



Activities by Turkish Partners

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Outline

- **Membership in Alliance**

- Middle East Technical University, Ankara
- Extending the Portal with
 - Credential Management Portlet
 - File Management Portlet
- and maintaining Turkish Portal, preparing samples workflows and guideline, data distribution tool for parameter study, etc.

at “<http://portal.grid.org.tr:8080/gridsphere/gridsphere>”

- **Grid Applications by P-GRADE Portal**

- G-PiP: Protein-protein interaction Prediction
 - Bilkent Univ., Ankara + Koc Univ., Istanbul
 - Development on Portal + GUI as a Portlet
- GridAE: Grid-based Artificial Evolution
 - Middle East Technical University, Ankara
 - GUI as a Portlet

- **Training and Dissemination Activities**

- Organized by ULAKBIM



Extending the Portal with Additional Portlets

- **Credential Management Portlet**
 - Credential manager for MyProxy complementing the existing Certificates Portlet
 - Supported MyProxy operations:
 - getting information about a previously stored MyProxy credential
 - changing passphrase of a MyProxy credential
 - removing a MyProxy credential



Credential Management Portlet

A screenshot of a web application window titled "Credential Manager". The interface includes several input fields: "hostname" and "port" at the top, "login" and "password" below them. Each field has an asterisk indicating it is required. Below the input fields is a message: "*: Cannot be left empty." The interface is divided into sections: "Information" (with an "Information" button), "Change password" (with "New Password" and "Confirm Password" fields and a "Change Password" button), and "Destroy" (with a "Destroy" button). At the bottom, there is a "Message:" field with the text "[Press a button.]". A callout box points to the "password" field.

**Provide MyProxy server
access details for the credential
involved:**

- Hostname
- Port number
- User name (from upload)
- Password (from upload)



Credential Management Portlet

A screenshot of the Credential Manager portlet interface. The window title is "Credential Manager". It contains several sections: a form for entering hostname, port, login, and password; an "Information" section with fields for Owner, Desc, Start Date, and End Date; a "Change password" section with "New Password" and "Confirm Password" fields; and a "Destroy" section with a "Destroy" button. A "Message" area at the bottom displays "[Press a button.]". Three red arrows point from text labels below to the "Information", "Change Password", and "Destroy" buttons.

Remove the credential from MyProxy server

Change MyProxy passphrase

Display information about MyProxy credential (owner, start date, end date, description)



Extending the Portal with Additional Portlets

- **File Management Portlet**
 - LCG File Catalog (LFC) Operations through Logical File Name (LFN)
 - listing contents of an LFC Name server
 - browsing directories of an LFC Name server
 - creating a new directory
 - removing a directory/file
 - displaying details (owner-group info, last modification, access rights) of a directory/file
 - changing access rights of a directory/file
 - renaming a directory/file



Extending the Portal with Additional Portlets

- **File Management Portlet**
 - File and Replica Management Operations
 - uploading a (local) file to a storage element
 - downloading a file from a storage element
 - listing replicas of a file, replicating a file to a storage element, deleting a replica of a file



File Management Portlet

- Listing LFC Host(s) of a VO
- Listing contents of an LFC Host

A screenshot of the File Manager portlet interface. The window title is "File Manager". It contains three dropdown menus: "Select Grid:" with "LCG2" selected, "Select VO:" with "trgridb" selected, and "Select LFC Host:" with "lfc.ulakbim.gov.tr" selected. Below the "Select LFC Host:" dropdown is a text input field labeled "or Enter". To the right of each dropdown is a button: "View" for the Grid, "View" for the VO, and "List" for the LFC Host. A "Message: null" status bar is at the bottom. Two red arrows point from the text labels below to the "View" and "List" buttons.

