

**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**

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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

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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.

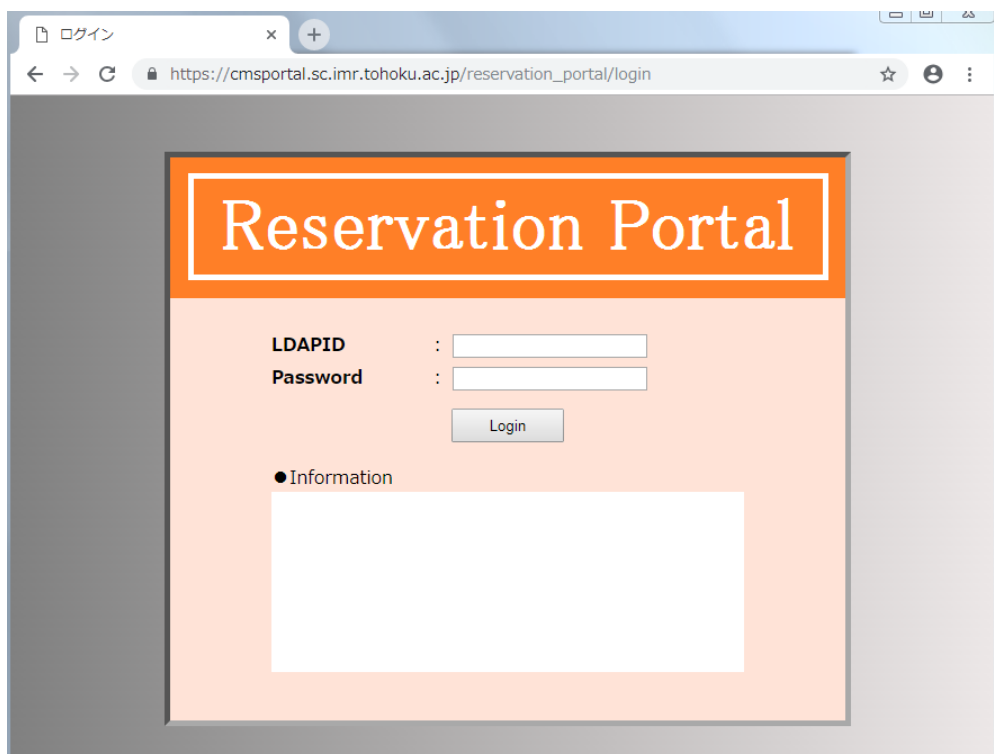
```
$ ssh vis
```

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://cmsportal.sc.imr.tohoku.ac.jp/reservation\_portal/login
```



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

Please refer to [the Reservation Portal User's Manual](#) 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
```

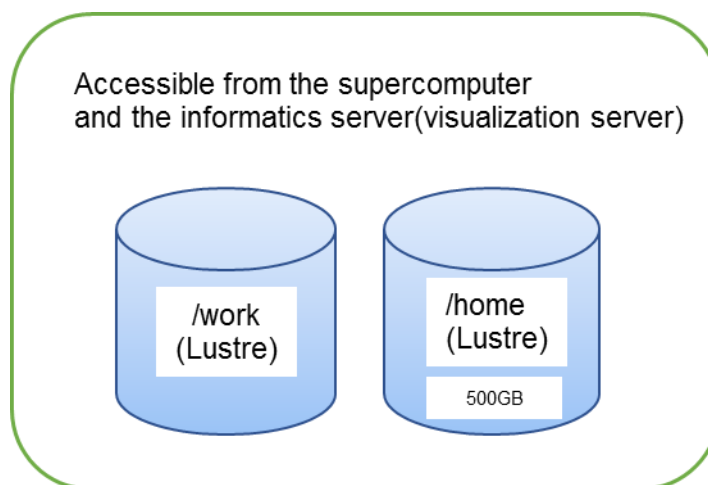
3

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

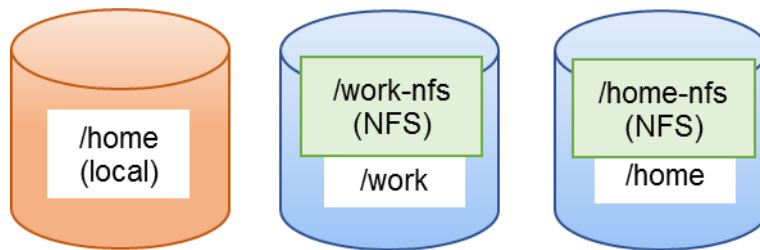
Accessible machine	Area	Quota	Description
①Supercomputer ②Accelerator server ③Informatics server	/home/UID	500GB	This area is user's home directory and stores data of supercomputing system.
①Supercomputer ②Accelerator server ③Informatics server	/work/xxx	none	This is Lustre area. Please use the scratch 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.
	/work/scratch/xxx	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
/home/UID	none	This area is user's home directory and local area of the virtual server. It has a small capacity, and will be deleted after the virtual server usage period ends. Therefore, please use /home-nfs and /work-nfs.
/home-nfs/UID	500GB	This area is NFS mounted on home area used by supercomputer.
/work-nfs	none	This area is NFS mounted on work area.

(*)UID : user account

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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 2021.102 2021.106 2022.103 2023.103	GUI
3	Mathematica	13.2.1	GUI
4	AVS/Express	8.5	GUI
5	QuantumATK NanoLab	2019.03 2019.12 2020.09 2021.06 2021.06-SP2 2022.03 2022.12-SP1	GUI
6	Molekel	5.4.0	GUI
7	MOLDEN	5.8	GUI
8	XCrySDen	1.5.60	GUI
9	ANSYS Mechanical CFD	2020R1 2021R1 2021R2 2022R2	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.

