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A Compact Computing Environment For A Windows PC Cluster Towards Seamless Molecular Dynamics Simulations

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Abstract —**A Windows PC cluster is focused for its high availabilities and fruitful functions such as a well-tuned MPI library and a fully-equipped job scheduler. However, the software tools are complicated for users who are not familiar with the Windows system. They don't want to pay much time to learn about the system because what they want is getting calculated results. Furthermore, there is not any tool to support visualization of calculated results. To support seamless molecular dynamics simulations from computations to visualization on a Windows cluster, a compact computing environment has been built by using Java. It provides hints for parallel computing and assists seamless job execution and its visualization. As a result, application users can proceed their computations without deep understandings of the Windows cluster.**

Keywords: Windows PC cluster, MS-MPI, job scheduler, Java RMI, molecular dynamics simulation

1 Introduction

It is now familiar to build and utilize a PC cluster by using a Windows server system [1]. The Windows system provides many useful software tools such as a well-tuned MPI [2] library named MS-MPI [1] and a powerful job scheduler.

Those software tools are available with a Windows GUI. However, most of the application users do not expect to encompass the expertise for the Windows cluster. As a result, they have difficulties in operation of their programs because of complexity in selection and utilization of appropriate functions of the system. Furthermore, there is not any support to check standard output/error of a running job in a GUI menu named Compute Cluster Job Manager of the job scheduler. Instead, a command line interface is available to check them, however, it is too complicated for non-expert users. It is also noticed that there is not any support for a visualization of calculated results.

To remove such difficulties, a compact and user-friendly computing environment which is available on a client PC is built to manipulate the Windows cluster. A computing environment has been built by using Java because Java is useful for building GUI applications and platform independent. It collects essential functions for a target molecular dynamics simulation to control a remote Windows cluster from a client PC. This environment consists of client and server programs and hides complexity of job execution on the Windows cluster from application users. The client program runs on a client PC, while the server program runs on a head node of a Windows cluster. A platform dependent part is encapsulated in the server program. This computing environment provides hints for parallel computing in a simple manner. Furthermore, it assists program job submission into the job manager of the Windows cluster.

In this paper, section 2 briefly explains the Windows cluster. Section 3 describes about motivations, details of its system architecture, and a user interface of the environment. Related work is also remarked in section 4, followed by summary of this work in section 5.

2 Brief Overview of a Windows PC Cluster

Typical configuration of a Windows PC cluster is illustrated in Figure 1. An Active Directory server is deployed for authentication of users and host name querying service (Fig. 1(1)). A user issues a job execution request from a client PC to a head node of a cluster by using a GUI-based job scheduler system named Compute Cluster Job Manager or a command line interface (CLI) (Fig. 1(2)). A logical job unit named a job container is created on the job scheduler. In general, users can add multiple tasks in the job container. Hereafter, I describe a job container as a job. Later, the job is submitted to the job scheduler. The scheduler authenticates information

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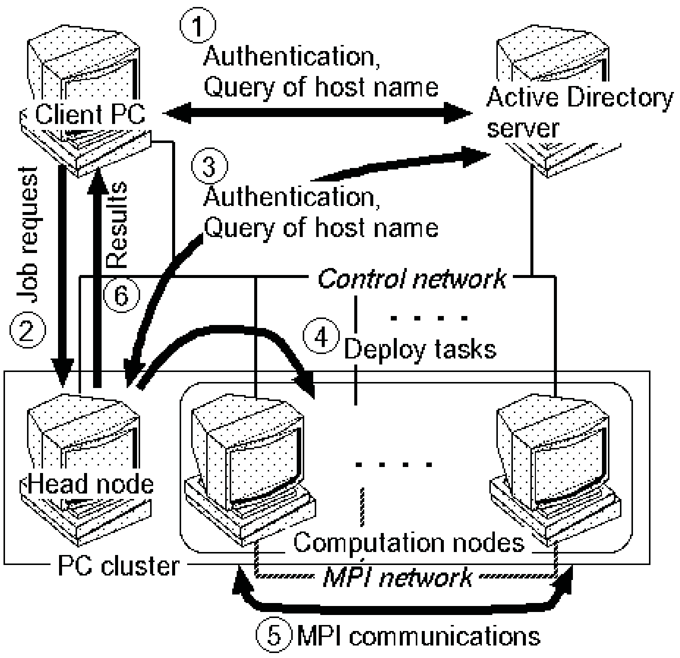


Figure 1: Typical configuration of a Windows PC cluster

such as a user ID about the submitted job (Fig. 1(3)). The job scheduler analyzes its request and tasks in the job are queued for computation.

