# 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

# 1 Outline of parallel computing and informatics servers

## 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<br>(17 servers: For calculating) | 5 servers |
| CPU | Intel Xeon Gold 6154<br>・Frequency ： 3.0 GHz<br>・Number of CPU cores :<br>18 Core<br>・Number of socket :<br>2 Sockets/Server | Intel Xeon Gold 6140<br>・Frequency : 2.3GHz<br>・Number of CPU cores :<br>18Core<br>・Number of socket :<br>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

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.

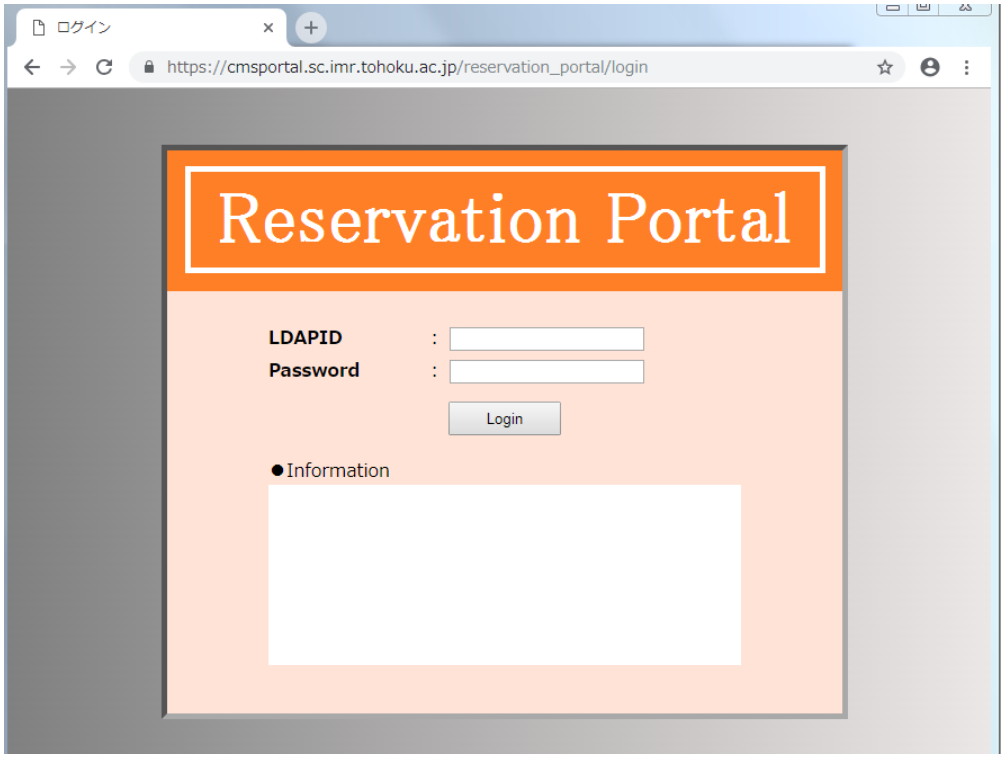
```
$ ssh vis
```

## 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
```

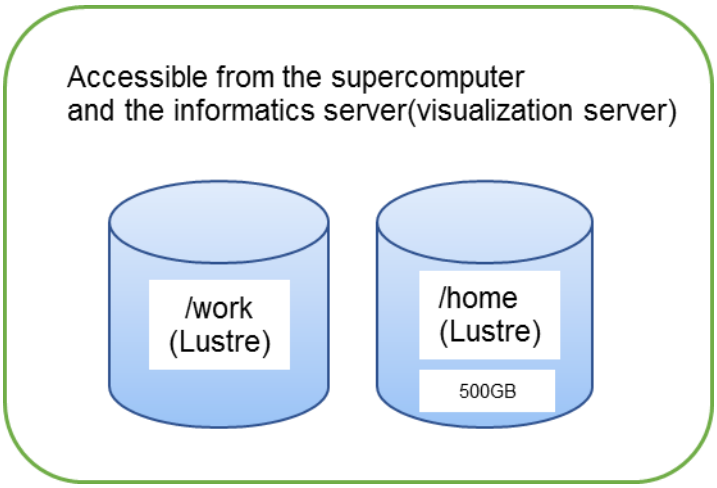
# 3

# 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

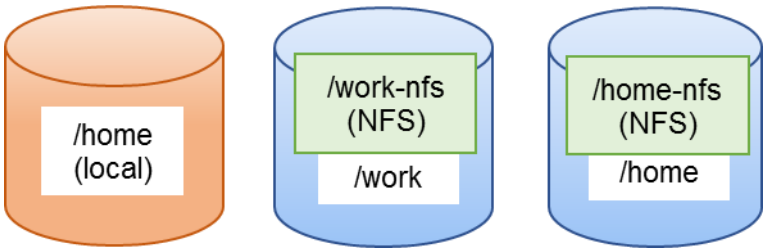
| Accessible machine | Area | Quota | Description |
|---|---|---|---|
| ①Supercomputer<br>②Accelerator server<br>③Informatics server | home/UID | 500GB | This area is user's home directory and stores data of supercomputing system. |
