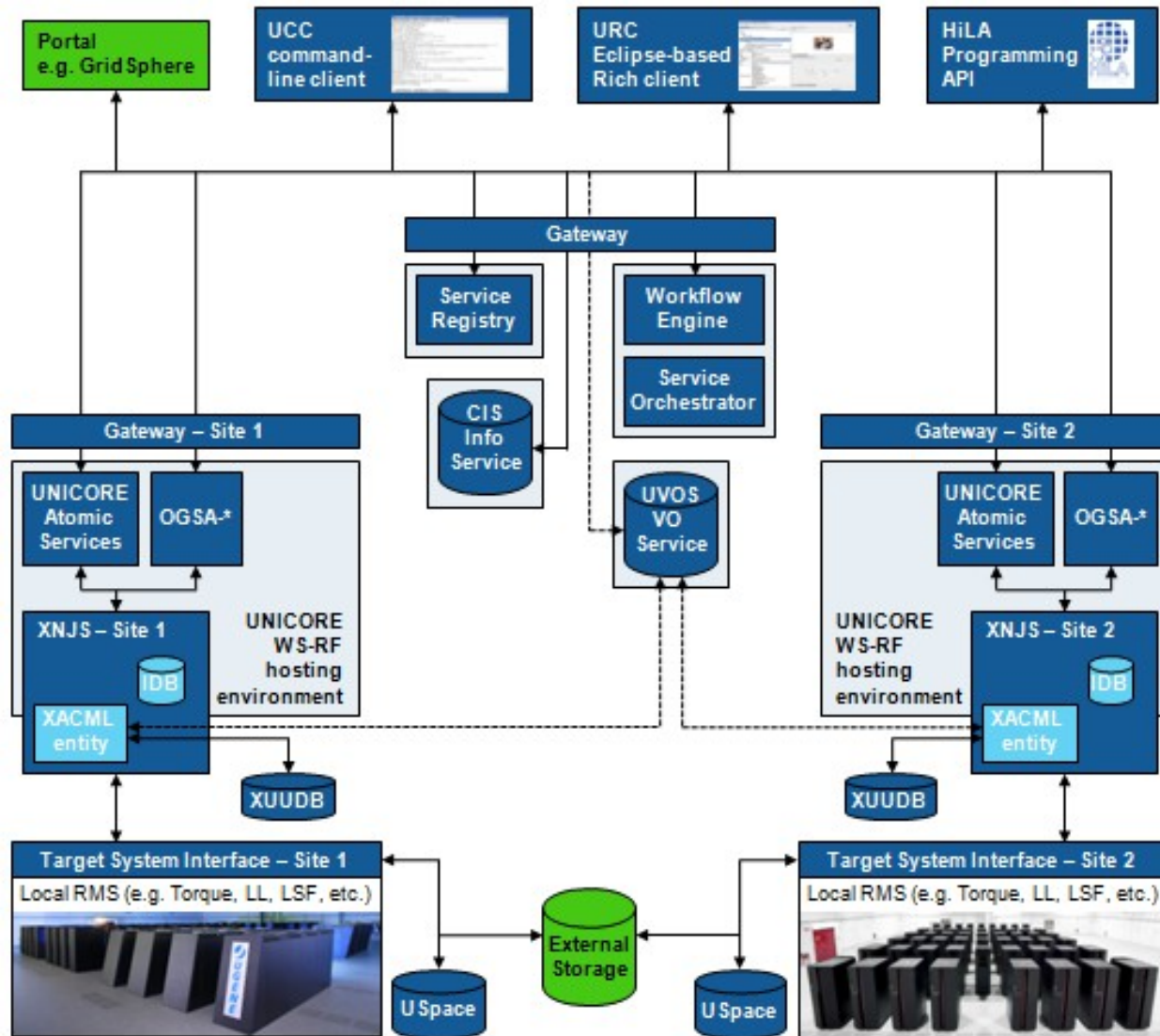
# UNICORE

- Submit Jobs to the Grid
  - Simple scripts
  - HTC *and* HPC
  - Complex workflows
  - Gridbeans
  - Portal client
- Manage Data on the Grid
  - Transfer files between sites and jobs
  - Metadata Storage
  - Drag 'n Drop

