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EDISON 플랫폼 시뮬레이션 시스템에서 전처리 및 후처리기 연계를 위한 인터페이스 개발☆

Interface Development for Pre and Post processor on EDISON Platform Simulation System

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ABSTRACT

The EDISON is a platform that supports numerical analysis for problem solving in computational science and engineering. We provide a cloud service for users, and provide an environment to access and execution of the simulation service on the web. For now, the EDISON platform provides simulation services for eight applied field on computational science engineering. Users can check the numerical analysis result by web in the computational science and engineering platform. In addition, various services such as community activity with other researchers, and the configuration of simulation environment by user 's needs can be provided. A representative service of the EDISON platform is a web-based simulation service that performs numerical analysis for problem solving of various computational science and engineering. Currently, EDISON platform provides workbench simulation service. It is the web-based simulation execution environment, and result analysis to provide simulation regardless of various personal computing resource or environment in each numerical analysis. In this paper, we build an interface for pre and post processor that can be used in conjunction with the workbench-based simulation service provided by EDISON platform. We provide a development environment with interface that is implemented by applying a pre and post processor optimized for the simulation service. According to simulation and execution are performed by linking the new workbench-based simulation service to the pre and post processor.

☞ 주제어 : 계산과학공학, 인터페이스, 전처리기, 후처리기, 시뮬레이션
☞ keyword : Computational Science and Engineering, Interface, Pre Processor, Post Processor, Simulation

1. Introduction

The EDISON platform[8-11] is a web-based platform that supports simulation and numerical analysis of problems in computational science and engineering. We have built a variety of simulation analysis programs that can not be support in personal computing resources or environments. EDISON platform provides a cloud computing based simulation services that users can easily access and use. One of the main services of EDIOSN platform is the workbench simulation service that can provide various combinations of web based simulation services to excute computational science and engineering simulation. In order to execute a single simulation, various services should be provided as combination, and a simulation environment optimized for the user should be configured and serviced according to the characteristics of each simulation on the workbench based simulation service[7][8].

Nowadays, EDISON platform service provides workbench service for configuring and providing simulation environment of various users. It works with workbench-based simulation service for interlocking of pre and post processor which is specialized each computaional science simuatlion is used as a applied disciplines. It is provided by implementing the interface for simulation environment to interlock workbench simulation service with pre and post processor. Therefore, an environment was provided to calculate simulation pre and

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and post processor of simulation. The development environment of simulation platform is connected development a module for users to provide a simulation service in conjunction with the workbench service. By providing an interface for inter-networking of analytical simulation to solve each computational science engineering problem. It is possible to provide simulation service in real time that interlock pre and post processor as a web-based service. The pre and post processor modules for executing the simulation can share the data throughout the simulation with a simple implementation through the interface provided by the EDSION platform. The visualization of the characterization data of each applied disciplines simulation are constructed and implemented with the interface for pre and post processor module linkage.

When running simulations in computational science and engineering on the EDISON platform through the interface of workbench-basd simulation service, the user can apply various pre and post processor algorithms to the workbench simulation tool for execution. This means that it is possible to provide a suitable simulation environment for scientific simulation developers. That can link optimized pre and post processors to each simulation and execute each simulation. Therefore, it is advantageous to provide development environment to simulation service as a web-based platform according to the demand and supply of various users.

In this paper, we build an interface that could be linkaged to workbench-based simulation service with pre and post processor. That can be used in conjunction with the workbench-based simulation service provided by EDISON platform. Built interface provide a service environment that is implemented by applying a pre and post processor optimized for the simulation environment. In addition, the simulation is executed and analyzed by linking the configuring workbench-based simulation service with the pre and post processor in real time.

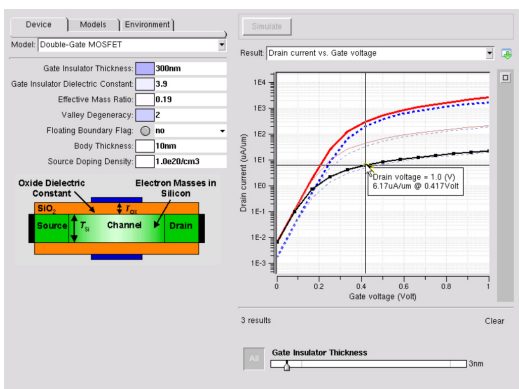
2. EDISON Platform

2.1 Platform for computational Science and Engineering

Computational science and engineering (CSE) is a multidisciplinary field lying at the intersection of mathematics and statistics, computer science, and core disciplines of science and engineering [1, 2].

CSE closes the centuriesold gap between theory and experiment by providing technology that converts theoretical models into predictive simulations. It creates a systematic method to integrate experimental data with algorithmic models. CSE has become the essential driving force for progress in science when classical experiments or conventional theory reach their limits [2].