Once enough CPUs can be assigned for a waiting job, the scheduler allocates vacant computation nodes for each task (Fig. 1(4)). For parallel computing, a well-tuned MPI library named MS-MPI [1] is provided. The library is based on an MPICH2 [3] implementation. After parallel computation by the computation nodes (Fig. 1(5)), status of a task is returned through the Compute Cluster Job Manager or the CLI (Fig. 1(6)).

3 Client Computing Environment For a Windows PC Cluster

3.1 Architecture

This system is developed to provide the following functions:

- Support of parameter settings such as a user ID, a program name, the number of CPUs, a work directory, and standard input/output/error
- Support of seamless job execution and visualization by encapsulating complicated Windows cluster operations
- Job and task monitoring

To provide a user-friendly interface for non-expert users, a GUI interface is essential. It is also remarked that portability is important issue. Therefore, Java SE Development Kit 6 [4] was selected to develop the computing environment.

An organization of developed Java classes is illustrated in Figure 2. This system has two parts; one is a server side part which runs on a head node of a PC cluster and the another is a client side part which runs on a client PC. The reason for such configuration is to provide a platform independent system in the client side. All the platform dependent properties are deployed in the server side.

Data communications between server and client are carried out by using Java's Remote Method Invocation (RMI). This system is available for a user in a Windows domain in which an Active Directory server runs.

The client side has two layers in implementation; one is a user application layer and the another is a lower interface layer. The application layer provides GUI menus for job creation, job submission, and monitoring a PC cluster and jobs in a seamless manner. The `JobMenuFrame` class provides such GUI menus and a user can specify several parameters here. A job list is created to store information about submitted jobs and associated tasks. The `JobMenuFrame` class creates the list at the start-up of this system with the help of a Java's `JTree` object.

On the other hand, the lower layer provides control methods for a Windows cluster. Some of the Java classes (`SubmitJob`, `MatchJob`, and `WatchCluster`) provide interfaces for an RMI server object (`CCSManageServer`) in the server side. Besides, the `MatchJob` and `WatchCluster` classes invoke threads which run in parallel with a main thread. The former checks status of a selected task by accessing a job list, while the latter checks the number of available CPUs by issuing a command to the cluster.

Both the `JobMenuFrame` and `MatchJob` classes fetch the job list. For job submission, several associated methods of the `JobMenuFrame` class are used. Once a job is created, a user can add several tasks in the associated job. A user can submit the job with the help of the `SubmitJob` class. Job submission to a remote Windows cluster is carried out by using Java RMI with the help of the `CCSManageServer` and `CCSManageImpl` classes on a remote Windows cluster. Later, the `JobMenuFrame` class stores information about the job and associated tasks in the job list. The `MatchJob` class fetches the list periodically to check status of a selected task.

The server side part has a role to receive RMI requests for job submission and so on from a client side application. The RMI server carries out operations for the Windows cluster. A request from the client side is analyzed and an associated Java method in the `CCSManageImpl` class is called in the RMI server. The Java class provides native interfaces to the Windows cluster with the help of the CLI. Each method in the class carries out job control,