# UNICORE in Recent Research

- *Combining HPC with Data-Intensive Research via UNICORE for Seismological Applications*, Michele Carpené (CINECA)
- *Experiences with Running Data Extraction Application using UNICORE*, Lara Flörke, Mathilde Romberg, Jülich Forschungszentrum
- *Experience with UNICORE Services for Multiscale Materials Modelling*, Michele Carpené, Super Computing Application & Innovation (SCAI), CINECA
- *UNICORE-based Workflows for the Simulation of Organic Light-Emitting Diodes*, Stefan Bozic, Ivan Kondov, Velimir Meded, Wolfgang Wenzel, Karlsruhe Institute of Technology, Germany
- Several more...
- Source: UNICORE Summits 2013, 2012  
<http://www.unicore.eu/summit/2013/schedule.php>  
<http://www.unicore.eu/summit/2012/schedule.php>

# UNICORE Architecture



Source: <http://www.unicore.eu/unicore/architecture.php>

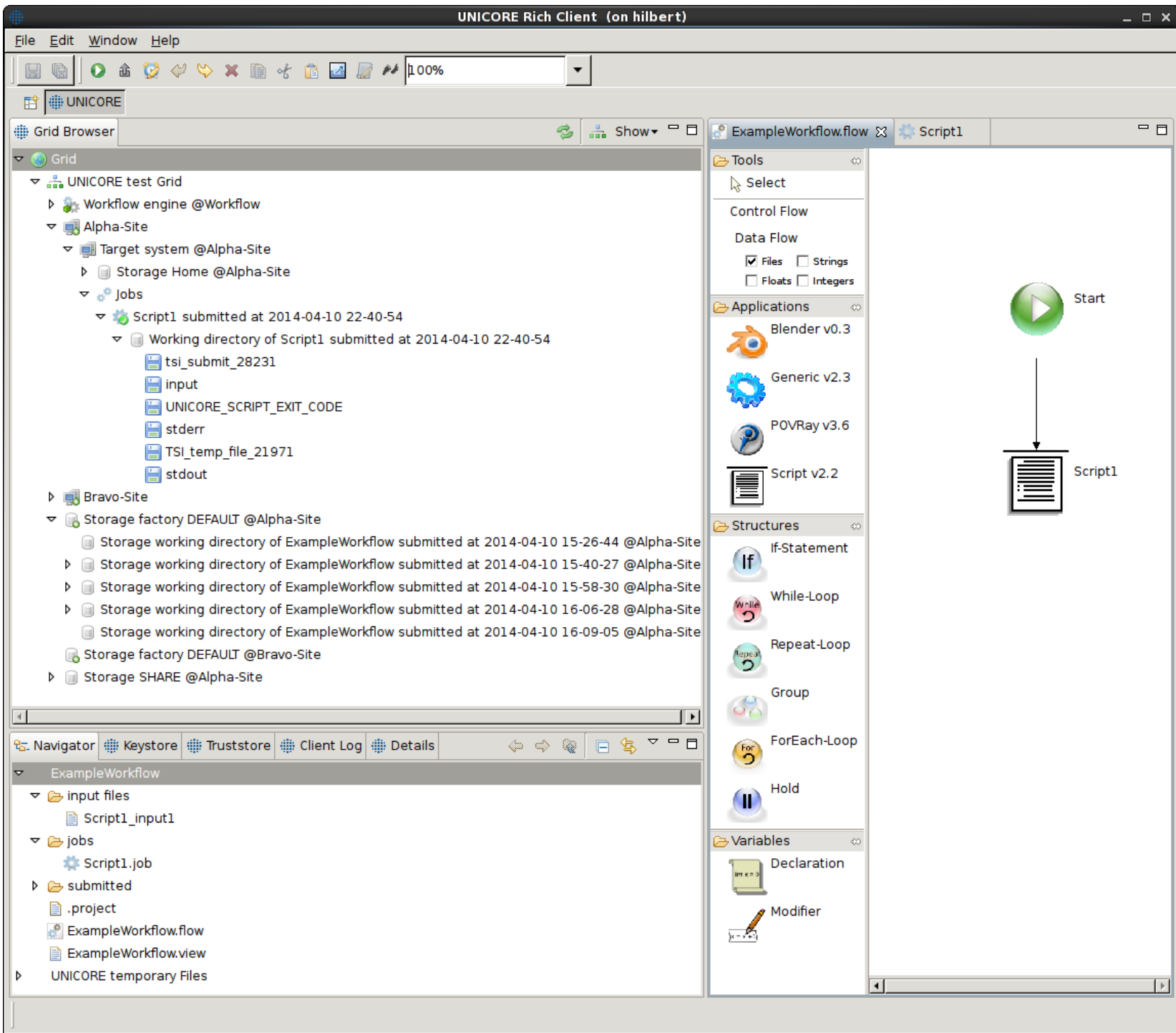