| ①Supercomputer<br>②Accelerator server<br>③Informatics server | work/xxx | none | This is Lustre area.<br>Please use the scratch if the sum of the output file exceeds 500GB.<br>Move the necessary data to user's home directory<br>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.<br>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. Because the capacity of this area is small, 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

# 4

# 4 Usage of applications

## 4.2 Applications on the virtual private server

## 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<br>6.1.1 | GUI |
| 2 | ADF-GUI | 2017.113<br>2018.105<br>2019.102<br>2019.304<br>2020.101 | GUI |
| 3 | Mathematica | 12.1.1 | GUI |
| 4 | AVS/Express | 8.5 | GUI |
| 5 | QuantumATK NanoLab | 2019.03<br>2019.12<br>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.

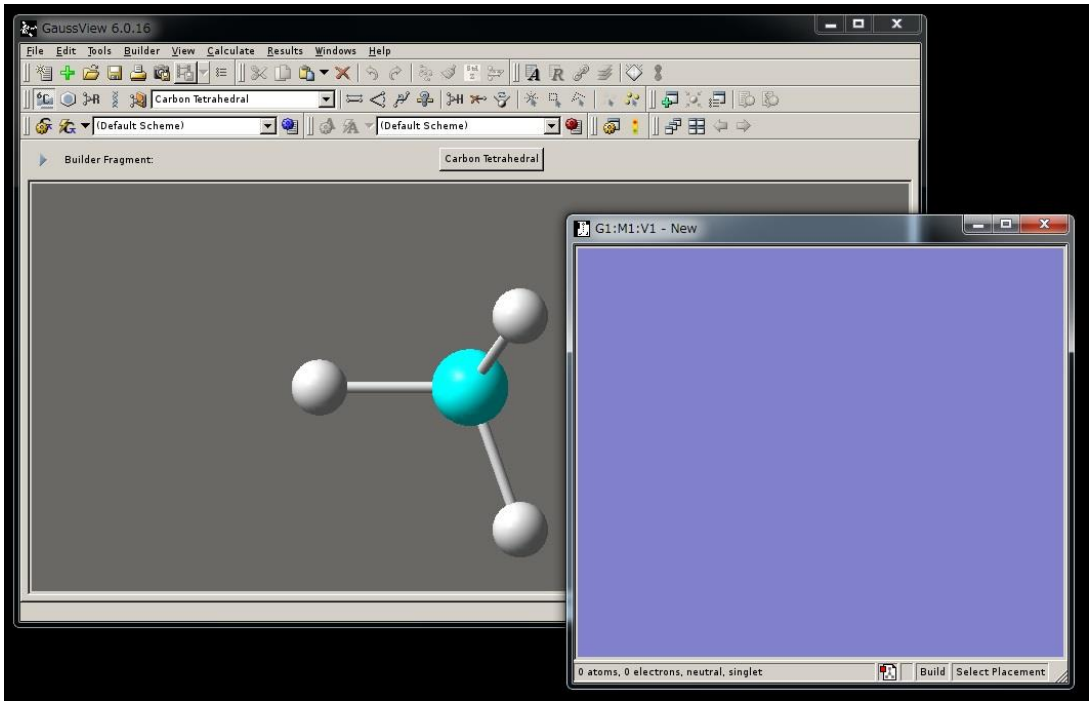
・6.0.16

```
$ gview
```

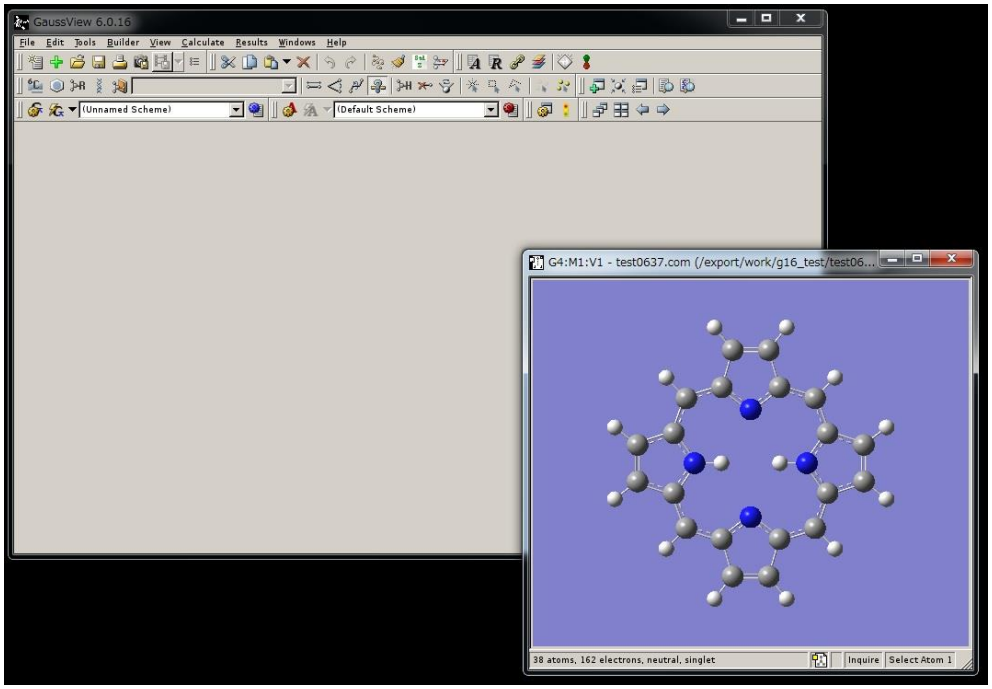
・6.1.1

```
$ 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.