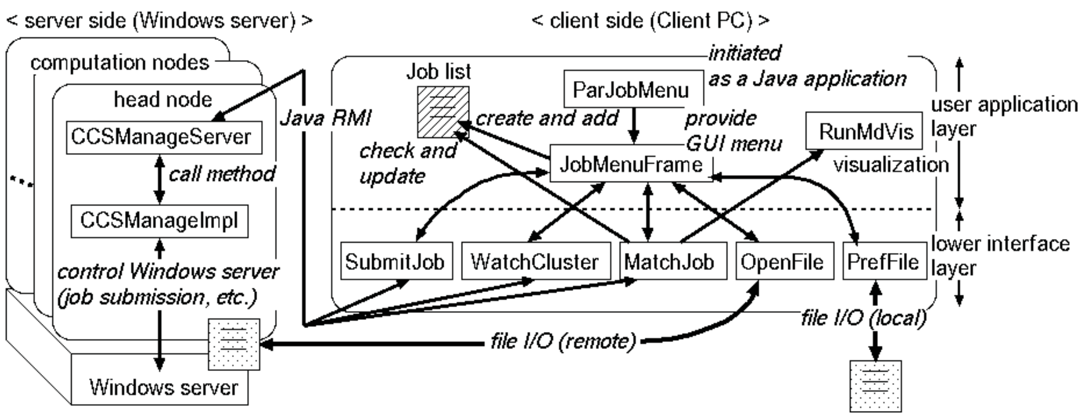


Figure 2: Organization of developed Java classes

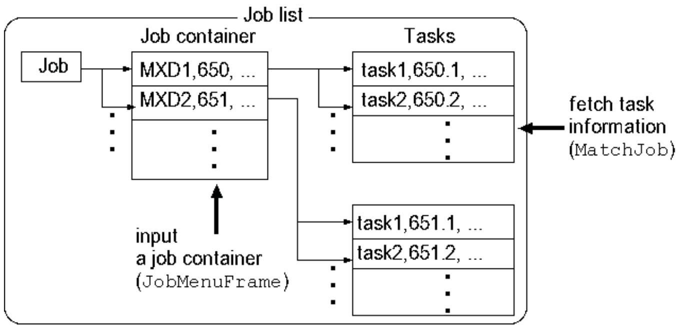


Figure 3: Data structure of a job list to hold information about submitted jobs and associated tasks

monitoring of job and a PC cluster system, and so forth.

Figure 3 depicts an example of a data structure of the job list. A tree node associated with a job is created under the root node, "Job". In this figure, MXD1 and MXD2 stand for names of jobs, where 650 and 651 stand for job IDs. Associated parameters such as the maximum number of CPUs, user ID, and so forth are registered with those parameters.

A child node is created for a task under associated job node so as to have a similar data structure in the Windows job manipulations. Associated parameters such as the number of CPUs to be used, a work directory, standard input/output/error are registered. With the help of this data structure, we can easily check a target job or a target task effectively.

3.2 Seamless job submission and visualization

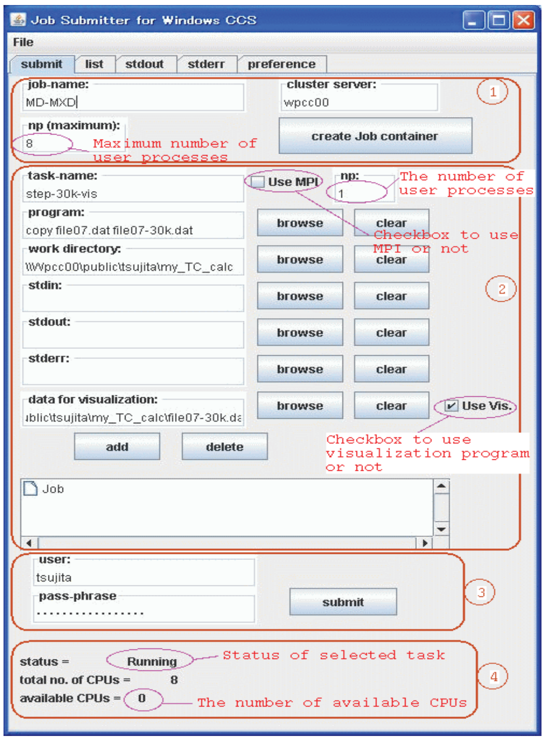
To start computation, users need to create a job to be passed to a job scheduler. A menu window provided by the `JobMenuFrame` class helps to create the job and associated tasks as shown in Figure 4 (a). In this menu, job creation, task creation, job submission, and status monitor are available. In the job creation (Fig. 4 (a): (1)), a user specifies a job name, name of a cluster's head node, and the maximum number of requested CPUs to be used. Later, pressing a button, "create Job container," creates a new job by using a method of the `SubmitJob` class. A corresponding icon for the job is indicated in the tree structure style list of this menu.