# UNICORE Components

- Gateway - entry point to UNICORE site
- Registry - collector of resource information
- Workflow engine - high level workflow execution
- Service Orchestrator - individual task brokering and execution
- UNICORE/X - provides access to computational and storage resources
- Target System Interface
  - Operates with LRMS (PBS, LSF, LL, SLURM)
  - Perl daemon on head node executed as root
- AuthN/AuthZ
  - X.509 PKI certs & proxies
  - Username/password
  - LDAP, Kerberos
  - XUADB
  - mapfile
  - XACML

# UNICORE Rich Client

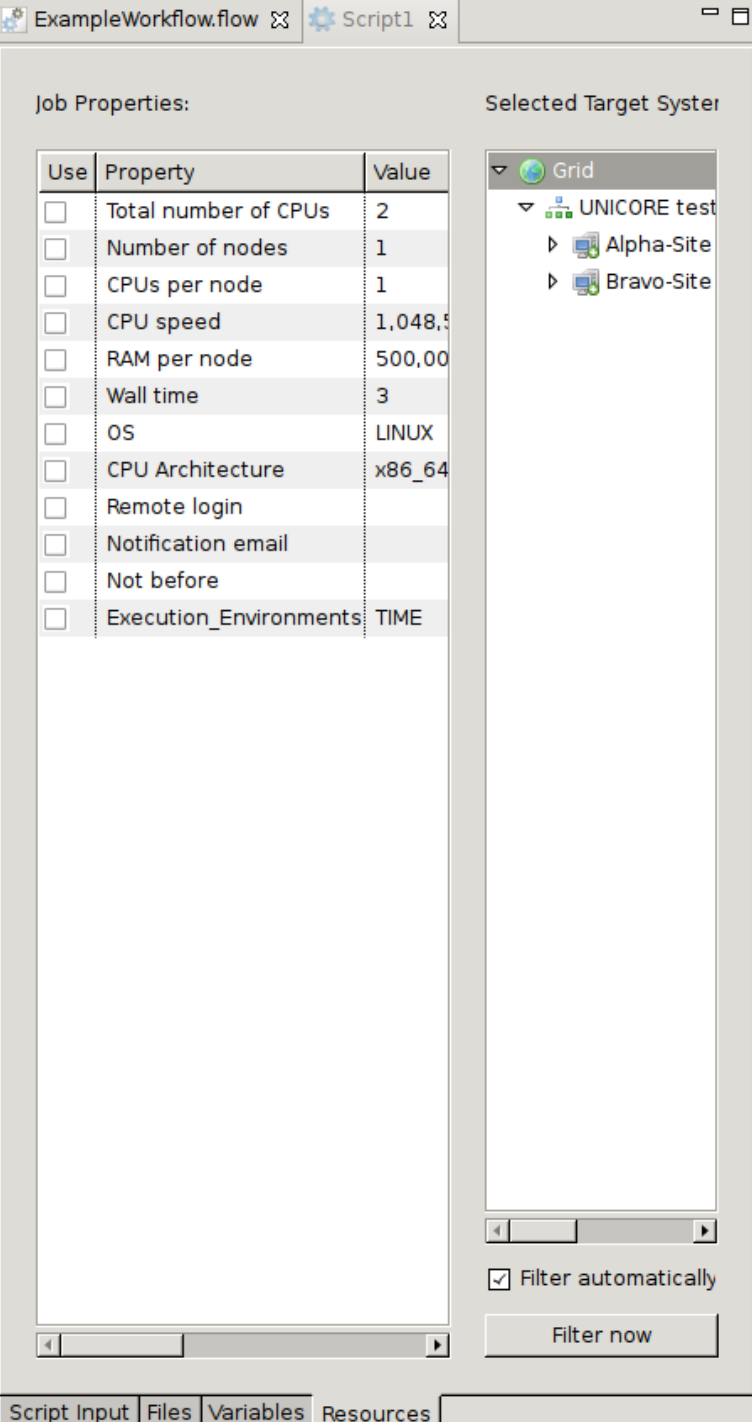
- Eclipse (Java) based client can run on desktop or server. Reasonable memory usage.
- Define and submit jobs
- Define and submit complex workflows
- Manage storage
- Manage multiple credentials
  - X.509 user and CA certificates
  - SURAGrid usage would load a VOMS proxy

