Institute for Materials Research, Tohoku University Parallel Computing & Informatics Server Manual

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Center for Computational Materials Science, Institute for Materials Research, Tohoku University

Contents

1	Outl	ine of parallel computing and informatics servers	1-3
	1.1	Specification	1-4
	1.2	Server configuration	1-4
2	Logi	in method	2-5
	2.1	Login method to visualization server	2-6
	2.2	Login method to the virtual private server	2-6
	2.2	.1 Reserving a virtual server	2-6
	2.2	.2 Login method to the virtual server	2-7
3	Outl	ine of storage	3-8
	3.1	Configuration of storage	3-9
4	Usa	ge of applications	4-11
	4.1	Applications on the visualization server	4-13
	4.1	.1 GaussView	4-14
	4.1	.2 ADF-GUI	4-16
	4.1	.3 Mathematica	4-17
	4.1	.4 AVS/Express	4-18
	4.1	.5 QuantumATK NanoLab	4-19
	4.1	.6 Molekel	4-21
	4.1	.7 MOLDEN	4-21
	4.1	.8 XCrySDen	4-22
	4.1	.9 ANSYS Mechanical CFD	4-22
	4.1	.10 VESTA	4-23
	4.2	Applications on the virtual private server	4-24
	4.2	.1 Gaussian16	4-26
	4.2	.2 GaussView	4-27
	4.2	.3 Mathematica	4-28
	4.2	.4 ANSYS Mechanical CFD	4-29
	4.2	.5 MATLAB	4-29
	4.2	.6 CRYSTAL	4-30
	4.2	.7 VASP	4-30
	4.2	.8 WIEN2k	4-31
	4.2	.9 SIESTA	4-31
	4.2	.10 ABINIT	4-31
	4.2	.11 CPMD	4-33

4.2.12 QUANTUM ESPRESSO	4-33
4.2.13 LAMMPS	4-33

1 Outline of parallel computing and informatics servers

1.1 Specification

1.2 Server configuration

1.1 Specification

The specification of the parallel computing and informatics server.

Server name	Virtual private server	Visualization server
Model name	HPE ProLiant DL360 Gen10	HPE ProLiant DL380 Gen10
Number of servers	29 servers (17 servers: For calculating)	5 servers
CPU	Intel Xeon Gold 6154 •Frequency : 3.0 GHz •Number of CPU cores : 18 Core •Number of socket : 2 Sockets/Server	Intel Xeon Gold 6140 Frequency : 2.3GHz Number of CPU cores : 18Core Number of socket : 2 Sockets/Server
Accelerator	-	-
Total amount of main memories	576 GiB/Server	576 GiB/Server

1.2 Server configuration

The configuration of the parallel computing and informatics server.

Server	Usage	Number of servers	Installation site
Virtual private server	For virtual machine	12	Center for computational materials science Room101
Visualization server	For visualizing	5	Center for computational materials science Room 101

2

2 Login method

- 2.1 Login method to visualization server
- 2.2 Login method to the virtual private server

2.1 Login method to visualization server

Log in the ssh relay server 'cms-ssh.sc.imr.tohoku.ac.jp'.

\$ ssh -l username cms-ssh.sc.imr.tohoku.ac.jp

Log in the vis of the visualization server.

\$ ssh vis

2.2 Login method to the virtual private server

2.2.1 Reserving a virtual server

Specify the following URL to log in the reservation portal. Please use Firefox or Chrome browser. Microsoft Edge and Internet Explorer are not available.

https://cms	sportal.sc.imr.tohoku.ac.jp/reservation_portal/login	
 ログイン 	× +	
← → C 🔒	https://cmsportal.sc.imr.tohoku.ac.jp/reservation_portal/login	☆ ⊖ :
	Reservation Portal LDAPID : Password : Login • Information	

You need ID and password of the supercomputing system to log in the reservation portal.

Please refer to <u>the Reservation Portal User's Manual</u> for details on how to reserve virtual servers.

When the virtual machine is ready, reservation portal will send an invitation e-mail to your entered e-mail address.