The HUBzero cyberinfrastructure lets scientific researchers work together online to develop simulation and modeling tools. Other researchers can then access the resulting tools using an ordinary Web browser and launch simulation runs on the national Grid infrastructure, without having to download or compile any code. HUBzero use has expanded to support a growing number of hubs for pharmaceutical engineering (pharmaHUB.org), heat transfer (thermalHUB.org), microelectromechanical systems (memsHUB.org), healthcare (IndianaCTSI.org), cancer care (cceHUB.org), engineering education (globalHUB.org), and nanotechnology (nanoHUB.org) [3]. nanoHUB.org served more than 56,000 users from 172 countries [4, 6].

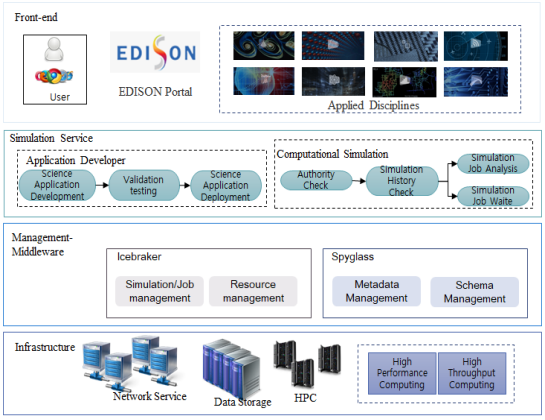


(Figure 1) nanoHUB FETtoy tool [5]

2.2 EDISON Platform

The EDSION platform is a web-based platform that supports simulation and numerical analysis of problems in computational science and engineering. The EDISON

platform now has a Science Apps for performing computational science engineering simulation in eight specialized areas. A variety of libraries are provided internally to run simulations on the web, and various services are provided for registration of Science Apps for simulation. The overall system architecture of the EDISON platform is shown in Figure 2 [8-11].



(Figure 2) EDISON Platform Architecture

Users of the EDISON platform can run registered science apps and share results regardless of the internal simulation runs. Although the process of developing and registering a science app in performing various simulations is procedural, the characterization of simulation execution to solve each computational science and engineering problem is not reflected in the workbench based simulation system. Therefore, there is a growing demand for pre and post processing that can interact with simulation services to analyze the data and the intent of numerical analysis programs to solve computational science and engineering problems.

The workbench based simulation system provides services that can be integrated and managed while segmenting the services of the required pre and post processor modules according to each simulation procedure for performing the simulation. Then, the developer can develop a pre and post processor module suitable for various simulations and connect them to the simulation service.

3. Configuration Simulation with Pre and Post Processor

3.1 EDISON Workbench-based Simulation

The EDSION workbench-based simulation system provides users with various web-based simulation services. It is possible to freely use services that support various simulation processes that require numerical analysis by connecting to the EDISON portal and executing computational science and engineering simulation.

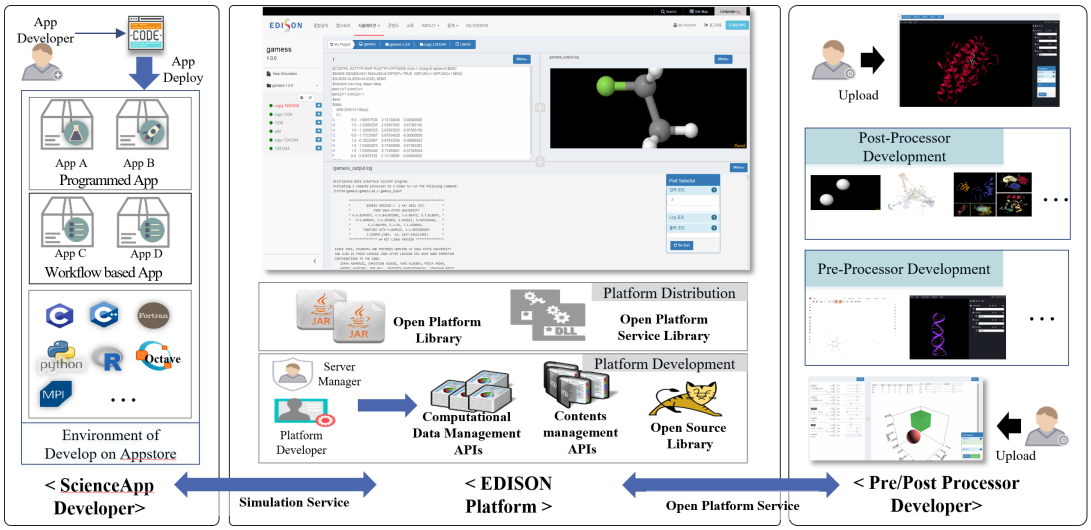
The services provided by the EDSION workbench can be classified into three broad categories.

