An Integrated Scientific Experiment Framework for Numerical Analysis in e-Science Environment

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***Abstract*—The analytical experiments for numerical analysis lead a sequence of complex scientific computations composing of numerical equations and require enormous computing resources with appropriate management tools. Currently most studies on e-Science environments for numerical studies focus on solving specific problems to drag out the best performance of matters and have less interest in providing a uniform framework to apply for diverse numerical domains, especially for fluid dynamics. This paper presents an integrated e-Science experiment framework which could be easily applicable to solve various numerical analyses in fluid dynamics. As a proof-of-concept, an integrated e-Science framework with diverse numerical analyses has been designed and implemented over UNICORE that runs over grid computing environment.**

***Keywords*-e-Science; PSE; scientific numerical analysis; UNICORE**

I. Introduction

The experimentation in numerical analysis needs highly efficient and enormous computational resources because these experiments are composed of computations of complicated numerical equations and computation-intensive operations. Many studies and developments have been proposed to support the various scientific computational applications in e-Science environments. But, already developed frameworks support e-Science environment only for analyzing specific computational model [1][2][3][4][5]. By constructing research environments which is defined per-application in specific e-Science environment, it is difficult to conduct research efficiently and access heterogeneous resource in absence of common interfaces even though they have similar processes. Also, as proceeding e-Science developments, common interfaces, and integrated environments are required to provide various analyze techniques to research and reuse it with demands of other applications requirements. Our research has focused on the integrated scientific experimental environment for numerical analysis, especially in fluid dynamics.

UNICORE (Uniform Interface to COmputing REsources) [6] has been developed for an integrated common environment. However, adding specific applications to UNICORE is difficult to general scientists or researchers because they have to develop interfaces for each their experiments using GridBean [7].

On developing a Problem Solving Environment (PSE) for numerical applications in fluid dynamics, we are principally concerned with the following requirements:

- Support research execution in diverse computing environment: it can be executed in personal computer or grid environments.
- Support an independent experimental environment on each research domain.
- Support pre-process for generating input files of numerical analysis.
- Support post-process for visualizing analyzed results.

In this paper, we describe a design and implementation of the PSE that aims to provide a numerical study environment that requires seamless access into grid resources through a common interface for diverse domains in fluid dynamics. To support scientific computational application, we developed a common and integrated e-Science environment based on UNICORE Rich Client supporting a user interface to each application using GridBean. In a precedent study [8], we implemented just one application in a domain, i.e. 1D Euler equation in compressible flows. It is hard to say as an integrated framework. So, in this work, we expand our target range of domains as compressible flows, turbulent flows and multiphase flows in fluid dynamics.

The rest of the paper is organized as follows. In Section 2, related works are reviewed. In Section 3, an execution scenario for numerical studies and design of PSE framework architecture are described. The implementation of PSE framework is presented in Section 4. Finally, conclusion and future work are stated in Section 5.

II. Related Work

In this section we shall briefly present some approaches that are representative for the areas of grid computing environment and e-Science projects which are based on Eclipse.

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A variety of scientific computational applications for numerical study have been developed, like FLOWGRID [5], and they have been executed on grid environment with functions of managing and monitoring computational jobs as well as supporting simulations. FLOWGRID is a grid application for solving Computational Fluid Dynamics (CFD) problems and FlowServe middleware [9] is provided for interactions on different interfaces. FLOWGRID is carried out targeting the specialized engineers only and limited in terms of extensibility.

One of the most well-known Eclipse-based e-Science environments is g-Eclipse [10], which is an integrated workbench framework to access the power of existing grid infrastructures. The g-Eclipse supports connectors between a user environment and many different grid middlewares (such as gLite, UNICORE, Globus toolkit) and provides tools to customize users experimental environments. However, g-Eclipse included as a plugin to existing eclipse IDE (Integrated Development Environment), is uncomfortable with complicated interfaces because there exists the irrelevance of the functions to users experimentations.

UNICORE [6] is a Grid computing technology providing grid software that combines resources of supercomputer centers and makes them available through the Internet. Within the UNICORE environment the user has a convenient way of using distributed computing resources without having to learn site or system specifics by a seamless way.

Also the UNICORE supports various clients for jobs creation, submission, and monitoring, both graphical and command-line oriented. The graphical UNICORE Rich Client referred to as URC used in our framework offers graphical editors for setting up job descriptions. Instead of editing text-based job descriptions, the user is provided high level interfaces which are tailored to the applications what he wants to execute on remote systems. And these graphical interfaces are developed using GridBean which provides pluggable interfaces.

Our framework is specifically supported in the UNICORE Rich client (URC) as adding scientific domain-specific plugins. Besides, the advantage of adopting open standards in UNICORE 6 allows for the seamless use of UNICORE components by other technologies.

