

The Integration of AJAX, Interactive X Windows Applications and Application Input Generation into the UCLA Grid Portal

SC07-GCE07

UGP Documentation at:
<http://www.ucgrid.org>

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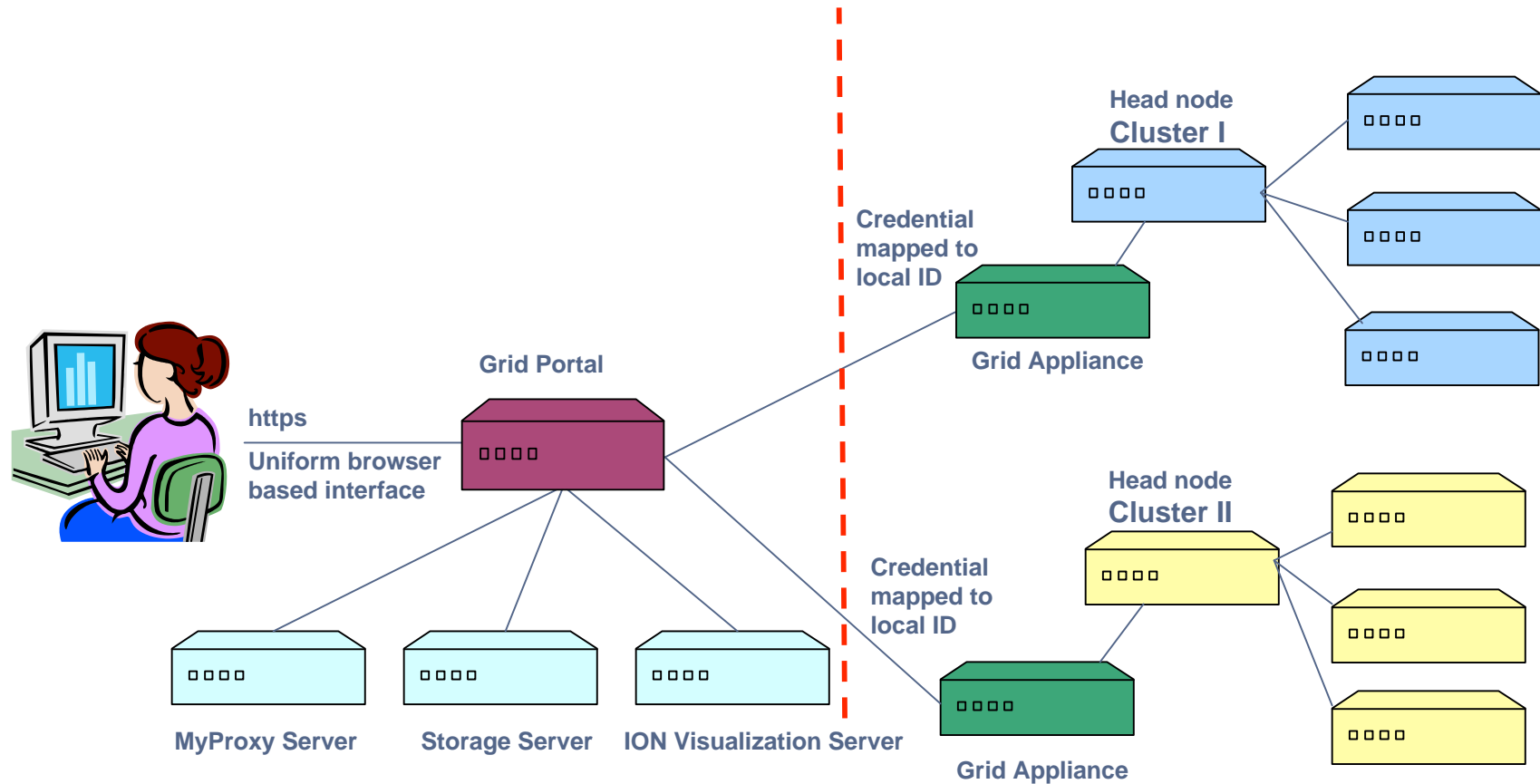
UGP (UCLA Grid Portal)

- Joins computational clusters into a Grid
- Services Provided
 - Resource Discovery
 - Data Manager
 - Batch Job Submittal/Status/Output
 - Interactive GUI applications (run on the clusters)
 - Grid Development Environment
- Simple Identity Management Interface

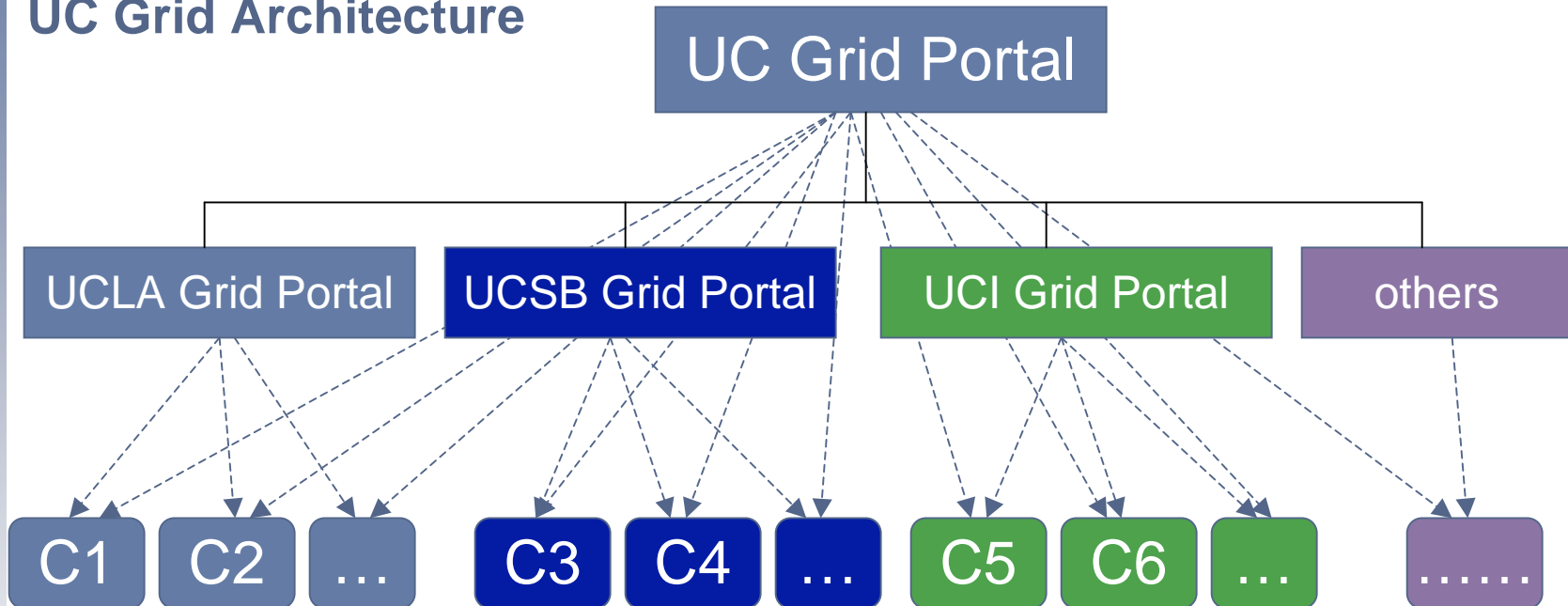
UGP (UCLA Grid Portal)

- Under development at UCLA since 2002.
- Web Portal built on top of:
 - Globus Toolkit 4.n -- Tomcat
 - MySQL -- Shibboleth
 - GridSphere Portlet Framework
- AJAX based interfaces built on top of the following toolkits:
 - Zimbra AJAX Toolkit
 - YUI (Yahoo User Interface)
 - GWT (Google Web Toolkit)