(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 2020.101

```
$ amsinput
```

・ADF 2019.304

```
$ adfinput
```

・ADF 2019.102

```
$ adfinput2019.102
```

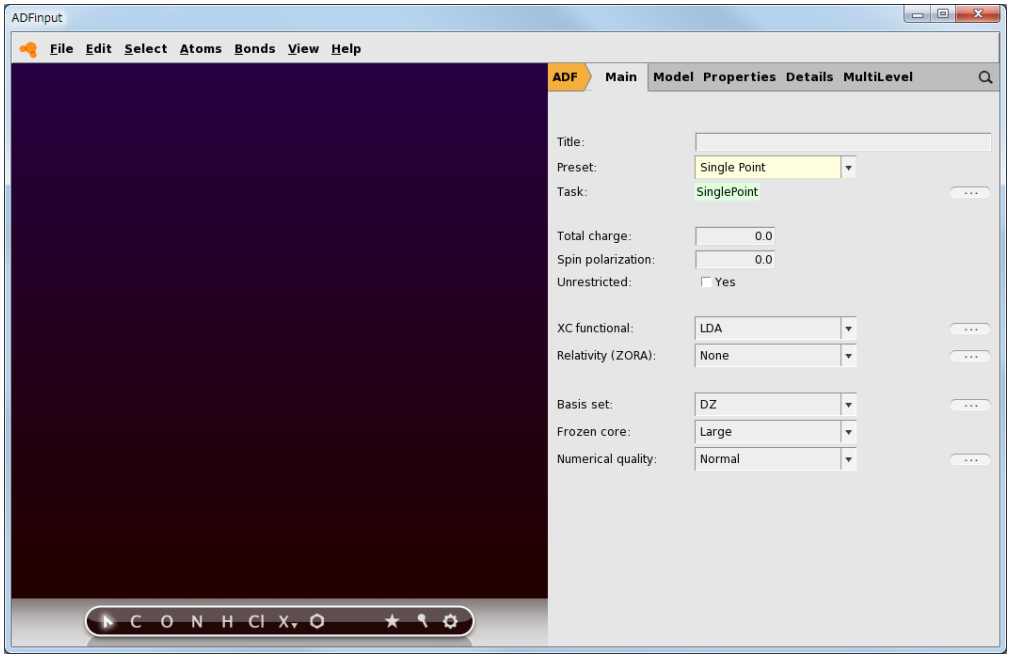
・ADF 2018.105

```
$ adfinput2018.105
```

・ADF 2017.113

```
$ adfinput2017.113
```

Application window launches into screen.



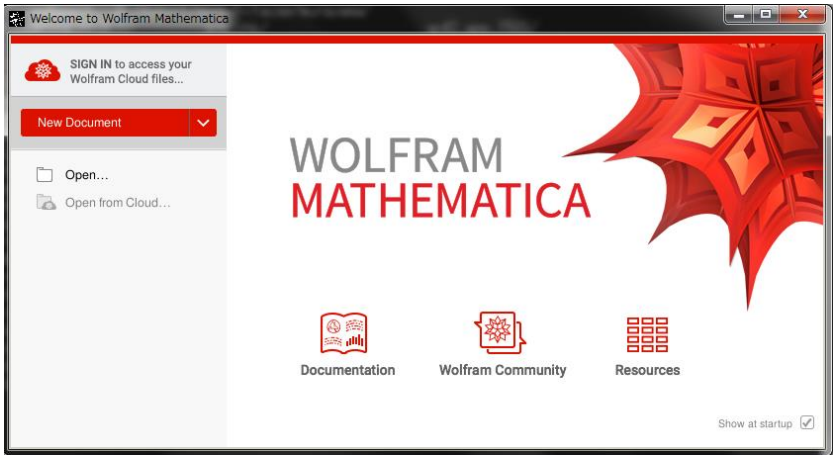
## 4.1.3 Mathematica

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

Execute the commands as follows.

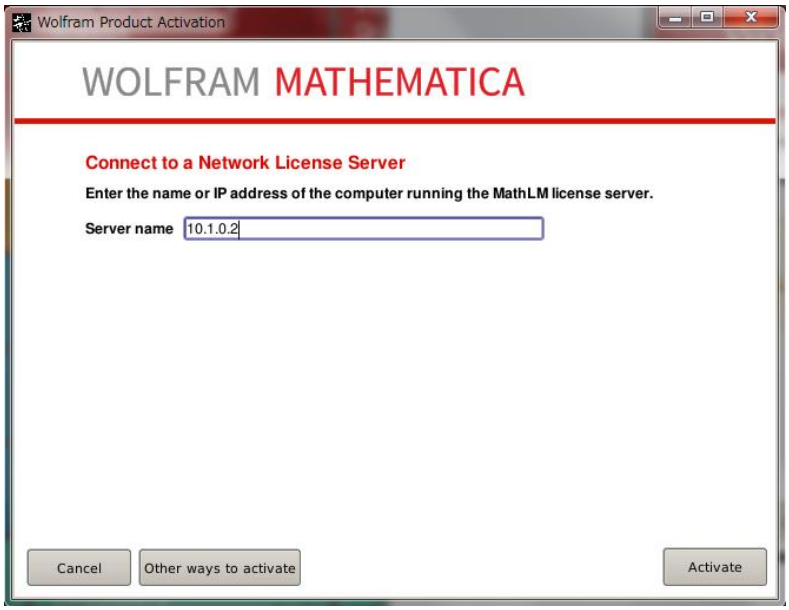
```
$ Mathematica
```

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.

