# *How to use "Chem" computers in TMU*

Theoretical/Computational chemistry lab.

**written by M. Abe in 2015**

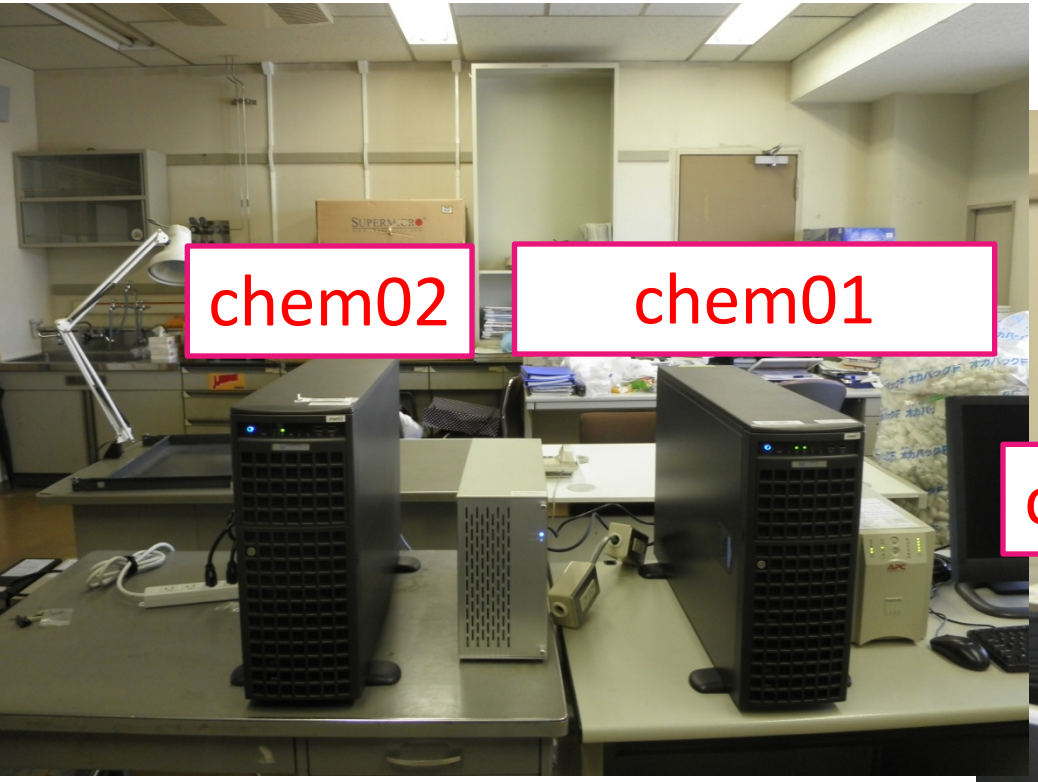
http://www.comp.tmu.ac.jp/chem_comp/chem_kanri.html