Single Campus Architecture



UC Grid Architecture



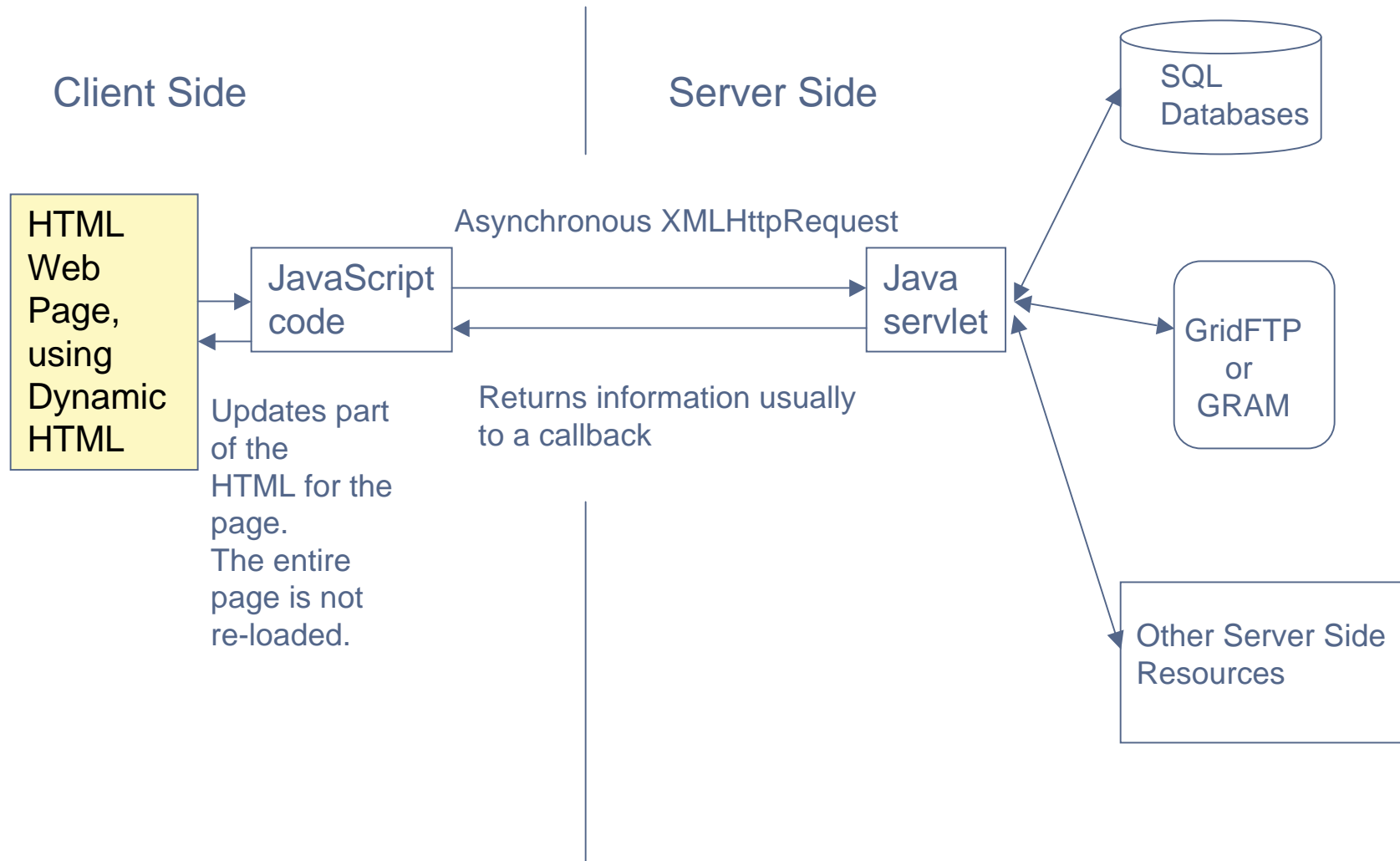
- User always applies from Campus Portal
- One Certificate Authority(CA) throughout UC Grid
- User CA is automatically created and pushed to myproxy server
- Simple account creation process (approval/denial workflow)
- Once the admin approves, the user is able to login to two portals instantly
- Enabled by Register Web Service and Sync Web Service in UC Grid Portal

Conventional Web Interfaces vs. AJAX Enabled User interfaces

AJAX

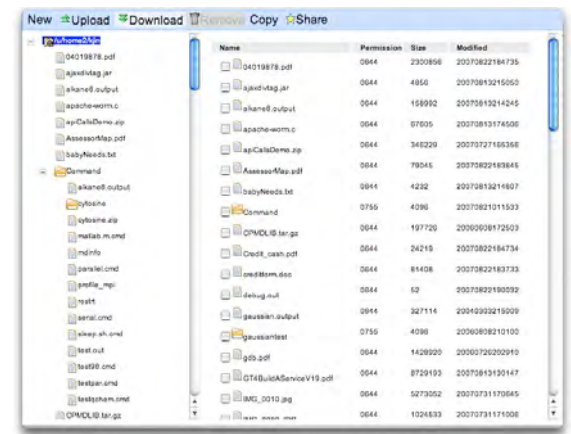
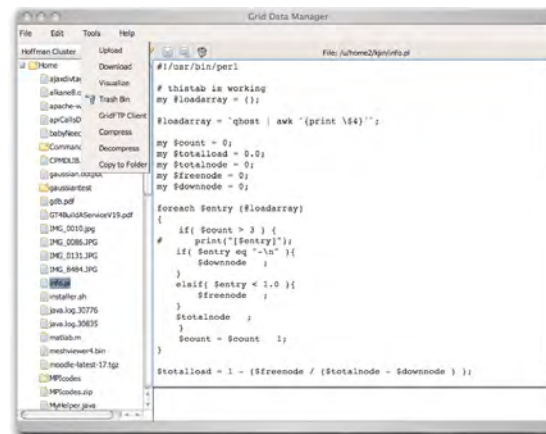
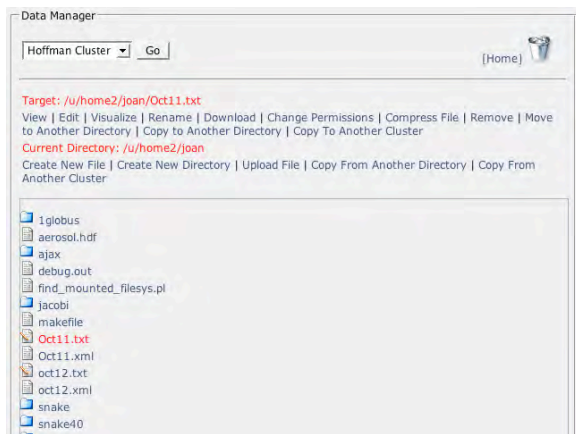
- AJAX = asynchronous JavaScript and XML
- JavaScript runs in the Browser
- Java code on the server processes the requests
- Asynchronous XMLHttpRequests used for communication
- Only part of the Web page is updated
- Interactivity gains and efficiency benefits (fewer clicks required)

How AJAX Works



AJAX Data Managers vs. HTML Data Manager

- AJAX Data Managers looks and work like a desktop data manager.



Conventional
Portlet
Cerca 2004

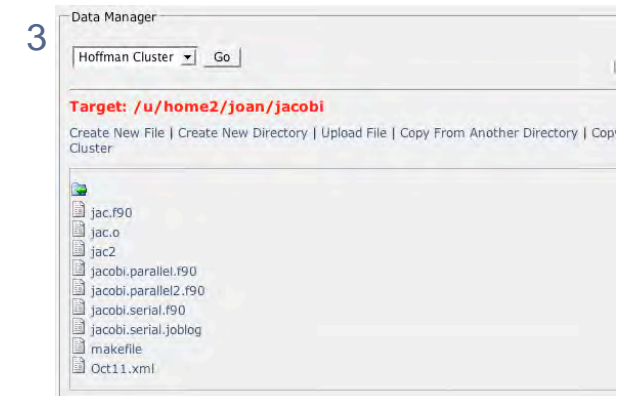
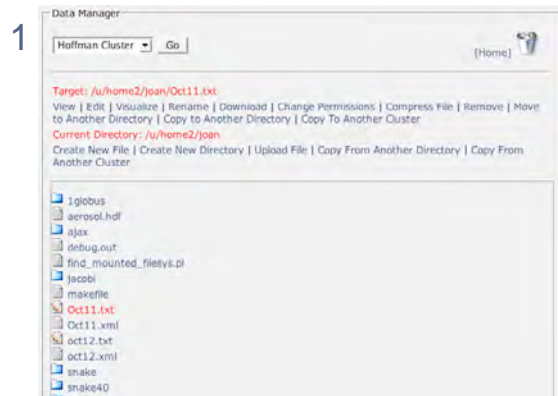
AJAX
Zimbra
Cerca 2005