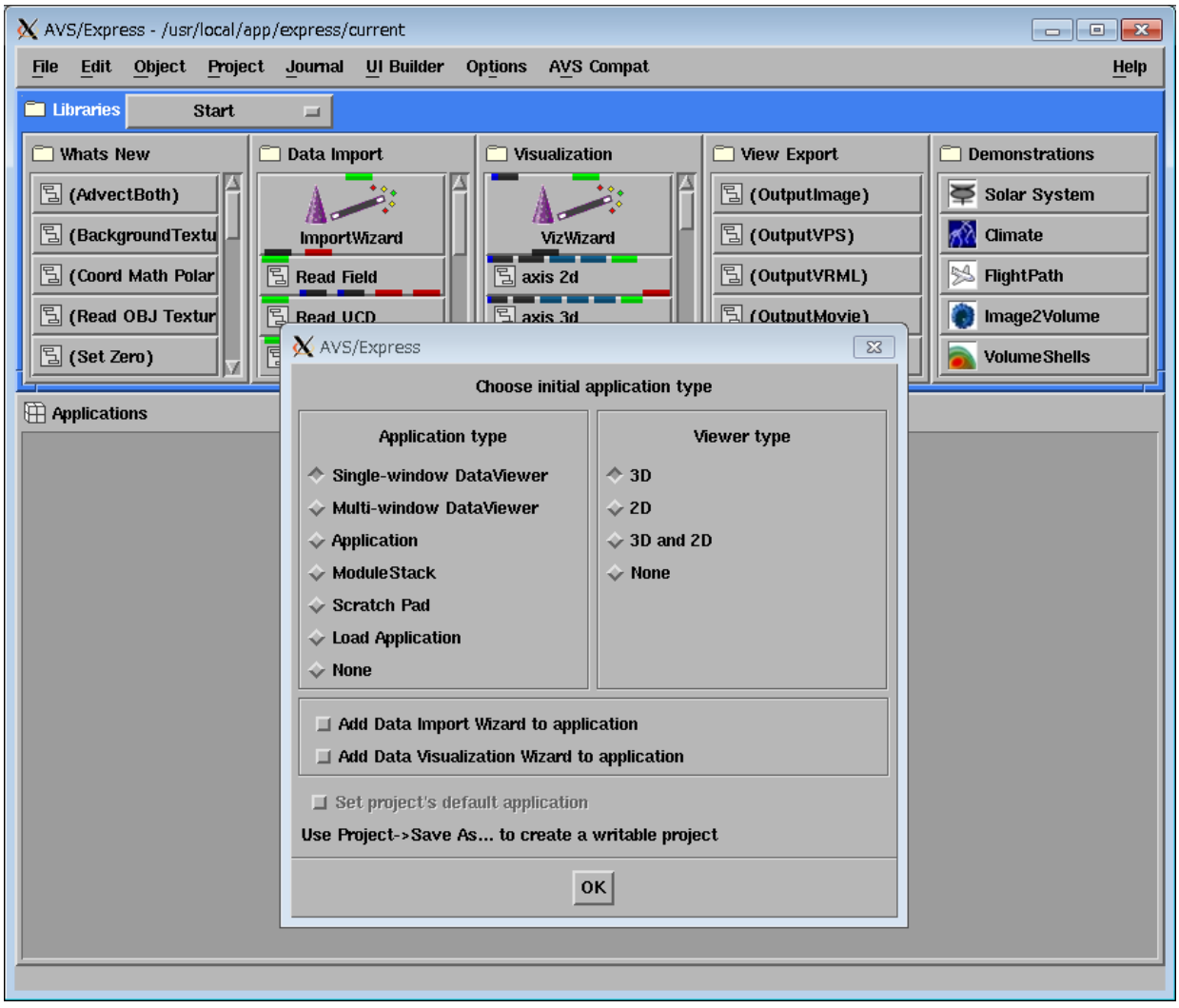
In the case developing applications using AVS, execute the commands as follows.

```
$ 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.

・2020.09

