Building Blocks for a Simple TeraGrid Science Gateway

-- A GISolve Approach

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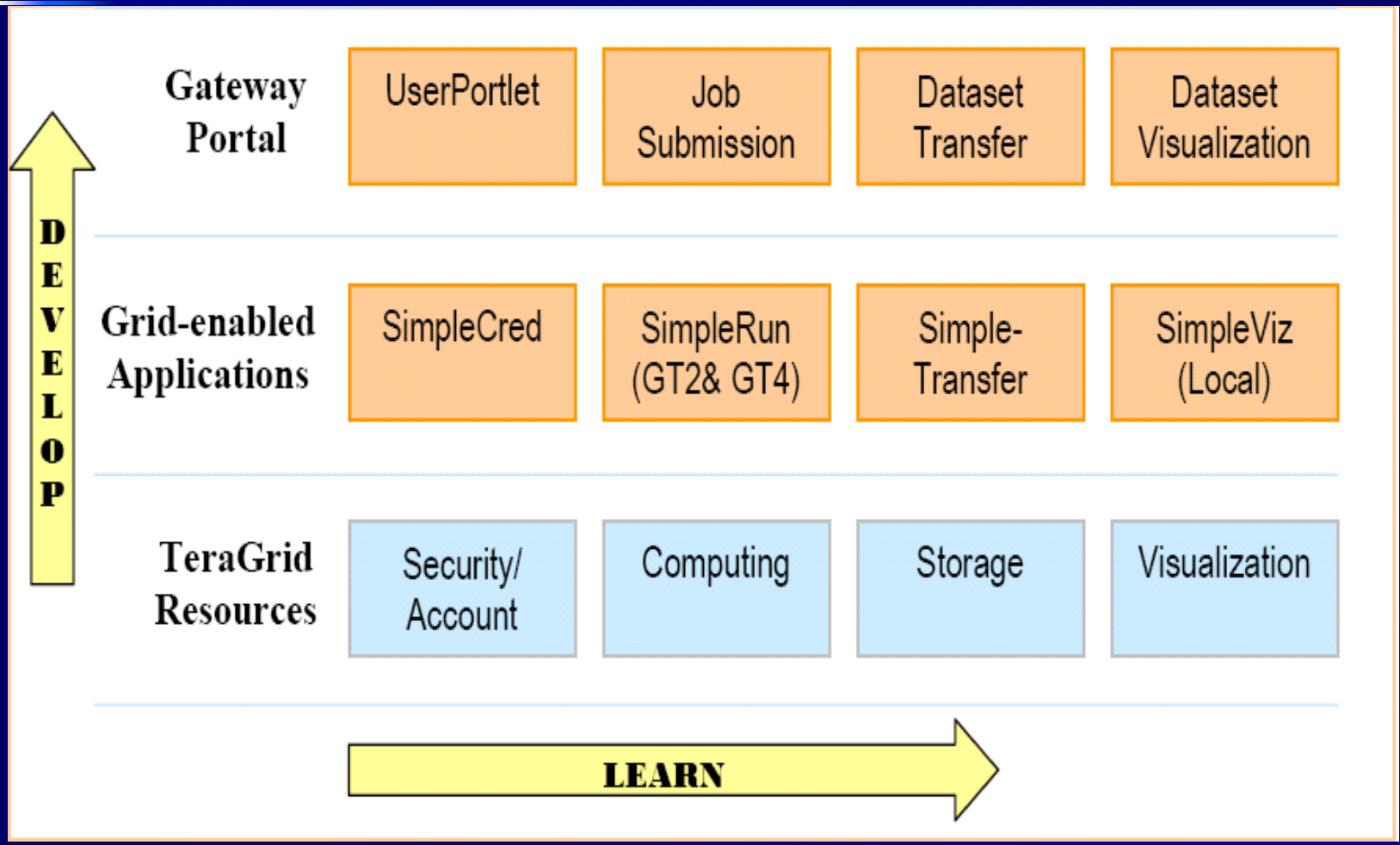
Objectives

- Use TeraGrid to support domain-specific scientific computing
- Develop Grid-enabled applications to access TeraGrid capabilities
- Create a GridSphere-based portal as a TeraGrid science gateway interface
- Develop JSR-168 compliant portlets to build gateway components
- Understand a GISolve-based workflow to steer analyses on TeraGrid

Overview


Gateway Portal
UserPortlet
Job Submission
Dataset Transfer
Dataset Visualization
Grid-enabled Applications
SimpleCred
SimpleRun (GT2& GT4)
Simple-Transfer
SimpleViz (Local)
TeraGrid Resources
Security/ Account
Computing
Storage
Visualization
DEVELOP
LEARN