AJAX
GWT
Cerca 2007

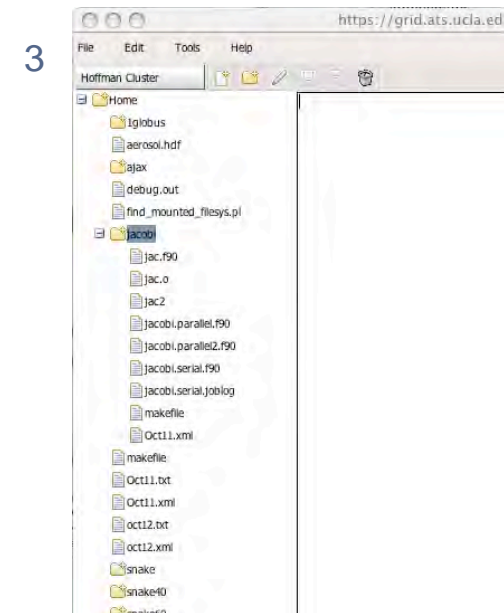
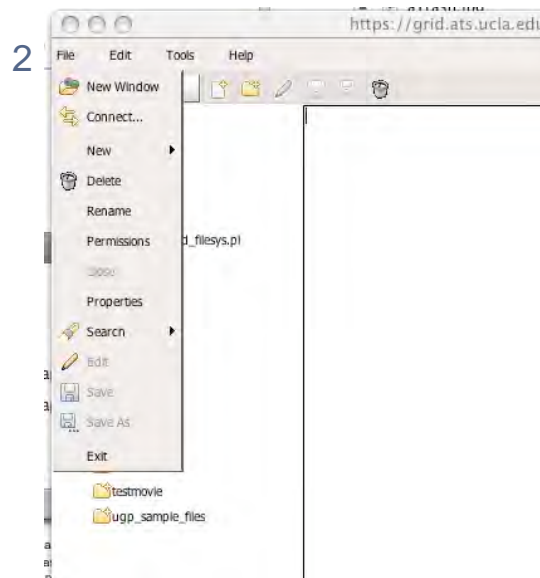
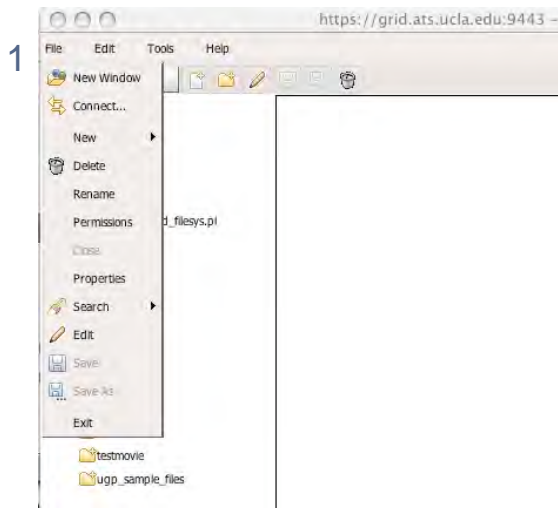
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- The user does not have to wait for the entire page to refresh with each click.

Conventional

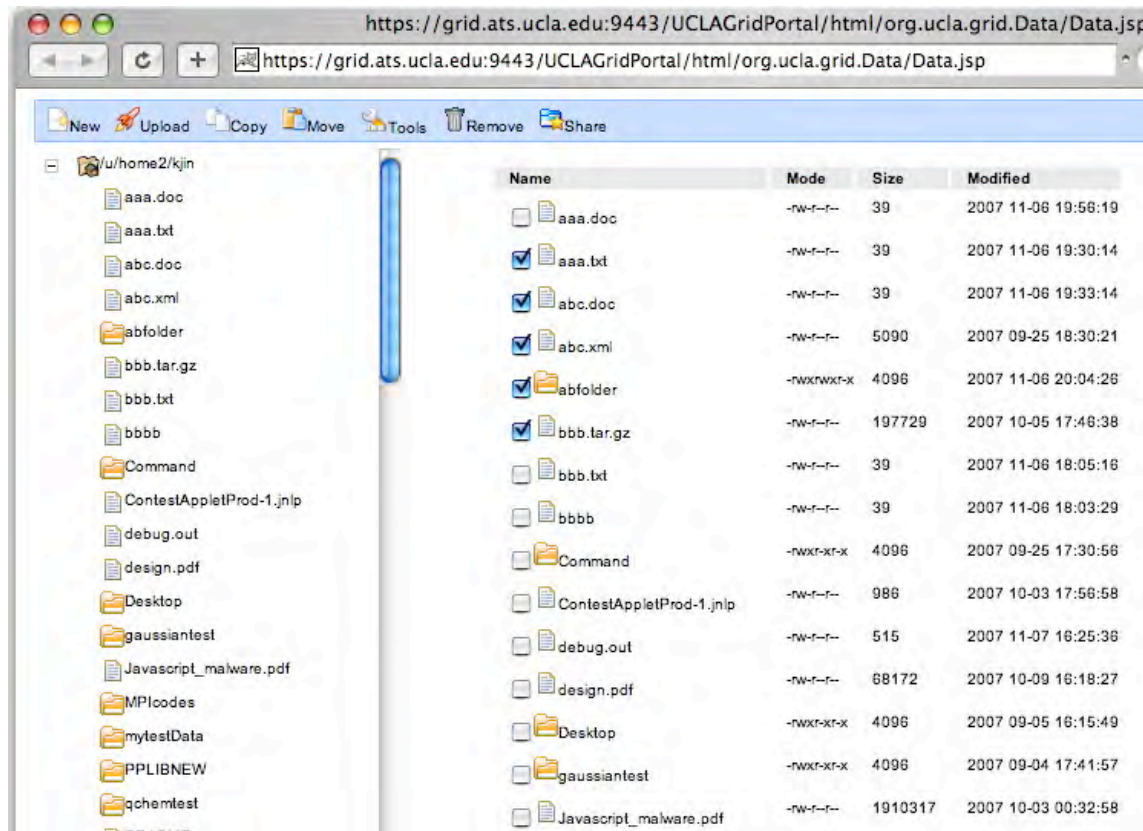


AJAX



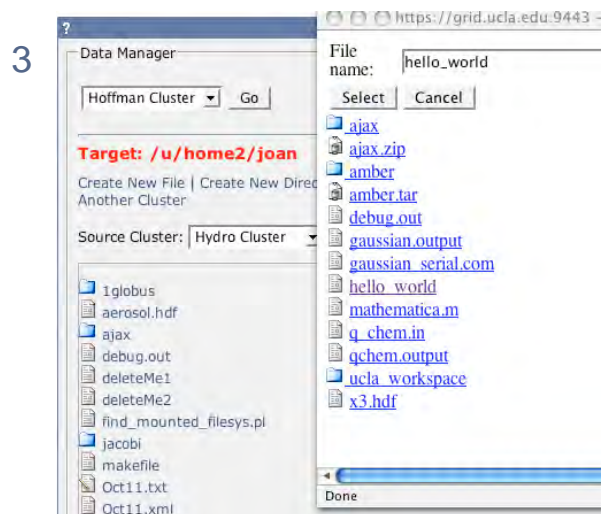
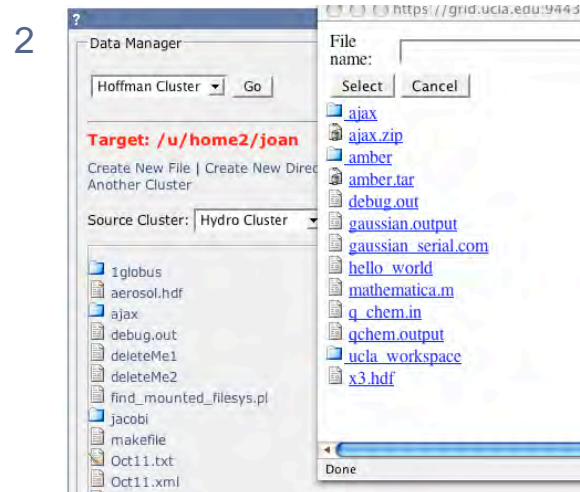
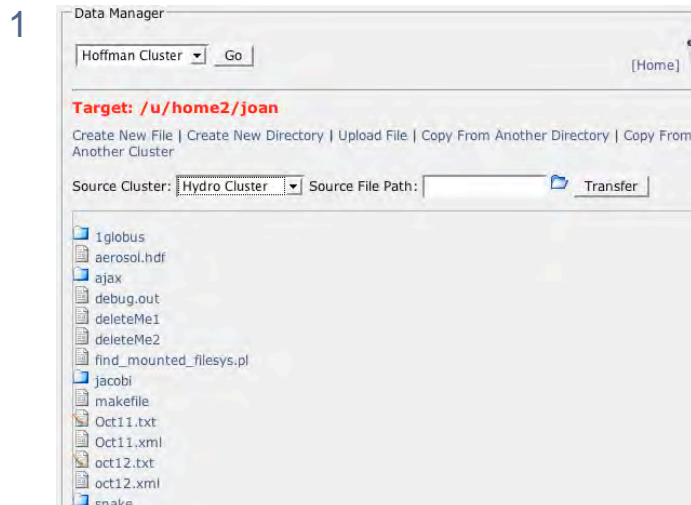
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- With AJAX we can do perform the same action on multiple files at once



- In order to attract users to Grid Portals we have to make them as easy to use as possible and offer increased functionality.

