Intelligent u-Learning and Research Environment for Computational Science on Mobile Device

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Abstract

In the 21st century, IT reform has led to the development of cyber-infrastructure owing to the outstanding enhancement of computer and network performance. The ripple effect has continued to increase. Accordingly, this study suggests a new computational research environment using mobile devices. In order to simplify the access of supercomputer, Science AppStore, task management and virtualization technologies are developed on mobile devices. User can be able to research by utilizing computational science SW such as compressible flow solver and nano device simulation tool that in installed on supercomputer in mobile environments. Also, this research environment makes it possible to monitor the simulation result and covers 14 university, 33 subjects, and 1,202 individuals.

Keywords: Computational Science, Research Environment, Mobile Device

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1. Introduction

Modern science is based on the three fundamental pillars: theory, experiment, and computation. Although the area of computation existed in science in the past, the position and importance of computation have changed so significantly that now it is in a higher position than theory and experiment. Traditionally, theory provides principles while experiment verifies them. In such a case, computation is merely an assistant means. With the development of computer performance, however, complicated computation that was impossible to implement in the past comes to be executable, and experiments can be replaced with computer simulations [1].

Computer simulations can saves time and budget necessary for actual experiments, and also enable experiments that would have been impossible before for technical and ethical reasons to be executable. That is why science and industry in the 21st century focus on computational science [2]. In addition, IT reform has led to the development of cyber-infrastructure owing to the outstanding enhancement of computer and network performance. The ripple effect has continued to increase.

Such a paradigm is drastically changing the basic frame of education and daily life [3]. In particular, simulations in utilization of supercomputer, high performance cluster and grid computing [4] have been utilized not only for research but also in various applicable areas such as education, society, medical science, economy, national defense, public sectors, etc [5]. Besides, advanced countries with a high level of simulation technology have continued to adopt recent science technology research products in education and research environments based on the academic and industry cooperation to strengthen the national science technology competitiveness and to train outstanding professional human resources.

Thus, this study suggests an intelligent computational research environment that can utilize cyber-infrastructure based computational science simulation software and contents such as high performance computing and networking in education and research anytime anywhere.

2. Computational Science Research Environment

2.1 Bottleneck of Multi-disciplinary Computational Science Research

Computational science consists of three parts, pre-processing, computation and post-processing. In each case, there are several types of tools, languages (e.g. Fortran, C, JAVA, and etc) and domain scientists (e.g. Mechanical engineering, Physics, and etc). In recent year, multi-disciplinary research such as combination of fluid and chemistry has been great progress. In order to improve the efficiency of complex or inter-disciplinary research, systematic and user-friendly ICT technology is very important. In the existing simulation environment as shown in Figure 1(a), a lot of time had to be consumed for preparation including learning various programming languages and Linux commands more than for the research itself. In contrast, systemized one-stop research environment goes beyond the existing method to type in each command in the console screen, and makes it so easy to implement a simulation by means of a web-based user interface as in Figure 1(b) that even beginners (e.g. undergraduate students or college students), and advanced functions are provided for experts to apply conveniently.

(a) Traditional in-house code simulation (As-Is) (b) Web based One-stop simulation (To-Be)

Fig. 1. Simulation type

2.2 Seamless ICT Architecture for Computational Science Research Environment

In this paper, seamless (or one-stop) ICT architecture to enable complex and multi-disciplinary research on mobile device is proposed. Basic functions of this architecture such as user-information management, visualization framework and task management are verified on supercomputer system using CFD(Computational Fluid Dynamics) problems[3].

This architecture has four main layers, cyber-infrastructure layer, middleware layer, application framework layer and research community layer, as shown in Figure 2. Application framework provides a web-based RESTful[6] interface for such services as user authentication, workflow, simulation S/W metadata inquiry, storage management, statistical service, and etc.

The middleware layer provides such services as simulation S/W metadata management, simulation data management that involves multiple calculation tasks, data history resource management, heterogeneous(physical and virtual) computing resource and visualizing resource coupling, and etc. Finally, cyber-infrastructure layer provides users with physical computing and network resources to implement simulations in a stable manner.