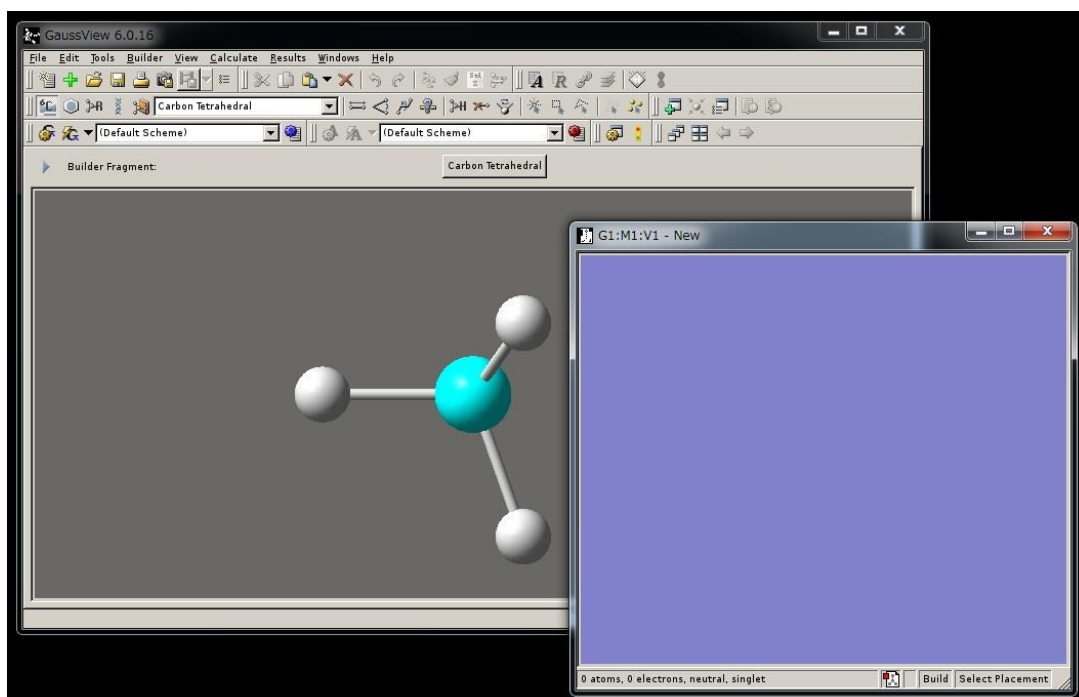
•6.0.16

```
$ gview
```

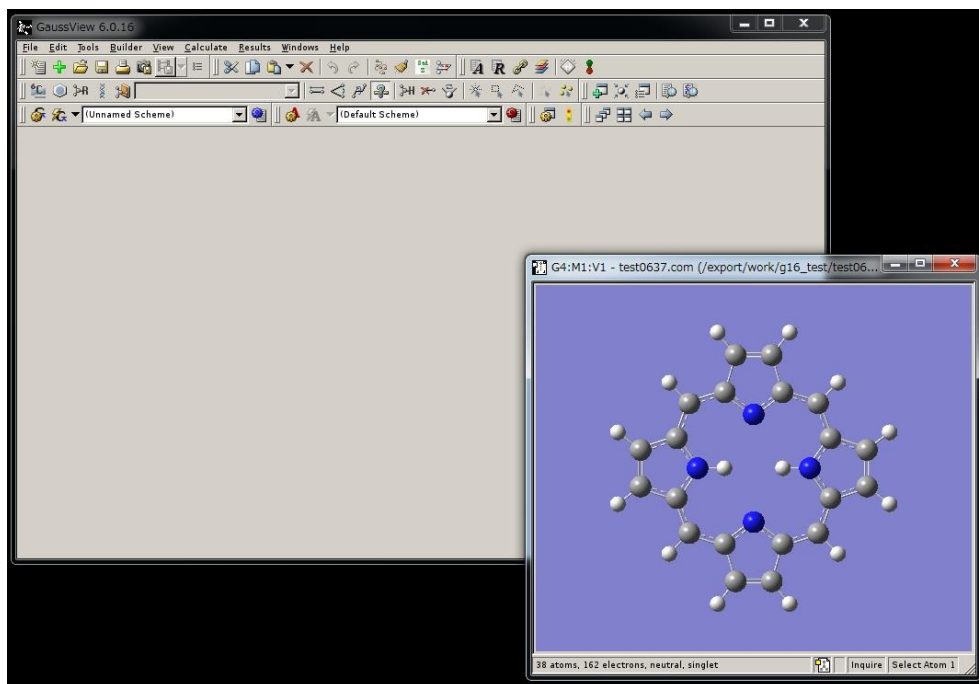
•6.1.1

```
$ gview-611
```

Application window launches into screen.



The examples of reading the Gaussian input files.



4.1.2 ADF-GUI

ADF will be available only to authorized users.

Please contact [our center](#) if you would like to use ADF.

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

(Example)

```
$ ssh -X -l username cms-ssh.sc.imr.tohoku.ac.jp  
> ssh -l username vis1.sc.imr.tohoku.ac.jp
```

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

Execute the commands as follows.

