

# *How to use “Chem” computers in TMU*

Theoretical/Computational chemistry lab.

**written by M. Abe in 2015**

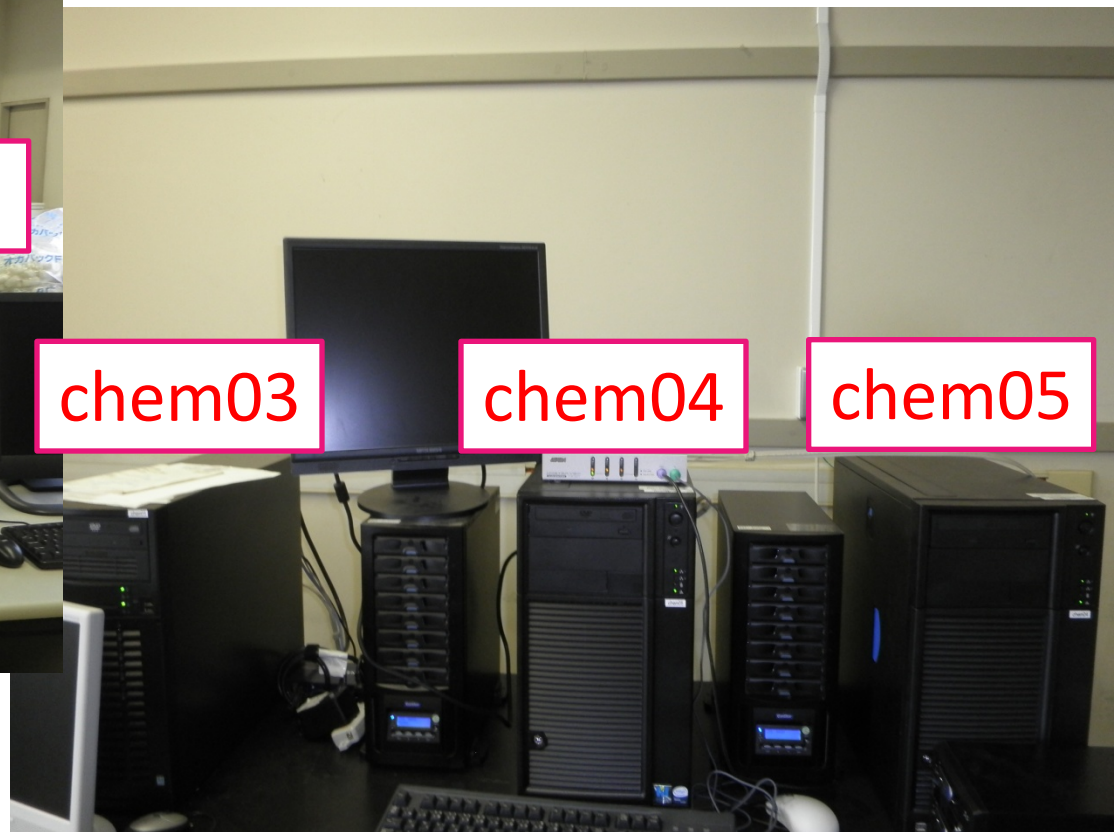
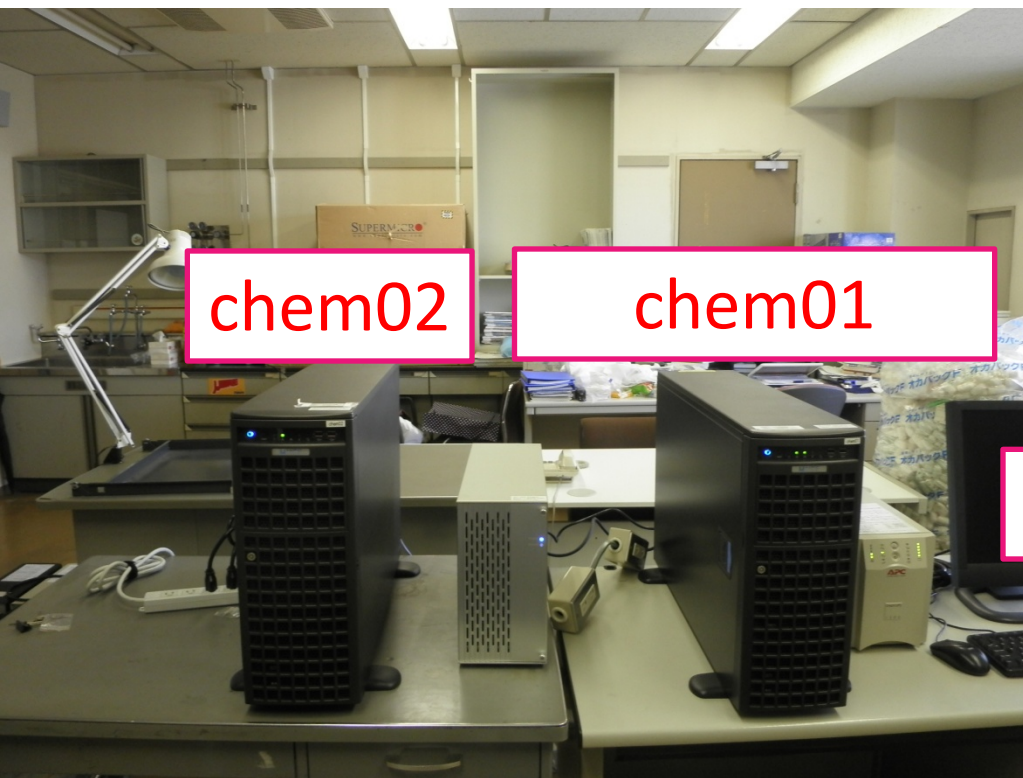
[http://www.comp.tmu.ac.jp/chem\\_comp/chem\\_kanri.html](http://www.comp.tmu.ac.jp/chem_comp/chem_kanri.html)