In the second one (Fig. 4 (a): (2)), a task name, a program name, a work directory, standard input/output/error, and the number of CPUs are specified in the menu. There are check boxes for an MPI program and visualization program. Once a user presses a button, "add," the task is registered in the selected job with the help of the `SubmitJob` class. Later, an icon which stands for the task is indicated under the associated job's icon in a tree structure manner.

In the third one (Fig. 4 (a): (3)), the job including tasks is passed to an RMI server program on a head node of a PC cluster by using a Java RMI with the help of the `SubmitJob` class when a user presses a button, "submit." In this operation, a user need to specify a user ID and a pass phrase. The RMI server receives the job and submits it into a job scheduler by using the CLI. If a user succeeds the submission, information of the job and associated tasks are registered in a job list which is indicated in a Job list menu as shown in Fig. 4 (b).

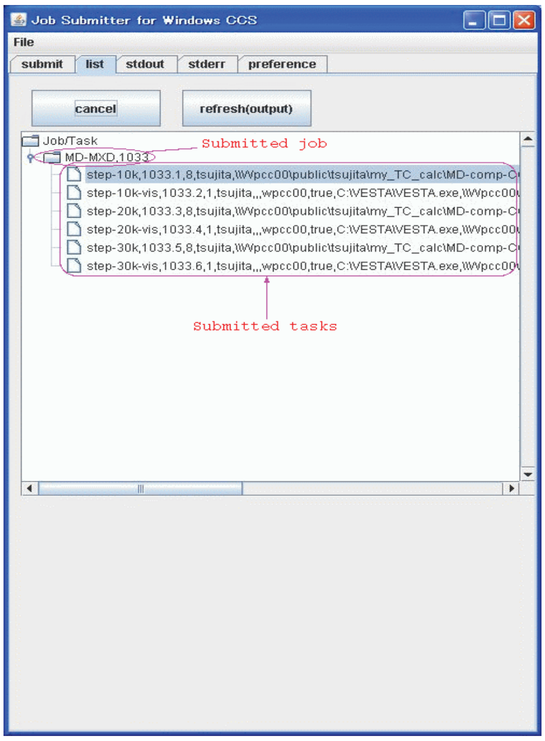
A user can check status of a selected task in the list (Fig. 4 (a): (4)) with the help of the `MatchJob` class. The total number of CPUs and available CPUs are also indicated here with the help of the `WatchCluster` class.

Standard output and error are indicated in tab menus, "stdout" and "stderr," respectively by using the `OpenFile` class. Users can see the outputs by selecting the target task in the Job list in Fig. 4 (b). Fig. 4 (c) shows an example of a standard output menu window with a running program. Pressing a button, "refresh(output)," updates the current output. If errors or warnings are reported from the Windows cluster in a standard error, those are indicated in the "stderr" menu


Job Submitter for Windows CCS
File
submit
list
stdout
stderr
preference
create Job container
Maximum number of user processes
Use MPI
The number of user processes
browse
clear
Checkbox to use MPI or not
Use Vis.
Checkbox to use visualization program or not
add
delete
submit
Status of selected task
The number of available CPUs
1
2
3
4