•ADF 2023.103

```
$ amsinput
```

•ADF 2022.103

```
$ amsinput2022.103
```

•ADF 2021.106

```
$ amsinput2021.106
```

•ADF 2021.102

```
$ amsinput2021.102
```

•ADF 2020.101

```
$ amsinput2020.101
```

•ADF 2019.304

```
$ adfinput
```

•ADF 2019.102

```
$ adfinput2019.102
```

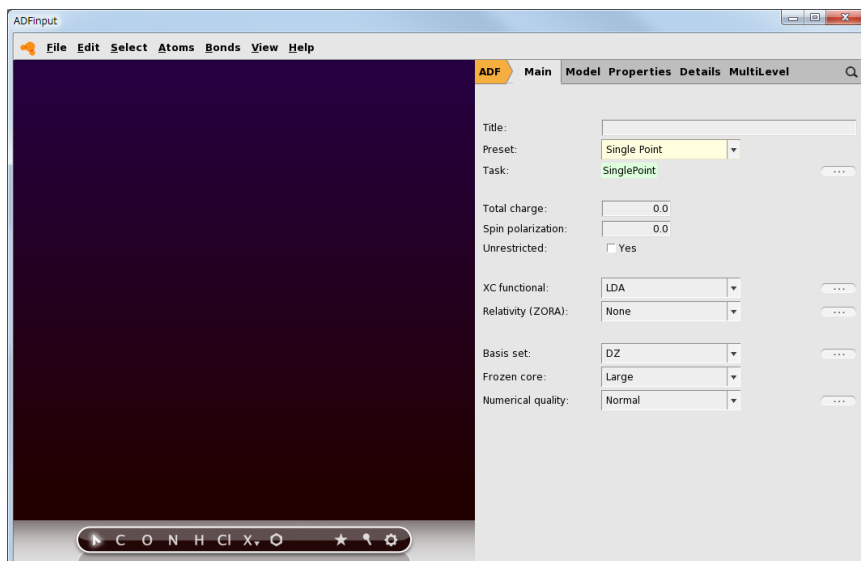
•ADF 2018.105

```
$ adfinput2018.105
```

•ADF 2017.113

```
$ adfinput2017.113
```

Application window launches into screen.



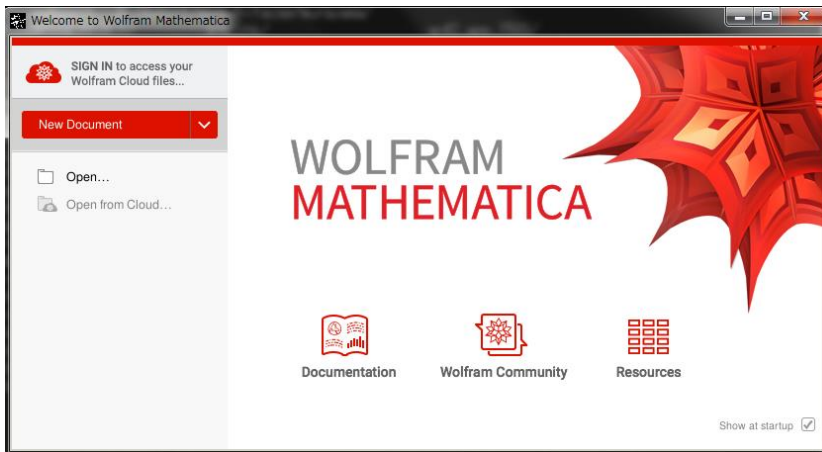
4.1.3 Mathematica

Please contact [us](#) if you want use Mathematica on your PC.

Execute the commands as follows.

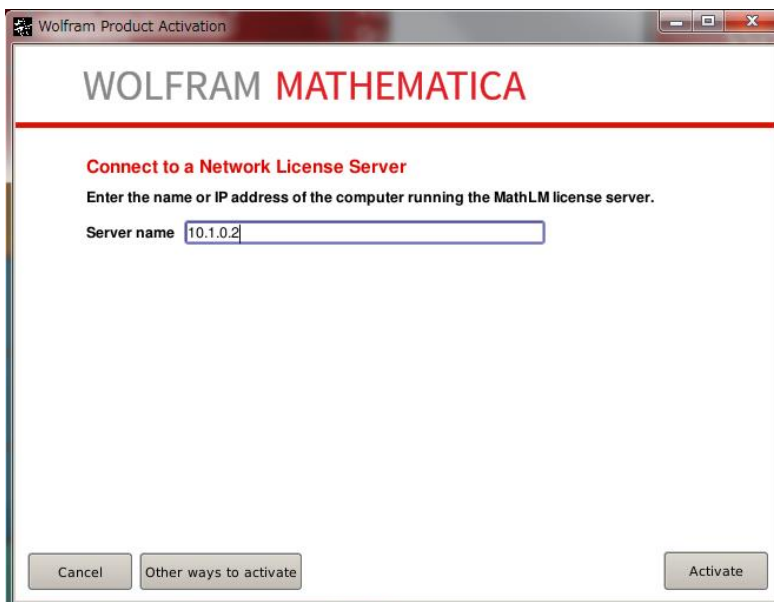
```
$ Mathematica
```

Application window launches into screen.



Note:

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



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.