Learning Curve

- Access TeraGrid resources
  - Accounts, computing and data storage
- Develop Java programs for TeraGrid access
  - JGlobus Cog programming
  - A simple visualization module
- Build a simple science gateway Grid portal
  - JSR-168 PortletAPI
  - GridSphere-based portlet development

Development Curve

- Command line
  - Running domain science application on TeraGrid
- Grid-enabled application development
  - Java programming
  - Application-specific SimpleGrid API
- Science gateway
  - SimpleGrid portal
  - A straightforward GIScience (Geographic Information Science) application workflow

Application Example

- DMS Spatial Analysis
  - Spatial interpolation based on the Dynamically Memorized Strategy (DMS)
- Application package
  - Binary executables
  - Sample datasets
  - Package directory layout
- Build user-friendly science gateway interfaces for scientists to perform DMS analysis transparently on TeraGrid

Technologies

- TeraGrid access
  - Globus Toolkit 4.0.1 (CTSS3)
    - MyProxy, GRAM, WS-GRAM, GridFTP
- Programming
  - Java Cog kit
    - JGlbous module
- Grid portal
  - GridSphere portal server
  - GridSphere-based portlet development framework
  - JSP and GridSphere Visual UI

Environments

- Three tutorial portal servers
  - grow-dev1.its.uiowa.edu
- Portal server software
  - SSH client and server
  - Globus Toolkit 4.0.1 client tools
  - Java J2SE 1.5
  - Ant 1.6.5
  - Apache httpd 2.0.52
  - Tomcat 5.5.23
  - GridSphere 3.0.5 (customized)
  - MySQL server 4.0.20
- TeraGrid sites
  - UC, NCSA, and SDSC

User Accounts

- TeraGrid training accounts
  - train01 – train19
  - Gateway head nodes:
    - tg-login.ncsa.teragrid.org
    - tg-login.uc.teragrid.org (through ncsa or sdsc)
    - Tg-login.sdsc.teragrid.org
- Portal accounts
  - train1 – train 19
  - Password is dispatched with tutorial materials
  - URL: https://${portal_server}/gridsphere/gridsphere

User Accounts (Cont'd)

- MySQL database accounts
  - Same user names as TeraGrid training accounts
  - Password same as your portal account password
- Tutorial server UNIX accounts
  - Same user names as TeraGrid training accounts
  - Password dispatched with tutorial materials
  - BASH shell environment
- Tutorial package
  - In $HOME/SimpleGrid

Exercise 1: Setup Development Environment

- Login to one of the three tutorial servers
  - SSH login: username@${tutorial_server}
- Environment setup

```
cd ~
# add simplegrid-env.sh in your .bashrc
vi .simplegrid-env.sh
```

Outline

- Part I: Basic TeraGrid services and tools
- Part II: SimpleGrid API development for Grid-enabled analysis
- Part III: SimpleGrid portal development

Part I: Basic TeraGrid Services and Tools

- Questions to answer
  - Where are your home directories on all 3 TeraGrid sites?
  - What is your grid certificate identity?
  - How do you create a grid proxy with a specified duration using MyProxy?
  - Are you able to transfer a sample dataset to a specified TeraGrid site?
  - How to submit a job and return immediately without waiting for its completion?

DMS Binary Package Deployment

- SSH login
- Setup your TeraGrid account environment

```
## content of your .soft setting
@teragrid-basic
# TeraGrid wide Globus 4 and Grid software suite
@globus-4.0
# Platform recommended development software suite
@teragrid-dev
```

- Deploy DMS binary package to all three sites

```
scp SimpleGrid/applications/dms.uc.tar.gz train1@tg-login.uc.teragrid.org:./
ssh train1@tg-login.uc.teragrid.org:./
tar xvfz ./dms.uc.tar.gz
```

