CoaxSim Grid: Developing Scientific Application Portal for a CFD Model

- International collaboration project between NCSA and KISTI -

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Intro.

- Grid Computing: Scalability & Accessibility
- What we have started from;
  - A Computational Fluid Dynamics modeling application
  - TG resources, GT4(pre-web service version)
  - Gridsphere, Grid Portlet (www.gridshpere.org)
  - eAIRS from KISTI
  - Two visiting scholars from KISTI and SWU, Korea
  - Supports from NCSA (MyProxy, Clumon, and other Cyberenvironment teams)
- What we have developed;
  - Customized grid services for the application (Job submission/monitoring, data management, etc.) on top of GridSphere framework and service modules from eAIRS of KISTI
  - CoaxSim Grid portal for the CFD application
  - A community-oriented problem solving environment for a scientific application in the context of grid portal.

eAIRS from KISTI

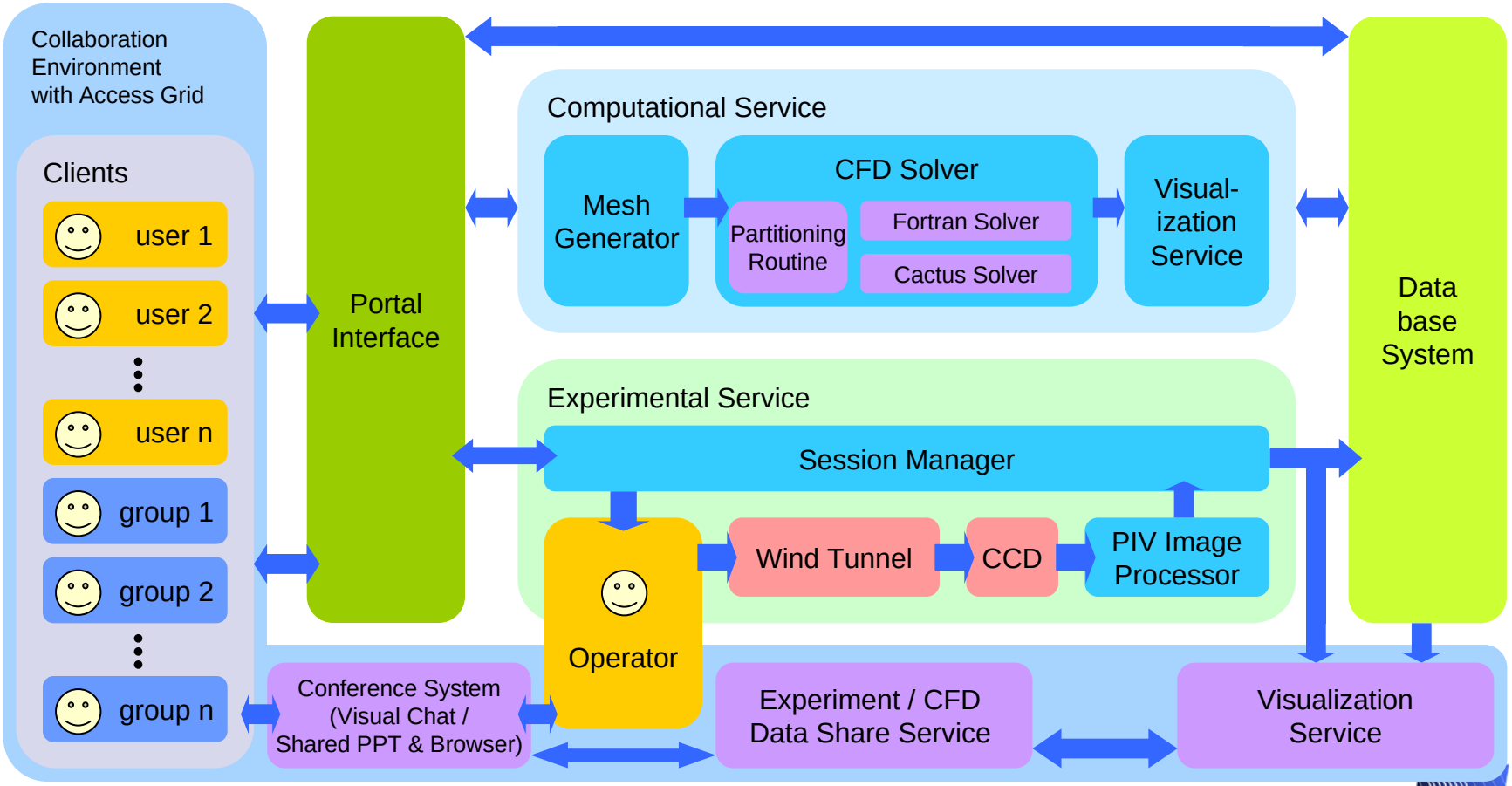
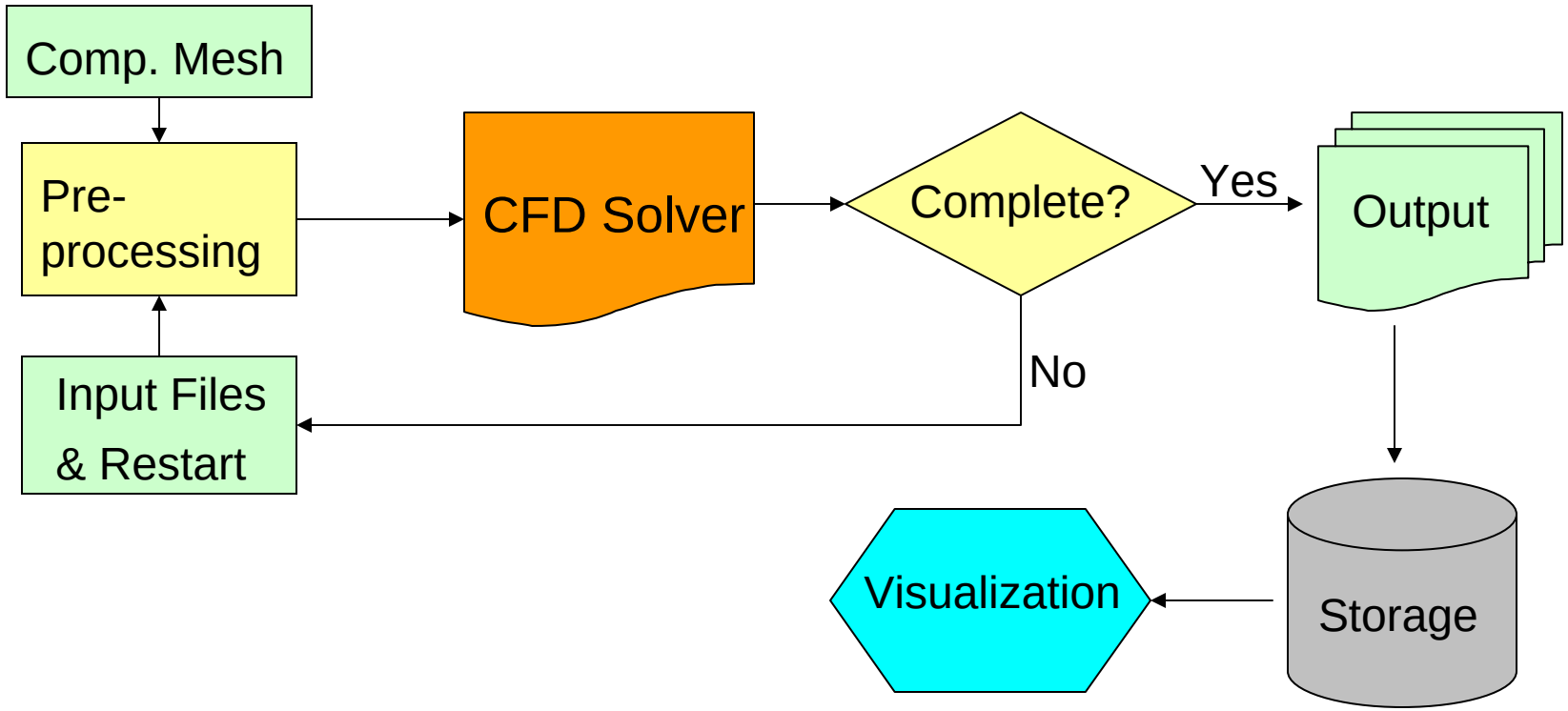