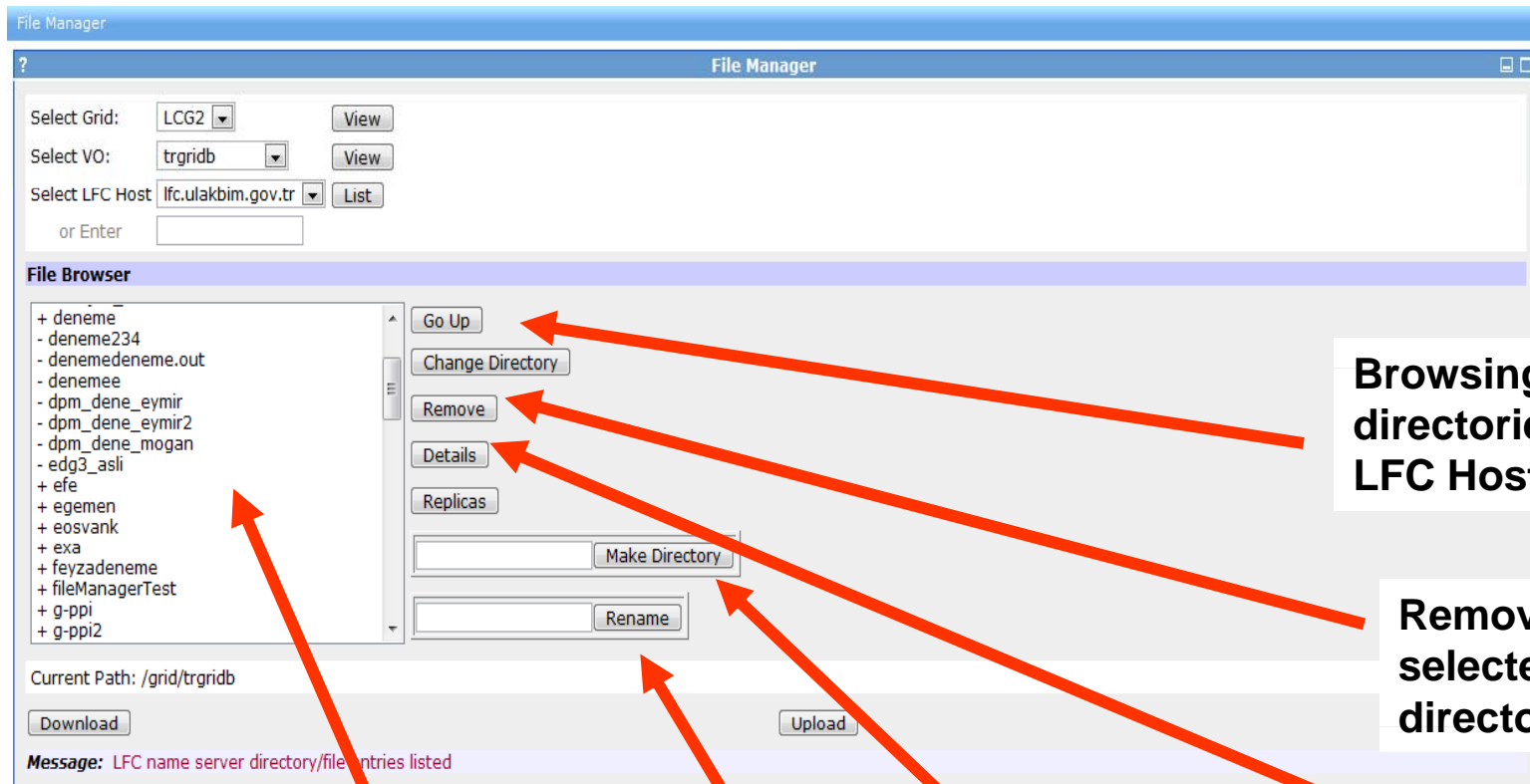
List LFC Host for the selected VO

List LFC directory/file entries for the selected (or entered) LFC Host



File Management Portlet

- LFC operations after listing the contents of an LFC Host



Browsing directories of the LFC Host

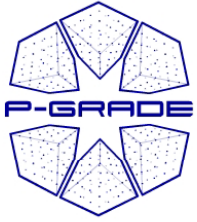
Remove the selected directory/file

Display details of a directory/file

Directory (starting with “+”) and file (with “-”) entries for the LFC host of “trgridb”