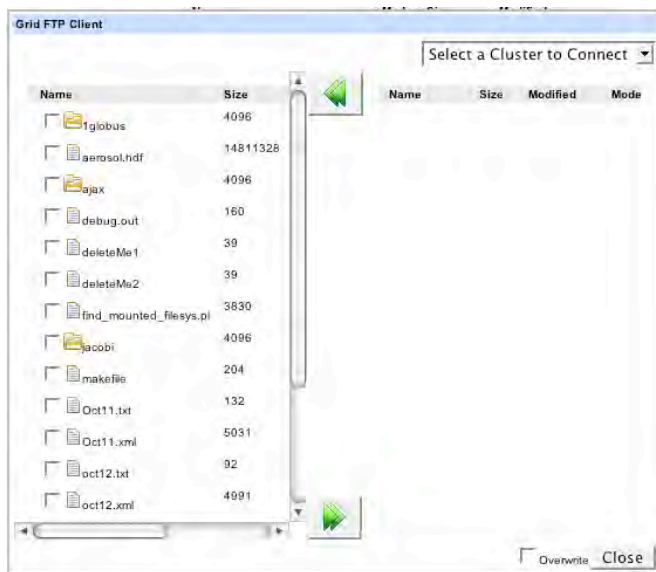
FTP -- Conventional



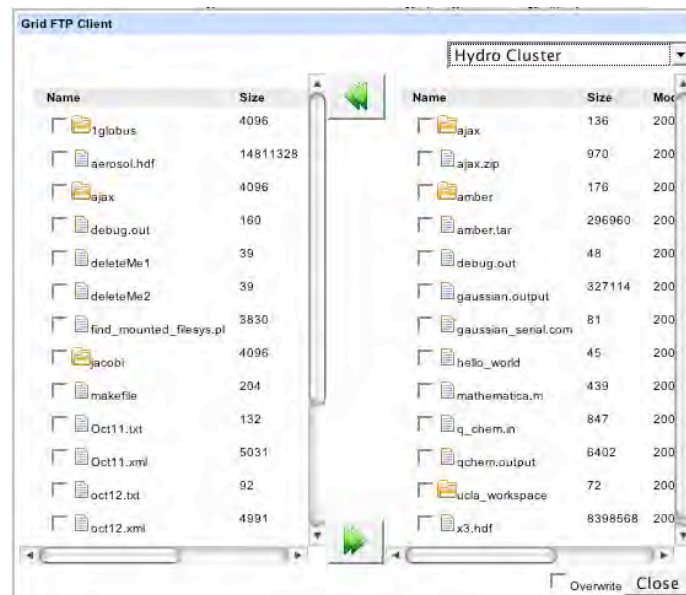
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AJAX FTP Client