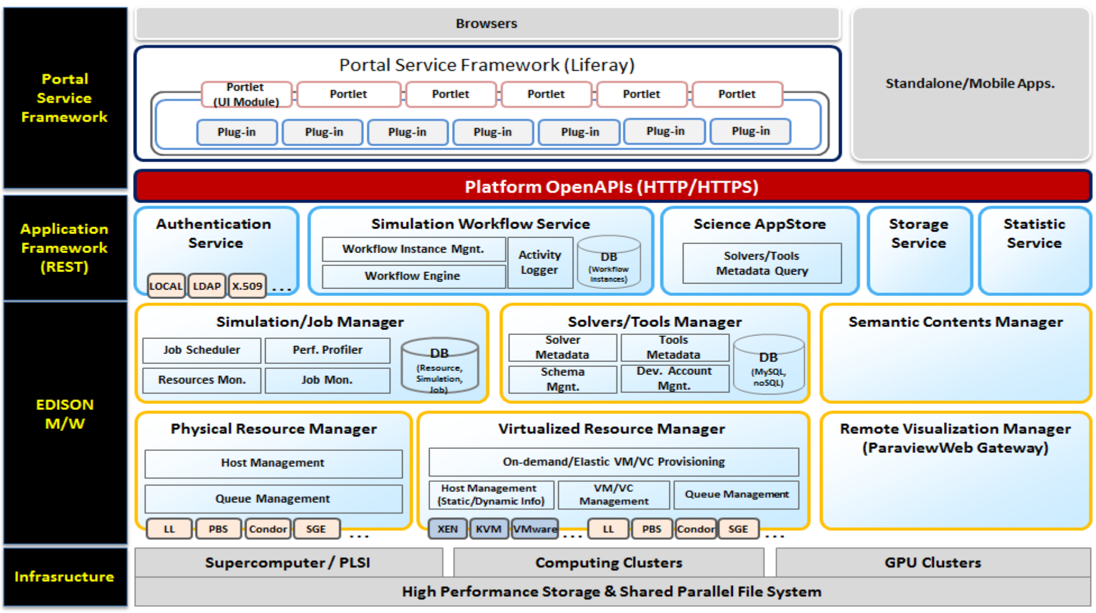

Fig. 2. Seamless ICT Architecture for Computational Science Simulation

3. ICT Framework for Computational Science Research on Mobile Device

It must overcome the various difficulties in order to implement computational science research on mobile device. In particular, it is necessary to novel research, such as data handling, computing technology, web technology and large data visualization. In this paper, Science Appstore(application framework), virtualization computing resource and task management framework is designed and developed on mobile device. The science Appstore technology provides the interface to store and manage multi-disciplinary simulation S/W, and create a large-scale computing resource based simulation environment. As shown in Figure 3, the virtualization computing resource and task management framework provide the coupling of various types of base environment, such as authentication and authorization, virtualization, task management, storage device administrator, and etc. This framework is extended to run on the web-based HTTP(s) REST interface.

The REST interface provided by the virtualization computing resource and task management framework includes the following:

1) User Management & Authentication

The system administrator authorized by the system in advance may register or delete a user. General users may acquire the system authentication by means of the login and logout interface, and may call on other service APIs by means of an authentication token presented upon successful authentication. Within the framework, a HTTP(s) BASIC based authentication mechanism is utilized for user authentication and authorization, and the administrator and common users have different access types.

2) Physical Server Management

To execute a simulation upon a user's request, the virtual machine and virtual cluster needs to be provisioned and registered to the shared pool. For this process, an Add and Delete function is provided for the physical server in which the virtual machine and virtual cluster will be operated. Common users are unable to access physical server management APIs while the permitted administrator only can use such APIs.