**Administrator: Minori Abe**

# Outline

- Specifications of Chem clusters
  - CPU, Memory, Hard disk size
- What you have to do first
  - Creation of your account
  - Settings for your PC
- What you have to do after you get your user ID
  - How to log in
  - Changing your password
- How to use Chem clusters
  - Brief instruction how to run Gaussian03 and Gaussian09 in Chem
  - Brief summary of LSF (Load Sharing Facility)
  - Basic commands for LSF
- Procedure of running Gaussain03 and Gaussian09
- Cautions

# These are chem01 ~ chem05!



Located in 8-547

Chem01, Chem02: latest and fastest, Chem03: poor,  
Chem04, Chem05: not bad

# Specifications of Chem clusters

Host name	CPU	CPU Clocks (GHz)	Core	Memory (GB)	HDD	Size	HDD	Size
chem01	Xeon X5690	<b>3.47</b>	<b>12</b>	<b>96</b>	/home	8TB	/scr	2TB
chem02	Xeon X5690	<b>3.47</b>	<b>12</b>	<b>96</b>	/scr	2TB		
chem03	Xeon W3520	<b>2.67</b>	<b>4</b>	<b>6</b>				
chem04	Xeon E5410	<b>2.33</b>	<b>8</b>	<b>16</b>	/work	500GB	/scr	1TB
chem05	Xeon E5450	<b>3.00</b>	<b>8</b>	<b>16</b>	/scr	500GB	/data	3.5TB

Chem01,Chem02: latest, Chem03: poor, Chem04,Chem05:not bad

# Preparation for Chem (1)

- **Get you user ID**

Please mail to Minori Abe [minoria@tmu.ac.jp](mailto:minoria@tmu.ac.jp) with 1. your name, 2. laboratory name, 3. student ID (if you have), 4. your grade (like M2) or your occupation, 5. your favorable user ID, but please include your name.