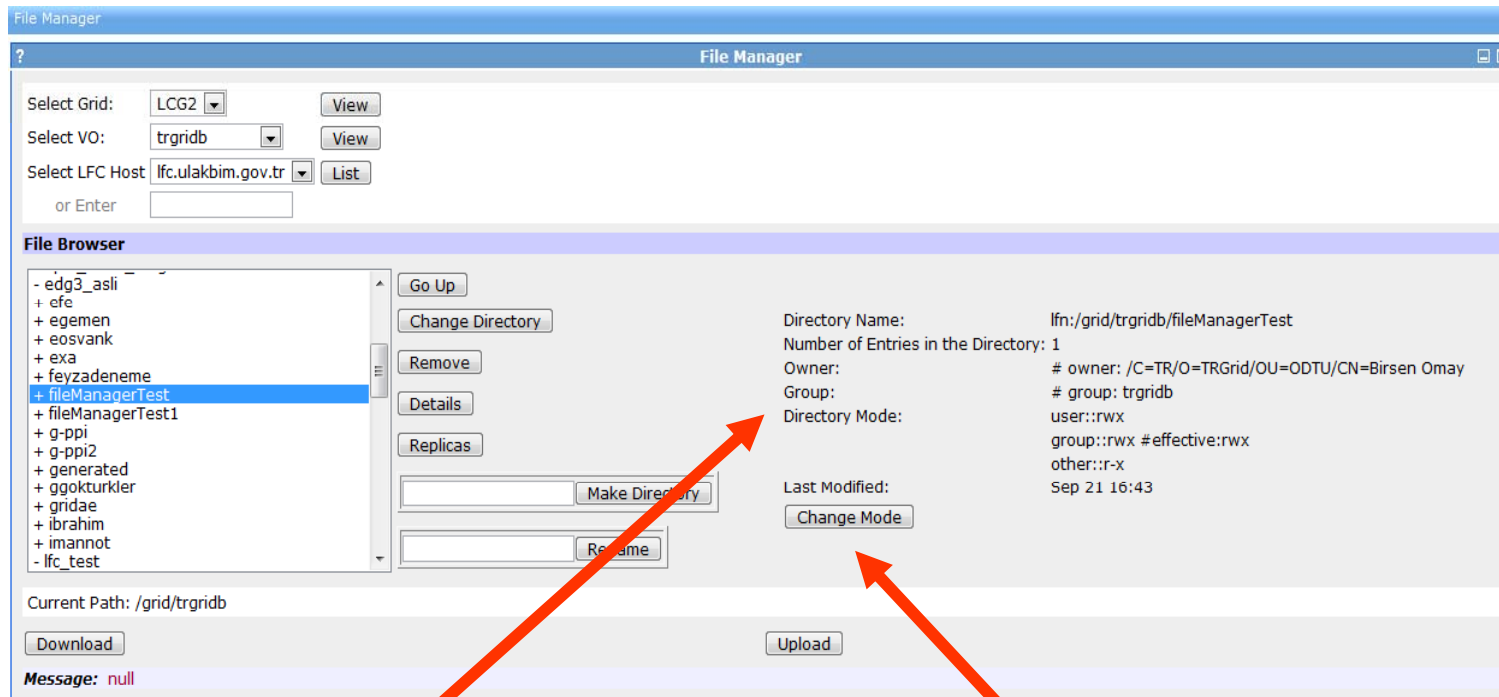
Rename a directory/file

Create a new directory



File Management Portlet

- Displaying details of an LFC item and changing mode of a director/file



Details displayed for the directory
“/grid/trgridb/fileManagerTest”

Change mode of the
directory/file



File Management Portlet

- Uploading a file to the listed LFC directory

A screenshot of the File Manager portlet interface. The window title is "File Manager". The main content area shows a path: "Select a file to upload to: /grid/trgridb/fileManagerTest/test1". Below this, there are several input fields and controls: "Storage Element:" with a dropdown menu showing "se.ulakbim.gov.tr"; "Upload Name:" with an empty text box; a "Browse..." button next to an empty file name field; and an "Upload" button. To the right, under "File Mode", there are three rows of checkboxes: "User:" (Read, Write, Execute, all checked), "Group:" (Read, Write, Execute, Read checked), and "Others:" (Read, Write, Execute, Read checked). A "Back" button is located at the bottom left. A status bar at the bottom shows "Message: null".