Figure - curtsey of of KISTI

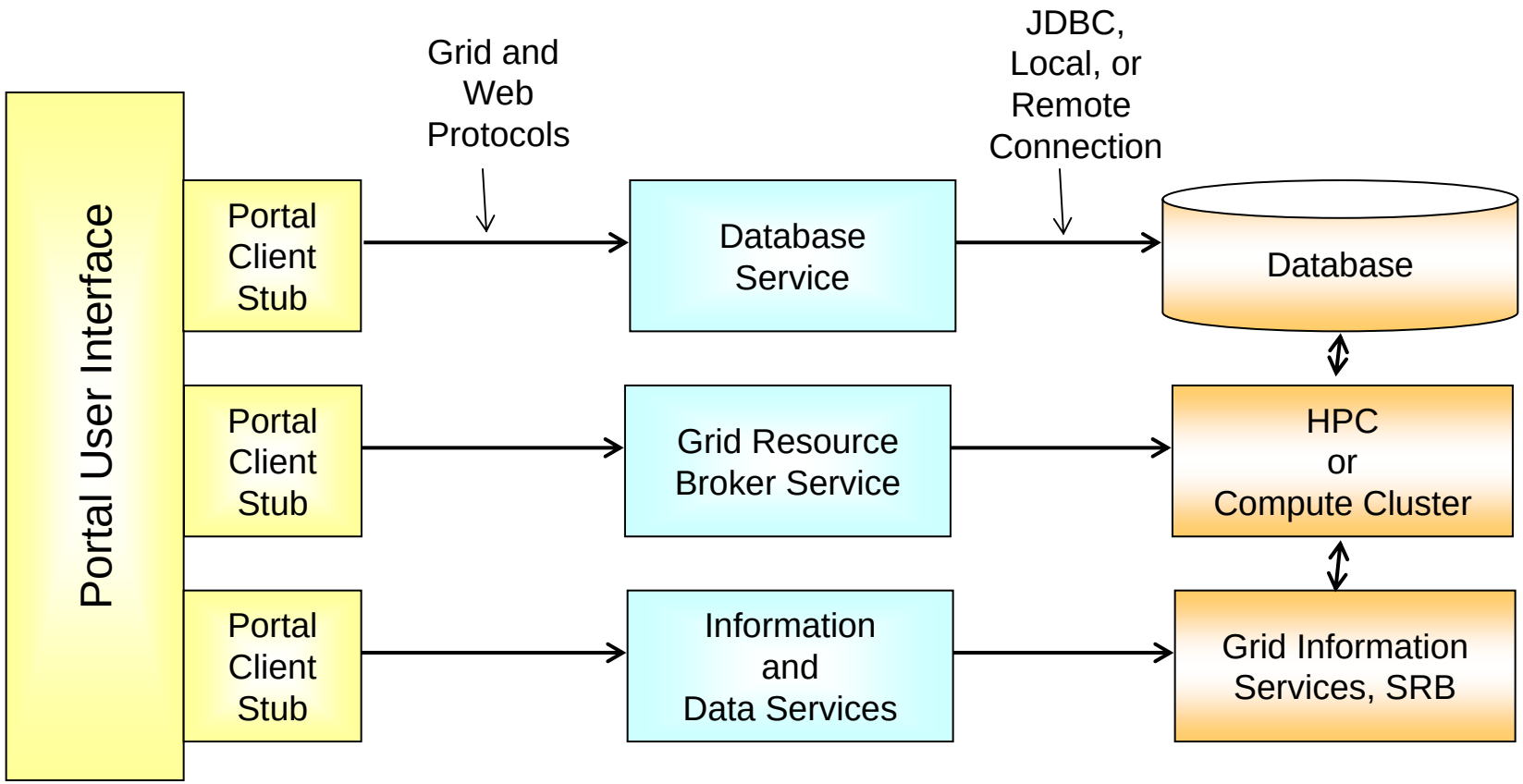
The CFD Application

- Computational Fluid Dynamics Modeling: Investigating combustion instability of injector flow in the liquid rocket engine
- MPI-parallelized using domain decomposition method
- Pre-process/Runs/Post-process/Visualization workflow
- User's requirements for the portal
  - Accessibility to the grid resources from local through the web.
  - Flexibility of managing input/output files
  - Capability on resources selection/registration
  - Clear job submission process and monitoring ability
  - Customized services for automated process of application runs and post processing
  - No worries on credential management, GT compatibility, resources heterogeneity, etc.

Application Scenario for Common CFD numerical modeling



Application Portal Architecture



Three-tiered architecture is accepted as de facto standard for accessing Grid and other services

Figure : curtsey of OGCE consortium

Portal Development

- Gridsphere framework, Grid Portlet w/ GT4
  - Provide basic functions: log-in, credentials, resource registry, file browsing, job submission, status check-up, etc.
  - Not sufficient enough when you want something special for your own application
  - Need to develop customized version of the basic functions
  - Upgraded: credential management, job submission/monitoring
  - Newly developed: application monitoring, file transfer modules

Log-In/Credential Management

- User credential is required for using Grid resources/services
  - The credential is retrieved from Myrpoxy repository
  - Once the initial setup is done, user can retrieve his/her credential with logging into the portal without typing proxy-init command
  - The credential is used for other services such as job submission and file management
- Used default Grid Portlet (v1.3) modules in the Gridsphere frame (2.0.1)
  - Login/Credential management
  - File browsing, upload & download
  - Job submission, status check