Get a Grid Proxy

```
[tomcat@grow-dev1 ~]$ myproxy-logon -l gisolve -t 100 -s myproxy.teragrid.org
Enter MyProxy pass phrase:
A credential has been received for user gisolve in /tmp/x509up_u502.

[tomcat@grow-dev1 ~]$ grid-proxy-info
subject  : /C=US/O=National Center for Supercomputing Applications/CN=Gisolve
Community User
issuer   : /C=US/O=National Center for Supercomputing
Applications/CN=Certification Authority
identity : /C=US/O=National Center for Supercomputing Applications/CN=Gisolve
Community User
type     : end entity credential
strength : 1024 bits
path     : /tmp/x509up_u502
timeleft : 99:59:54  (4.1 days)
```

http://teragrid.org/userinfo/access/

Transfer a Sample Dataset

```
[tomcat@grow-dev1 test]$ globus-url-copy
file:/home/tomcat/SimpleGrid/simplegrid/webapp/storage/samples/sample
gsiftp://gridftp-hg.ncsa.teragrid.org:2811/~/sample1

[tomcat@grow-dev1 test]$ ssh gisolve@tg-login.ncsa.teragrid.org

tg-login2 ac/gisolve> ls -l sample1
-rw-r--r--    1 gisolve  lpt       1116491 2007-05-29 21:28 sample1
```

http://teragrid.org/userinfo/data/transfer_location.php

http://teragrid.org/userinfo/data/gridftp.php

GRAM Job Submission

- RSL (for UC)

```
&(jobType="single")
(count=1)
(host_count="1")
(project=TG-SES070007N)
(directory="/home/gisolve/gisolve/DMS/release")
(executable=/home/gisolve/gisolve/DMS/release/process.pl)
(arguments="500" "500" "20" "/home/gisolve/sample1" "/home/gisolve/result1")
(stdout="stdout.gisolve.test")
(stderr="stderr.gisolve.test")
```

- Commands

```
$ globusrun -b -f ./gt2.rsl -r tg-grid.uc.teragrid.org:2120/jobmanager-pbs
globus_gram_client_callback_allow successful
GRAM Job submission successful
https://tg-grid1.uc.teragrid.org:50004/19686/1180493030/
$ globus-job-status https://tg-grid1.uc.teragrid.org:50004/19686/1180493030/
DONE
```

WS-GRAM Job Submission

- RSL (XML)

```
<job>
   <factoryEndpoint
         xmlns:gram="http://www.globus.org/namespaces/2004/10/gram/job"
         xmlns:wsa="http://schemas.xmlsoap.org/ws/2004/03/addressing">
      <wsa:Address>
https://tg-login1.uc.teragrid.org:8443/wsrf/services/ManagedJobFactoryService
      </wsa:Address>
      <wsa:ReferenceProperties>
         <gram:ResourceID>PBS</gram:ResourceID>
      </wsa:ReferenceProperties>
   </factoryEndpoint>
   <executable>/home/gisolve/gisolve/DMS/release/process.pl</executable>
   <directory>/home/gisolve/gisolve/DMS/release</directory>
   <argument>500</argument>
   <argument>500</argument>
   <argument>20</argument>
   <argument>/home/gisolve/sample1</argument>
   <argument>/home/gisolve/result1</argument>
   <stdout>/users/gisolve/gisolve/DMS/results/stdout.sample1</stdout>
   <stderr>/users/gisolve/gisolve/DMS/results/stderr.sample1</stderr>
</job>
```

WS-GRAM Job Submission

- Command: globusrun-ws -submit -f rsl_xml_file

http://teragrid.org/userinfo/jobs/globus.php

Analysis Process

- Get a grid proxy
- Transfer a dataset to specified TeraGrid sites
- Submit Grid jobs to run DMS binary executables against the transferred dataset
- Collect results back
- Visualize results
  - Will be shown later

Part II: SimpleGrid API Development for Grid-enabled Analysis

- How to do Part I in a programming way?
- Purpose
  - Automate the access to TeraGrid resources as a Grid-enabled application
- Package
  - Location: SimpleGrid/simplegrid/src/
  - SimpleGrid API for DMS analysis
    - org.gisolve.demo.app.*
    - org.gisolve.demo.grid.*
    - org.gisolve.demo.util.*
  - Libraries
    - All jars from ${GLOBUS_LOCATION}/lib
      - Particularly cog-jglobus.jar
    - JFreeChart libraries for visualization

http://www.globus.org/cog/manual-user.pdf

Get a Grid Proxy

- Class
  - org.gisolve.demo.grid.security.SimpleCred
- Two methods to get a proxy
  - Load an existing valid proxy file
    - SimpleCred::load()
  - Create a proxy by contacting with a MyProxy server
    - SimpleCred::logon()
- Export proxy to a file
  - SimpleCred::export()

Transfer a Sample Dataset

- Class
  - org.gisolve.demo.grid.data.SimpleTransfer
- Local<->remote transfer
  - SimpleTransfer::remote2local()
  - SimpleTransfer::local2remote()
- Third-party transfer
  - Refer to Cog manual (version 1.1)

http://wiki.cogkit.org

GRAM Job Submission

- Class
  - org.gisolve.demo.grid.job.SimpleRunGT2
  - org.gisolve.demo.grid.job.SimpleRSL
- RSL generation
  - Application specific
- GT2 job submission
  - Use batch mode in which a call returns immediately with a job handle