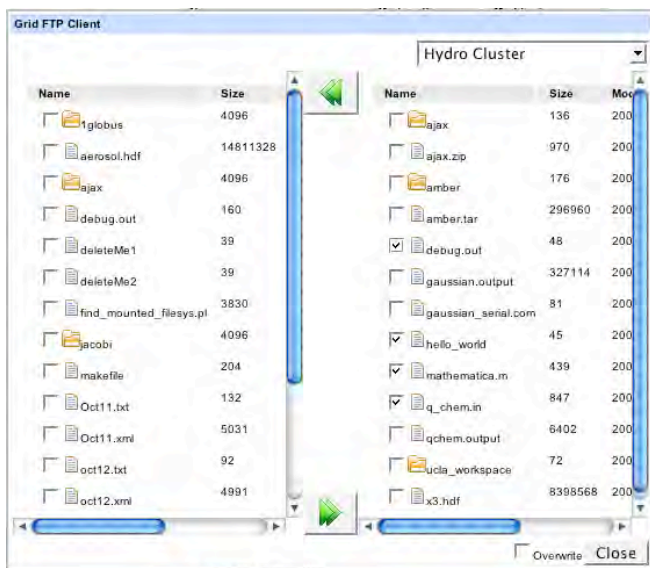
1



2

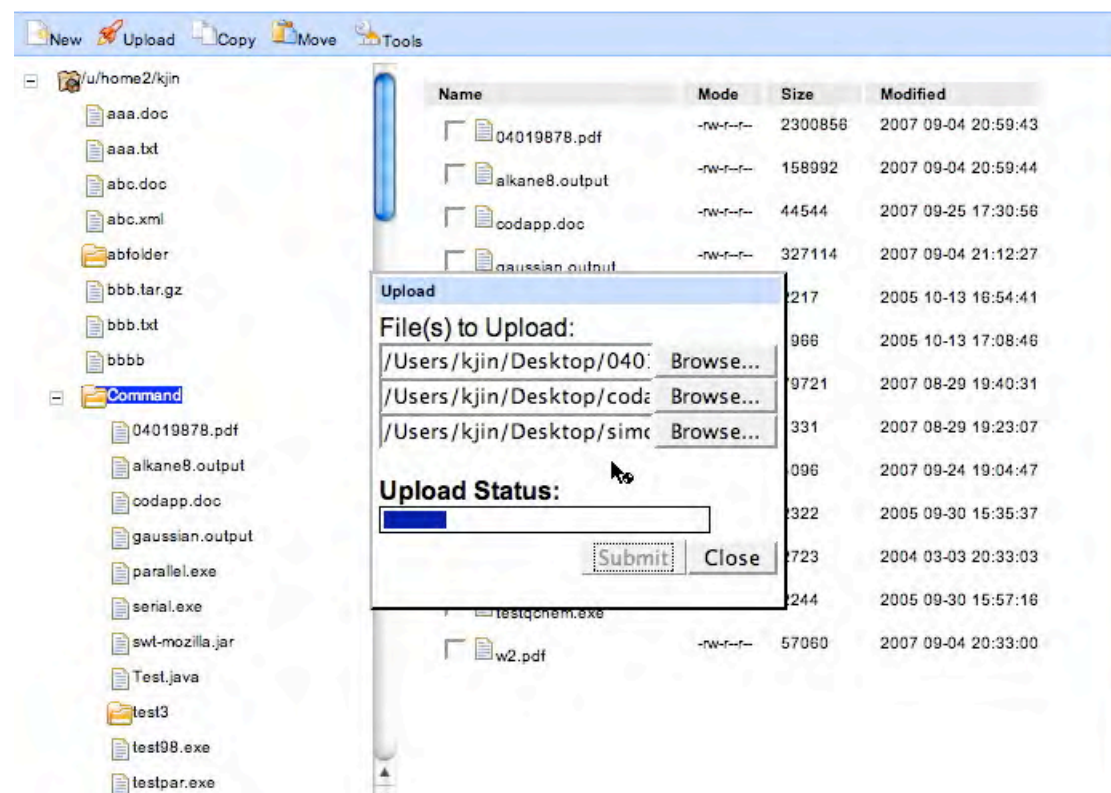


3

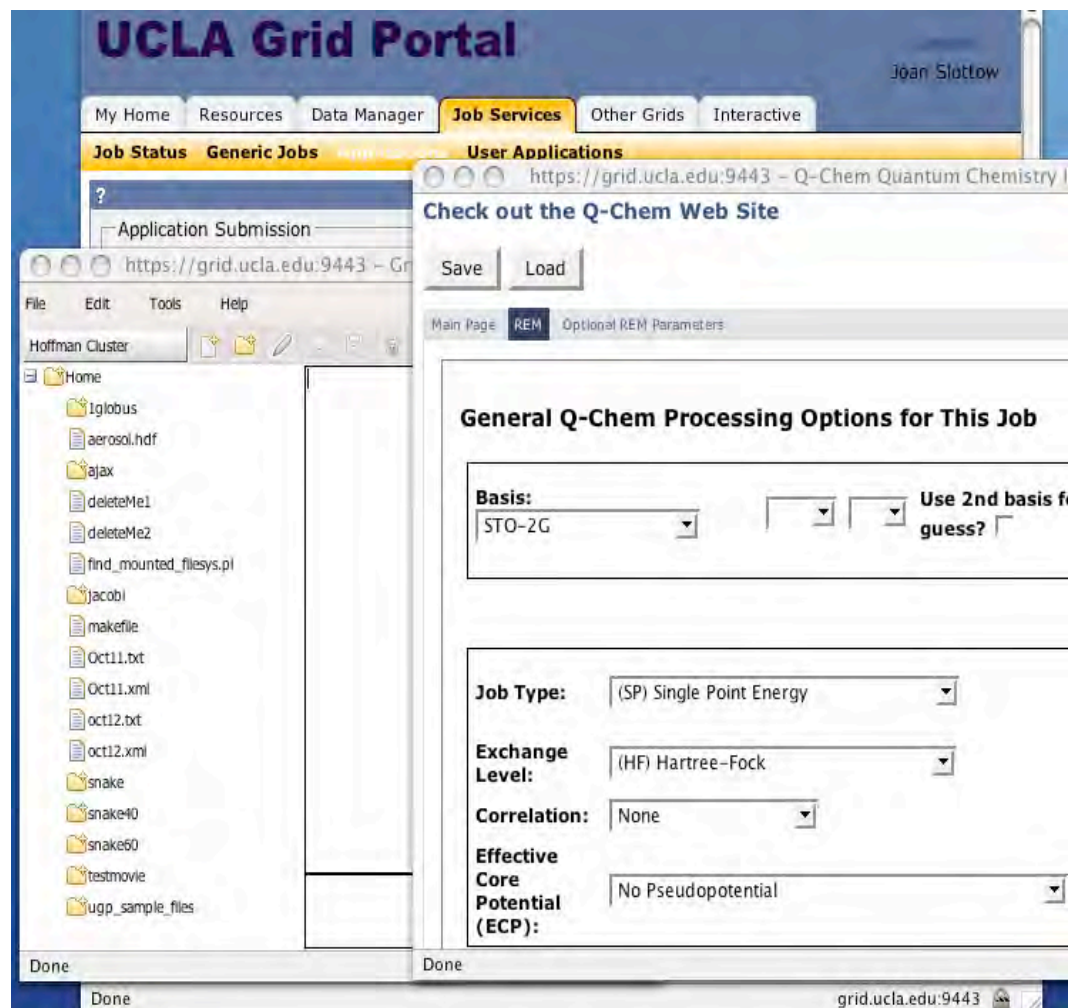


Progress bar

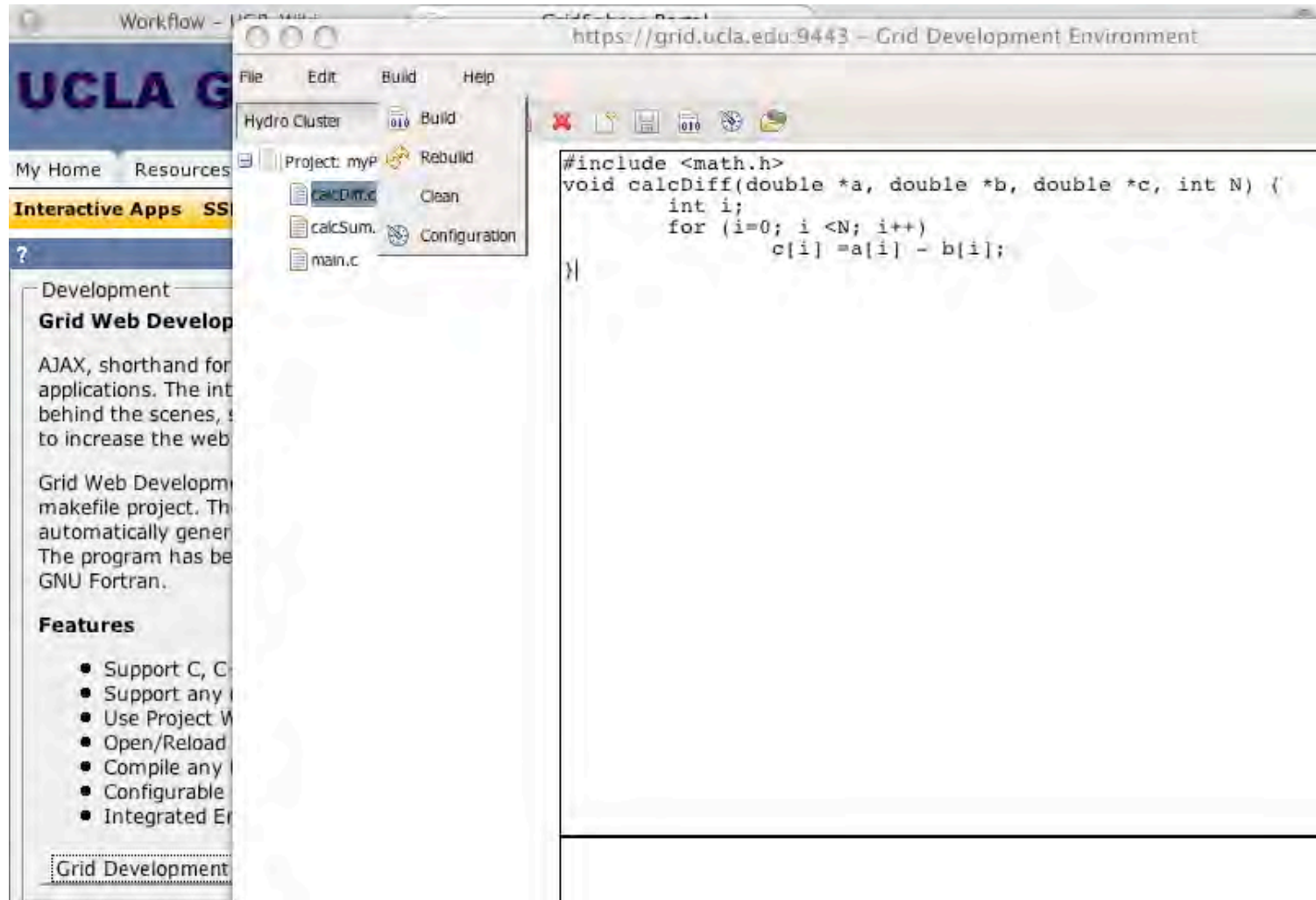
- See the upload progress at real time
- Could not do it without AJAX



Work with overlapping windows



Grid Development Environment (GDE)



Auto Completion

The screenshot shows a web form titled "Job Services" with a "Generic Job Submission" section. The form includes the following fields and options:

- Submit to:** A dropdown menu currently showing "Hoffman Cluster".
- Job To Submit:** A section header with the instruction "Required entries have **bold** labels."
- Job Name:** A text input field with a placeholder text "Just a name you give".
- Executable:** A text input field with a dropdown menu open, showing a list of executable commands. The first item, "Command/parallel.exe", is highlighted in yellow. The list includes:
 - Command/parallel.exe
 - Command/serial.exe
 - Command/test98.exe
 - Command/testqchem.exe
 - Command/testpar.exe
 - Command/cytosine
 - Command/matlab.exe
- Arguments:** A text input field with a placeholder text "The file name of you".
- Directory:** A text input field with a placeholder text "me used in your job which is not specified as a". Below this field is a list of instructions:
 - Directory is the directory in directory.
 - If Directory is omitted, your
 - If Directory is specified but
- JobType:** A dropdown menu currently showing "Serial".