The file to be uploaded

Name of the new file
on LFC

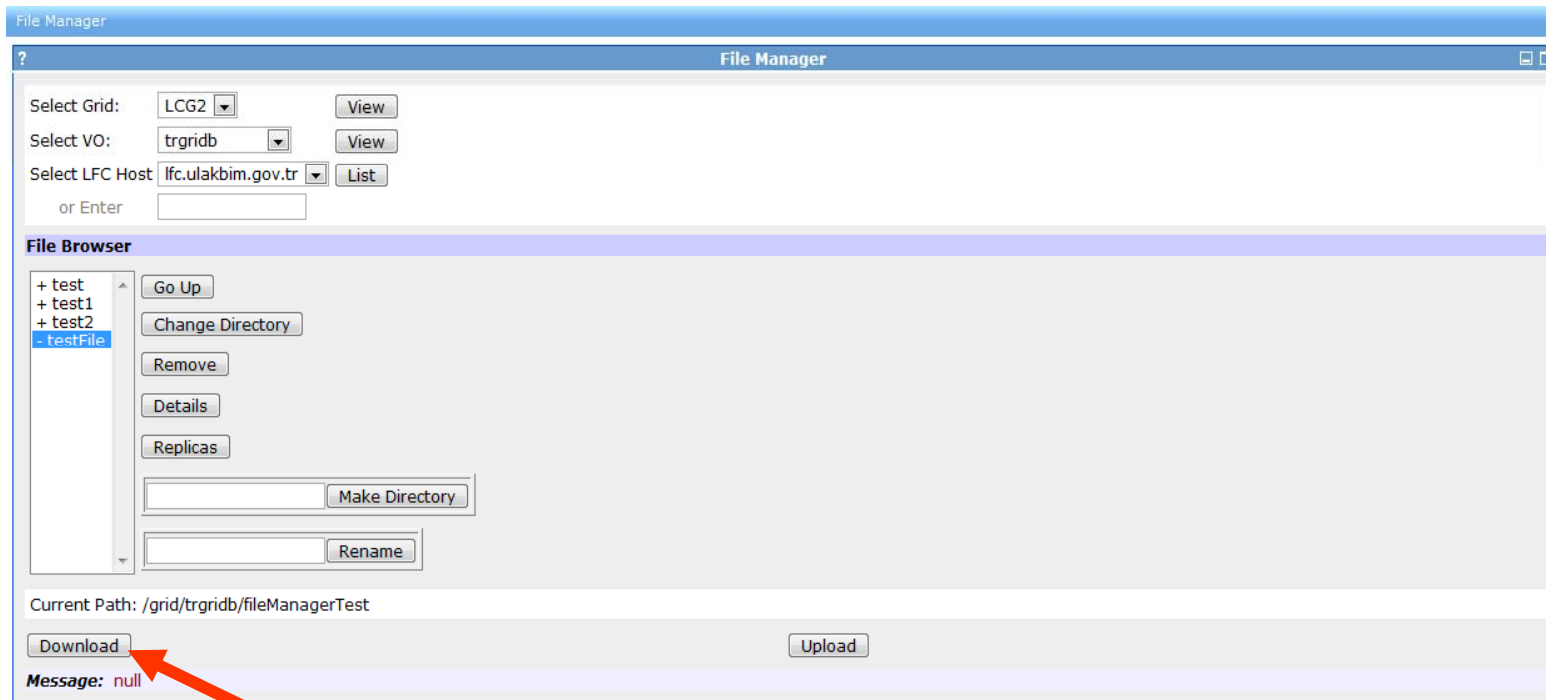
Storage element that the file
is to be uploaded to

Access modes for the
new file



File Management Portlet

- Downloading a file



Download the selected file



File Management Portlet

- Replica Management: Listing replicas of a file, replicating a file and deleting a replica