# UNICORE Rich Client



# UNICORE Rich Client

Requesting job properties  
via checkboxes



The screenshot displays the UNICORE Rich Client interface. The window title bar shows 'ExampleWorkflow.flow' and 'Script1'. The main area is divided into two panels: 'Job Properties' and 'Selected Target System'.

**Job Properties:**

| Use                      | Property               | Value   |
|--------------------------|------------------------|---------|
| <input type="checkbox"/> | Total number of CPUs   | 2       |
| <input type="checkbox"/> | Number of nodes        | 1       |
| <input type="checkbox"/> | CPUs per node          | 1       |
| <input type="checkbox"/> | CPU speed              | 1,048,5 |
| <input type="checkbox"/> | RAM per node           | 500,00  |
| <input type="checkbox"/> | Wall time              | 3       |
| <input type="checkbox"/> | OS                     | LINUX   |
| <input type="checkbox"/> | CPU Architecture       | x86_64  |
| <input type="checkbox"/> | Remote login           |         |
| <input type="checkbox"/> | Notification email     |         |
| <input type="checkbox"/> | Not before             |         |
| <input type="checkbox"/> | Execution_Environments | TIME    |

**Selected Target System:**

- Grid
  - UNICORE test
    - Alpha-Site
    - Bravo-Site

At the bottom of the 'Selected Target System' panel, there is a 'Filter automatically' checkbox (checked) and a 'Filter now' button. The bottom of the window features a tabbed interface with 'Script Input', 'Files', 'Variables', and 'Resources' tabs.

# UNICORE - Single Task

The screenshot shows the UNICORE workflow editor interface. The top bar displays the workflow name 'ExampleWorkflow.flow' and the current task 'Script1'. On the left, there is a sidebar with various tool categories: Tools (Select), Control Flow, Data Flow (Files, Strings, Floats, Integers), Applications (Blender v0.3, Generic v2.3, POVRay v3.6, Script v2.2), Structures (If-Statement, While-Loop, Repeat-Loop, Group, ForEach-Loop, Hold), and Variables (Declaration, Modifier). The main workspace contains a workflow diagram with a green play button icon labeled 'Start' connected by an arrow to a document icon labeled 'Script1'.