- Cannot do it without AJAX

Interactive GUI Applications

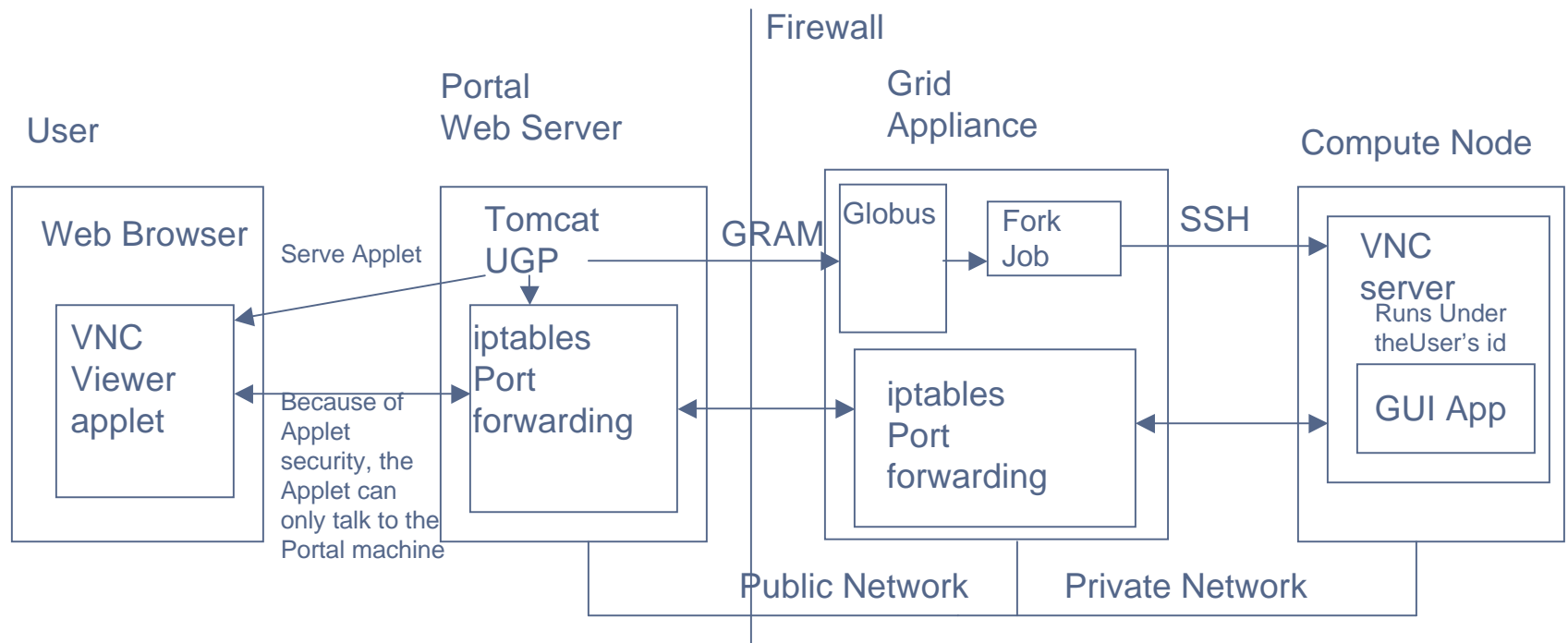
**Run on the cluster compute
nodes**

Interactive Applications via VNC

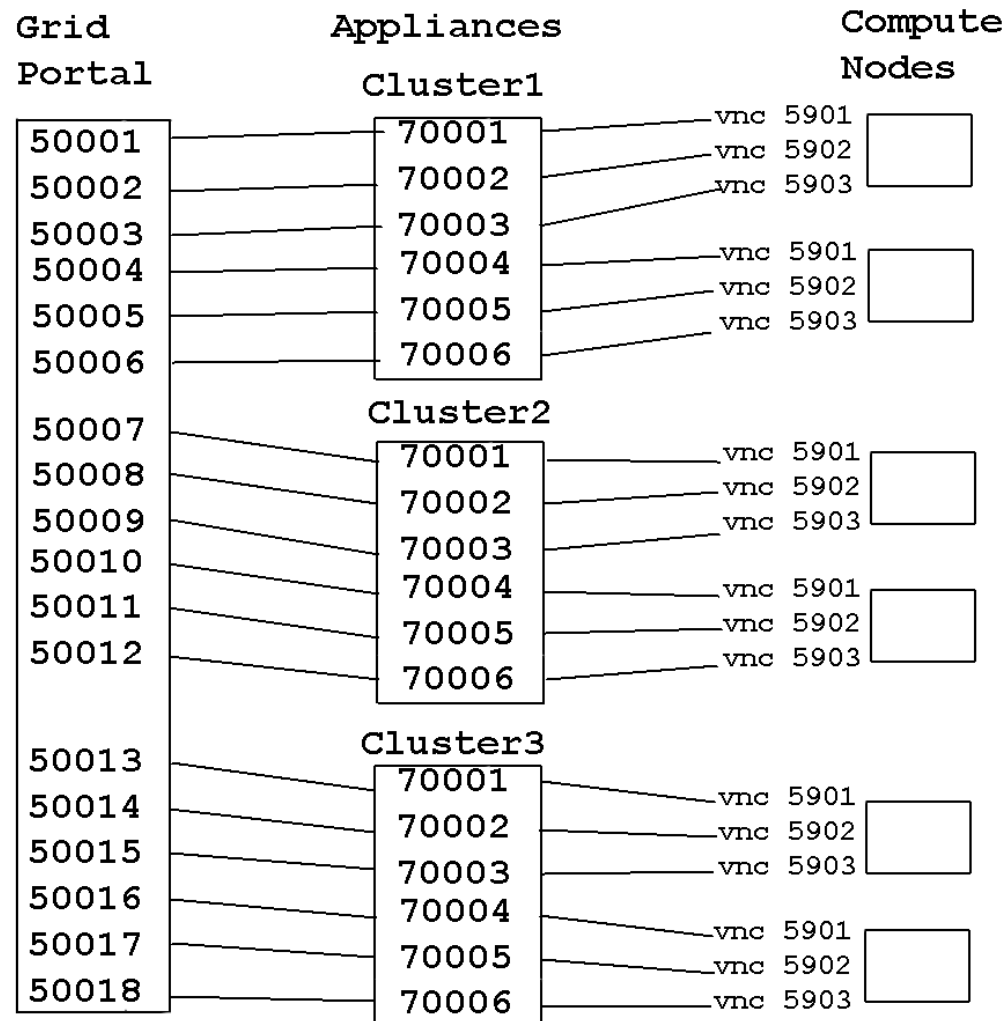
- Previous work in this area:
 - Purdue University's nanoHUB
 - University of Florida's In-VIGO
 - University of Texas Advanced Computer Center (TACC)

Interactive applications via VNC Design Diagram

There is 1 Grid Portal
One Grid Appliance per cluster
Multiple VNC servers can be
Running on an Appliance simultaneously



iptables set up for VNC



Interactive Matlab

The screenshot displays the UCLA Grid Portal interface. On the left, a sidebar lists various interactive applications under the heading "Interactive Application". The "Hoffman Cluster" section includes "Xterm" and "Matlab". The "CNSI Cluster" section includes "Xterm". The "Hydro Cluster" section includes "Xterm". The "Dawson Cluster" section includes "Xterm". Below this list, there is a table with columns "Application Name" and "h". The "Matlab" application is listed. At the bottom of the sidebar, it says "Page 1 out of 1 | 1 |" and "Refresh".

The main window shows the MATLAB 7.4.0 (R2007a) interface. The title bar reads "MATLAB 7.4.0 (R2007a)". The menu bar includes "File", "Edit", "Debug", "Desktop", "Window", and "Help". The toolbar contains icons for file operations and help. The "Current Directory" is set to "/u/home2/joan". The "Shortcuts" section includes "How to Add" and "What's New". The "Current Directory" and "Workspace" panes are visible. The "Command Window" shows the prompt ">>". The "Command History" pane shows the following commands:

```
%-- 8/17/07 7:10 AM --%
%-- 8/17/07 7:23 AM --%
```

A user can have up to n simultaneous interactive sessions.

Reconnect, kill, timeout

The screenshot displays the UCLA Grid Portal interface. On the left, the 'Interactive Applications' section lists available resources:

- Hoffman Cluster**
 - Xterm
 - Matlab
- CNSI Cluster**
 - Xterm
- Hydro Cluster**
 - Xterm
- Dawson Cluster**
 - Xterm

On the right, a terminal window titled 'joan@n22:~' shows the output of the 'ls' command:

```
[joan@n22 ~]$ ls
1globus      ajax          jacobi        May31.txt    snake        snake60
aerosol.hdf  debug.out     June4.txt     May31.xml    snake40      testmovie
[joan@n22 ~]$
```

At the bottom, a table provides details for the active session:

| Application Name | Appliance Name | Portal Port | User Name | Start Time | Kill | Reconnect |
|------------------|---------------------------|-------------|-----------|------------------------------|------|-----------|
| Xterm | hoffmangrid2.ats.ucla.edu | 50001 | joan | Fri Aug 17 07:21:00 PDT 2007 | | |

appForm

Application Form for batch jobs

Purpose of appForm

- For batch job submittal.
- User --> form --> input file for the application.
- Designed for the novice/occasional user of the application.