```
$ quantumatk
```

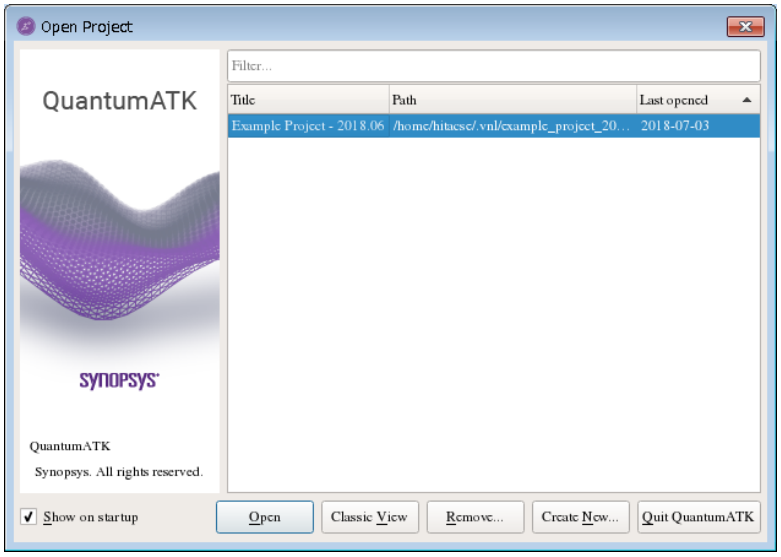
・2019.12

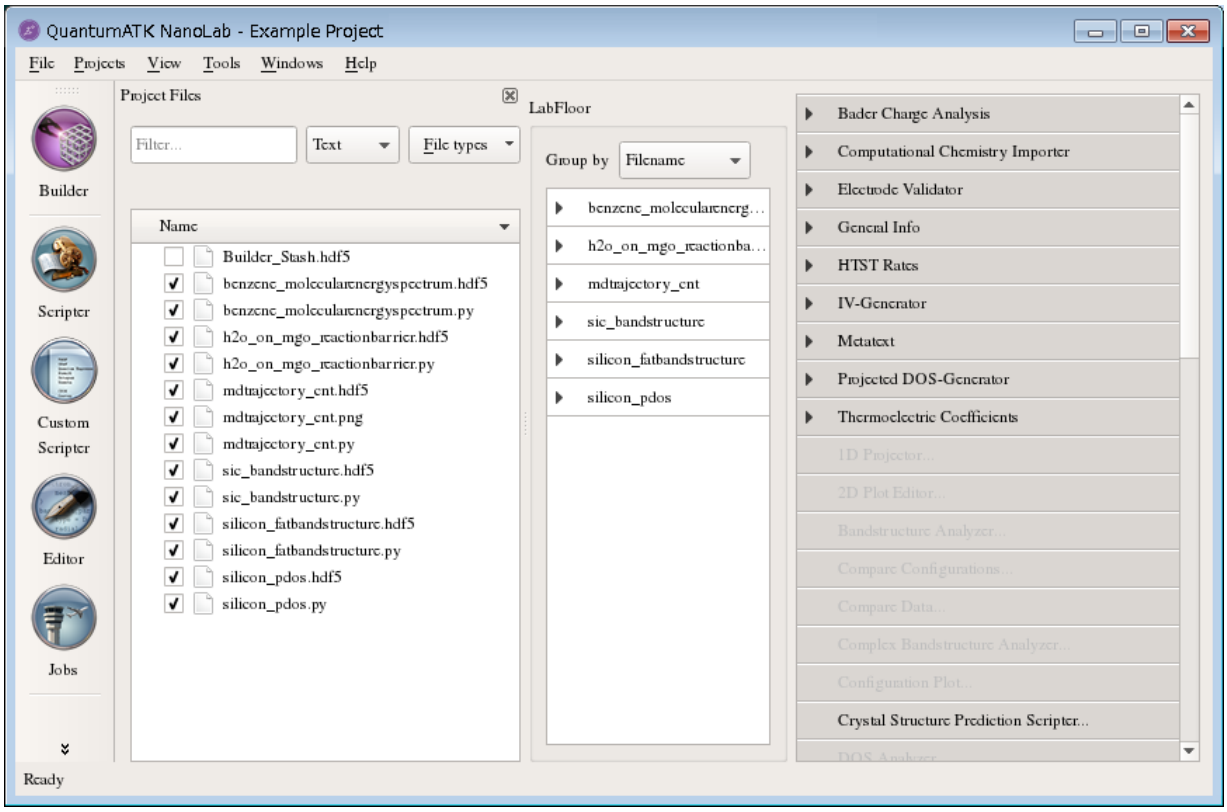
```
$ /usr/local/app/QuantumATK/QuantumATK-Q-2019.12/bin/quantumatk
```

・2019.03

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

Application window launches into screen.



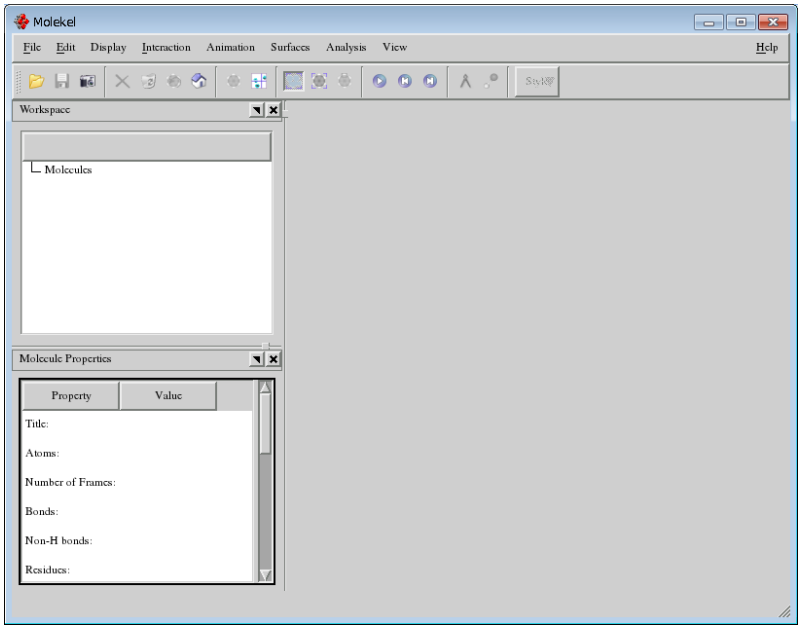


## 4.1.6 Molekel

Execute the commands as follows.

```
$ molekel
```

Application window launches into screen.

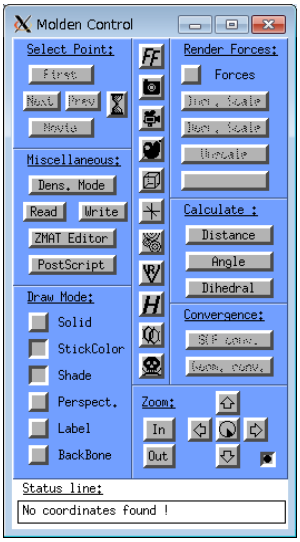



## 4.1.7 MOLDEN

Execute the commands as follows.

```
$ molden
```

Application window launches into screen.

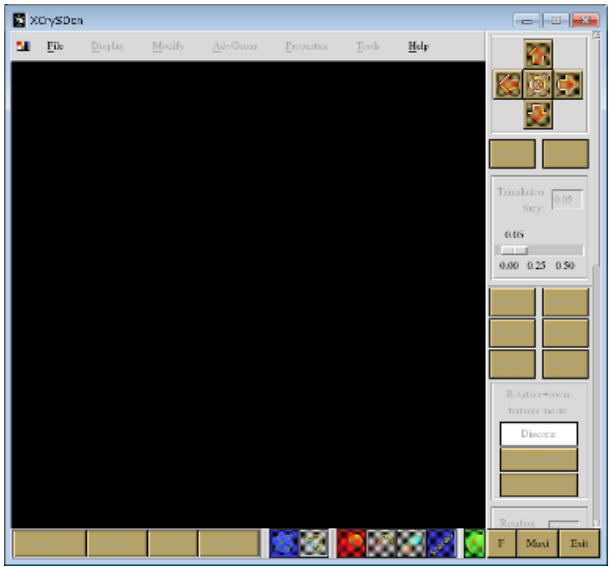



## 4.1.8 XCrySDen

Execute the commands as follows.