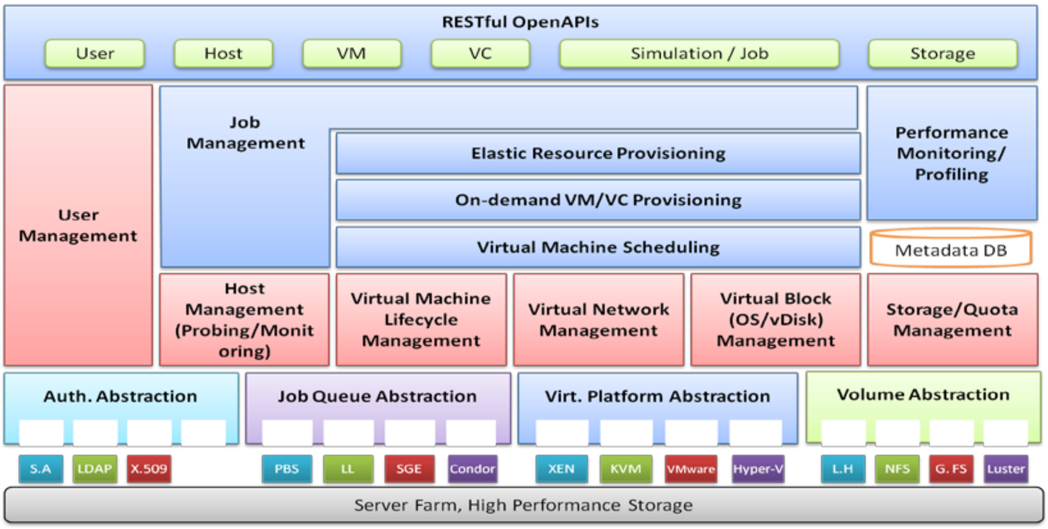

Fig. 3. Virtualized Resource Management Framework

3) Simulation Management

A simulation is of a virtual parent concept that includes a task group. The simulation management API is used for parameter study task group management, simulation creation/information inquiry/deletion/modification, and etc.

4) Task Management

A user may create a virtual parent concept of simulation entity, and then submit or manage tasks. As for a task submission, a user may state the task title, task type (sequential or parallel), interpreter, and interpreter parameter in XML (or JSON) and then call on the API to be submitted.

The status and cancel API is used for the monitoring or execution cancelation of the submitted task. Upon completing the task execution successfully, the user can check the metadata of the output files.

Among the supported RESTful OpenAPIs as shown in Figure 3, APIs used for service on mobile device are User, Simulation and Job, and Storage component. 'User' manages the user login and logout information while Simulation and Job manages simulation list, job list, and job status information. Lastly, 'Storage' stores result files after the simulation task management.

As explained above, OpenAPIs-utilized mobile framework consists of Science Appstore(S.AppStore) to provide simulation SW(solver) information of each computational science area and monitoring of jobs in progress for the simulation.

5) Virtual Machine Provisioning

This is an API to provision virtual machines/virtual clusters to the physical servers registered by the administrator. Both the administrator and common users are allowed to access, and they may request virtual machine provisioning with the number of processors and amount of memory specified. In addition, they may inquire details of the provisioned virtual machines, and the owner of the virtual machine may suspend or resume the virtual machine.

4. Implementation and Validation

This study presents an intelligent mobile environment where cyber-infrastructure based computational science simulation SW and contents can be utilized for education and research anytime anywhere. In particular, to evaluate the availability and functionality of the virtualization computing, task management framework and Science Appstore, a pilot service of the nano-physics area is conducted on mobile device.

1) Problem Formulation

The environment proposed in this paper has limited to single simulation environment. In order to improve this simulation environment, we would handle sequential and large scale of simulations on the environment. It needs to adjust precedence of input data and output data of each simulation, to consider capacities of resources which would be used in each simulation, and finally to schedule all jobs properly.

This problem can match widely known as the Resource Constrained Project Scheduling Problem (RCPSP). RCPSP is the problem of scheduling of project jobs based on the precedence and resource capacity constraints, which is to minimize the whole jobs makespan.

The RCPSP is known to be NP-hard, and, as increasing the number of jobs, running time increases exponentially. To improve this problem, we apply branch-and-cut algorithm to RCPSP[8-16].

Many prominent models for RCPSP have been introduced, and one of them, which consider to minimize total makespan(see Talbot(1982)), looks as follows :

$$\text{Minimize} \sum_{t=es_{n+1}}^{ls_{n+1}} t x_{n+1,t} \tag{1}$$

$$\text{Subject to} \sum_{t=es_i}^{ls_i} (t+d_i) x_{i,t} \le \sum_{t=es_j}^{ls_j} t x_{j,t} \quad \forall (\mathrm{i}, \mathrm{j}) \in \mathrm{A}, \tag{2}$$

$$\sum_{t=es_i}^{ls_i} x_{i,t} = 1 \quad \forall \mathrm{i} \in \mathrm{N}, \tag{3}$$

$$\sum_{i=1}^{N} r_{i,t} \sum_{s=\max(t-d_i, es_i)}^{\min(t-1, ls_i)} x_{i,t} \le R_{kt} \quad \forall \mathrm{k} \in \mathrm{R}^{\mathrm{K}} \text{ and } \mathrm{t} = 1, \ldots, \mathrm{T}, \tag{4}$$

$$x_{i,t} \in \{0,1\} \quad \forall \mathrm{i} \in \mathrm{N}; \mathrm{t} = 1, \ldots, \mathrm{T}, \tag{5}$$