Goals

- Must Work through the Grid Portal
- Easy to add additional applications

Technologies Used

- XSLT, XML, YUI

Previous Work

- Purdue/nanoHub Rappture
- San Diego Supercomputer Center (SDSC) and National Biomedical Computation Resource (NBCR) Project Gemstone

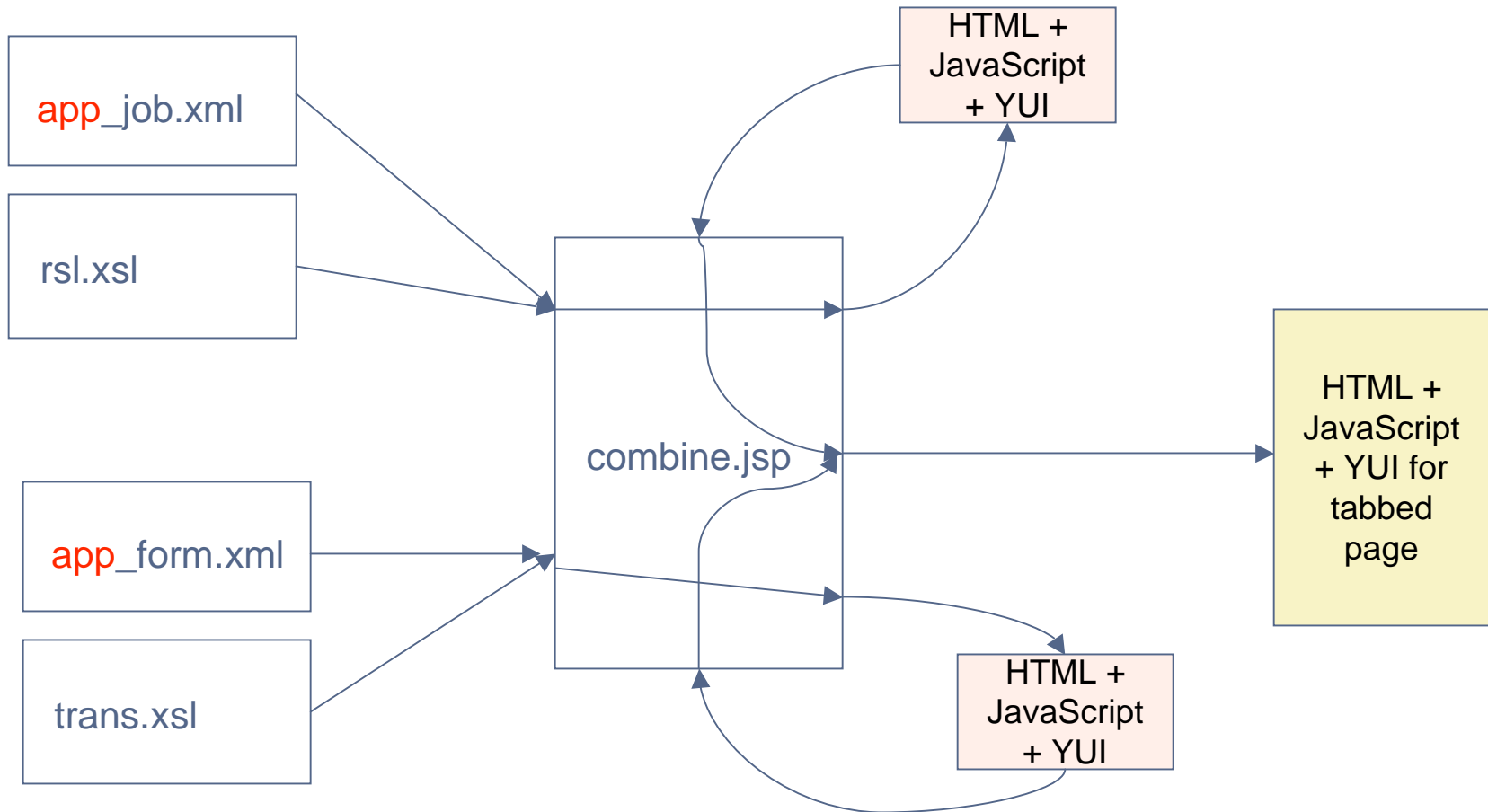
appForm uses YUI tabview

The screenshot displays a web application interface for job submission. On the left is a navigation sidebar with a tree view under 'Application Submission' containing 'Predefined Applications' and a list of application types like 'Hoffman Cluster' (Gaussain03-Parallel, Gaussain03-Serial, XMD-Serial, Mathematica, Q-Chem, Stata, Matlab, Amember8, Amber8-Parallel) and 'CNSI Cluster' (Gaussain03-Serial). The main content area features a YUI tabview with two tabs: 'Job Parameters' (active) and 'Input Generator'. The 'Job Parameters' tab contains a 'Submit Job' button and a form with the following fields and instructions:

- Submit to:** Hoffman Cluster
- Application Description:** Ab initio quantum chemistrypackage Instructions to use arguments, namely the inputfile name and scratch dire added by default. Users need to add only the input file
- Job Name:**
- Executable:**
- Arguments:**
- Directory:**
 - If you specify a directory, your job will be run in that director
 - If you don't specify a directory, your job will run in your hom
 - Unless an absolute path is specified for any file used in the jo directory specified or your home directory, if omitted.
- Directory:**
- Stdin:**
- Job Type:**
- Job Requirements:**
 - For serial jobs, the number of processors must be one.
 - Some schedulers terminate jobs that have reached their ma maximum elapsed time.
- Number of Processors:**
- Max Time (in hours):**
- Max Memory:**

Two tabs, one for GRAM rsl (resource specification language) one for appForm

How appForm Works



`app_job.xml`, `app_form.xml` and `app_form_input.xsl` must be written for each app.

Dynamic HTML used to change the form

1

This screenshot shows the 'Input Generator' tab of the Q-Chem Quantum Chemistry Input Page. The page has a top navigation bar with 'Submit Job', 'Job Parameters', and 'Input Generator' tabs. Below the navigation bar, there is a description of Q-Chem and a link to the Q-Chem Web Site. The main form area contains a 'Title for this run' field with 'Q-Chem' entered. Below this is a section titled 'How the Molecule will be Specified' with instructions on how to provide a molecule description. A dropdown menu labeled 'In the form' is selected. Underneath, there is a 'Molecule Description' section with 'Charge' set to 0 and 'Multiplicity' set to 1. At the bottom, there is a 'Coordinates' field with a placeholder text 'A list of the form: atom x y z'.

2

This screenshot shows the 'Input Generator' tab of the Q-Chem Quantum Chemistry Input Page, but with a different configuration. The top navigation bar is the same. The main form area contains the same 'Title for this run' field with 'Q-Chem' entered. Below this is the 'How the Molecule will be Specified' section, but the dropdown menu is now set to 'From a file'. Underneath, there is a section titled 'Read Molecule Description from a File' with instructions on how to select a file. A 'Molecular Description File Name' field is present, followed by a 'Select File' button.

Input Generator tab can itself be divided into multiple tabbed pages

Tabs superior to pages, the user can go back and fourth between the tabs without loss of input values

YUI Dialogs used for file selection

3

Q-Chem Quantum Chemistry Input Page

Q-Chem is a modern ab initio electronic structure program, that is capable of performing first principles ground and excited states of

Check out the Q-Chem

Save

Load

Main Page REM Optional REM Pa

Title for this run

Q-Chem

How the Molecule

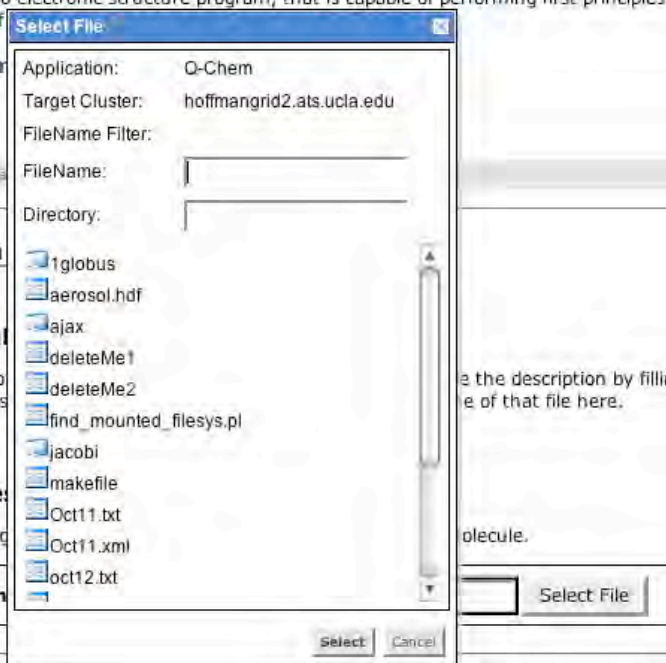
You are required to provide a description of the molecule, or, if your molecule description is already in a file, you can select the file on the target cluster.