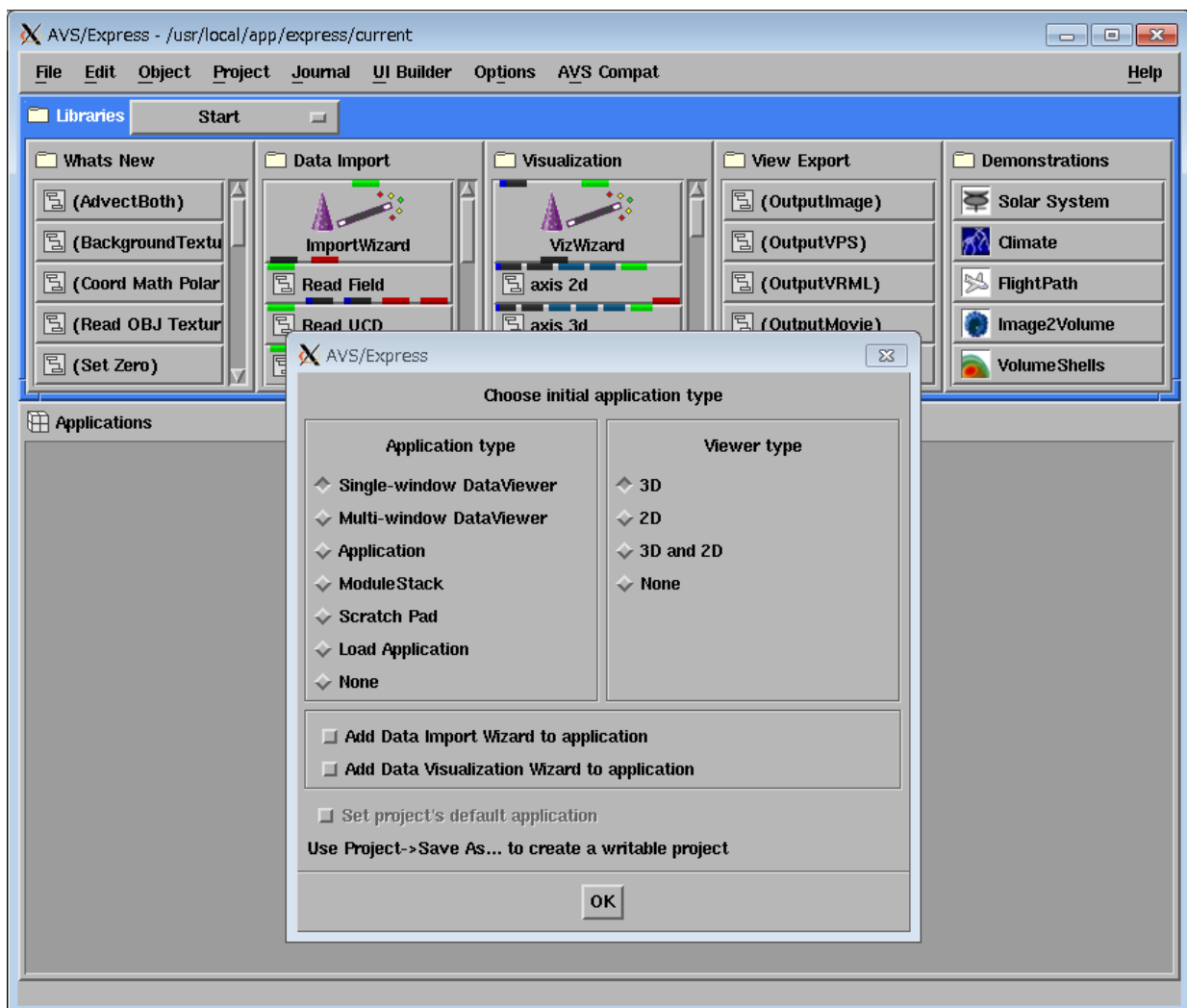
In the case developing applications using AVS, execute the commands as follows.

```
$ 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.



4.1.5 QuantumATK NanoLab

Please contact [us](#) if you want to use it on your Windows PC.

Execute the commands as follows.

•2022.12-SP1

```
$ quantumatk
```

•2022.03

```
$ /usr/local/app/QuantumATK/QuantumATK-T-2022.03/bin/quantumatk
```

•2021.06-SP2

```
$ /usr/local/app/QuantumATK/QuantumATK-S-2021.06-SP2/bin/quantumatk
```

•2021.06

```
$ /usr/local/app/QuantumATK/QuantumATK-S-2021.06/bin/quantumatk
```

•2020.09