Table 1. Symbol Definition

Symbol	Definition
d_i	Duration for each job i
$x_{i,t}$	A binary variable which equals zero unless job i is assigned a completion time in period t. Then, $x_{i,t} = 1$, else 0
es_i	Earliest completion time of job i
ls_i	Latest completion time of job i
$r_{i,k}$	Amount of renewable resource k required job i each period in process ($r_{ik} > 0$)
R_{ik}	Amount of renewable resource k currently available in period t ($R_{kt} > 0$)

The constraints (2) present the precedence which each pair of jobs has, and constraints (3) secure that each job is performed exactly once. Constraints (4) take the resources relation that each job uses in simulation not to exceed the amount of each resource available in certain period.

This kinds of mixed inter problem(MIP) can be solve using branch-and-cut algorithm, which improves branch-and-bound algorithm and strengthens relaxation of linear programming adding new valid equalities called cutting plane before branching sub-solution. Branch-and-cut algorithm improves the performance than branch-and-bound algorithm does, but still has exponential running time increasing the number of variables.

In order to deal with large size of variables for solving MIP models, branch-price-and-cut algorithm has been used, which adds column generation algorithm to branch-and-cut algorithm. Column generation algorithm is an algorithm for solving large size of linear program which means that it deals with only useful and important values. It begins with decomposition of original to new formulation known as master problem, adds the value to problem, and the relaxation is re-optimized. Therefore, to schedule large scale of simulations, a customized branch-price-and-cut algorithm suited to scheduling problem(RCPSP) is needed.

2) RCPSP Solvers

To check the performance of RCPSP, experiments was done with original MIP solvers – SCIP 3.0.1 to perform branch-and-cut algorithm and GCG 1.1.0 to perform branch-price-and-cut algorithm. GCG uses its own common decomposition method. Our test is on Intel Xeon Processor E5630 2.53GHz(16GB memory) and uses single mode data sets from PSPLIB web page**.** **Table 2** shows the results using SCIP and GCG solvers.

When scheduling small size of jobs, both solvers perform very highly, but in the case of large size of jobs over 90, it takes very time consuming running time. Compared to the results using SCIP(branch-and-cut), the results using GCG(branch-price-and-cut) underperform despite using branch-price-and-cut algorithm, because its own decomposition method doesn't work as the most appropriate decomposition method to RCPSP. When decomposing certain problem, it is necessary to choose or implement decomposition method with problem, because it works well according to the structure of problem.

Analyzing the process of problem solving, GCG solving RCPSP often handles too many variables than SCIP.

Table 2. SCIP & GCG Test Result

Dataset (3,6,9,12)	J30		J60		J90		J120	
	SCIP	GCG	SCIP	GCG	SCIP	GCG	SCIP	GCG
J*01_1	0.01	0.00	0.01	0.04	0.54	0.63	-	-
J*01_2	0.01	0.03	0.05	0.02	0.05	0.12	-	-
J*01_3	0.01	0.01	0.02	0.02	0.41	37.74	-	-
J*01_4	0.02	0.01	0.04	0.14	4.39	681.98	-	-
J*01_5	0.01	0.03	0.02	0.03	0.36	0.79	-	-
J*01_6	0.01	0.01	0.22	0.55	0.96	7.20	102.20	-
J*01_7	0.00	0.01	0.09	2.43	0.29	3.66	65.33	-
J*01_8	0.01	0.01	0.08	0.06	814.29	Aborted	-	-
J*01_9	0.01	0.01	0.03	0.03	2.28	7.01	1423.35	-
J*01_10	0.01	0.01	0.02	0.03	0.21	0.35	-	-
J*02_1	0.02	0.01	0.02	0.03	0.00	0.11	5.17	-
J*02_2	0.01	0.01	0.01	0.02	0.02	0.13	38.12	232.91
J*02_3	0.01	0.01	0.01	0.02	0.02	0.03	87.64	-
J*02_4	0.00	0.01	0.01	0.03	0.02	0.07	0.11	3.25
J*02_5	0.00	0.01	0.01	0.02	0.03	0.09	2.66	-
J*02_6	0.00	0.01	0.01	0.02	0.03	0.14	13.04	79.87