After creating your use ID, the administrator will send an email with your user ID and initial password.

Your email address is added in our mailing list ([chemcomputer-ml@ml.tmu.ac.jp](mailto:chemcomputer-ml@ml.tmu.ac.jp)) and important information such as power cut will be noticed via the mailing list.

# Preparation for Chem (2)

- What you need to set up in your own PC (Windows case)

- ◆ Install of TTSSH and WinSCP

<http://ttssh2.sourceforge.jp/>



<http://winscp.net/eng/docs/lang:jp>



WinSCP

- ◆ Install of Gaussian09W and GaussView

This is optional but if you are not familiar with Linux Gaussian, we recommend to install it to create inputs and see outputs.

You can borrow the CD of Gaussian09W and GaussView in the office of the chemistry department in TMU.

# After getting you ID (1)

## ● How to log in Chem (Chem01 is log in machine)

Use your PC connecting to TMU network; start TTSSH and write the below IP address in host name.

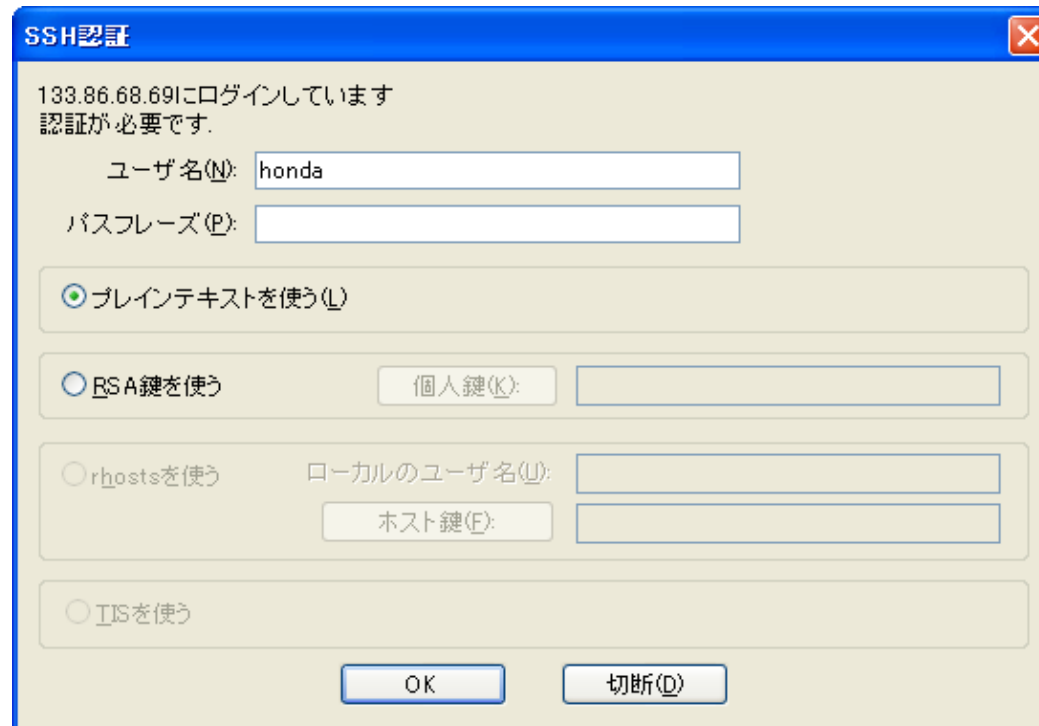
**133.86.68.69**

Tick SSH in service and write 22 in TCP port.



# After getting you ID (2)

Write your user ID and password.