GRAM Job Submission: MPI

- MPI on TeraGrid
  - User “softenv | grep mpi” to see different MPI settings
- MPI job submission through Globus
  - Specify “count” element in RSL
    - “count” is the number of processes to spawn
  - Specify “host_count” element in RSL
    - “host_count” is the number of CPUs for MPI execution
  - “count = host_count” means each CPU runs one MPI process
  - Specify “jobType=mpi” in RSL

WS-GRAM Job Submission

- Class
  - org.gisolve.demo.grid.job.SimpleRunGT4
  - org.gisolve.demo.grid.job.SimpleRSL
- RSL generation
  - Application specific
- GT4 job submission
  - Use batch mode in which a call returns immediately with a job handle
  - Note that it uses a different globus package org.globus.exec.*

http://www.globus.org/toolkit/docs/4.0/execution/wsgram/developer-index.html#id2563059

How to Write RSL?

- RSL schema
  - http://globus.org/toolkit/docs/4.0/execution/wsgram/schemas/gram_job_description.html
- GT2 and GT4 schema comparison
  - http://www.globus.org/toolkit/docs/4.0/execution/wsgram/WS_GRAM_Migrating_Guide.html

Exercise 2

- Test SimpleGrid API
  - Source simplegrid-env.sh
  - SimpleGrid/bin/runTest2.sh

Part III: SimpleGrid Portal Development

- Science gateways to TeraGrid
  - Provide an online access points to TeraGrid
  - Aggregate domain science application-level capabilities
  - Hide the complexity of using TeraGrid
  - Portal is commonly used to meet such needs
- Focus
  - Provide transparent access to TeraGrid for domain scientists
  - Build application-oriented workflow inside portal for easy access by users
  - Technical details for portlet development
    - GridSphere
    - PortletAPI
    - GridSphere-based portlet development

GridSphere

- Features
  - http://www.gridsphere.org
  - Open source
  - PortletAPI (JSR-168) compliant
  - Object persistence support through Hibernate
- GridSphere 3.0.5
  - Download: https://svn.gridsphere.org/
  - Requirements: java, ant, tomcat, mysql
  - Build: ant install
    - Be sure to change hibernate.properties, build.properties
    - Copy mysql jdbc driver to ${CATALINE_HOME}/common/lib/
  - Development using Eclipse
    - Instructions will be added in our online documentation