Dataset (3,6,9,12)	J30		J60		J90		J120	
	SCIP	GCG	SCIP	GCG	SCIP	GCG	SCIP	GCG
J*02_7	0.01	0.01	0.01	0.03	0.01	0.06	36.27	1.37
J*02_8	0.01	0.01	0.01	0.05	0.04	0.09	22.46	1.31
J*02_9	0.01	0.01	0.01	0.05	0.03	0.08	27.53	1149.34
J*02_10	0.01	0.01	0.02	0.02	0.02	0.25	19.48	6.53
J*03_1	0.01	0.01	0.01	0.02	0.01	0.05	7.49	3.64
J*03_2	0.01	0.01	0.01	0.03	0.01	0.08	0.16	0.25
J*03_3	0.00	0.02	0.01	0.02	0.01	0.07	0.06	0.26
J*03_4	0.00	0.02	0.00	0.01	0.02	0.09	43.18	1.03
J*03_5	0.00	0.02	0.00	0.02	0.01	0.03	70.65	0.28
J*03_6	0.00	0.02	0.02	0.02	0.00	0.14	0.00	0.41
J*03_7	0.01	0.00	0.00	0.02	0.01	0.05	0.12	0.57
J*03_8	0.00	0.02	0.01	0.04	0.01	0.05	0.68	0.31
J*03_9	0.00	0.02	0.03	0.02	0.01	0.07	0.10	0.12
J*03_10	0.01	0.01`	0.01	0.02	0.01	0.02	0.03	0.26

3) Implementation and Validation

The nano-physics pilot service utilize the simulation solver shown in **Table 3** and covers 14 university, 33 subjects (**Table 4** and **Table 5**, delete duplicate content), and 1,202 individuals. 3,053 simulations in total were involved.

These simulation tools and SW is implemented and validated to EDISON (Education-research Integration through Simulation On the Net) project funded by MSIP(Ministry of Science, ICT and Future Planning).

Table 3. Nano-Physics Simulation S/W

Simulation S/W Name	Feature
An electronic structure calculation SW for Single-band Effective Mass based 3-D Finite Structure	Semi-conductor 3-D representation Multi-dimensional confinement Handling Mass calculation through parallelization
A single particle energy level interpretation SW for 1-D Potential Well	Basic calculation of energy level interpretation in quantum mechanics and semiconductor engineering Enhancement of educational effect by comparing the hand-induced analytical solution (2th/3rd grade college students) Applicable to various potential barrier profiles
SW for Drift-Diffusion based bulk P/N Junction Diode characteristic interpretation	Electrical charge/voltage self-consistent calculation based on Continuity Equation & Poisson Equation Electrostatic calculation of Step Junction and linear/Gaussian Doping Junction
SW for 6/8 band k.p based nanowire & quantum well electronic structure calculation	Confined semiconductor sub-band structure confined in an actual space Mass calculation function through MPI parallelization

Simulation S/W Name	Feature
SW for Nanowire FET element performance & characteristic analysis	NEGF-Possion based program for Ballistic, Square Nanowire problems Mass calculation function through MPI parallelization
Carbon Nano-Tube FET element simulation SW	NEGF-Possion utilized program for Ballistic, CNT Nanowire (MOSFET, Schottky Barrier, Tunnel-FET) problems Mass calculation function through MPI parallelization
Nano MOS element characteristic interpretation SW	Quantum-mechanical calculation of a gate leakage current in 1-D MOScap Simulation of a gate stack that consists of two substances
Electronic energy band structure conversion & visualization SW	Electronic energy band structure visualized based on the information after the primary principle calculation and saved as an image file
DFT based electronic structure calculation in utilization of SIESTA package	Structure optimization, molecular dynamics simulation, band structure calculation Mass calculation function through parallelization
Carbon Nano-Tube Modeler	Carbon Nano-Tube structure creation and download
Graphene Nanoribbon modeler	Graphene Nanoribbon structure creation and download
1D finite square-well bound state calculation SW	1-dimensional Schrödinger equation 1-dimensional potential energy quantization
2 dimensional elastic collision simulation of 2 objects	Law of conservation of momentum after a collision without any external force Scattering angle of particle collision depending on the mass
Tersoff potential energy calculation program	3-dimensional atomic structure calculation Calculation in utilization of Tersoff potential
Tersoff potential stress calculation program	3-dimensional atomic structure calculation Stress tensor calculation

Fig. 4 shows the mobile-EDISON main screen. Mobile-EDISON main screen displays the information on Nano-Physics, Computational Chemistry, which are frequently used for a simulation in EDISON and computational science areas.

Fig. 4. mobile-EDISON main screen

Fig. 5. Science Appstore main screen

Fig. 6. Simulation Monitoring Screen

Fig. 7. Job Monitoring Screen

Fig. 5 shows the Science Appstore screen. Science Appstore provides solver information for interpretation, screen information on the solver output, and solver output file information.