The image shows a screenshot of an SSH authentication dialog box titled "SSH認証". The dialog box has a blue title bar with a close button (X) in the top right corner. The main content area is light beige and contains the following text and controls:

- Text: "133.86.68.69にログインしています 認証が必要です。"
- Text: "ユーザ名(N):" followed by a text input field containing "honda".
- Text: "パスワード(P):" followed by a text input field.
- Radio button: "プレーンテキストを使う(L)" (selected).
- Radio button: "RSA鍵を使う" followed by a "個人鍵(K):" label and a text input field.
- Radio button: "rhostsを使う" followed by a "ローカルのユーザ名(U):" label and a text input field, and a "ホスト鍵(F):" label and a text input field.
- Radio button: "IISを使う".
- Buttons: "OK" and "切断(D)" at the bottom.

If you succeed in log in, the following prompt appears

**chem01:<USERID>\$**

After you complete log in, please change your password.



# After getting you ID (3)

- **How to change your password**

Write the following command in TTSH

**yppasswd**

Then you will be asked to write your present password and new password (twice).

```
chem01:<USERID>$ yppasswd
Changing NIS account information for USERID on chem00.chem.metro-u.ac.jp.
Please enter old password:
Changing NIS password for USERID on chem00.chem.metro-u.ac.jp.
Please enter new password:
Please retype new password:

The NIS password has been changed on chem00.chem.metro-u.ac.jp.
```

**You must change your password in the first log in.**

# Calculation Flow of running Gaussian09

① Create input file for Gaussian in your PC (using GaussView)

② Access chem01(133.86.68.69) with WinSCP → transport your input file to the following directly  
**~/g03jobs**

③ Log in  
133.86.68.69 with TTSSH

Change directly to "g03jobs"  
**cd g03jobs**

Run your Gaussian job  
**g09job \*\*\*.gjf \*\*\*.out**

④ Check you job  
**list**

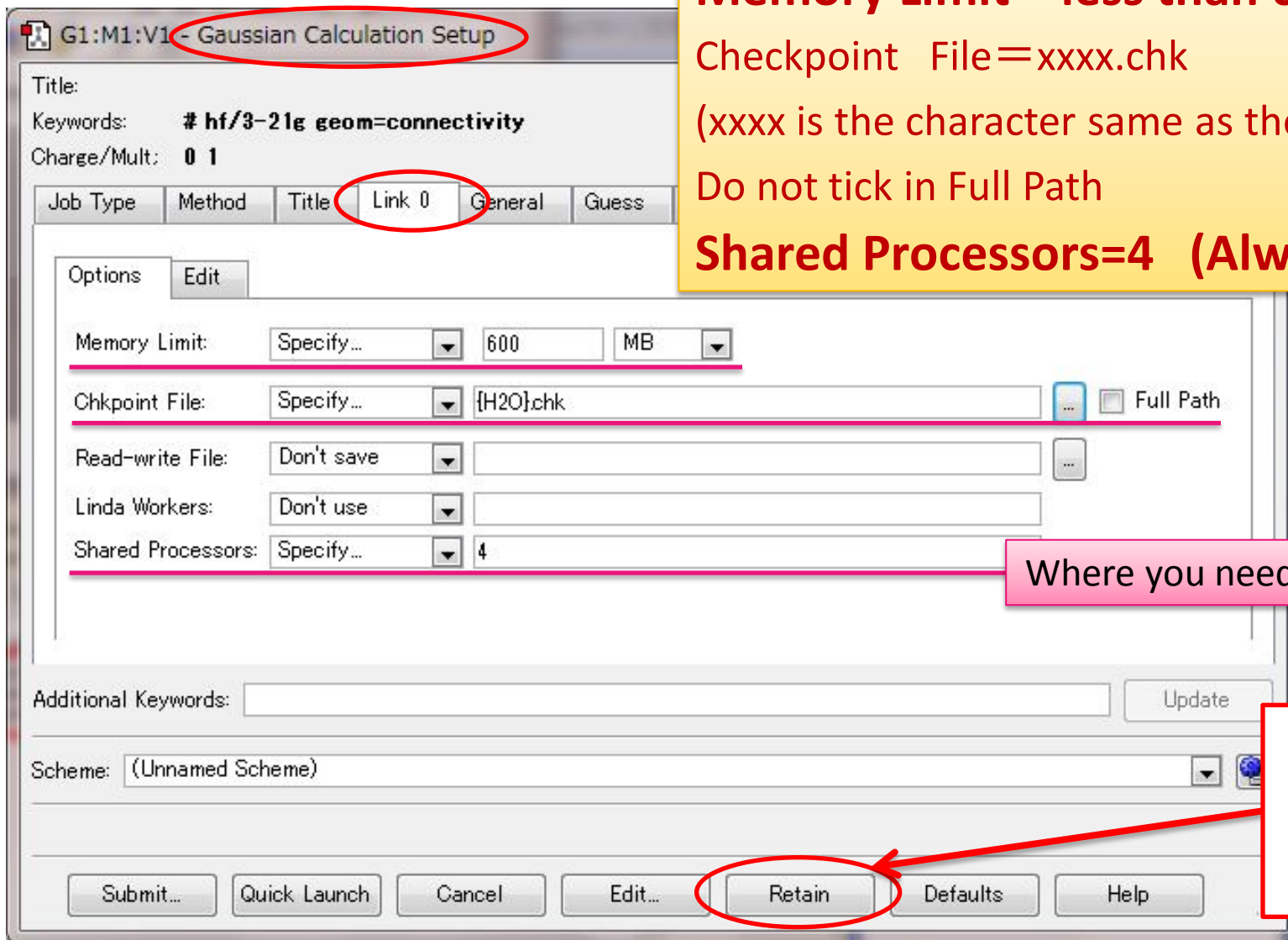
After the calculation is over, create fchk file to see MOs in your PC  
**formchk \*\*\*.chk**