The screenshot shows the File Manager portlet interface. At the top, the title bar reads "File Manager". Below it, the file path is displayed: "File: /grid/trgridb/fileManagerTest/test1/uploadTest". A section titled "Replicas" contains a text area with the URL: "srm://se.ulakbim.gov.tr/dpm/ulakbim.gov.tr/home/trgridb/generated/2007-09-21/file5bd5b0f1-8d23-4450-b6fe-d3cd866f6431". Below the replicas list are three buttons: "Delete", "Replicate", and "Back". The "Storage Element" dropdown menu is set to "se.ulakbim.gov.tr". At the bottom, a message field shows "Message: null".

Replicas of the file
“/grid/trgridb/fileManagerTest/test1/uploadTest”

Replicate the file on the
selected storage element

Delete the selected replica of the file



G-PiP: Protein-protein interaction Prediction Application

- Discovers protein-to-protein interactions in a protein database given interface templates
- Consists of two computational phases:
 - Surface extraction of input proteins
 - Matching surfaces to left or right partners of an interface template



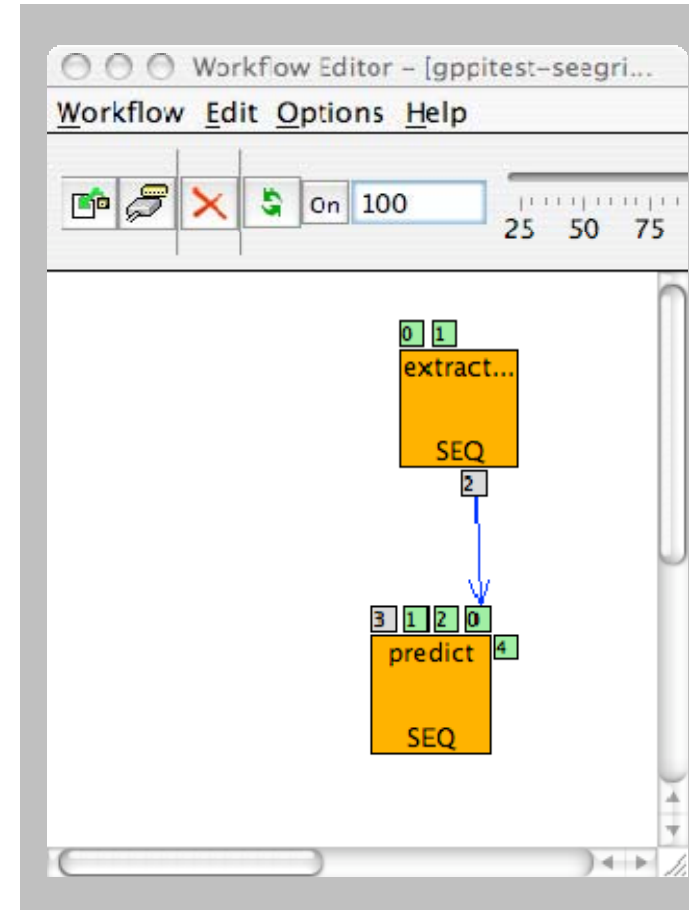
Serial version on P-GRADE Portal

- We took the python MPI code and made a serial version, and split the two phases
- We modified input and output such that we can use remote files within P-GRADE:
 - Input directories are archived as “*tar*”
 - Required linux bioinformatics tools are packed in another archive and supplied as input