III. Design of Integrated Scientific Experiment Framework

A. Framework Scenario for numerical study

A numerical analysis environment for target domains such as compressible flows, turbulent flows and multiphase flows require pre-process, simulation process, and post-process. Figure 1 shows a scenario of using our PSE framework. At first, the user installs our PSE program on PC and then selects a method of numerical studies to be performed. In pre-process step, the user can generate or upload input files that are proper for the selected numerical study. When it is finished, in simulation process step, the user configures solving conditions such as experiment method. The user selects resource to submit the job and then a JSDL (Job Submission Description Language) file which specified by GridBean model about a job definition and attributes will be submitted and executed at the previously selected resource. If the job execution is finished, the user can check whether the execution is finished, and then he can download output files. As a post-process step, graphical view is also offered for output files which require visualization.

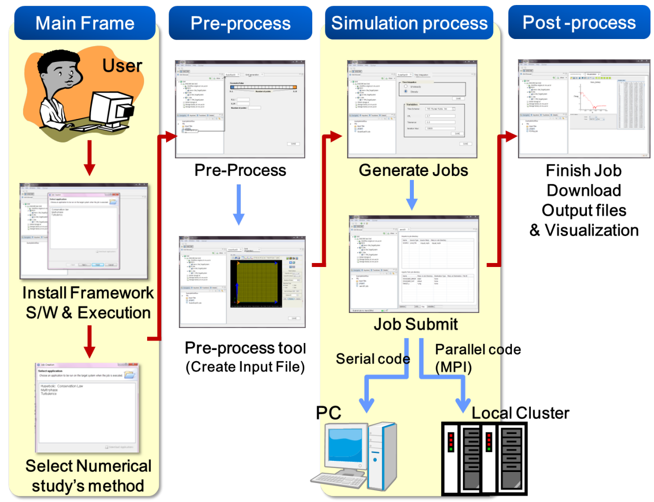

Figure 1. Scenario for numerical study

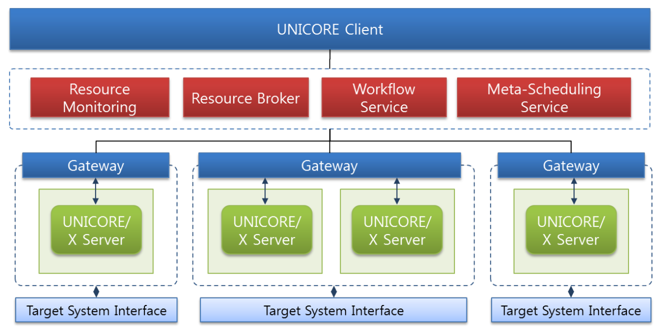

Figure 2. Framework Architecture

B. Integrated Scientific Experiment Framework Architecture

The overall architecture of the framework based on UNICORE is depicted in Figure 2. If the user submits a job or a workflow for specific application using PSE framework interfaces based on URC, Resource Broker receives the requests from UNICORE Client and collects the necessary information (such as application name, resource information; number of nodes, number of cores) through Resource Monitoring to choose the set of acceptable machines. If well suited resource (s) is selected, the job with user information is authenticated by Gateway and forwarded to web services

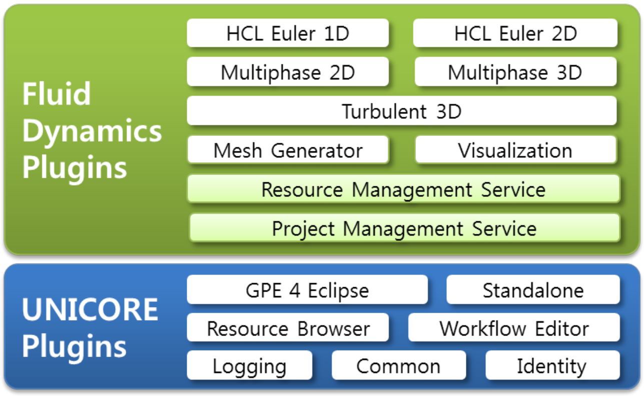

Figure 3. Client Architecture

interfaces offered by UNICORE/X server and executes it on Target System Interface. The workflow job is supported by Workflow Service module that interacts with Resource Broker and Meta-Scheduling Service. The Meta-Scheduling Service collects information across all pre-selected resources about availability, user policies, and cost parameters.

Figure 3 shows entire plugins architecture in client-side, it is made up of two layers, the one is basic UNICORE plugins that constitute the core of the URC and the other is Fluid Dynamics plugins that consist of applications for three research domains. Descriptions of basic UNICORE plugins can be found in other publication [11].

The following list contains short descriptions of Fluid Dynamics Plugins about what each plugin does:

- HCL Euler 1D / HCL Euler 2D: Plugins for the numerical study of compressible flows.
- Multiphase 2D / Multiphase 3D: Plugins for the numerical study of multiphase flows.
- Turbulent 3D: A plugin for the numerical study of turbulent flows.
- Mesh Generator: A plugin for generating input files and setting up boundary conditions of pre-processing that may be used for the applications.
- Visualization: A plugin for post-process to visualize the experiment results.
- Resource Management Service: A module to add job properties for specific application and provides filters that find resources with certain types or attributes.
- Project Management Service: A module to management history of experiments such as execution information, simulation results, errors, log files and user descriptions.