```
$ /usr/local/app/QuantumATK/QuantumATK-R-2020.09/bin/quantumatk
```

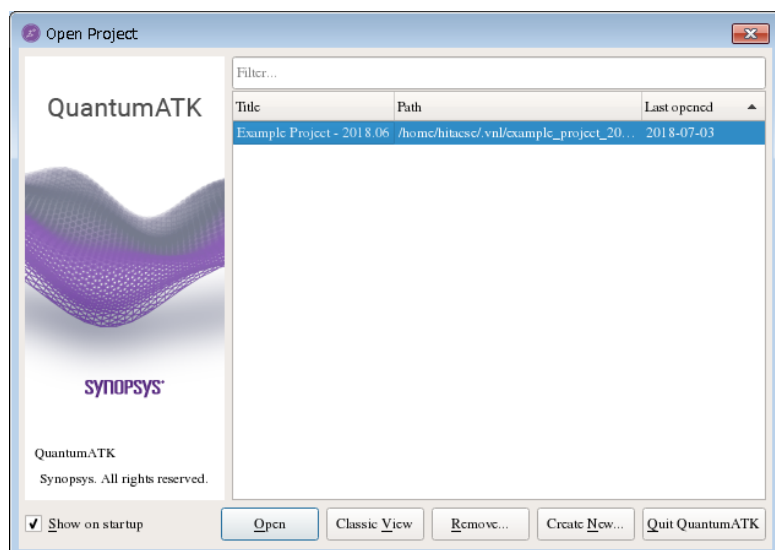
•2019.12

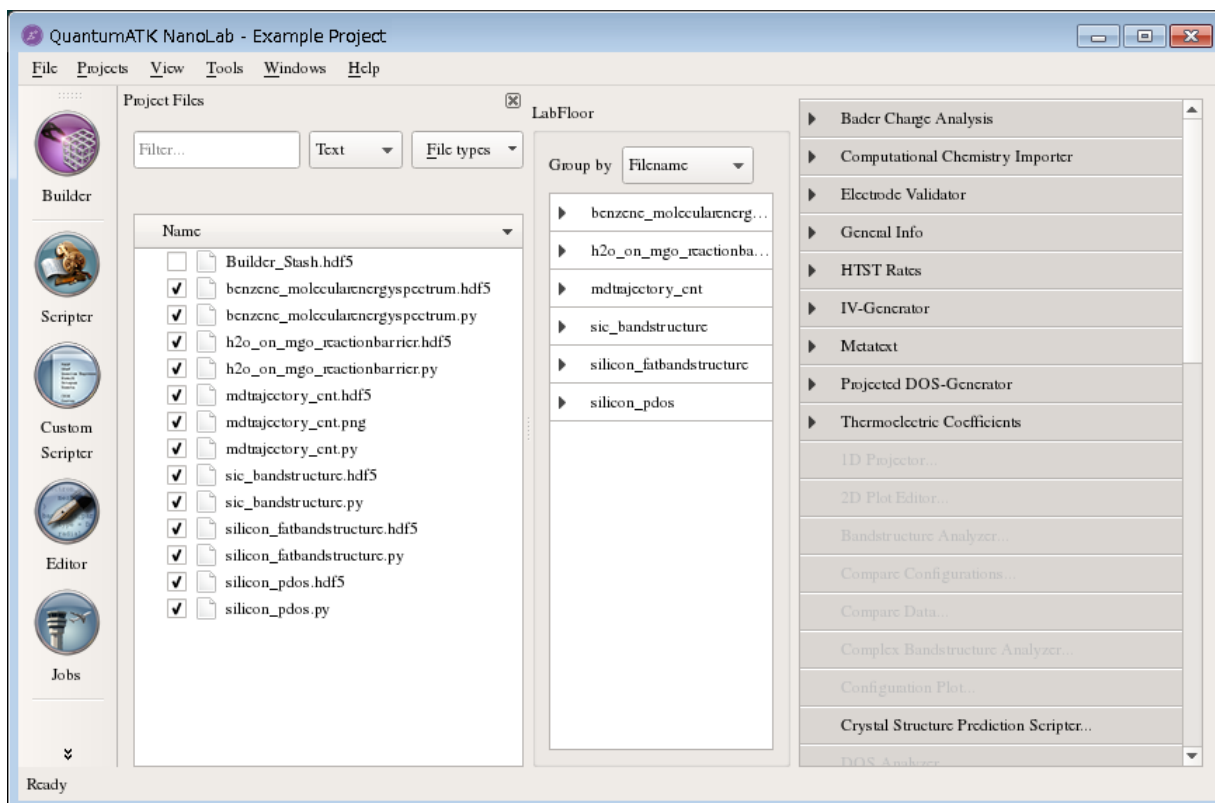
```
$ /usr/local/app/QuantumATK/QuantumATK-Q-2019.12/bin/quantumatk
```

•2019.03

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

Application window launches into screen.



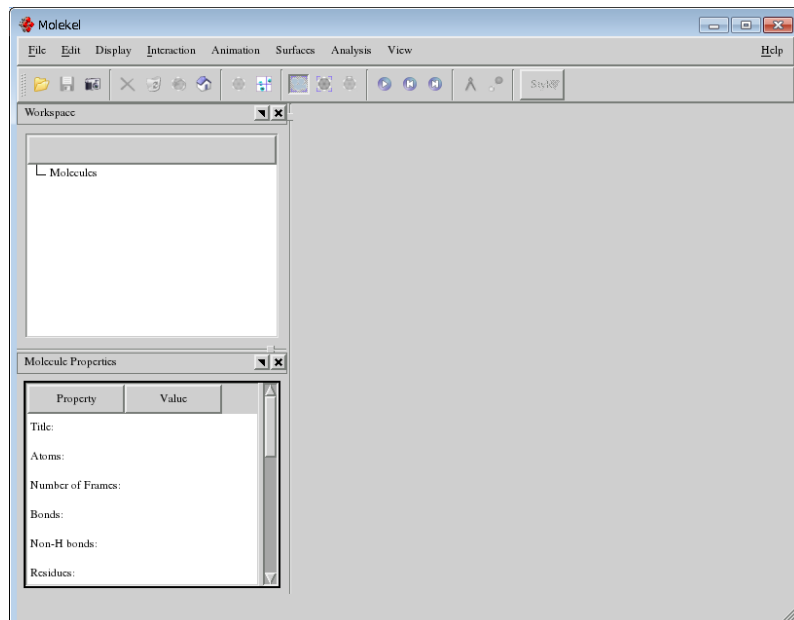


4.1.6 Molekel

Execute the commands as follows.

```
$ molekel
```

Application window launches into screen.

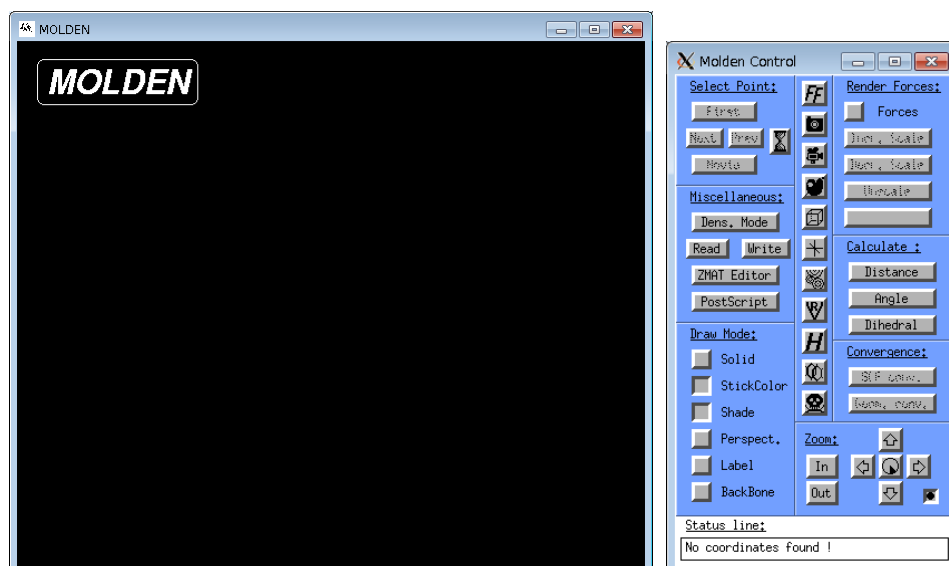


4.1.7 MOLDEN

Execute the commands as follows.