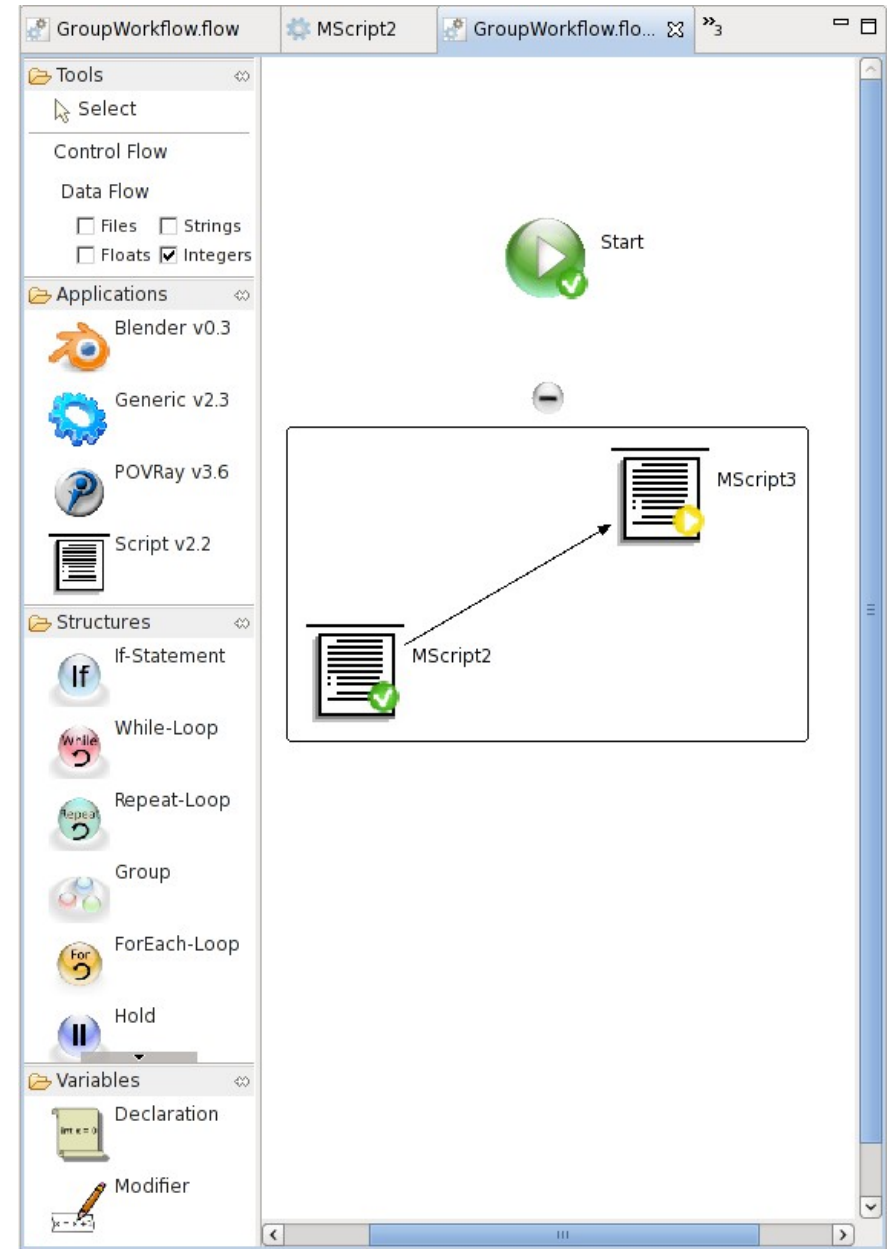
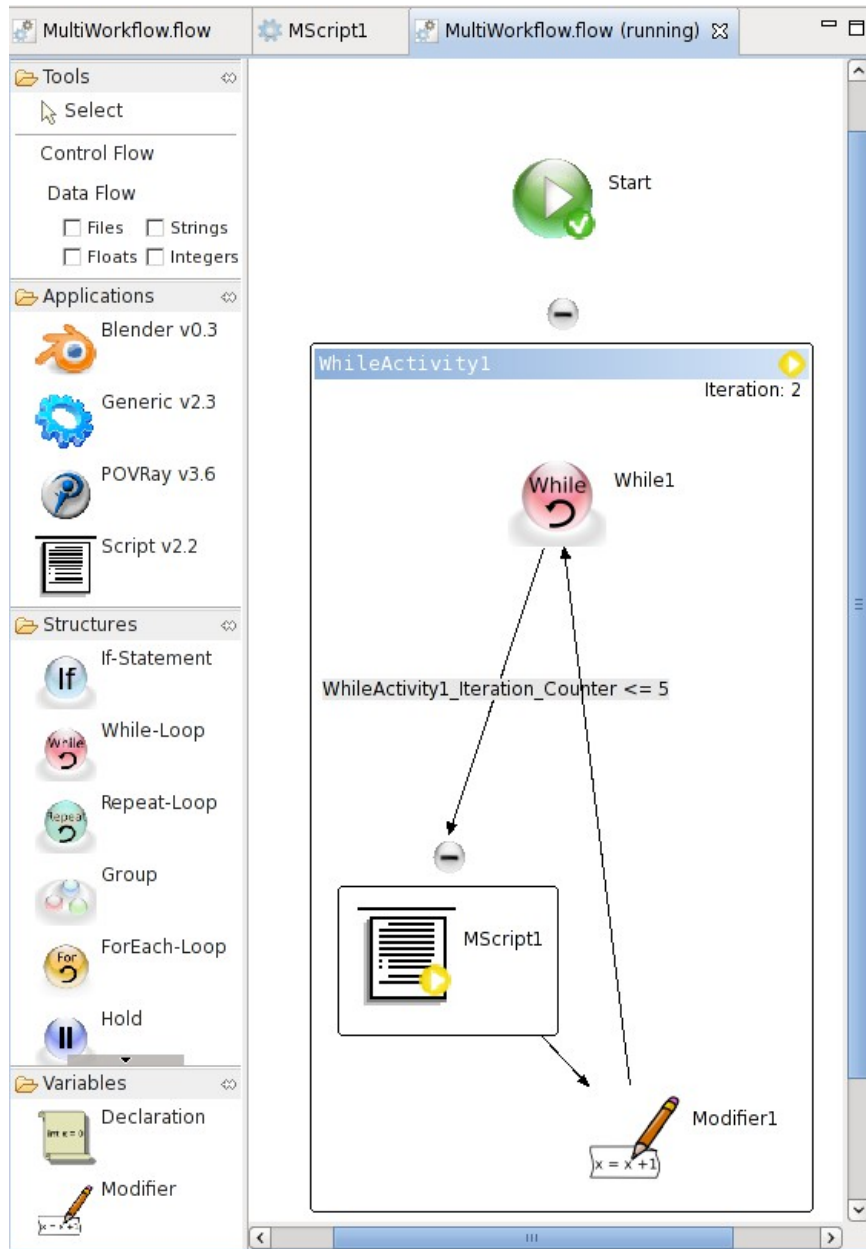
The screenshot shows the UNICORE script editor interface for the 'Script1' task. The top bar shows the workflow name 'ExampleWorkflow.flow' and the task name 'Script1'. Below the bar, there are configuration fields: 'Job name: Script1', 'Options: [empty]', 'Arguments: [empty]', 'Interpreter: Bash shell', and 'Version: any version'. The main area is a code editor with a 'File Edit' menu and the following script content:

```
hostname
echo TZ=$TZ
TZ=CST6CDT date
echo "-----"
env
echo "-----"
sleep 30
TZ=CST6CDT date
exit 0
```