IV. Implementation

To implement user interfaces of PSE in three other domains, we developed applications specific plugins per each application using GridBean that is presented above Section 3. Within these plugins, components are organized

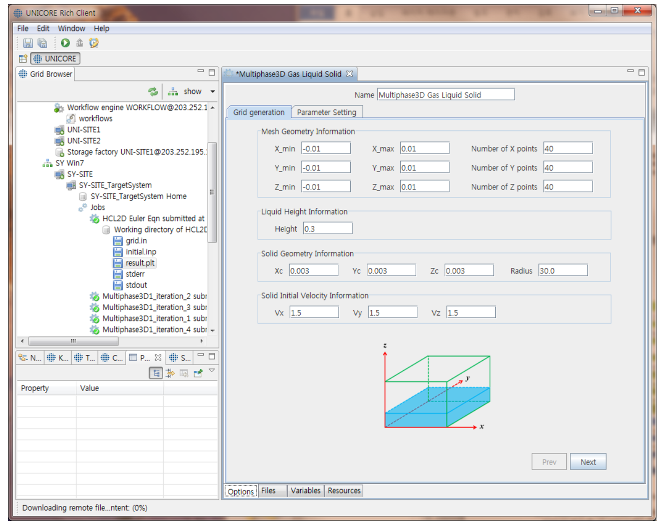

Figure 4. An Integrated Scientific Experiment Tool

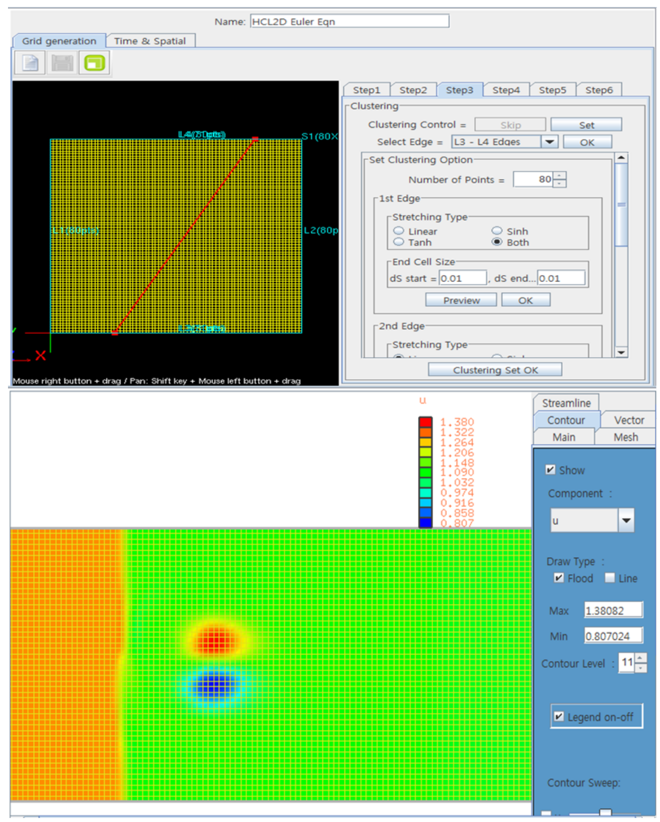

Figure 5. A Mesh Generator and a Visualization Tool

dynamically by providing functions to control events of the experiment. For a specific example of user interfaces, to execute the Multiphase 3D numerical study of the multiphase flows is shown in Figure 4. Figure 5 depicts a mesh generator for pre-processing and a visualization tool for post-process in HCL 2D Euler numerical study. Moreover, with the aim

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of an integrated workbench framework, applications in three other domains can be accessed through a uniform manner within a PSE.

Basically user interfaces of the framework consist of one or more plugin modules and one data model depends on each of numerical studies method. But, there are a lot of methods and parameters which need to experiment.

For users convenience, we developed interface to be organized dynamically by controlling event about the experiment method selection. To dynamically configure parameters when experimental methods are selected in each application, we classified parameters as commonly applied ones and additional ones instead of defining a set of parameters in each experimental method. Defining parameter sets like this, makes management of parameters more efficient and accurate.

In case of middleware, we used most of UNICORE, and we modified IDB (Incarnation DB) which saved applications information such as name, version, location of an executable file, and parameters required for the job execution. Also, in order to provide resources among authorized users only, we generated authorization keys for each application and its information is managed through XUUDB.

V. Conclusion and Future Work

In this paper, we presented a design of the integrated scientific experiment framework supporting numerical analysis in fluid dynamics within e-Science environments. The framework adopting three numerical analysis applications is implemented as a proof-of-concept within the Eclipse-based UNICORE Rich Client. The implementation contains a mechanism to define sequences of simulations and the framework can conveniently add other numerical analysis models. A common execution environment to support various applications that are in diverse domains is important. Hence, this framework is expected to improve their experiments efficiency, convenience and reusability of technologies.

In the future, we will expand our framework to support more complex experiments and more diverse numerical study methods. Also we plan to develop a resource selection algorithm reflecting requirements of application and properties of resources.

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