First, as a simulation job management for each user, it is a function to create or delete a history of a simulation job executed by a user. The second is a preprocessing function to execute the simulation. It includes the ability to enter or edit a pre processing data before running the simulation. The third is a post processing service that can confirm and analyze the results of the completed simulation result data.

As mentioned above, the workbench simulation service provides users with the ability to run and manage computational science engineering simulations. Although the pre and post processor for basic simulation execution is provided, the environment required for each simulation differs for each simulation which configures specialized each simualtion analysis for computation science simulation with pre and post processor. Therefore, we provide simulation interface and communicating with workbench-based simulation service for simulation and data analysis service.

3.2 The Workbench based Development Process

The EDSION workbench simulation system is divided into three parts: a developer of the Science App who perform numerical analysis in computational science and engineering, a platform developer, and a pre and post processor developer. The EDISON platform provides interfaces for registering and developing necessary pre and post processors which be connected with science applications registration and simulation environments. As well as developing platform for executing simulation and delivering the results of science



(Figure 3) Workbench Based Simulation System Architecture[7]

app's simulation on computational science and engineering.

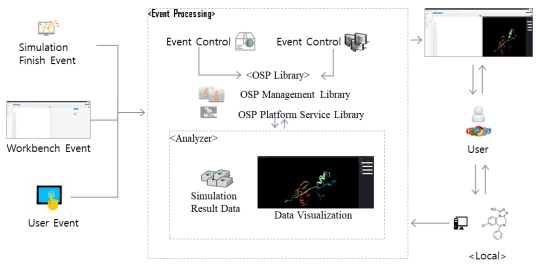
Respectively, we defined a procedure to provide a more optimized environment to simulate on the web through linkage between pre processor and post processor of each science app, and provided workbench-based simulation service to users.

As shown in Figure 3, the workbench-based simulation service is serviced by the entire EDISON platform can provide users with simulation environments built by various developers. We provide the necessary libraries and interfaces for developer of pre and post processor associated with workbench-based simulation. We also have defined procedures to be applied automatically to the workbench simulation environment [7, 8].

3.3 Coupling Process of Pre and Post Processor with Simulation Service

The process of the computational science and engineering simulation service configuration, includes conjunction with the pre and post processor in executing, using the EDISON platform is shown in Fig 4.

When a user runs a simulation on the EDSION platform, the work of each simulation is processed and the final simulation results can be passed back to the user. The pre



(Figure 4) Processing of Simulation on EDISON Platform

and post processor developed in this process is linked to the EDISON workbench-based simulation service based on event processing.

First, the data is edited according to the procedures and data characteristics of the internal module, and optimized user input and preprocessing are performed. When the preprocessing is completed, the simulation job is generated according to the simulation of the user and the high-performance HPC of the server is executed.

Second, when the simulation is finished, the workbench simulation service sends an event to the post processing module that the simulation is finished so that the user can perform post processing. The post processing module that accepts these events receives the event and can receive and

confirm the simulation result data.

Finally, the user can receive the process of analyzing and post processing the simulation result data.

4. Test and Analyze Simulation Service

4.1 Interface for Pre and Post Processor

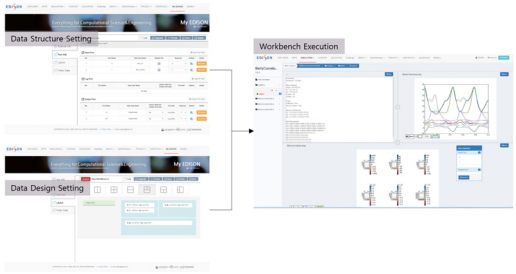
The interface to run the actual simulation service is built on the Liferay 6.2 portlet, and the developer can construct on a JavaScript based interface.

Figure 5 is a schematic diagram to linkage of the pre and post processing of chemical structure files in the actual EDSION platform. On the workbench simulation service, pre and post processor has been called as a module, and executing the simulation and extracting the simulation result.

As you can see in Figure 5, the end user can connect to the EDISON portal to run the simulation and analyze the results. As shown in the figure above, users can add pre and post processor functions for simulation data processing according to various file formats in computational chemistry. Each step of EDISON platfrom simulation service is matched with EDISON workbench-based simulation execution process.