Serial version on P-GRADE Portal

- Resulting simple two-stage workflow



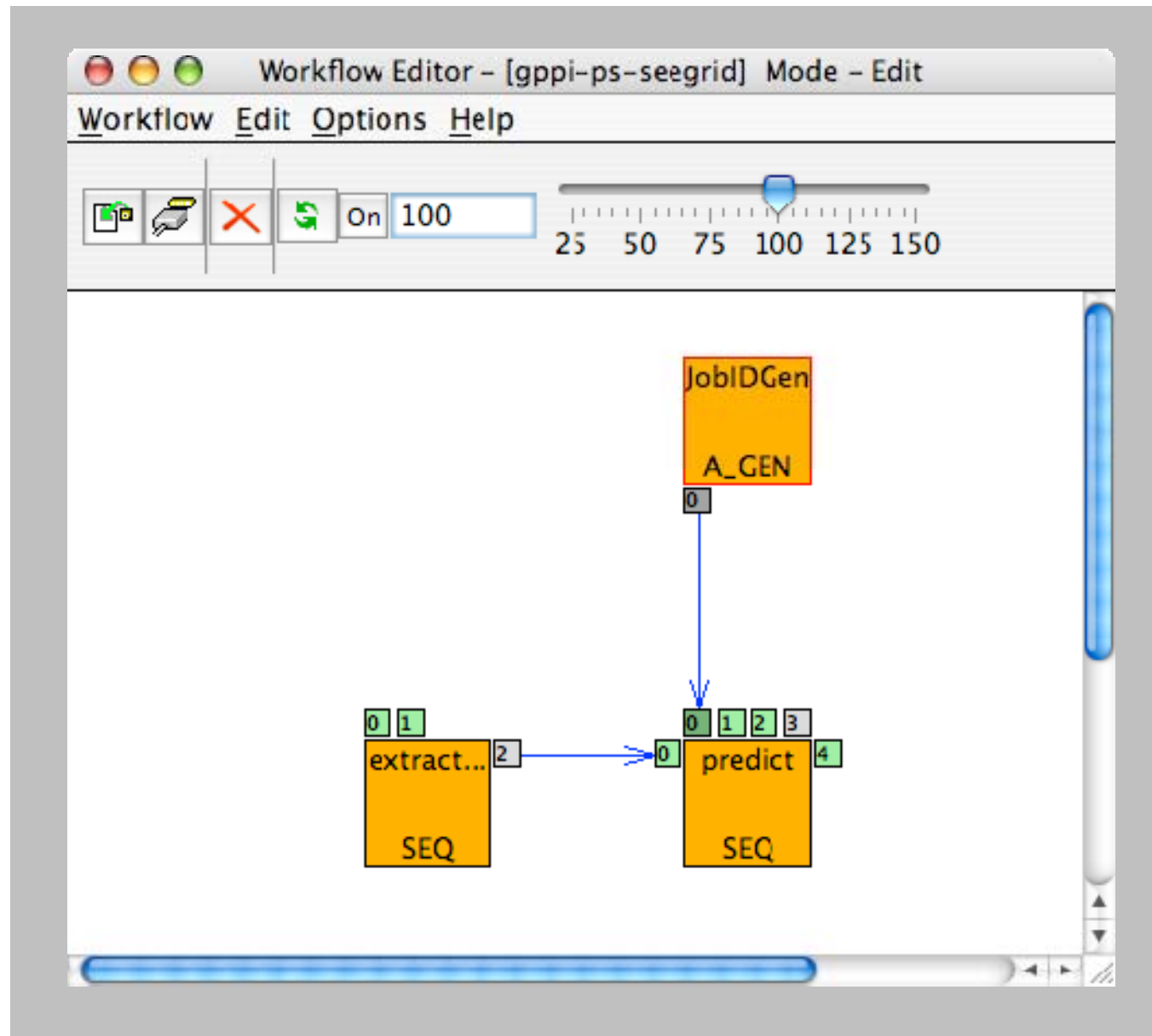


Parameter Study Version

- For parallelism we use the parameter study feature in P-GRADE Portal
- An auto-generator constructs a list of process ID's
- After surface extraction (cheaper), we want to parallelize the matching task
- Each job matches a portion of proteins



PS Workflow





Next version

- The current version is in testing
- We are developing a smarter version
 - A custom generator that will partition the input proteins
 - much less file copy overhead
 - A collector that will construct a single XML file as output



Training and Dissemination

- P-GRADE Portal lecture and hands-on during the Grid training sessions
 - Ankara; July 10, 2007
 - Istanbul; March 16, 2007
 - Ankara; February 13, 2007
 - Ankara; October 26, 2007
- P-GRADE Portal Inductive Presentation during the 2nd Turkish National Grid Workshop
 - Ankara; March 2, 2007