```
$ xcrysden
```

Application window launches into screen.



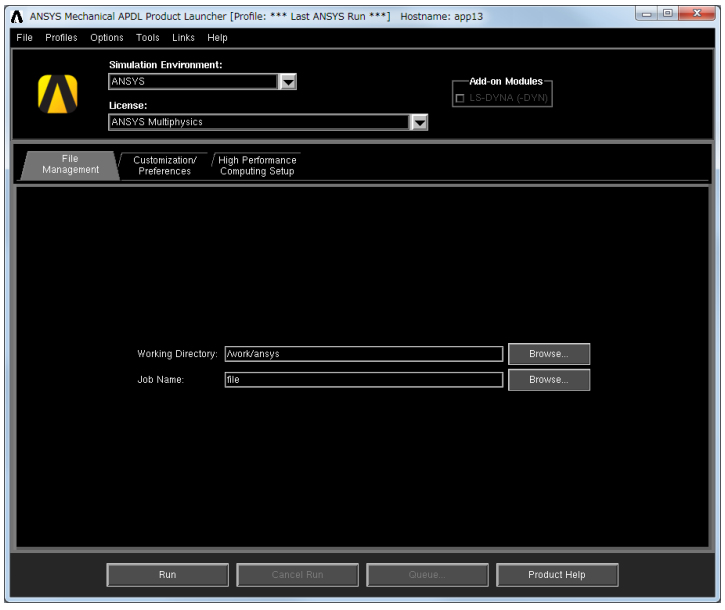

## 4.1.9 ANSYS Mechanical CFD

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

Execute the commands as follows.