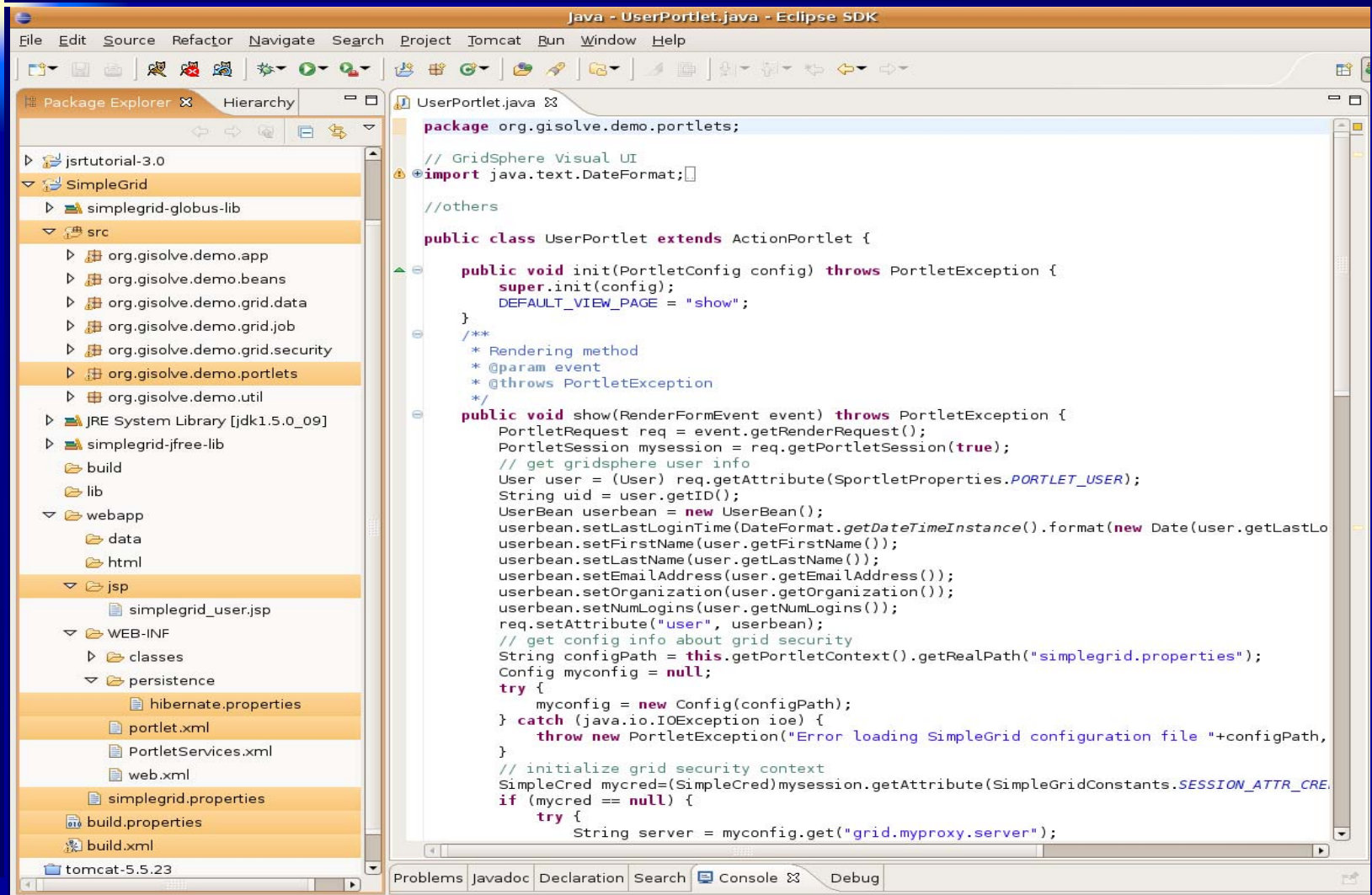
Exercise 3

- Demo
  - GridSphere interface
  - New portlet project creation

SimpleGrid Portlets

- Location: SimpleGrid/simplegrid
- Two portlets
  - UserPortlet
    - Display user information
    - Initialize or renew grid proxy
      - Automatic renewal after initialization
  - DMSPortlet
    - DMS workflow control
    - Build user interfaces for DMS analysis
- Each tutorial user will build and deploy their version of SimpleGrid portlets (project name is simplegrid_${USER})

Introduction to SimpleGrid Development



SimpleGrid Project Layout

- src/org.gisolve.demo.portlets
  - Portlet action classes
- lib/
  - Libraries for Globus and JFreeChart
- webapp/jsp/
  - JSP pages for user interface rendering
- webapp/WEB-INF/persistence/hibernate.properties
  - Configuration for backend database access
- webapp/WEB-INF/portlet.xml
  - Portlet definition
    - Defines unique portlet id, the portlet class, etc.
- webapp/simplegrid.properties
  - SimpleGrid specific configuration about Grid resources
  - Loaded at the first time the UserPortlet is visited
- build.xml
  - Ant build file to compile, deploy, and install SimpleGrid portlets to GridSphere
  - Need to change if you have your own libraries or packages developed
- build.properties
  - Define project name and location of GridSphere where SimpleGrid finds dependent GridSphere java classes and PortletAPI (javax.portlet.*) definitions

Runtime Configurations

- simplegrid.properties

Portlet Container

- PortletAPI (JSR-168 specification)
  - Portlet specification
  - What are not defined?
    - Object persistence: store portlet status in permanent storage
    - Portlet rendering method
      - JSP, Velocity, GridSphere Visual UI (JSP taglib), Java Server Face
- GridSphere: JSR-168 compliant portlet container
  - Implemented javax.portlet.*
  - Hibernate as object persistence technologies
  - JPS-based Visual UI rendering
  - What are not standardized?
    - ActionPortlet based on Visual UI
    - Portlet service framework (from WebSphere)
  - Other open source portlet containers
    - Apache Jetspeed/Pluto, Sakai

PortletAPI (JSR-168 Specification)

- Sample portlet
  - GridSphere jsrtutorial: ActionHelloworld
- Portlet modes
  - VIEW (doView()): the default display mode
  - EDIT (doEdit()): preference/configuration editing
  - HELP (doHelp()): help information
- Base portlet: GenericPortlet
- PorletURL
  - Generate actionURL and renderURL in response page

http://www.gridsphere.org/gridsphere/gridsphere/guest/download/r/

PortletAPI (JSR-168 Specification)