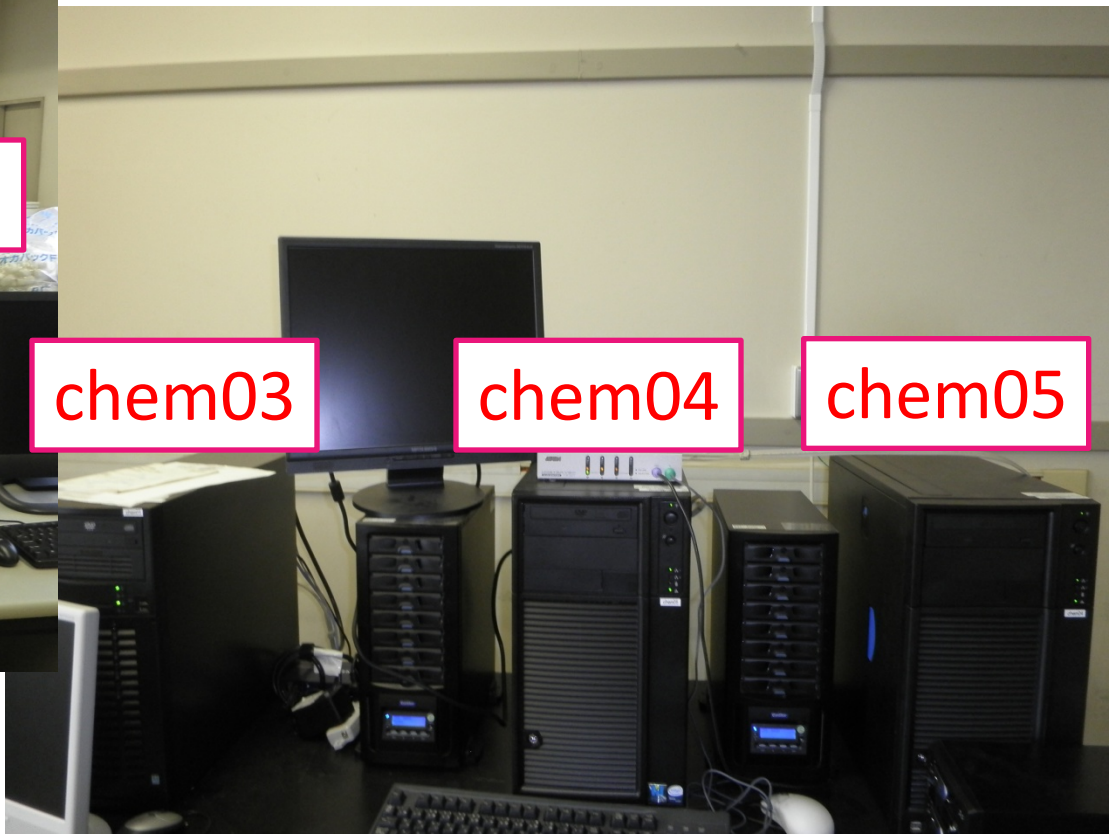
Administrator： Minori Abe

# 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 | **3.47** | **12** | **96** | /home | 8TB | /scr | 2TB |
| chem02 | Xeon X5690 | **3.47** | **12** | **96** | /scr | 2TB | | |
| chem03 | Xeon W3520 | **2.67** | **4** | **6** | | | | |
| chem04 | Xeon E5410 | **2.33** | **8** | **16** | /work | 500GB | /scr | 1TB |
| chem05 | Xeon E5450 | **3.00** | **8** | **16** | /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
  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) 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


◆**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)**

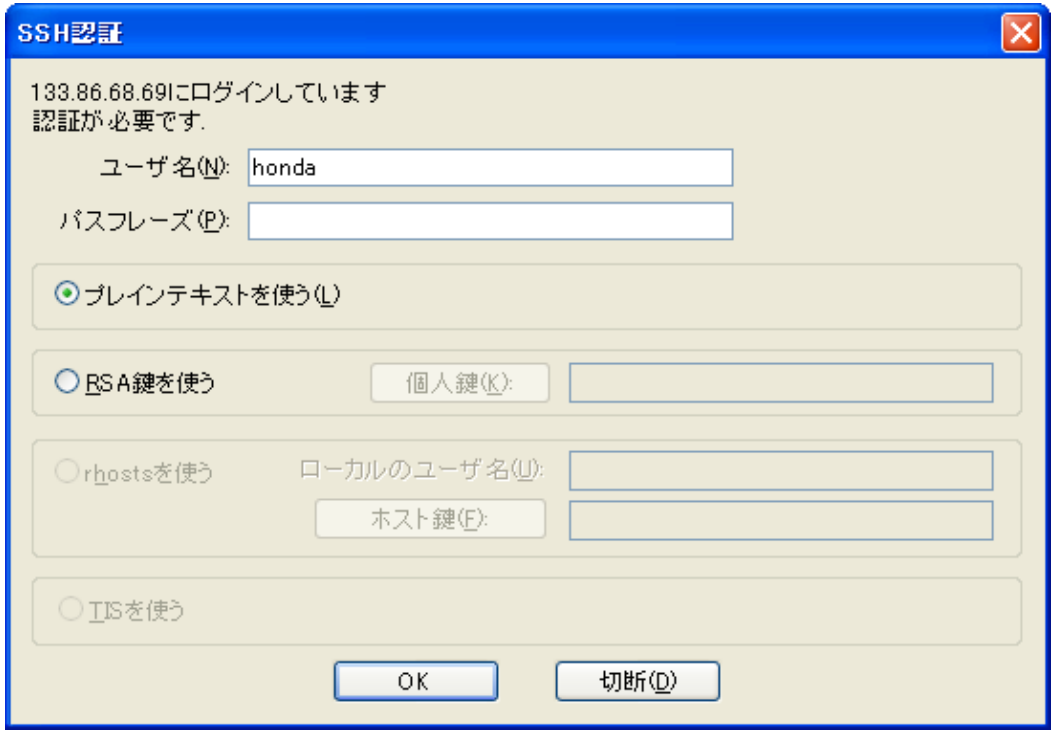
Use your PC connecting to TMU network; start TTSSH and write the below IP address in host name.