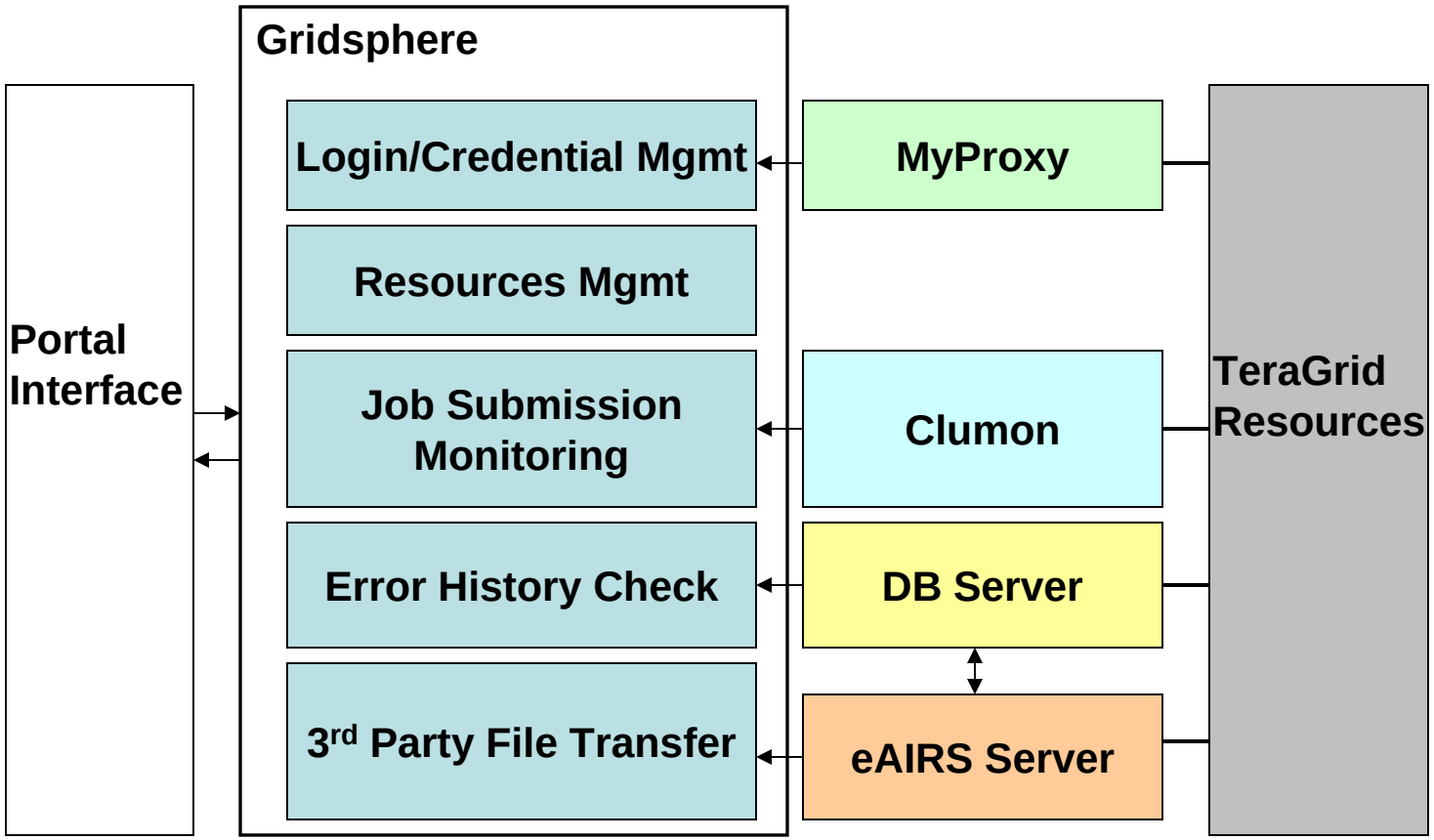
Job Submission/Monitoring Process

- Job Submission
  - Select Grid service/Resource/Application Details
  - GRAM job submission with RSL scripting
  - Generate unique job id and hand it over to Clumon Server, able to track the job status by linking GRAM job number and PBS job id.
- Job Monitoring with Clumon
  - Cluster Monitoring System at NCSA
  - Display the information for the job submitted through the CoaxSim Portal.

Cutomized Portlet Modules for Application

- Real-time error check-up capability
  - Displays residual value along the run time
  - Enable users to check up info on the application side
- Third-party file transfer using gridFTP
  - Hold on to the user credential
  - Output file transfer from TG machine to MSS in background process
  - DB server store meta data and provide them whenever the portal displays info on screen
  - Enable downloading selected files from MSS to local workstation

Current Portal Structure



Demo

Special Features

- Automatic credential update on the portal
- Updated Job Submission Interface
- Job monitoring with Clumon (GRAM-PBS connection)
- Real-time error check-up capability on portal
- Output data file management with 3rd-party file transfer using gridFTP module
- Customized UI for user-oriented usability

Conclusion

- A scientific application portal has been developed: Numerical CFD model + Gridsphere/Portlet + eAIRS from KISTI.
- NCSA-KISTI international collaboration will benefit both sides mutually by further developing/upgrading the portal project.
- A community-oriented, application-specific portal still demands lots of customizing, programming, and supports.
- Things are getting better, and more standardized technologies are blooming.
- Expecting another big learning curve once the WS-GT4 rolls out.

Lessons Learned, Future Work

- Need active merging of available technology : PURSE, MyProxy, Trebuchet, etc.
- Still required lots of work for bypassing problems caused by “being-developed or being-implemented, being-tested” services (MDS4, WS-GT4, etc)
- File management challenge remains.
- Better design is desired for a GENERIC 3rd-party file transfer module.