- PortletRequest
  - Get parameters from portlet container
    - ActionRequest
      - Used in action processing
    - RenderRequest
      - Used in rendering
- PortletResponse
  - Pass parameters to portlet container
    - ActionResponse
      - Parameters set in ActionResponse will be passed to RenderRequest
    - RenderResponse
      - Used in rendering response page
- Action processing
  - processAction(ActionRequest, ActionResponse)
- Default rendering
  - doView(RenderRequest, RenderResponse)

PortletAPI (JSR-168 Specification)

- Portlet definition (portlet.xml)

```
<portlet>
    <description xml:lang="en">SimpleGrid user portlet</description>
    <portlet-name>SimpleGridUserGisolve</portlet-name>
    <display-name xml:lang="en">SimpleGrid user gisolve</display-name>
    <portlet-class>org.gisolve.demo.portlets.UserPortlet</portlet-class>
    <expiration-cache>0</expiration-cache>
    <init-param>
      <name>aname</name>
      <value>avalue</value>
    </init-param>
    <supports>
      <mime-type>text/html</mime-type>
      <portlet-mode>view</portlet-mode>
      <portlet-mode>edit</portlet-mode>
      <portlet-mode>help</portlet-mode>
    </supports>
    <supported-locale>en</supported-locale>
    <portlet-info>
      <title>SimpleGrid User home for gisolve</title>
      <short-title>simplegrid-gisolve</short-title>
      <keywords>simplegrid, gisolve, user</keywords>
    </portlet-info>
    <portlet-preferences>
      <preference>
       ……
      </preference>
    </portlet-preferences>
</portlet>
```

Portlet Development

- Questions
  - How to direct actions to corresponding action methods?
    - Avoid a big processAction()
  - How to get parameters from PortletRequest?
  - How to render response pages?
  - How to communicate between portlets?

Portlet Development

- GridSphere Visual UI
  - Rendering: JSP tag-lib
  - Action: ActionPortlet
- Velocity
  - Rendering: Velocity templates
  - Action: VelocityPortlet

http://www.gridsphere.org/gridsphere/docs/TagGuide/TagGuide.html

http://www.collab-ogce.org/ogce2/velocity-portlets.html

Exercise 4

- Deploy your SimpleGrid project (simplegrid_${USER}) to gridsphere container
  - Use “ant install” for a fresh install
  - Use “ant deploy” for update (it does not clear database content)
  - Look at $CATALINA_HOME/webapps/simplegrid_${USER}/WEB-INF/lib to see project jars generated by deployment
- How does Gridsphere know your project?