Example:

【予約管理ポータル】仮想マシン利用開始のお知らせ
username 様
ご予約頂いておりました仮想マシンが本日より利用可能となりました。
ご利用期間は
2018-06-18 ~ 2018-06-29
となります。
以下の仮想マシンがご利用になれます。
先頭マシンが SSH 接続可能となっております。
2台目以降は先頭マシンを踏み台として接続してください。
Name: RESERVE-16-000
IP: XXX.XXX.XXX XXX
User: username
PW: QyWWZAGX
初期パスワードは利用開始後に変更してください。

2.2.2 Login method to the virtual server

Log in the ssh relay server 'cms-ssh.sc.imr.tohoku.ac.jp'.

```
$ ssh -l username cms-ssh.sc.imr.tohoku.ac.jp
```

Specify the user name and IP address described in the invitation e-mail.

```
$ ssh -l username XXX.XXX.XXX.XXX
```

3 Outline of storage

3.1 Configuration of storage

3.1 Configuration of storage

The configuration of the storages in the supercomputing system is as follows.



List of storage area

Accessible machine	Area	Quota	Description
 ①Supercomputer ②Accelerator server ③Informatics server 	home/UID	500GB	This area is user's home directory and stores data of supercomputing system.
 Supercomputer Accelerator server Informatics 	work/xxx	none	 This is Lustre area. Please use the scratch if the sum of the output file exceeds 500GB. Move the necessary data to user's home directory and remove the unnecessary data from this area.
server work/scratch/ xxx none		none	This is Lustre area aimed for outputting a temporary file, such as a Gaussian. Be careful that if your file is not accessed more than one month, the file is automatically deleted.

(*)UID:user account

xxx: Any directory or file that the user has created.

(*)The files not accessed more than one month are automatically deleted in scratch area of /work.

The configuration of the storages in the virtual server is as follows.



List of storage area

Area	Quota	Description
		This area is user's home directory and local area of the
home/UID	none	virtual server. Because the capacity of this area is small,
		please use /home-nfs and /work-nfs.
home of // IID	FOOCD	This area is NFS mounted on home area used by
nome-nis/UID	200GB	supercomputer.
work-nfs	none	This area is NFS mounted on work area.

(*)UID:user account

4

4 Usage of applications

- 4.1 Applications on the visualization server
 - 4.1.1 GaussView6
 - 4.1.2 ADF-GUI
 - 4.1.3 Mathematica
 - 4.1.4 AVS/Express
 - 4.1.5 QuantumATK NanoLab
 - 4.1.6 Molekel
 - 4.1.7 MOLEDEN
 - 4.1.8 XCrySDen
 - 4.1.9 ANSYS Mechanical CFD
 - 4.1.10 VESTA

4.2 Applications on the virtual private server

- 4.2.1 Gaussian16
- 4.2.2 GaussView6
- 4.2.3 Mathematica
- 4.2.4 ANSYS Mechanical CFD
- 4.2.5 MATLAB
- 4.2.6 CRYSTAL
- 4.2.7 VASP
- 4.2.8 WIEN2k
- 4.2.9 SIESTA
- 4.2.10 ABINIT
- 4.2.11 CPMD
- 4.2.12 QUANTUM ESPRESSO
- 4.2.13 LAMMPS

4.1 Applications on the visualization server

The following applications are available on the visualization server.

#	Application	Version	Execution type
1	GaussView 6	6.0.16 6.1.1	GUI
2	ADF-GUI	2017.113 2018.105 2019.102 2019.304 2020.101	GUI
3	Mathematica	12.1.1	GUI
4	AVS/Express	8.5	GUI
5	QuantumATK NanoLab	2019.03 2019.12 2020.09	GUI
6	Molekel	5.4.0	GUI
7	MOLDEN	5.8	GUI
8	XCrySDen	1.5.60	GUI
9	ANSYS Mechanical CFD	2020R1	GUI
10	VESTA	3.4.6	GUI

The SSH terminal and X11 software are necessary on Windows. The X11 software is necessary on Macintosh.

Log in a visualization server (vis.sc.imr.tohoku.ac.jp) by using ssh command with option "-X". (Example)

\$ ssh -X -l username cms-ssh.sc.imr.tohoku.ac.jp > ssh -l username vis.sc.imr.tohoku.ac.jp

4.1.1 GaussView

Execute the commands as follows.

•6.0.16

\$ gview			
•6.1.1			
\$ gview-611			

Application window launches into screen.



The examples of reading the Gaussian input files.



4.1.2 ADF-GUI

Log in a visualization server (vis1.sc.imr.tohoku.ac.jp) by using ssh command.



Notice: The SSH terminal and X11 software are necessary on Windows. The X11 software is necessary on Macintosh.

Execute the commands as follows.

•ADF 2020.101		
\$ amsinput		
•ADF 2019.304		
\$ adfinput		
•ADF 2019.102		
\$ adfinput2019.102		
•ADF 2018.105		
\$ adfinput2018.105		
•ADF 2017.113		
<pre>\$ adfinput2017.113</pre>		

Application window launches into screen.