⑤ Download the output file (\*\*\*.out) and fchk file (\*\*\*.fchk) to your PC with WinSCP

Analyze your output file and fchk file using GaussView in your PC

# (1) Create your input file with GaussView

## Modification of Gaussian Calculation Setup



**Memory Limit = less than 6 GB**

Checkpoint File = xxxx.chk

(xxxx is the character same as the input file xxxx.gjf)

Do not tick in Full Path

**Shared Processors=4 (Always 4 please)**

Where you need to change

After click "Retain",  
choose the "file" tab in  
Gaussview, and click  
"save as" and save.

## (2) Transfer your input file to chem01(133.86.68.69) by WinSCP

The screenshot shows the WinSCP interface with two panels. The left panel displays the local PC's file system, and the right panel displays the remote server's file system. A green arrow labeled "Drag & Drop" points from the local file list to the remote file list. A pink callout box points to the "g03jobs" directory in the remote panel, with the text "Please change here to 'g03jobs'".

**Files in your PC**

名前	拡張子	サイズ	種類	更新日時
Final_THF.gjf		3,369	GJF ファイル	2012/01/...
Final_THF_2.gjf		3,376	GJF ファイル	2012/02/...
Final_THF_ion.gjf		5,206	GJF ファイル	2012/01/...
FINAL_THF_ION.LOG		13,885	テキストドク...	2012/01/...
G_Plum_2-.g...			ファイル	2012/02/...
G_Plum_N.g...			ファイル	2012/02/...
G_Plum_NHC.gjf		3,600	GJF ファイル	2012/02/...
G_Plum_NHC_NHC...		4,689	GJF ファイル	2012/02/...
G_Plum_NHC_NHC...		10,243	GJF ファイル	2012/02/...
G_Plum_THF.gjf		3,363	GJF ファイル	2012/02/...
GeC4H4.gjf		2,472	GJF ファイル	2012/02/...
GeC4H4-2.gjf		2,468	GJF ファイル	2012/02/...
H2O_inp.chk		536,576	回復されたフ...	2012/09/...
H2O_inp.gjf		312	GJF ファイル	2012/09/...
H2O_INP.LOG		22,319	テキストドク...	2012/09/...
L1.gjf		365	GJF ファイル	2012/09/...
NHC.jpg		208,717	JPEG イメージ	2012/04/...