```
$ molden
```

Application window launches into screen.

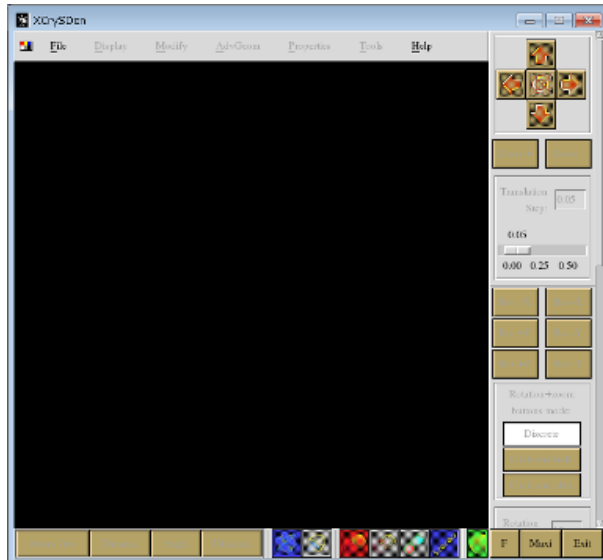


4.1.8 XCrySDen

Execute the commands as follows.

```
$ xcrysdn
```

Application window launches into screen.



4.1.9 ANSYS Mechanical CFD

Please contact [us](#) if you want to use it on your PC.

Execute the commands as follows.

•2022R2