ADFinput			
🔫 <u>F</u> ile <u>E</u> dit <u>S</u> elect <u>A</u> toms <u>B</u> onds <u>V</u> iew <u>H</u> elp			
	ADF Main Model	l Properties Details MultiLeve	al Q
	Title:		
	Preset:	Single Point	
	Task:	SinglePoint	
	Total charge:	0.0	
	Unrestricted:	T Yes	
	XC functional:	LDA 🔻	
	Relativity (ZORA):	None	
	Basis set:	DZ v	
	Frozen core:	Large 🔻	
	Numerical quality:	Normal	

4.1.3 Mathematica

Please contact us if you want use Mathematica on your PC.

Execute the commands as follows.

\$ Mathematica

Application window launches into screen.



Note:

On the first execution of Mathematica, the activation window may appear.

Wolfram Product Activation	
WOLFRAM MATHEMATICA	
Connect to a Network License Server Enter the name or IP address of the computer running the MathLM license server. Server name 10.1.0.2	
Cancel Other ways to activate	Activate

Enter the license server's IP address 10.1.0.2 and push 'Activate' button for the activation. If you cannot enter IP address in the field, push 'other ways to activate' button, select 'network license' as authorization method, and enter the license server's IP address.

4.1.4 AVS/Express

Please contact us if you want to use it on your PC.

In the case developing applications using AVS, execute the commands as follows.

\$ express -mavs -nohw

In the case not developing application but only use GUI, execute the commands as follows.

\$ express.static -mavs -nohw

Application window launches into screen.

X AVS/Express - /usr/local/app/e	express/current		- • •
<u>File Edit Object Project</u>	Journal <u>UI</u> Builder Options A <u>V</u> S	Compat	<u>H</u> elp
🗖 Libraries 🛛 Start	-		
Libraries Start Whats New (AdvectBoth) (BackgroundTextu) (Read OBJ Textu) (Set Zero) Applications	Data Import ImportWizard Read Field AvS/Express Choose initial a Application type Single-window DataViewer Multi-window DataViewer Application Module Stack Scratch Pad Load Application None	ion View Export (Output/VPS) (Output/VPS) (Output/VRML) (Output/VRML) (Output/VRML) Viewer type 3D 2D 3D and 2D None	Demonstrations Solar System Climate FlightPath Image2Volume VolumeShells
	Add Data Import Wizard to appli Add Data Visualization Wizard to	cation b application	
	☐ Set project's default application Use Project->Save As to create a	writable project	

4.1.5 QuantumATK NanoLab

Please contact us if you want to use it on your Windows PC.

Execute the commands as follows.

•2020.09

\$ quantumatk

•2019.12

\$ /usr/local/app/QuantumATK/QuantumATK-Q-2019.12/bin/quantumatk

•2019.03

\$ /usr/local/app/QuantumATK/QuantumATK-P-2019.03/bin/quantumatk

Application window launches into screen.

🥝 Open Project			×
	Filter		
QuantumATK	Tide	Path	Last opened 🔺
	Example Project - 2018.06	/home/hitacse/.vnl/example_project_20.	. 2018-07-03
Synopsys:			
QuantumATK			
Synopsys. All rights reserved.			
✓ Show on startup	Open Classic V	icw <u>R</u> emove Create <u>N</u> ew	Quit QuantumATK



4.1.6 Molekel

Execute the commands as follows.

\$ molekel

Application window launches into screen.

🏘 Molekel	- • •
<u>File</u> <u>Edit</u> Display Interaction Animation Surfaces Analysis View	<u>H</u> clp
🔁 🖟 🕺 🖉 🖉 🐨 🕷 🔛 🔛 🔤 🖉 🐨 🖉 🐨	
Workspace X	
L Molecules	
Molecule Properties	
Property Value Title:	
Atoms:	
Number of Frames:	
Bonds:	
Non-H bonds:	
Residues:	
	1

4.1.7 MOLDEN

Execute the commands as follows.

\$ molden

Application window launches into screen.



4.1.8 XCrySDen

Execute the commands as follows.

\$ xcrysden

Application window launches into screen.



4.1.9 ANSYS Mechanical CFD

Please contact us if you want use Mathematica on your PC.

Execute the commands as follows.



Application window launches into screen.