**Files in Chem01**

名前	拡張子	サイズ	更新日時	パーミッ...
..			2013/02/28 1...	rwX----- k
H2O_inp.gjf		312	2012/09/27 1...	rw-r--r-- k

Please change here to "g03jobs"

Drag & Drop

# (3) Submit your job

Log in 133.86.68.69 by TTSSH (see p.7 and 8)

After login

purple: you need to write

black: respond from the computer

chem01:<USERID >% cd g03jobs

Change your directly

/home/chem/USERID /g03jobs

Confirmation of your current directly

chem01:<USERID >% ls

Show what are located in the current directly

H2O.gjf

You can confirm your input is here

chem01:<USERID >% g09job H2O.gjf H2O.out

Submission of your job

Job <4603> is submitted to default queue <normal>.

Confirmation of your  
job submission

chem01:<USERID >%list

Confirmation of the  
current status of your job

# Summary of how to submit your job

## ● How to use Gaussian09 in chem

You need to put your input in g03jobs directly and you should also be in the g03jobs directly. Then use the command **g09job** to run it.

**g09job input\_file\_name out\_put\_file\_name**

For example,

**g09job h2o.gjf h2o.out**

Your job of h2o.gjf is automatically assigned to an available computer. Output file (.out and .chk) will be created in g03jobs directly.

You can specify the computer for your job as follows. (For ex, chem02)

**g09job h2o.gjf h2o.out chem02**

If you want to use Gaussian03 version, use g03job command.

**g03job h2o.gjf h2o.out**

# Local rules in our LSF

- LSF (Load Sharing Facility)

LSF is a management system for job submission.

## Local rules in chem

Single user can calculate at most three jobs at the same time.

If you submit the fourth job though the other three are still running, it assigned as “pending” and it will run after your any job will be finished.

You can submit your jobs as much as you like but it will be proceeded one by one.

# How to confirm the current status of your job (1)

“list” is a command to show the current status of chem computers in our LSF. If you write “list” and enter,

JOBID	USER	STAT	QUEUE	FROM_HOST	EXEC_HOST	JOB_NAME	SUBMIT_TIME
1260	aaa	RUN	normal	chem01. chem	4*chem02. ch	job001. chk	May 15 11:00
1261	aaa	RUN	normal	chem01. chem	4*chem01. ch	job002. chk	May 15 11:01
1263	bbb	RUN	normal	chem01. chem	4*chem02. ch	optAA. chk	May 15 13:00
1264	ccc	RUN	normal	chem01. chem	4*chem01. ch	nmrBB. chk	May 15 13:38
1262	aaa	PEND	normal	chem01. chem		job003. chk	May 15 11:02

If the person with userID=ddd submit his/her job as `g09job test.gjf test.out`, then,...

JOBID	USER	STAT	QUEUE	FROM_HOST	EXEC_HOST	JOB_NAME	SUBMIT_TIME
1260	aaa	RUN	normal	chem01. chem	4*chem02. ch	job001. chk	May 15 11:00
1261	aaa	RUN	normal	chem01. chem	4*chem01. ch	job002. chk	May 15 11:01
1263	bbb	RUN	normal	chem01. chem	4*chem02. ch	optAA. chk	May 15 13:00
1264	ccc	RUN	normal	chem01. chem	4*chem01. ch	nmrBB. chk	May 15 13:38
1262	aaa	PEND	normal	chem01. chem		job003. chk	May 15 11:02
1265	ddd	PEND	normal	chem01. chem		test. chk	May 15 18:30



# How to confirm the current status of your job (2)

- g03kill (Job ID) is a command to cancel your job.

Note that even you run g09job, killing command is “g03kill”!