From a file

Read Molecule Description

Select the file on the target cluster.

Molecular Description



This layout was accomplished simply by specifying the xml for the form

1

Save Load

Optional Parameter Forms

All displayed options are defaults. Only change if you know what you're changing.

| | |
|---|--|
| Show Self Consistent Field (SCF) Controls: | Show Reaction Path Following Options: |
| Show Density Functional Theory (DFT) Options: | Show NMR Calculation Options: |
| Show Large Molecules Options: | Show Wavefunction Analysis and Molecular Properties Options: |
| Show Correlated Methods Options: | Show Resource Control Options: |
| Show Excited States Options: | Show Miscellaneous Symmetry Options: |
| Show Geometry Optimization Options: | Show Printing Options: |
| Show Vibrational Analysis Options: | |

2

Save Load

Optional Parameter Forms

All displayed options are defaults. Only change if you know what you're changing.

| | |
|---|--|
| Show Self Consistent Field (SCF) Controls: | Show Reaction Path Following Options: |
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| Show Geometry Optimization Options: | Show Printing Options: |
| Show Vibrational Analysis Options: | |

Large Molecule Options

| | | |
|------------------------------------|--|--|
| (cfmm_order) CFMM Order | -1 | Use multiple expansions of order n in CFMM Calculation |
| (grain) Perform CFMM Calculation?: | Program decides best value | CFMM is a useful linear scaling method for very large molecules. |
| (lin_k) Use Link?: | Use Link whenever CFMM is used | |
| (omega) Omega: | | Controls the degree of attenuation of the 2-electron Coulomb operator. Omega = n/1000. |
| (pao_method) PAO | Use FP&D only for local MP2 calculations | Controls the evaluation of polarized atomic orbitals |

Dynamic Visual Feedback

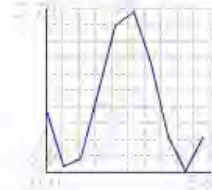
JMathPlot used
via AJAX to
generate the
graphs from the
numbers in the
form

Density Parameters in X

For LINEAR $n(\text{dir}) = 1 + \text{amplitude} * (\text{dir}/\text{scale} - \text{shift})$; For SINE $n(\text{dir}) = 1 + \text{amplitude} * \sin(\text{dir} * \text{scale} - \text{shift})$; For GAUSSIAN $n(\text{dir}) = 1 + \text{amplitude} * \exp(-((\text{dir}-\text{shift})/\text{scale})^2/2.)$

| | | |
|--------------------------|----------------------------------|--|
| Density Amplitude | <input type="text" value="5.0"/> | Amplitude of density compared to uniform background. |
| Density Scale | <input type="text" value="8.0"/> | Scale length for spatial coordinate. |
| Density Shift | <input type="text" value="2.0"/> | Shift of spatial coordinate. |

X Plot

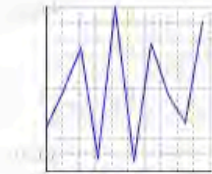


Density Parameters in Y

For LINEAR $n(\text{dir}) = 1 + \text{amplitude} * (\text{dir}/\text{scale} - \text{shift})$; For SINE $n(\text{dir}) = 1 + \text{amplitude} * \sin(\text{dir} * \text{scale} - \text{shift})$; For GAUSSIAN $n(\text{dir}) = 1 + \text{amplitude} * \exp(-((\text{dir}-\text{shift})/\text{scale})^2/2.)$

| | | |
|--------------------------|----------------------------------|--|
| Density Amplitude | <input type="text" value="1.0"/> | Amplitude of density compared to uniform background. |
| Density Scale | <input type="text" value="1.0"/> | Scale length for spatial coordinate. |
| Density Shift | <input type="text" value="5.0"/> | Shift of spatial coordinate. |

Y Plot





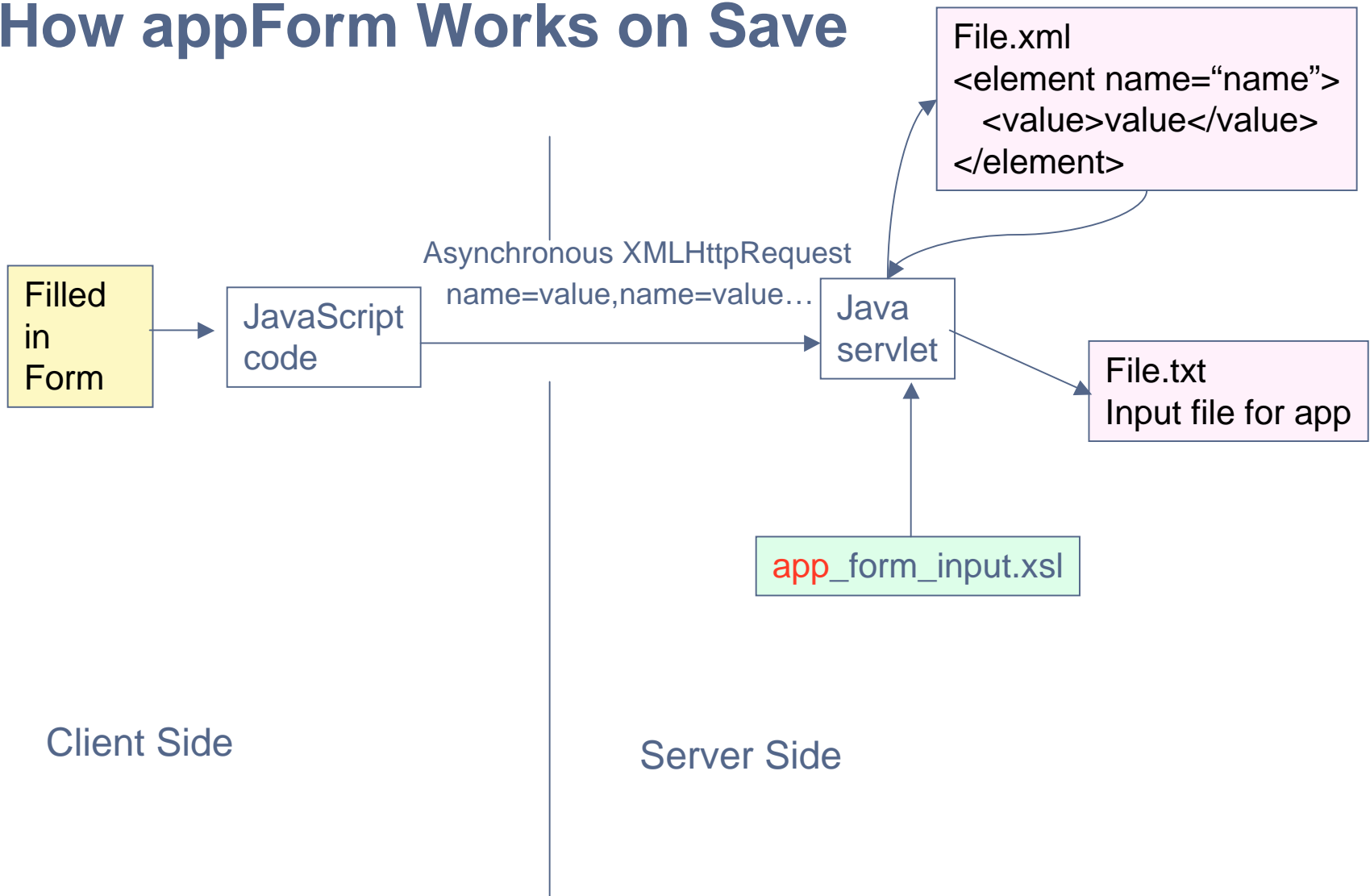
Save Button

saves the input in both .xml application input format.

Load Button

loads the .xml and populates the form.

How appForm Works on Save



To add an application:

1. **Define your job submission Interface via XML** (simple)
2. **Define your input generation interface via XML** (simple but takes doing)
3. **Traslate to the application input your input format via XSLT** (More complicated but can copy and modify existing translator)

Interested in UGP?

UGP documentation, download, wiki
<http://www.ucgrid.org>

Or catch Prakashan, Kejian or myself.