GridSphere-based Portlet Development

- Visual UI taglib for rendering

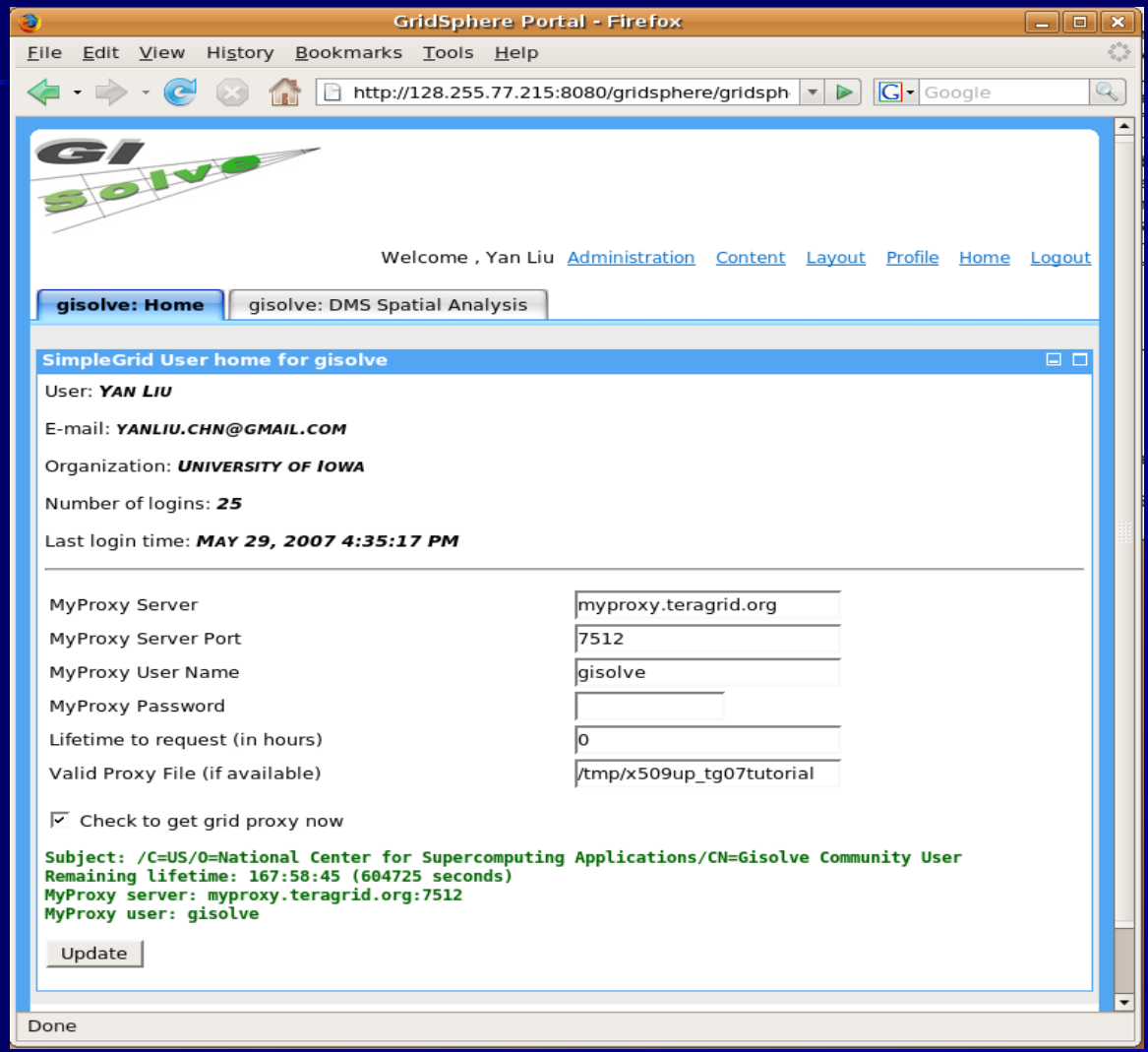
```
<%@ taglib uri="/portletUI" prefix="ui" %>
<%@ taglib uri="http://java.sun.com/portlet" prefix="portlet“ %>
<portlet:defineObjects/>
```

- Portlet class
  - Extend ActionPortlet
  - All beans are constructed from ActionFormEvent or RenderFromEvent
  - Get PortletRequest and PortletResponse from FormEvent
  - Use setNextState() to point to JSP page in rendering methods
  - Use setNextState() to point to rendering method in action methods

Example: UserPortlet

- UserPortlet::show()
  - Default rendering method which displays user information and grid proxy configuration in JSP
  - In JSP, Bean is used to render the values of user forms
    - Java code is embedded to directly access RenderRequest for grid proxy information
- UserPortlet::configSimpleCred()
  - Action method to retrieve grid proxy either from MyProxy server or locally from a valid proxy file

UserPortlet Interface



Velocity-based Portlet Development

- Portlet definition
  - Initial template name
  - velocity.properties
- Action class
  - Get parameters: ActionRequest.getParameter()
  - Rendering: VelocityContext.put(name, object)
  - Action methods: called based on their names through Java Reflection
- Velocity template