```
$ /usr/local/app/ansys/v222/ansys/bin/launcher
```

•2021R2

```
$ launcher
```

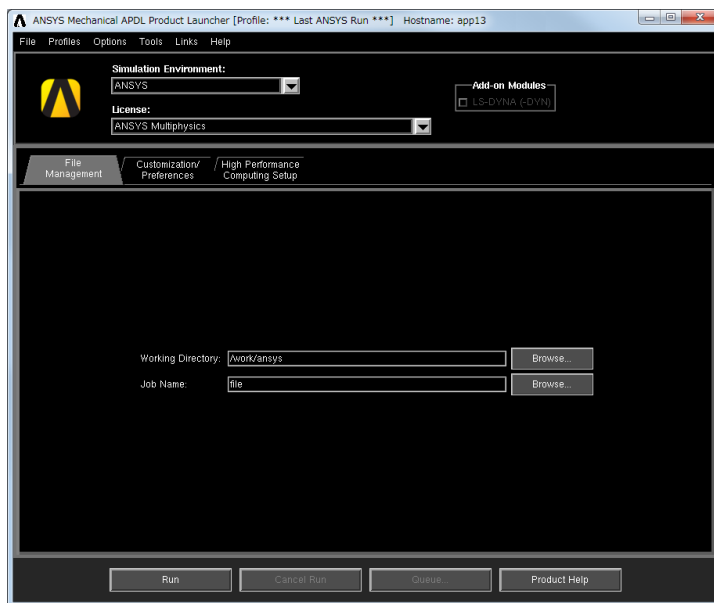
•2021R1

```
$ /usr/local/app/ansys/v211/ansys/bin/launcher
```

•2020R1

```
$ /usr/local/app/ansys/v201/ansys/bin/launcher
```

Application window launches into screen.

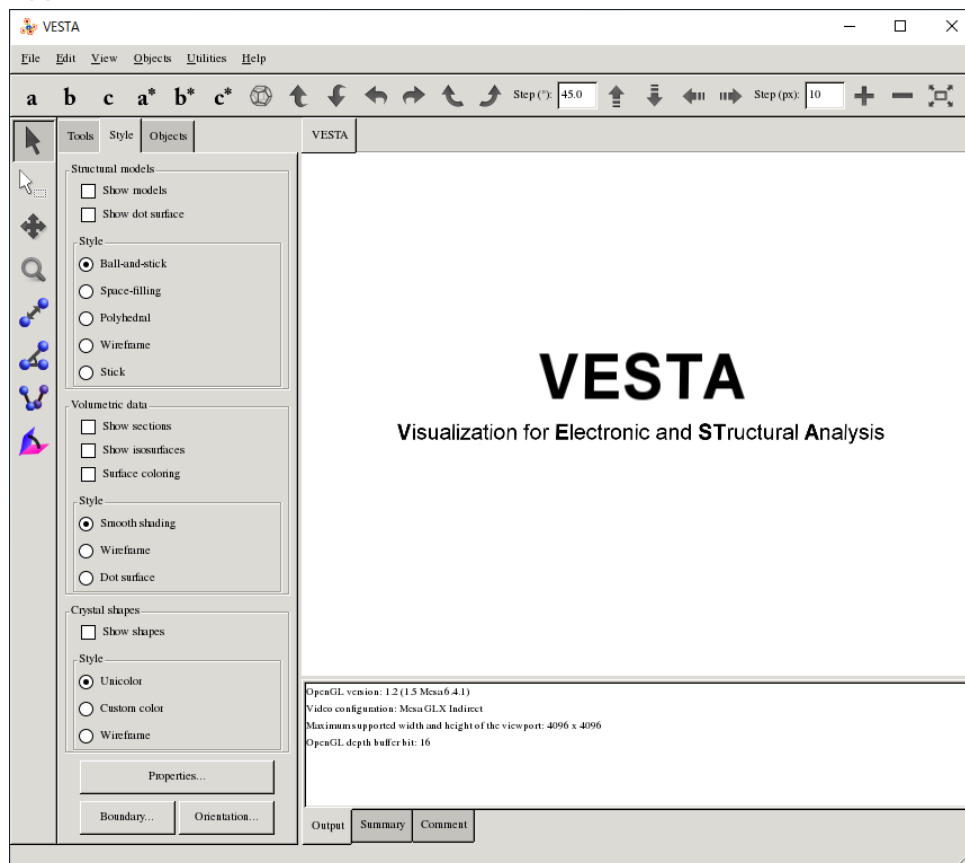


4.1.10 VESTA

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	13.2.1	GUI
4	ANSYS Mechanical CFD	2022R2	GUI
5	MATLAB	R2020a R2021a	GUI
6	Crystal	17	MPI SMP
7	VASP	4.6 5.4 6.2.1	MPI
8	WIEN2k	17.1 19.1	SMP
9	SIESTA	4.0 4.1.5	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)

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

* 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)

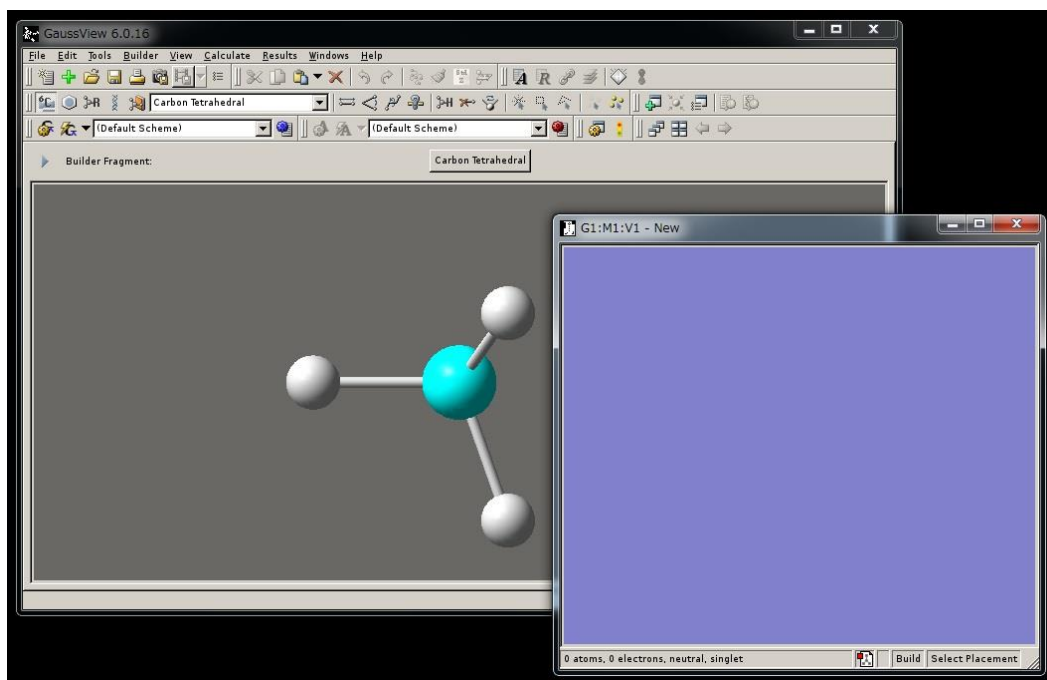
```
source /usr/local/app/Gaussian/g16.profile
g16 test0000.com
```

4.2.2 GaussView

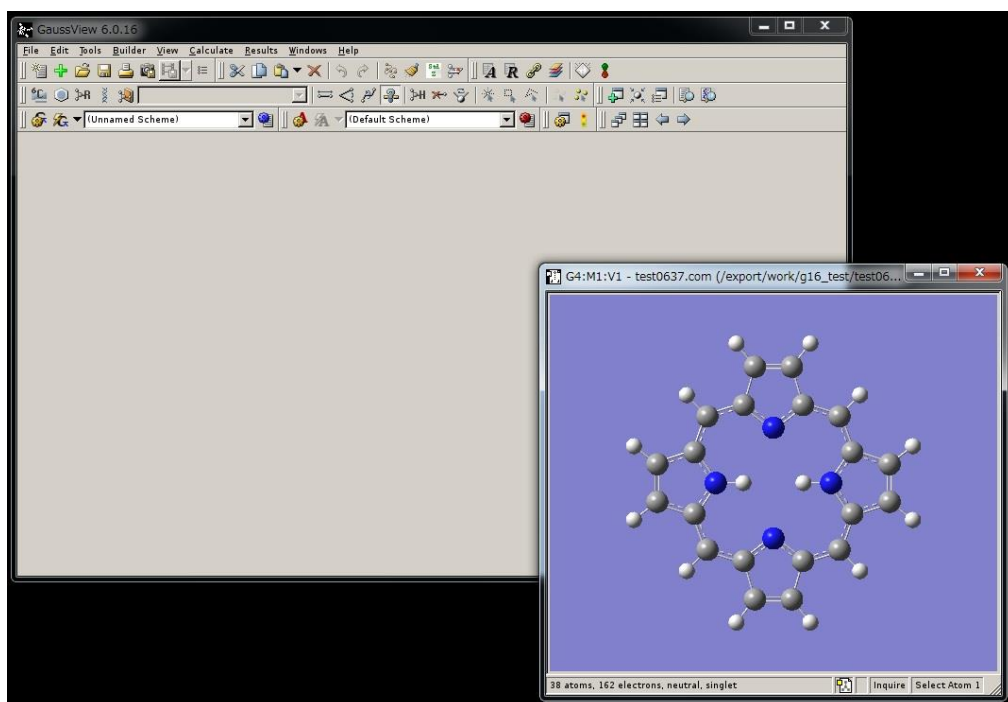
Execute the commands as follows.