**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.




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 Creat 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

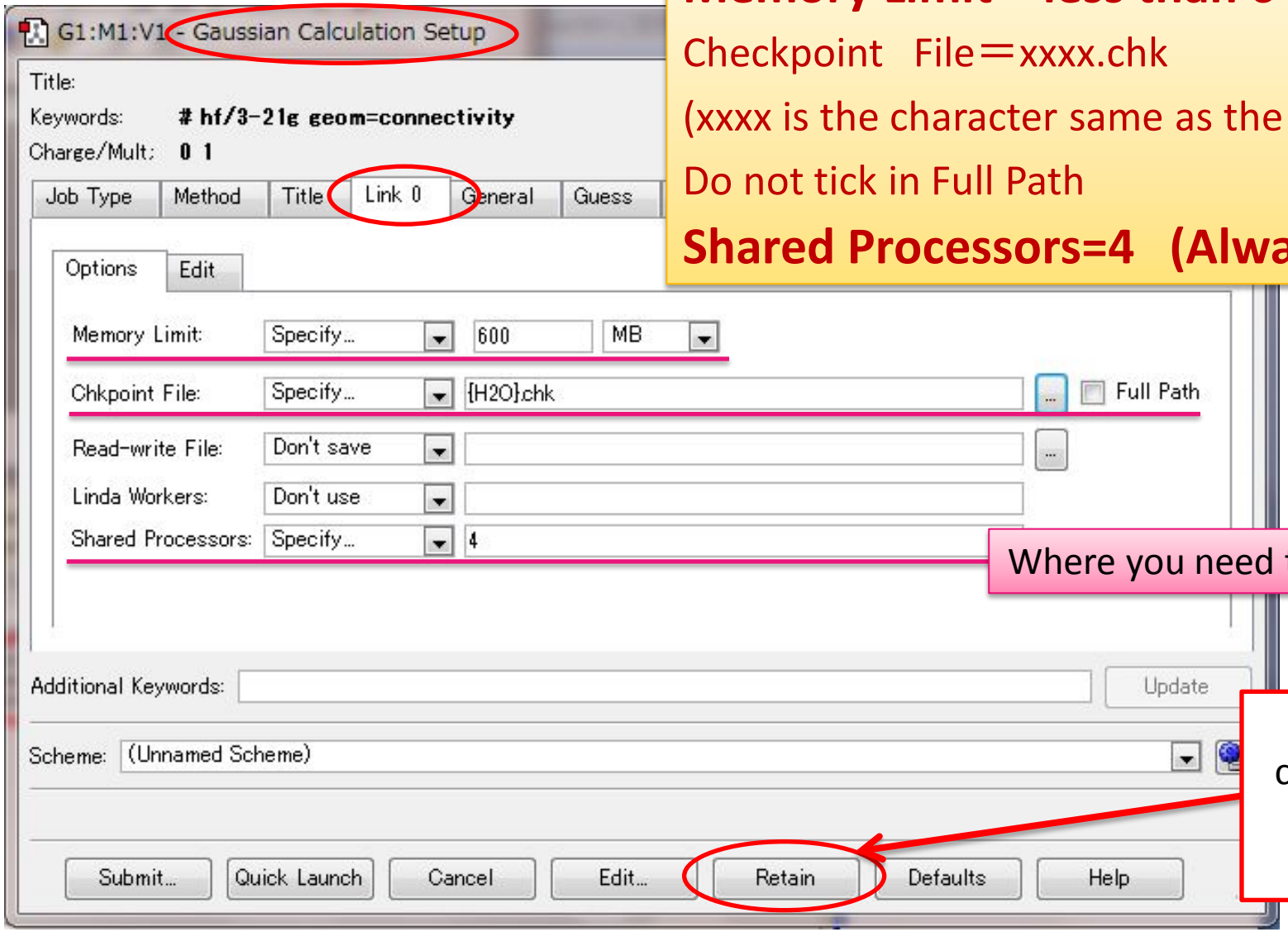
**Memory Limit = less than 6 GB**

Checkpoint File＝xxxx.chk

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