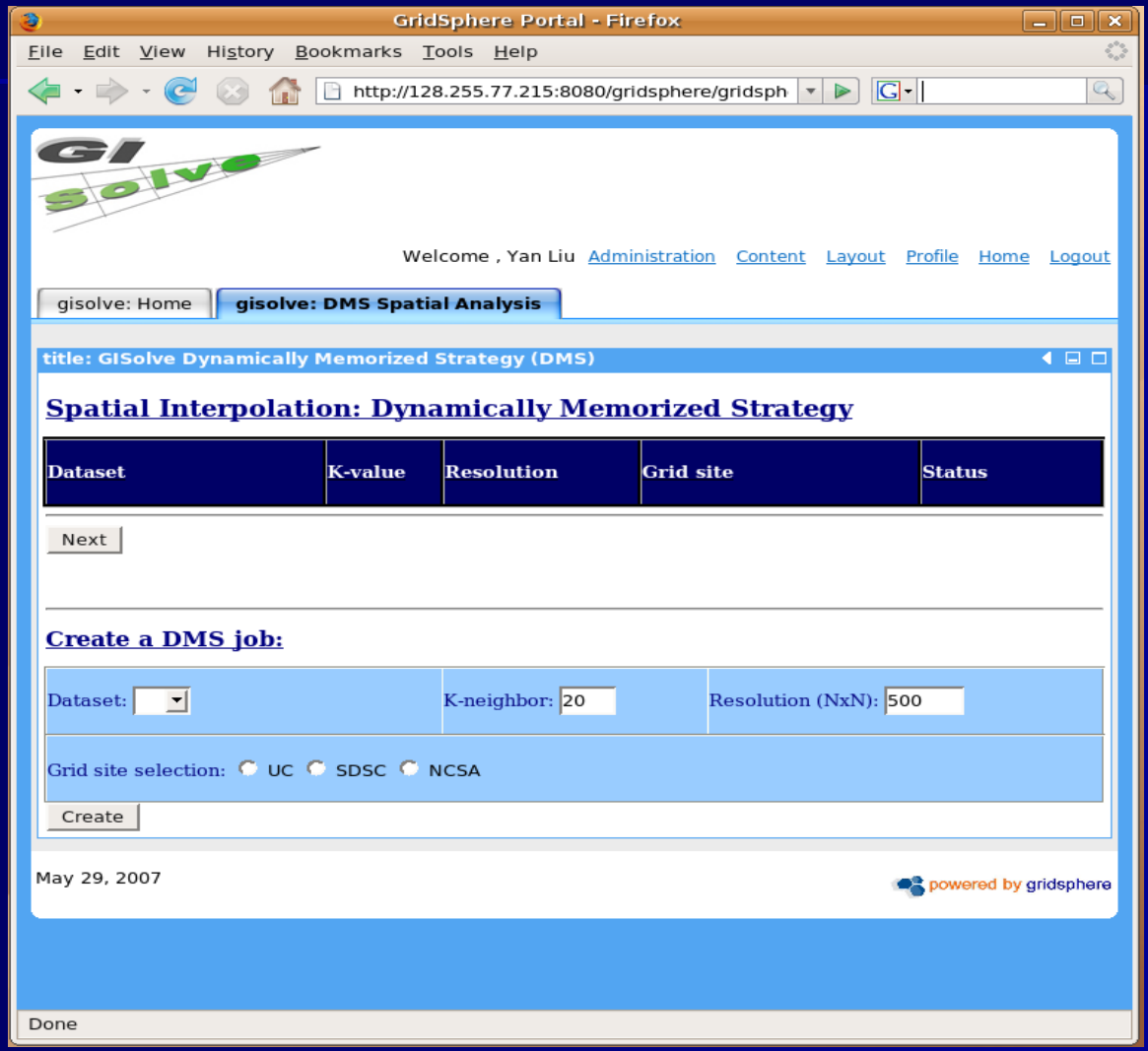
```
#if( !$gisolve_portal_error_info.equals("") )
   <pre><p><font face="Arial Narrow“ color="red">$gisolve_portal_error_info</font><p></pre>
<hr>
#end
<form name="dms0002" method="POST" action="$actionURL">
  <input type="submit" value="Return“ name="actionMethod_doDms_return">
</form><hr><p>
```

http://velocity.apache.org/engine/releases/velocity-1.5/user-guide.html

DMS Analysis Workflow in Portal

- Workflow control is done by keeping state information in PortletSession as attributes
- Portlet communication
  - Need to coordinate two portlets
    - PortletSession.getAttribute(name, PortletSession.APPLICATION_SCOPE)
    - PortletSession.setAttribute(name, value, PortletSession.APPLICATION_SCOPE)
- Learn how SimpleGrid remembers current status of each job

DMSPortlet Interface



Exercise 5

- Run DMS portlet and get visualization results
  - Result page plots results after the analysis
  - Do you see your job is running on TeraGrid?
    - Refresh job status
    - Verify it by using “qstat | grep gisolve” to see the status of your job
  - Thread in SimpleGrid portlets
    - File transfer and result visualization access the same portal server and are time-consuming
    - Threads are used to respond to user requests quickly

Visualization on TeraGrid

- SimpleGrid uses JFreeChart for simple local visualization
- We are evaluating the integration between GISolve and ParaView on TeraGrid to support advanced visualization

http://tg-portal.uc.teragrid.org/

Summary

- SimpleGrid provides basic components to develop science and engineering gateways
  - This tutorial includes code, links, and examples
  - Based on a real-world GIS application
- SimpleGrid is also used in GISolve, TeraGrid GIScience gateway
- Gateway server setup instructions and additional materials will be provided in GISolve/TeraGrid online documentation

Q & A

- Questions and comments?
- Thanks!