Ex. If a person with userid=aaa write “g03kill 1260” and enter,

JOBID	USER	STAT	QUEUE	FROM_HOST	EXEC_HOST	JOB_NAME	SUBMIT_TIME
1260	aaa	RUN	normal	chem01.chem	4*chem02.ch	job001.chk	May 15 11:00
1261	aaa	RUN	normal	chem01.chem	4*chem01.ch	job002.chk	May 15 11:01
1263	bbb	RUN	normal	chem01.chem	4*chem02.ch	optAA.chk	May 15 13:00
1264	ccc	RUN	normal	chem01.chem	4*chem01.ch	nmrBB.chk	May 15 13:38
1262	aaa	PEND	normal	chem01.chem		job003.chk	May 15 11:02
1265	ddd	PEND	normal	chem01.chem		test.chk	May 15 18:30

Job 1260 is cancelled and another job waiting in the queue (in this case JobID 1265 by ddd) is now submitted and running.

JOBID	USER	STAT	QUEUE	FROM_HOST	EXEC_HOST	JOB_NAME	SUBMIT_TIME
1261	aaa	RUN	normal	chem01.chem	4*chem01.ch	job002.chk	May 15 11:01
1263	bbb	RUN	normal	chem01.chem	4*chem02.ch	optAA.chk	May 15 13:00
1264	ccc	RUN	normal	chem01.chem	4*chem01.ch	nmrBB.chk	May 15 13:38
1265	ddd	RUN	normal	chem01.chem	4*chem02.ch	test.chk	May 15 18:30
1262	aaa	PEND	normal	chem01.chem		job003.chk	May 15 11:02

# Confirmation of termination of your job

With “list” command, if your job is not shown, then the calculation is over.

Ex. JOBID : 1260, USER : aaa is now disappear.

JOBID	USER	STAT	QUEUE	FROM_HOST	EXEC_HOST	JOB_NAME	SUBMIT_TIME
1261	aaa	RUN	normal	chem01.chem	4*chem01.ch	job002.chk	May 15 11:01
1263	bbb	RUN	normal	chem01.chem	4*chem02.ch	optAA.chk	May 15 13:00
1264	ccc	RUN	normal	chem01.chem	4*chem01.ch	nmrBB.chk	May 15 13:38
1262	aaa	PEND	normal	chem01.chem		job003.chk	May 15 11:02
1265	ddd	PEND	normal	chem01.chem		test.chk	May 15 18:30

chem01:<USERID>% ls

Show the file list in this directly

4603.out H2O.chk H2O.fchk H2O.gjf H2O.out

Please confirm these files are created.

4603.out : Job report (does not relate with gaussian output)

H2O.chk: checkpoint file

**H2O.fchk : formatted checkpoint file**

H2O.gjf : input file

**H2O.out: output file**

Check point file written by text format  
and readable in any circumstance.

# File transfer from chem01(133.86.68.69) to your PC by WinSCP

The screenshot shows the WinSCP interface with two panes. The left pane shows the local PC's file system (D: ローカルディスク) with a list of files including GJF files and logs. The right pane shows the remote server's file system (/home/chem/kawamura/g03jobs) with files like H2O.out, 4603.out, H2O.gjf, H2O.fchk, and H2O.chk. A pink box highlights the files in the local pane, and a green arrow labeled 'Drag & Drop' points from the local pane to the remote pane. A green box at the bottom right indicates the files in the remote server.