ANSYS Mechanic	cal APDL Product Launche	r [Profile: *** Last ANSYS Ru	n ***] Hostname: app13		
	Simulation Environments ANSYS License: ANSYS Multiphysics		Add-on	Modules N.A. (-DYN)	
File Management	Customization/ / Preferences	ligh Performance Computing Setup			
	Working Directory:	Avork/ansys		Browse	
	Job Name:	die		Browse	
	Run	Cancel Run	Queue	Product Help]

4.1.10 VESTA

Execute the commands as follows.

\$ VESTA-gui

Application window launches into screen.



4.2 Applications on the virtual private server

The following applications are available on the virtual private server.

#	Application	Version	Execution type
1	Gaussian 16	Rev B.01 Rev C.01	SMP
2	GaussView 6	6.0.16	GUI
3	Mathematica	12.1.1	GUI
4	ANSYS Mechanical CFD	2020R1	GUI
5	MATLAB	R2020a	GUI
6	Crystal	17	MPI SMP
7	VASP	4.6 5.4	MPI
8	WIEN2k	17.1 19.1	SMP
9	SIESTA	4.0	MPI
10	ABINIT	8.8.2 8.10.3	MPI
11	CPMD	4.1 4.3	MPI
12	Quantum Espresso	6.2.1 6.4.1	MPI
13	LAMMPS	31 Mar 2017 5 Jun 2019	MPI

The SSH terminal and X11 software are necessary on Windows. The X11 software is necessary on Macintosh.

Log in a virtual server by using ssh command with option "-X".

(Example)



* XX.XX.XX.XX: IP address of the virtual server

4.2.1 Gaussian16

Available executables

Version	Settings
B.01	source /work/app/Gaussian/g16.profile
C.01	source /work/app/Gaussian/C.01/g16.profile

Prepare input files of Gaussian 16(***.com) in the working directory.

The following input file calculates geometry optimization for hexacarbonyl. It specifies Hartree-Fock method and 3-21G basis set.

(Example)

\$ ls -l /usr/local/app/Gaussian/example.com
-rw-r--r- 1 root root 420 Jul 12 16:33 /usr/local/app/Gaussian/example.com

•The number of threads

Specify 'CPU=0-N' in the input file for parallelization. In the case of 'NProc=N is specified, the job cannot run in parallel normally.

(Example) CPU=0-31

Execute the commands as follows.

```
source /usr/local/app/Gaussian/g16.profile
g16 input file
```

(Example)

source /usr/local/app/Gaussian/g16.profile
g16 test0000.com

4.2.2 GaussView

Execute the commands as follows.

\$ gview

Application window launches into screen.



The examples of reading the Gaussian input files.



4.2.3 Mathematica

Please contact us if you want to use it on your PC.

Execute the commands as follows.

\$ Mathematica

Application window launches into screen.



Note:

On the first execution of Mathematica, the activation window may appear.

Wolfram Product Activation	
WOLFRAM MATHEMATICA	
Connect to a Network License Server Enter the name or IP address of the computer running the MathLM license server.	
Server name 10.1.0.2	
Cancel Other ways to activate	Activate

Enter the license server's IP address 10.1.0.2 and push 'Activate' button for the activation. If you cannot enter IP address in the field, push 'other ways to activate' button, select 'network

license' as authorization method, and enter the license server's IP address.

4.2.4 ANSYS Mechanical CFD

Please contact us if you want use Mathematica on your PC.

Execute the commands as follows.

\$ launcher

Application window launches into screen.



4.2.5 MATLAB

Please contact us if you want use MATLAB on your PC.

Execute the commands as follows.

\$ matlab

Application window launches into screen.

MATLAB				
HOME PLOTS APPS			8 1 1 1 5 6 5 0 %	arch Documentation 🛛 🔎 🛣
New Open Dicestration San Data Works	New Variable Open Variable	Oreferences Layout St Path ENVIRONM DAT	Community Help Add-Ons • RISOURCES	
	(م •
Name Size Date Modif / Tyme	Command Window			() ()
	Academic License			
Details ^				
Workspace 💿				
Name c. Yalut				
Ready				

4.2.6 CRYSTAL

Execute the commands as follows.

```
source /usr/local/app/Crystal/current/utils17/cry17.bashrc
runmpi17 MPI tasks input file
```

(Example)

```
source /usr/local/app/Crystal/current/utils17/cry17.bashrc
runmpi17 2 test11
```

4.2.7 VASP

VASP is available for users who have a license. If you have the license and want to use VASP, contact <u>our center</u>. After checking the license, VASP is ready for you.