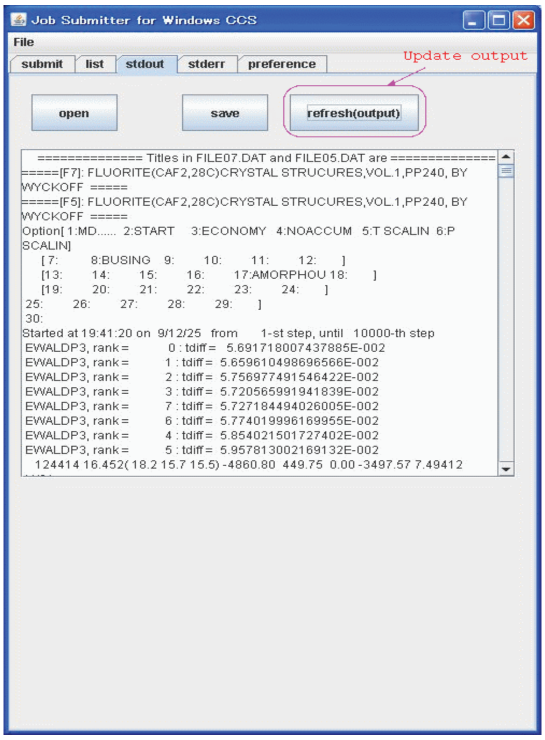
job-name: MD-MXD
cluster server: wpcc00
np (maximum): 8
task-name: step-30k-vis
np: 1
program: copy file07.dat file07-30k.dat
work directory: \\Wpcc00\public\tsujita\my_TC_calc
stdin:
stdout:
stderr:
data for visualization: ıblic\tsujita\my_TC_calc\file07-30k.dε
Job
user: tsujita
pass-phrase: ....
status = Running
total no. of CPUs = 8
available CPUs = 0

(a) Job submission menu



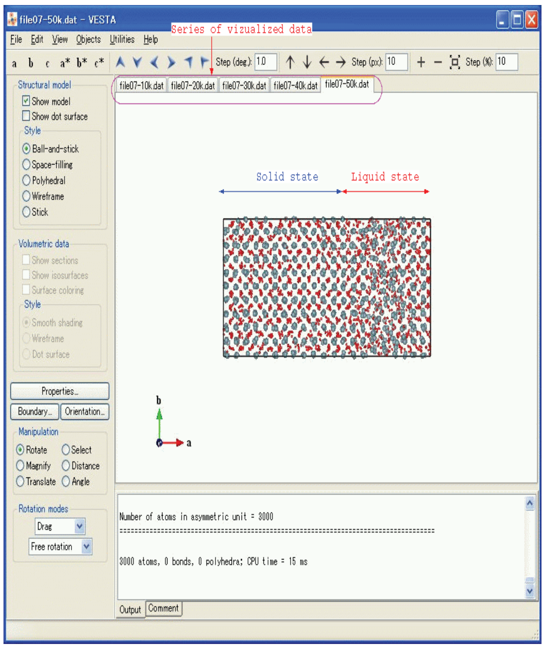
```
Job/Task
  MD-MXD,1033
    step-10k,1033.1,8,tsujita,\\Wpcc00\public\tsujita\my_TC_calc\MD-comp-C
    step-10k-vis,1033.2,1,tsujita,,,wpcc00,true,C:\VESTA\VESTA.exe,\\Wpcc00\
    step-20k,1033.3,8,tsujita,\\Wpcc00\public\tsujita\my_TC_calc\MD-comp-C
    step-20k-vis,1033.4,1,tsujita,,,wpcc00,true,C:\VESTA\VESTA.exe,\\Wpcc00\
    step-30k,1033.5,8,tsujita,\\Wpcc00\public\tsujita\my_TC_calc\MD-comp-C
    step-30k-vis,1033.6,1,tsujita,,,wpcc00,true,C:\VESTA\VESTA.exe,\\Wpcc00\
```