**Necessary files for analysis  
In GaussView**

**Drag & Drop**

**Files in your PC**

**Files in Chem01 (g03jobs directly)**

名前	拡張子	サイズ	種類	更新日時
Final_THF.gjf		3,369	GJF ファイル	2012/01/...
Final_THF_2.gjf		3,376	GJF ファイル	2012/02/...
Final_THF_3.gjf		5,386	GJF ファイル	2012/01/...
Final_THF_4.gjf		5,386	GJF ファイル	2012/01/...
Final_THF_5.gjf		5,386	GJF ファイル	2012/01/...
Final_THF_6.gjf		5,386	GJF ファイル	2012/01/...
Final_THF_7.gjf		5,386	GJF ファイル	2012/01/...
Final_THF_8.gjf		5,386	GJF ファイル	2012/01/...
Final_THF_9.gjf		5,386	GJF ファイル	2012/01/...
Final_THF_10.gjf		5,386	GJF ファイル	2012/01/...
G_Plum_NHC.gjf		3,600	GJF ファイル	2012/02/...
G_Plum_NHC_NHC...		4,689	GJF ファイル	2012/02/...
G_Plum_NHC_NHC...		10,243	GJF ファイル	2012/02/...
G_Plum_THF.gjf		3,363	GJF ファイル	2012/02/...
GeC4H4.gjf		2,472	GJF ファイル	2012/02/...
GeC4H4-2.gjf		2,468	GJF ファイル	2012/02/...
H2O_inp.chk		536,576	回復されたフ...	2012/09/...
H2O_inp.gjf		312	GJF ファイル	2012/09/...
H2O_INP.LOG		22,319	テキスト ドキ...	2012/09/...
L1.gjf		365	GJF ファイル	2012/09/...
NHC.jpg			イメージ	2012/04/...

名前	拡張子	サイズ	更新日時	パーミッ...
..			2013/03/01 1...	rw-x-----
H2O.out		33,135	2013/02/28 1...	rw-r--r--
4603.out		1,061	2013/02/28 1...	rw-r--r--
H2O.gjf		296	2013/02/28 1...	rw-r--r--
H2O.fchk		17,133	2013/02/28 1...	rw-r--r--
H2O.chk		638,976	2013/02/28 1...	rw-r--r--

# Summary of job running

- Create your input in your PC and transfer it to chem01
- in TTSSH,
  - ✓ Go to g03jobs directly (`cd ~/g03jobs`)
  - ✓ Submit your job with `g03job` or `g09job` command  
(`g09job h2o.gjf h2o.log`)
  - ✓ Confirm your job status by “list” command
  - ✓ If you want to cancel, kill your job with “`g03kill (Job number)`”
  - ✓ Confirm your output or `fchk` are created with “ls” command.
- Back transfer the result files to your PC and analyze them by Gaussview

# Caution (Specification of memory size)

Host name	CPU clocks	# of Core	# of Job	Memory (GB)
chem01	<b>3.47</b>	<b>12</b>	<b>2</b>	<b>96</b>
chem02	<b>3.47</b>	<b>12</b>	<b>3</b>	<b>96</b>
chem03	<b>2.67</b>	<b>4</b>	<b>1</b>	<b>6</b>
chem04	<b>2.33</b>	<b>8</b>	<b>2</b>	<b>16</b>
chem05	<b>3.00</b>	<b>8</b>	<b>2</b>	<b>16</b>

Only a 4-core parallel job can run.

(max number of jobs)

=(number of core)/4

However, only 2 jobs can run at a time in chem01 because it is the login machine and assigned as home directly.

Memory size per one job

Chem01 → 48GB

Chem02 → 32GB

Chem03 → 6GB

Chem04,05 → 8GB

If you specify the computer, you can run your job with the above memory size, beyond 6 GB. (But be careful please!)

# Caution (Access from outside of TMU)

You cannot log in Chem01 from outside of TMU directly.

If you have an account in other TMU server, you can log in to Chem01 via the server. In this case, first you have to log in to any account in TMU by TTSH and type

```
ssh USERID@133.86.68.69
```

Then you can log in to chem01.

To transfer your file, type

```
scp filename USERID@133.86.68.69:~/g03jobs
```

in TTSSH from the intermediate server then you can put your file to chem01.

# If you need any help

- Please feel free to contact to

Minori Abe

[minoria@tmu.ac.jp](mailto:minoria@tmu.ac.jp)

8<sup>th</sup> building room 571 (internal tel: 3582)

Theoretical / computational chemistry laboratory