Available executables

Version	Path
VASP4.6.36	/usr/local/app/VASP4/current/vasp
VASP4.6.36 Gamma point ver.	/usr/local /app/VASP4/vasp.4.6_gamma/vasp
VASP5.4.4 Standard ver.	/usr/local /app/VASP5/current/bin/vasp_std
VASP5.4.4 Gamma point ver.	/usr/local /app/VASP5/current/bin/vasp_gam
VASP5.4.4 non-collinear ver.	/usr/local /app/VASP5/current/bin/vasp_ncl

Execute the commands as follows.

```
mpirun [ -np MPI total tasks ][-ppn MPI tasks per node ] -hostfile hostfile
$ /usr/local/app/VASP4/current/vasp
```

(Example)

mpirun -np 2 -hostfile hostfile /usr/local/app/VASP4/current/vasp

4.2.8 WIEN2k

WIEN2k is available for users who have a license. If you have the license and want to use WIEN2k, contact <u>our center</u>. After checking the license, WIEN2k is ready for you.

Available executables

Version	Path
17.1	/work/app/WIEN2k/current
19.1	/work/app/WIEN2k/WIEN2k_19.1

Execute the commands as follows.

```
export SCRATCH=/work-nfs/$USER/scratch
export WIENROOT=/usr/local/app/WIEN2k/current
export PATH=$WIENROOT:$PATH
```

wien2k Script Option

(Example)

```
export SCRATCH=/work-nfs/$USER/scratch
export WIENROOT=/usr/local/app/WIEN2k/current
export PATH=$WIENROOT:$PATH
```

```
run_lapw -cc 0.0001 -NI
```

4.2.9 SIESTA

Execute the commands as follows.

mpirun [-np MPI total tasks | -ppn MPI tasks per node] -hostfile hostfile
/usr/local/app/SIESTA/current/Obj/siesta < input file > output file

(Example)

```
mpirun -np 2 -hostfile hostfile /usr/local/app/SIESTA/current/Obj/siesta <
input.fdf > siesta.out
```

4.2.10 ABINIT

Available executables

Version	Path
8.8.2	/usr/local/app/ABINIT/current/src/98_main/abinit
8.10.3	/usr/local/app/ABINIT/abinit-8.10.3/src/98_main/abinit

Execute the commands as follows.

mpirun [-np MPI total tasks | -ppn MPI tasks per node] -hostfile hostfile
/usr/local/app/ABINIT/current/src/98_main/abinit < input file</pre>

(Example)

mpirun -np 2 -hostfile hostfile

/usr/local/app/ABINIT/current/src/98_main/abinit < input.files</pre>

4.2.11 CPMD

CPMD is available for users who have own license.

To use CPMD, obtain the license on <u>CPMD web site</u> and contact our center.

After checking the license, CPMD is ready for you.

Available executables

Version	Path
4.1	/usr/local/app/CPMD/current
4.3	/usr/local/app/CPMD/CPMD4.3

Execute the commands as follows.

mpirun [-np MPI total tasks][-ppn MPI tasks per node] -hostfile hostfile
/usr/local/app/QuantumESPRESSO/current/bin/pw.x < input file > output file

(Example)

mpirun -np 2 -hostfile hostfile

/usr/local/app/QuantumESPRESSO/current/bin/pw.x < cluster4.in > qe.out

4.2.12 QUANTUM ESPRESSO

Available executables

Version	Path
6.2.1	/usr/local/app/QuantumESPRESSO/current
6.4.1	/usr/local/app/QuantumESPRESSO/qe-6.4.1

Execute the commands as follows.

mpirun [-np MPI total tasks][-ppn MPI tasks per node] -hostfile hostfile
/usr/local/app/QuantumESPRESSO/current/bin/pw.x < input file > output file

(Example)

mpirun -np 2 -hostfile hostfile
/usr/local/app/QuantumESPRESSO/current/bin/pw.x < cluster4.in > qe.out

4.2.13 LAMMPS

Available executables

Version	Path
31 Mar 17	/usr/local/app/ LAMMPS/current
5 Jun 19	/usr/local/app/ LAMMPS/lammps-5Jun19

Execute the commands as follows.

mpirun [-np MPI total tasks][-ppn MPI tasks per node] -hostfile hostfile
/usr/local/app/LAMMPS/current/src/lmp_intel_cpu_intelmpi < input file > output
file

(Example)

mpirun -np 2 -hostfile hostfile
/usr/local/app/LAMMPS/current/src/lmp_intel_cpu_intelmpi < in.ij > lammps.out