At the same time as the first simulation is executed, various events are generated in the workbench simulation service. Each modular of pre and post processor receives or processes the workbench simualtion event. It will unusable render the simulation services currently available on the

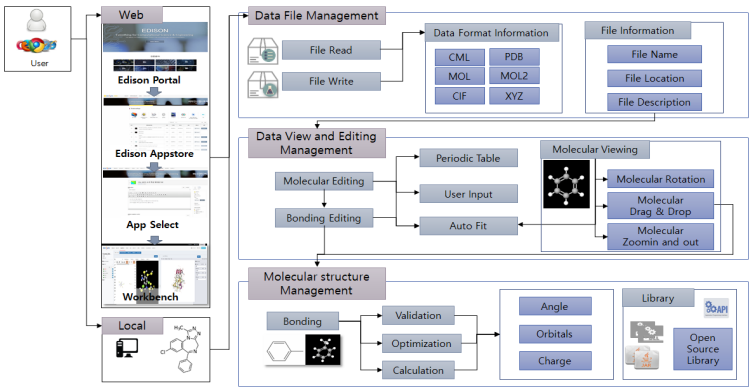
EDISON platform, if the pre and post processor failure to handle the events provided by the workbench-based simulation service. After developing and registering the pre and post processor through the internal interface, the simulation service that is organically linked to the workbench simulation service can be used.



(Figure 4) Processing of Simulation on EDISON Platform

The process of developing a pre and post processor to improve the simulation service and applying it to the workbench-based simulation environment is shown in Figure 6.

The EDSION workbench simulation system is divided into three parts: a developer of the Science App who perform numerical analysis in computational science and engineering, a platform developer, and a pre and post processor developer. The EDISON platform provides interfaces for registering and developing necessary pre and post processors which be



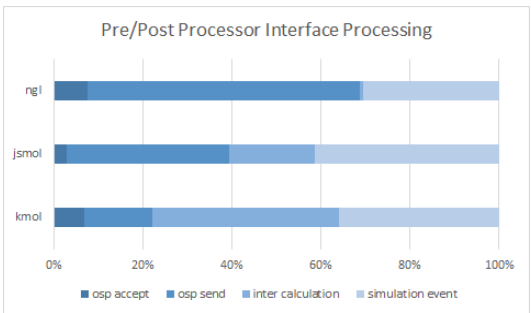
(Figure 5) Construction Pre/Post Processor and Simulation linkage

connected with science applications registration and simulation environments. As well as developing platform for executing simulation and delivering the results of science app's simulation on computational science and engineering.

Respectively, we defined a procedure to provide a more optimized environment to simulate on the web through linkage between pre processor and post processor of each science app, and provided workbench-based simulation service to users.

4.2 Evaluation Pre and Post Processor

Figure 7 shows the system analysis results of several pre and post processors deployed on the EDISON platform. It is the analysis result of three representative pre and post processors that are newly developed and interworked with the workbench service.



(Figure 7) Communication with Workbench Simulation Service

In the case of Ngl, it is a module that can be post process the molecular structure of protein. It includes the ability to use visualization and post processing when the results are received using the workbench simulation service. Since it mainly includes the post processor function of the simulation, the main function is the service that is calculated independently and brings the simulation result. Therefore, 'osp accept' and 'osp send' communication is 68.7%, mainly accepting and processing.

In the second case of Jsmol, it is a post processor that post processes the molecular structure. The simulation results show the molecular structure and include various post processing functions. Since the result includes the function of accepting and processing the result data similar to ngl, the procedures of 'osp accept' and 'osp send' take up a great deal of about 39.4% during the entire processing procedure.

Last case of processor, in the case of kmol, it is possible to pre process and post process modules in computational chemistry. It can represent the molecular structure and atomic structure of computational chemistry, and includes the ability to analyze and process the data. Unlike the two pre and post processors above, kmol includes data analysis and editing functions, so the 'inter calculation' part, which should be handled internally within the module, accounts for about 41.7%.

5. Configuration Simulation with Pre and Post Processor

Thus far, we have designed and constructed interfaces for front-end processing linkage on the EDSION platform. When the actual simulation is executed in the workbench, the module of the developed pre / post processor can be provided in an organic manner with the workbench based simulation service. We have been able to service on the EDSION platform in conjunction with the modules individually developed for the simulation service through the provided interface and to test and analyze the improved simulation services.

According to the analyzed results, each pre and post processing module should continuously update the service through communication with the workbench simulation service to provide the user with various post processing analyzing module. Therefore, it is designed and constructed to provide simulation preprocessing and post-processing functions through an interface for organically communicating. As a result, the current EDISON platform can provide a service by linking a wide variety of pre and post processors to the execution of each simulation. A professional researcher with actual computational science and engineering domain knowledge can construct a process that can contribute to the platform service environment.

Currently, the EDISON platform is building a project based collaborative research platform for sharing simulation services and solving common computational science simulation problems. In accordance with this development

order, future research will build a content sharing system for sharing code of simulation service and sharing pre and post processor. We expect it will improve simulator connection with other research fields and use services in combination.

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