```
$ launcher
```

Application window launches into screen.

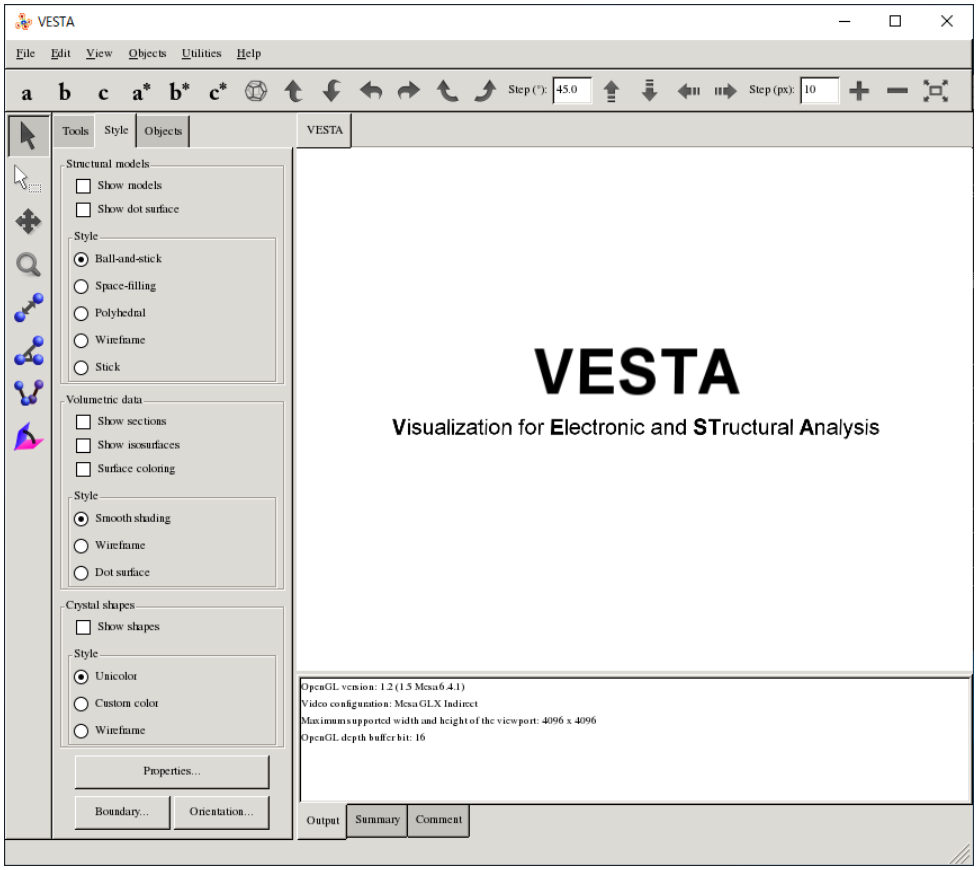


## 4.1.10 VESTA

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<br>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<br>SMP |
| 7 | VASP | 4.6<br>5.4 | MPI |
| 8 | WIEN2k | 17.1<br>19.1 | SMP |
| 9 | SIESTA | 4.0 | MPI |
| 10 | ABINIT | 8.8.2<br>8.10.3 | MPI |
| 11 | CPMD | 4.1<br>4.3 | MPI |
| 12 | Quantum Espresso | 6.2.1<br>6.4.1 | MPI |
| 13 | LAMMPS | 31 Mar 2017<br>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)

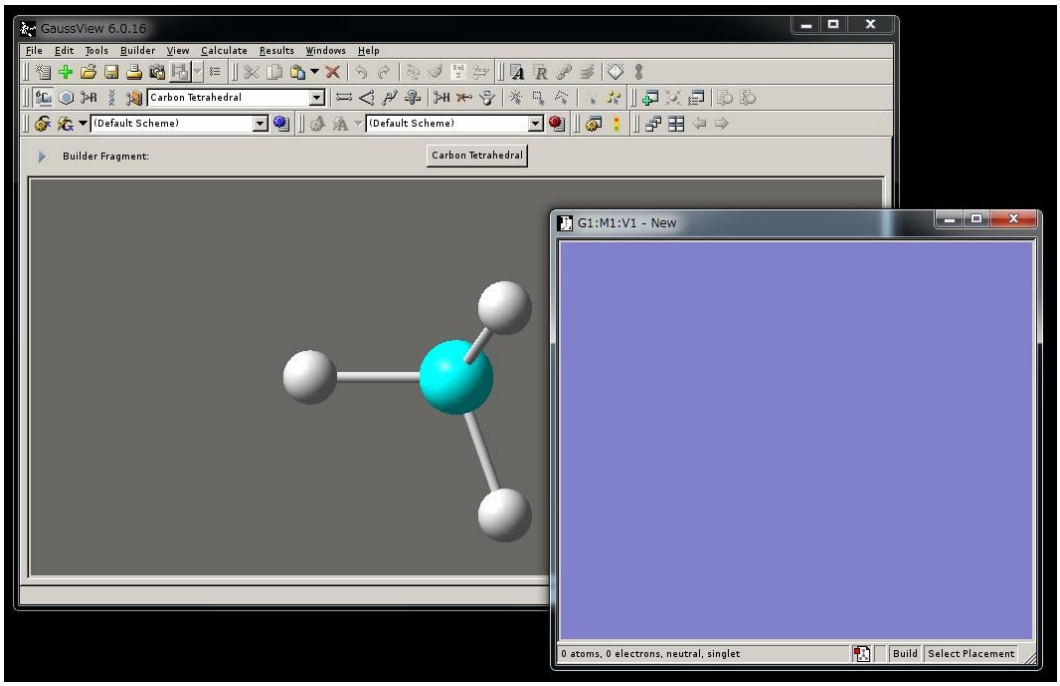
```
source /usr/local/app/Gaussian/g16.profile
g16 test0000.com
```

## 4.2.2 GaussView

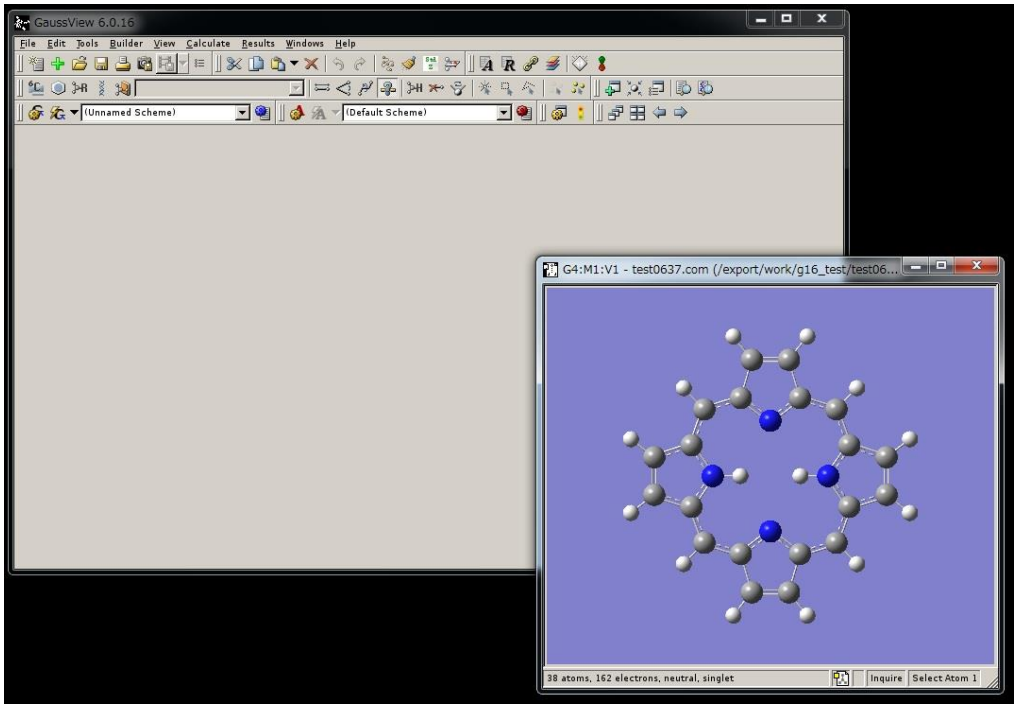
Execute the commands as follows.