```
$ gview
```

Application window launches into screen.



The examples of reading the Gaussian input files.



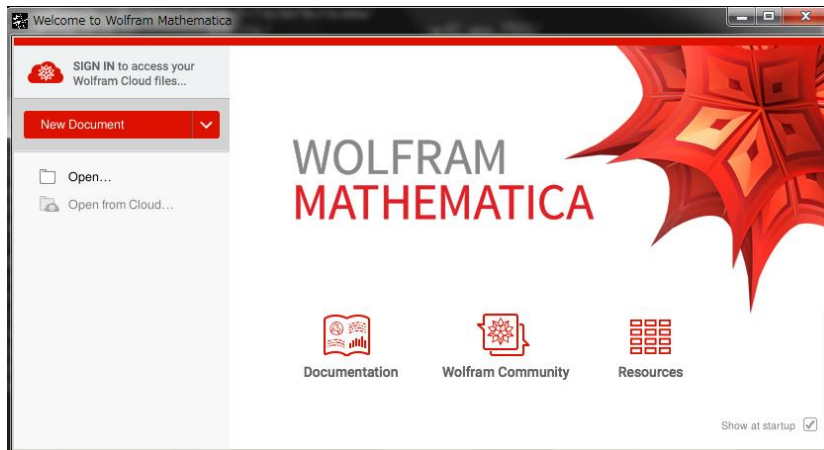
4.2.3 Mathematica

Please contact [us](#) if you want to use it on your PC.

Execute the commands as follows.

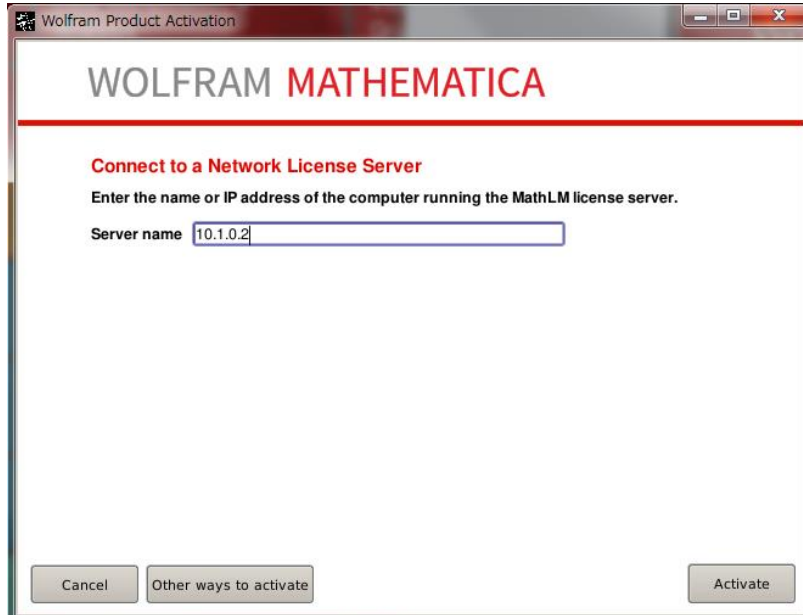
```
$ Mathematica
```

Application window launches into screen.



Note:

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



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

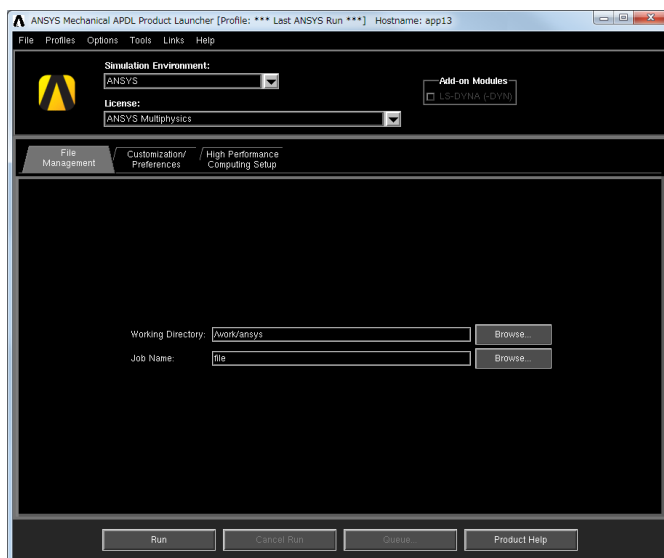
Please contact [us](#) if you want to use it on your PC.

Execute the commands as follows.

•2022R2

\$ launcher

Application window launches into screen.



4.2.5 MATLAB

Please contact [us](#) if you want to use it on your PC.

Execute the commands as follows.

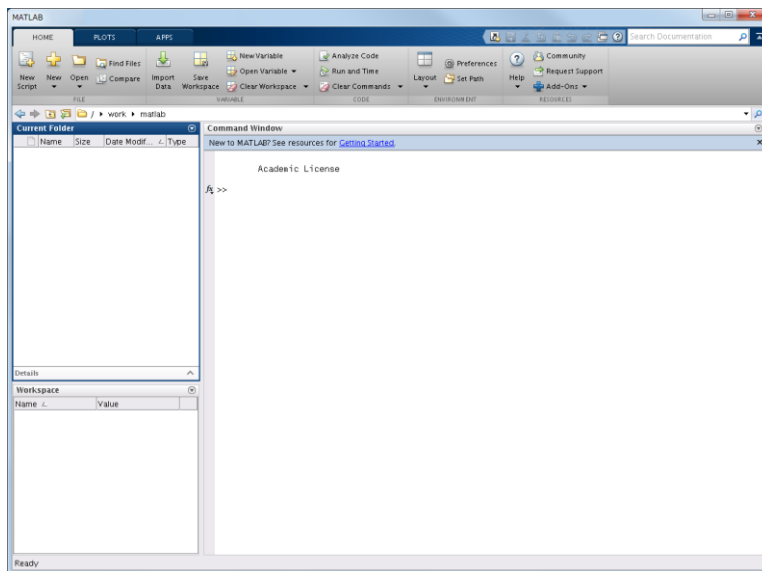
•R2021a

```
$ matlab
```

•R2020a

```
$ /usr/local/app/matlab/R2020a/bin/matlab
```

Application window launches into screen.



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 [our center](#). 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
VASP6.2.1 Standard ver.	/usr/local/app/VASP6/current/bin/vasp_std
VASP6.2.1 Gamma point ver.	/usr/local/app/VASP6/current/bin/vasp_gam
VASP6.2.1 non-collinear ver.	/usr/local/app/VASP6/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 [our center](#). 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

Available executables

Version	Path
4.0	/usr/local/app/SIESTA/current/Obj/siesta
4.1.5	/usr/local/app/SIESTA/siesta-4.1.5/Obj/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
```

(Example)

```
mpirun -np 2 -hostfile hostfile  
/usr/local/app/ABINIT/current/src/98_main/abinit < input.files
```

4.2.11 CPMD

Please contact [our center](#) if you would like to use CPMD.

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 > lammeps.out
```