(b) List of submitted jobs and tasks



```
 ============== Titles in FILE07.DAT and FILE05.DAT are ==============
=====[F7]: FLUORITE(CAF2,28C)CRYSTAL STRUCURES,VOL.1,PP240, BY
WYCKOFF  =====
=====[F5]: FLUORITE(CAF2,28C)CRYSTAL STRUCURES,VOL.1,PP240, BY
WYCKOFF  =====
Option[ 1:MD......  2:START    3:ECONOMY   4:NOACCUM   5:T SCALIN  6:P
SCALIN]
   [ 7:       8:BUSING    9:       10:       11:       12:      ]
   [13:       14:       15:       16:       17:AMORPHOU 18:       ]
   [19:       20:       21:       22:       23:       24:      ]
 25:       26:       27:       28:       29:      ]
 30:
Started at 19:41:20 on  9/12/25   from      1-st step, until   10000-th step
 EWALDP3, rank =          0 : tdiff =   5.691718007437885E-002
 EWALDP3, rank =          1 : tdiff =  5.659610498696566E-002
 EWALDP3, rank =          2 : tdiff =  5.756977491546422E-002
 EWALDP3, rank =          3 : tdiff =  5.720565991941839E-002
 EWALDP3, rank =          7 : tdiff =  5.727184494026005E-002
 EWALDP3, rank =          6 : tdiff =  5.774019996169955E-002
 EWALDP3, rank =          4 : tdiff =  5.854021501727402E-002
 EWALDP3, rank =          5 : tdiff =  5.957813002169132E-002
   124414 16.452( 18.2 15.7 15.5) -4860.80  449.75  0.00 -3497.57 7.49412
```

(c) GUI to check standard output



```
Number of atoms in asymmetric unit = 3000
================================================================
3000 atoms, 0 bonds, 0 polyhedra; CPU time = 15 ms
```

(d) Visualization of calculated results by using an existing visualization program, VESTA [5]

Figure 4: Examples of GUI menus in a client computing environment

window which has the same GUI.

After computations, we may have a molecular image by an existing visualization program named VESTA [5]. Here we can see several images obtained through 10,000 to 50,000 steps computations (10,000 steps each) to know melting temperature regarding stable and unstable conditions. In this example, solid and liquid parts are isolated at first. By facing the both parts at some temperature, we may know melting point of this material after a sort of computation steps. The developed computing environment is very helpful for this kind of computations.

4 Related Work

There are many implementations to manage parallel computations on PC clusters. Condor [6] provides a chance to develop, implement, and deploy mechanisms to realize high throughput computing on large collections of distributed computing resources. A job scheduler named Condor Central Manager deploys a submitted job to unused computer. Each computer carries out an allocated job and returns results to the job scheduler.

Sun Grid Engine [7] also enables resource management and job scheduling as the Condor system does. However, Condor has much functions than Sun Grid Engine because Condor aims at managing non-dedicated cluster systems. Whereas the Sun Grid Engine is more limited to the job resource management and monitoring in a closed cluster computing system.

Recently, a Windows PC cluster was deployed as a computing resource in the National Grid Service [8] by using a modified Globus [9] infrastructure named CCS Globus gateway [10]. Furthermore, its work-flow system provides usability in application user's computations.

Those systems described above are very powerful for a large scale PC cluster or a grid computing environment, however, users are required to be familiar with underlying system architectures. Besides, an administrative user should arrange configurations of both the hardware and the software. The computing environment in this paper aims to provide a compact and user-friendly computing environment for a small Windows cluster. It does not require any special servers and software, except for preparing a Java software. This computing environment enables non-expert users to utilize a Windows cluster without higher skills.

5 Summary

A compact computing environment for a Windows PC cluster has been developed to assist parallel computations for molecular dynamics simulations. This system consists of server and client programs to hide complex Windows cluster dependent mechanisms from a user level application. Inter-communications between server and client parts are realized by using Java RMI. The server program is deployed on a head node of a PC cluster, while the client program runs on a client PC. Once a user sends requests for their parallel computations from a client part to a server part by using this computing environment, the server part proceeds requested operations in cooperation with the Windows cluster. In this computing environment, users can easily submit their jobs and identify job status without deep understandings about the Windows cluster. Standard output and error of running tasks are seamlessly indicated on the computing environment. After computations, we can visualize calculated results in cooperation with an existing Windows native program in a seamless manner.

As a future work, preparing a menu to choose parameters for MD simulation runs is considered. Besides, extension to other cluster systems such as a Linux-based PC cluster is considered. Furthermore, secured connection in Java RMI between client and server parts is also considered.

Acknowledgment

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