```
$ gview
```

Application window launches into screen.




The examples of reading the Gaussian input files.



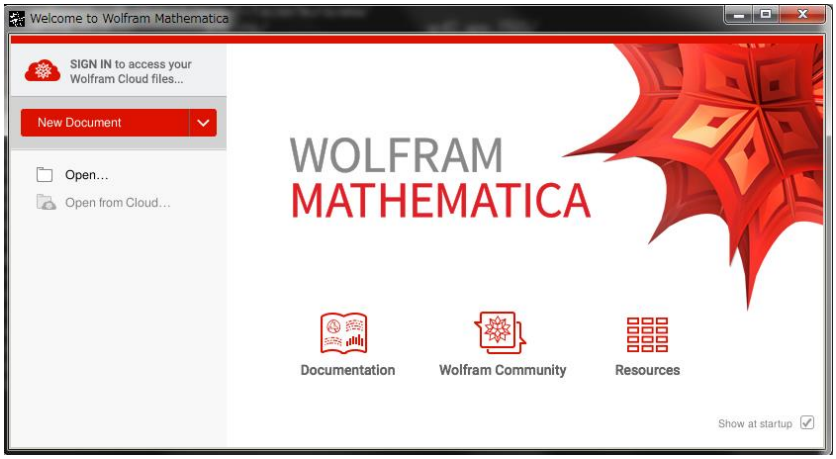
## 4.2.3 Mathematica

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

Execute the commands as follows.

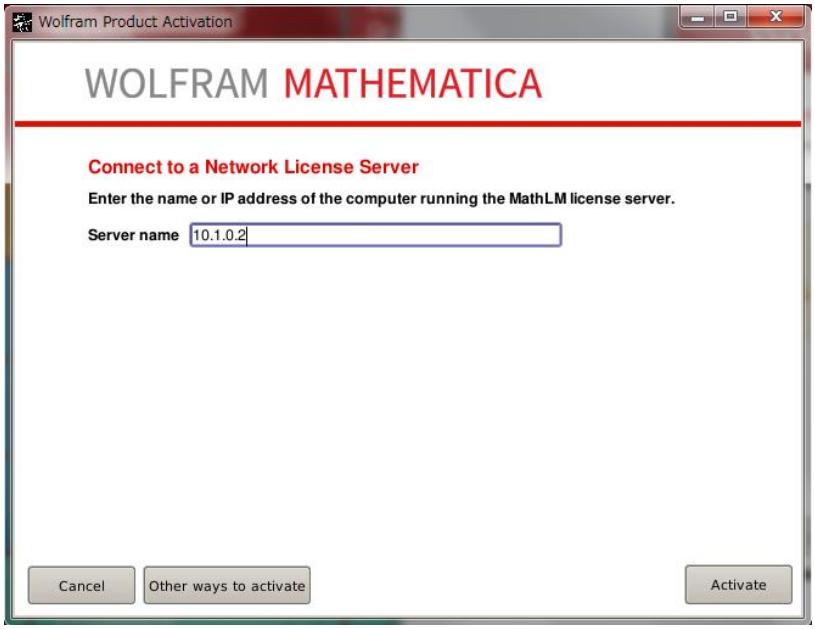
```
$ Mathematica
```

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.

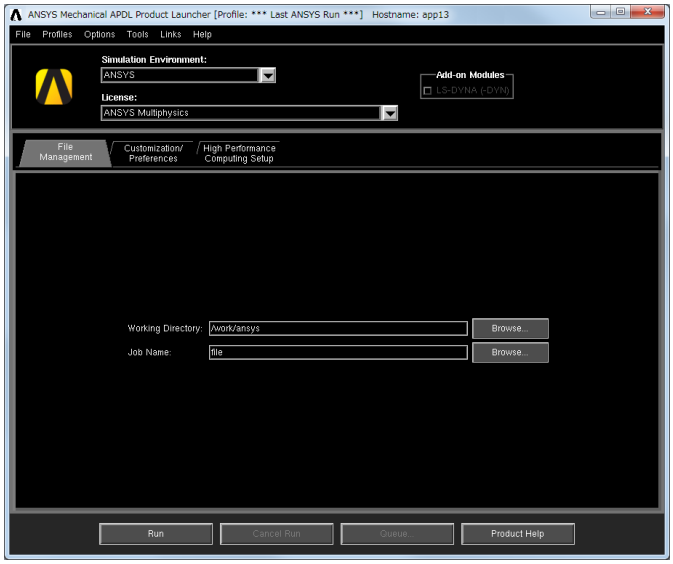
## 4.2.4 ANSYS Mechanical CFD

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

Execute the commands as follows.

```
$ launcher
```

Application window launches into screen.



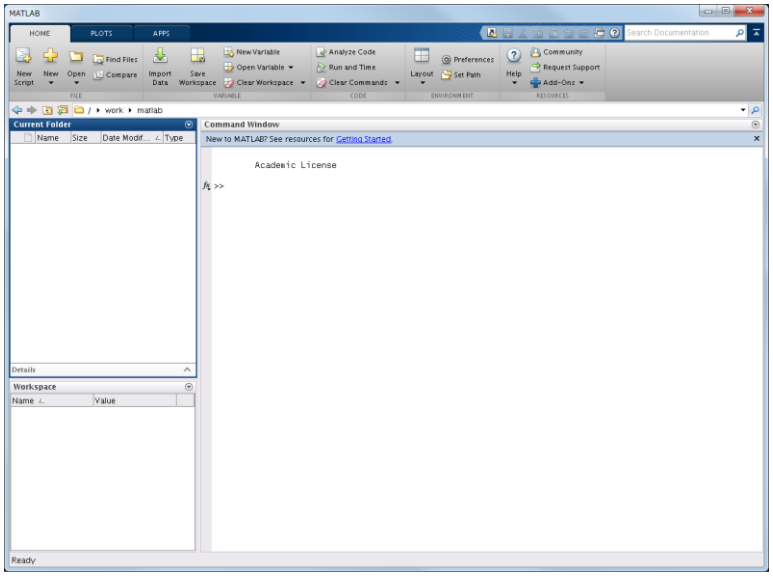

## 4.2.5 MATLAB

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

Execute the commands as follows.

```
$ matlab
```

Application window launches into screen.



## 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 |

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

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

CPMD is available for users who have own license.

To use CPMD, obtain the license on CPMD web site 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
```