Below the code editor, the file path is shown: 'File: /u/steve/UNICORE-Client-6.6.1/workspace/ExampleWorkflow/input files/Script1\_input1'. At the bottom, there are four checkboxes for execution options: 'Run in debug mode', 'Run with profiling', 'Run with timing', and 'Verbose execution'. The bottom bar contains tabs for 'Script Input', 'Files', 'Variables', and 'Resources'.



# UNICORE Multitask Workflows



# UNICORE Multi Scripts

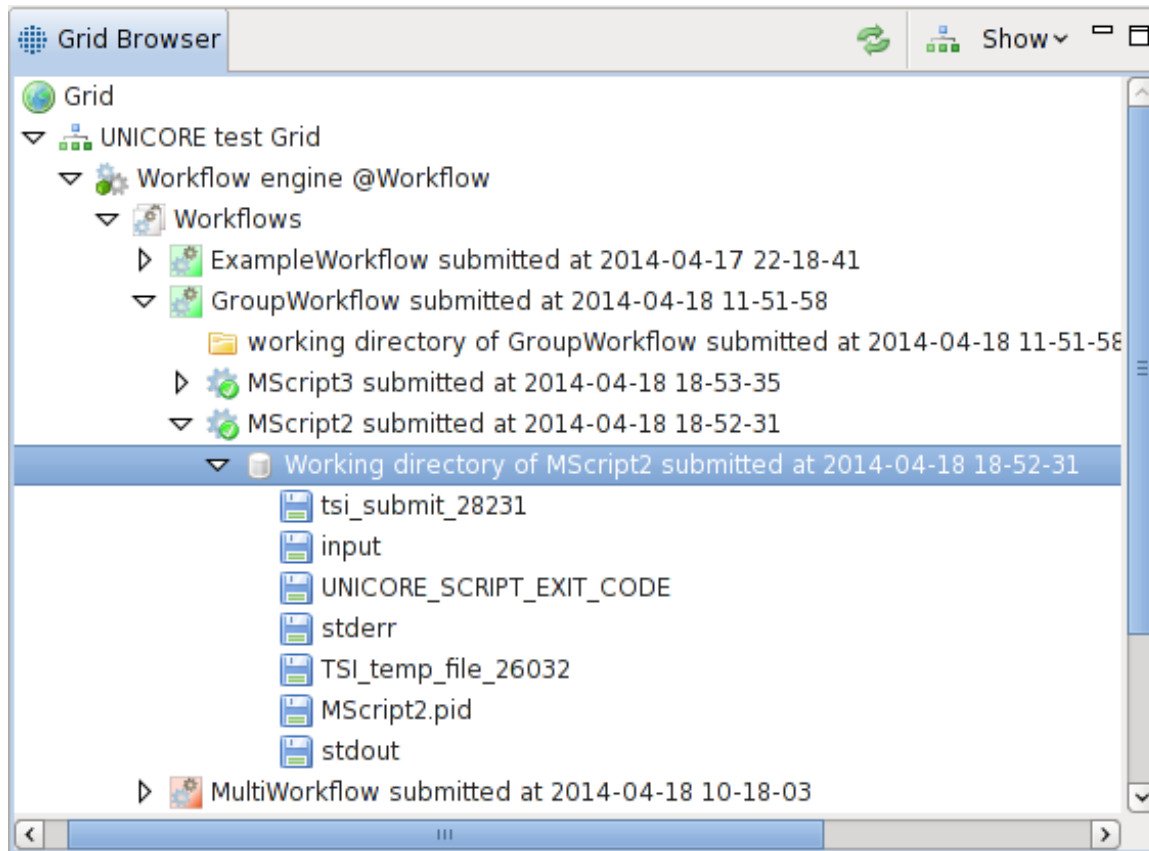
## MScript2

```
echo "MScript2 started at `date` on `hostname`"
echo "args=$*"
echo "I am `id`"
echo "pwd=`pwd`"
echo "-----"
env
echo "-----"
echo MScript2 PID = $$ > MScript2.pid
cp MScript2.pid /home/shared/filespace/SMS/Vmulti
sleep 10
echo "MScript2 ended at `date` on `hostname`"
exit 0
```