Fig. 6 shows the simulation monitoring screen where the simulation list and simulation information related to the computational science simulation is provided.

Fig. 7 shows the status of jobs being implemented in each simulation. The status of jobs is classified into 6 types: Initialized (Submitted included), Queued, Running, Success, Fail, and Canceled. In monitoring, jobs that are queued or running may be cancelled. As a simulation job is completed, the result may be checked through KiwiViewer.

We provided trial service(**Table 4** and **Table 5**) using EDISON Nano-Physics during courses and conduct a survey about satisfaction to teaching assistants. A total of 515 teaching assistants answered the survey, who were 137 of the 169 users in the second semester in 2012 and 378 of the 1,029 users in the first semester in 2013.

Table 4. Currently Available Subjects of nano physics Pilot Service(2nd sem, 2012)

School	Subject
KAIST	Introduction to Physical Electronics
Seoul National University	Electronic Properties of Materials
Sungkyunkwan University	Industrial Mathematics Electronic Physics
Korea University	Measurement Techniques for Nano Elements
Sookmyung Women's University	quantum mechanics 2 Computer-based Physics Quantum Physics 1 General Physics 1
Sejong University	Physics Colloquium Seminar 4

Table 5. Currently Available Subjects of nano physics Pilot Service(1st sem, 2013)

School	Subject
KAIST	Introduction to Physical Electronics Electronic Design Lab. Electrical Engineering Quantum Mechanics Special Topics in Physics 1
Seoul National University	Dielectric Thin Film stuff Semiconductor Physics Stuff Modern Physics
Sungkyunkwan University	Industrial Mathematics Electronic Physics
Korea University	Electronic Circuit Nano Engineering
Sookmyung Women's University	quantum mechanics 2 Computer-based Physics Quantum Physics 1 General Physics 1
Sejong University	Seminar 4 Introductory Physics1 General Physics Laboratory Experiments1-01 General Physics Laboratory Experiments1-02
Chungnam National University	Quantum Mechanics

Analyzing the ratio about participation to survey, there are more undergraduate students which represent 334(65%) than graduate students which represent 179(35%). Also, in the result of satisfaction survey(**Table 6**), it turned out that users are relatively largely satisfied with convenience of simulation generation and execution function, understanding of physical phenomenon and user support service 2nd sem 2012.

Table 6. Research Result of nano physics Pilot Service

Survey Content	2nd sem, 2012	1st sem, 2013
Was the process of simulation generation easy? (Entering parameters of simulations, uploading user-defined file, etc)	74.0	76.1
Was it easy to access the result of executed simulation?	72.4	72.7
Was it easy to understand every variety of physical phenomenon in courses using EDISON_Nanophysics?	65.0	60.0
Did you think that user support service is useful to apply the system? (User Support Service : visualization tool, supply of manual about simulation tool, visit to learning place field, and processes of problem solving)	78.0	70.1
How often did you use this system during this semester?	34.5	35.1
How satisfied were you with the progress of practice and execution of assignment?	73.7	71.1

5. Conclusion

In the existing simulation environment a lot of time had to be consumed for preparation including learning various programming languages and Linux commands more than for the research itself.

In this paper, ICT architecture to enable complex and multi-disciplinary computational research on mobile device is proposed. The proposed system support several types of languages (e.g. Fortran, C, JAVA), Web UI and computing resources. This is one-stop computational environment. Researcher can execute a number of simulation SW and data simultaneously with no user interruption. To develop intelligent research environment, AppStore concept is designed and implemented on mobile device as a new technology. Also, virtualization, data and task management technology is developed. All of components and contents are applied to the nano-physics and computational chemistry pilot mobile service.

The nano physics pilot service utilizes the simulation solver and covers 14 university, 33 subjects, and 1,202 individuals. Currently, this system provides the simulation monitoring service only for the nano-physics area, but it is expected that the service range will be expanded to various other areas such as CFD(Computational Fluid Dynamics), and etc.

Future work will be to implement new decomposition method and pricing tool appropriate to RCPSP. Also, as adding heuristics Heterogeneous Earliest Finish Time(HEFT) algorithm or new cutting plane, scheduling of large sale of simulations can be improved.

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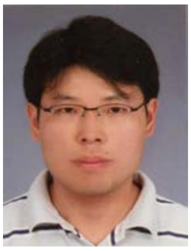

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