## MScript3

```
echo "MScript3 starting at `date` on `hostname`"
echo "args=$*"
cd /home/shared/filespace/SMS/Vmulti
if [ -f MScript2.pid ]; then
    echo "Found MScript2.pid in `pwd`"
    cat MScript2.pid
else
    echo "Could not find MScript2.pid in `pwd`"
fi
sleep 15
echo "MScript3 ended at `date`"
exit 0
```

# UNICORE Grid Browser



# UNICORE

- On the down side ...
  - Written in Java, except for TSI
  - Servers consume 630MB in base configuration
  - As with all Java apps, log information isn't very helpful
  - Uses pkcs12 certificate format - merely inconvenient
  - Steep admin curve, failed to get local UNICORE7 site running.
    - Registry started by offered no services
    - Perl IO:Socket:SSL interface between UNICORE/X and TSI broken.
  - Installation documentation is good but needs work



# UNICORE

- Installed on XSEDE  
[www.xsede.org/software/unicore](http://www.xsede.org/software/unicore)
- Actively developed: 7.0.2 release 2014-03-31
- Server bundle: 136MB tgz file
- Rich Client: 93MB zip file
- UNICORE Summit: Leipzig, June 24, 2014

Would UNICORE be useful in SURGrid?

**UNICORE**

***Live Demo***



# Taverna

*(more details in upcoming SURAGrid monthly call)*

- Client similar to UNICORE
- Runs as Tomcat webapp
- Uses sudo to run java as other users (*scary*)
- Grid use cases:
  - caGrid - OSG & caBIG
  - EGEE, EMBRACE, KnowARC, SIMDAT, ...
  - <http://www.taverna.org.uk/introduction/taverna-in-use/grid/>



# Taverna

The screenshot shows the Taverna Workbench 2.2.0 interface. At the top is a menu bar with options: File, Edit, Insert, View, Workflows, Advanced, Help. Below the menu bar is a toolbar with various icons for workflow design and execution. The main workspace is divided into several panels:

- Service panel:** Located on the left, it contains a list of services with their URLs, such as Biomart, Soaplab, and WSDL. A green box labeled "Services Panel" highlights this area.
- Workflow Explorer:** Located at the bottom left, it shows a tree view of the current workflow, including input ports, output ports, services, data links, control links, and merges. A green box labeled "Workflow Explorer" highlights this area.
- Workflow diagram:** Located on the right, it displays the visual representation of the workflow. A green box labeled "Workflow Diagram" highlights this area.

Annotations with arrows point to various parts of the interface:

- Tool bar:** Points to the toolbar below the menu bar.
- Menu bar:** Points to the menu bar at the top.
- Diagram configuration options:** Points to a toolbar within the workflow diagram area.
- Perspective:** Points to the "Design" tab in the top-left panel.





# Taverna

## ***Homework Assignment***

1) Visit <http://www.taverna.org.uk> and check out capabilities

2) Check out video at <http://bit.ly/1hUG3pp> (taverna.org.uk)  
OnlineHPC: HTML5 / mxgraph workflow builder for Taverna

2a) Apply for account at [onlinehpc.com](http://onlinehpc.com) (Russia)



*... even more workflow options:*

- Pegasus - <http://pegasus.isi.edu/>
- BOSCO - <http://bosco.opensciencegrid.org/>
- SHIWA - <http://www.shiwa-workflow.eu/>
- Condor DAGs on OSG Connect - <http://osgconnect.net/>
- Local Condor DAGs w/ OSGMM - <http://osgmm.sourceforge.net/>
- EMI-WMS - <https://wiki.italiangrid.it/twiki/bin/view/WMS/WebHome>
- Homegrown scheduler with SGVO BDII query

*... just to name a few!*



## Moving Forward on Workflows

- Install UNICORE6 instance on TAMU\_Calclab
  - Integrate with SURAGRID VOMS
  - Add TAMU\_BRAZOS and other interested resources
- Install Taverna instance on TAMU\_Calclab
  - *Ditto*
  - Taverna demo for SURAGRID monthly call
- Working group for Workflow Management?
- Target new users at SURAGRID member sites

***Q?***

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