Do not tick in Full Path

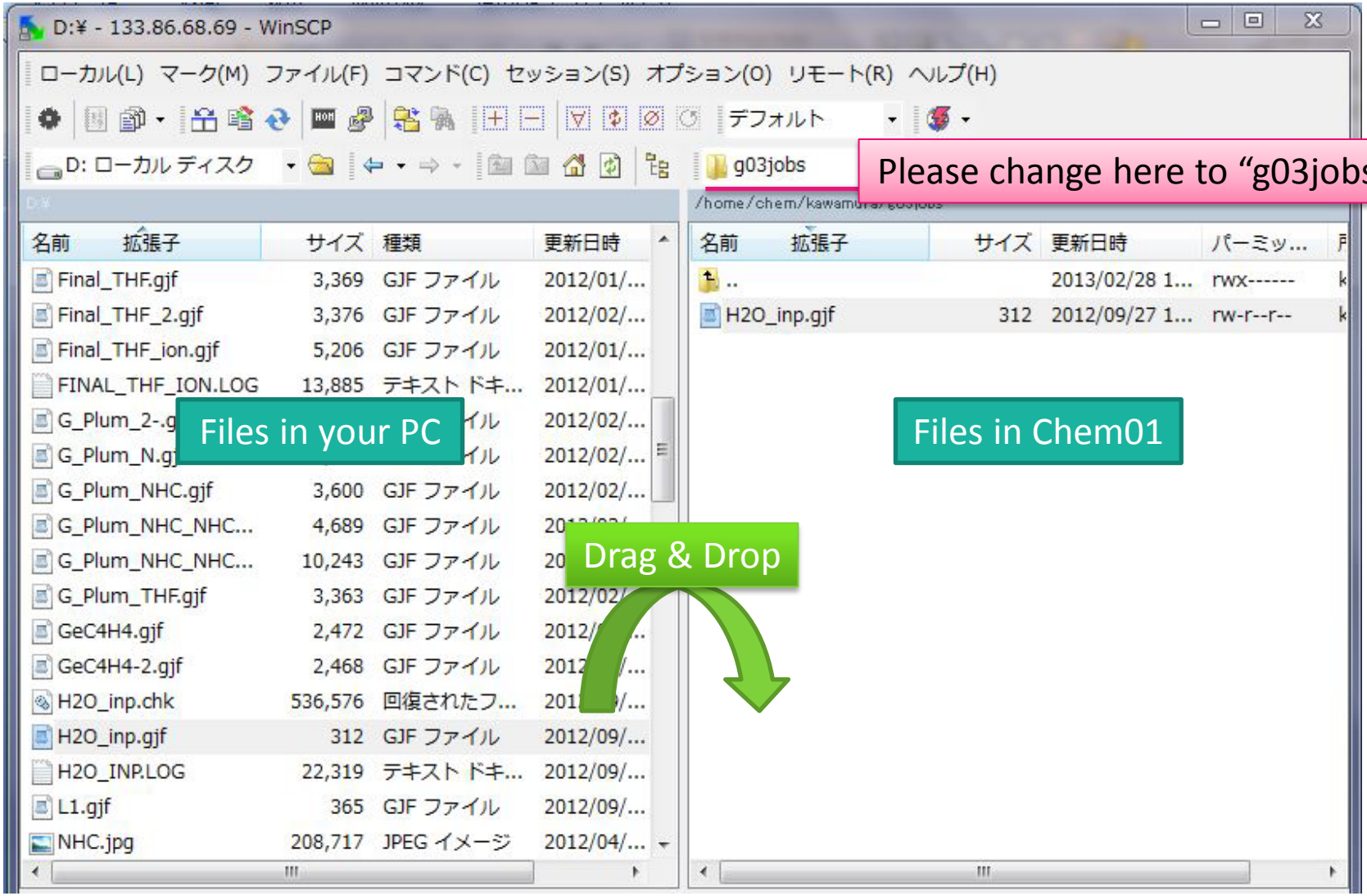
**Shared Processors=4 (Always 4 please)**




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



# (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 threes 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

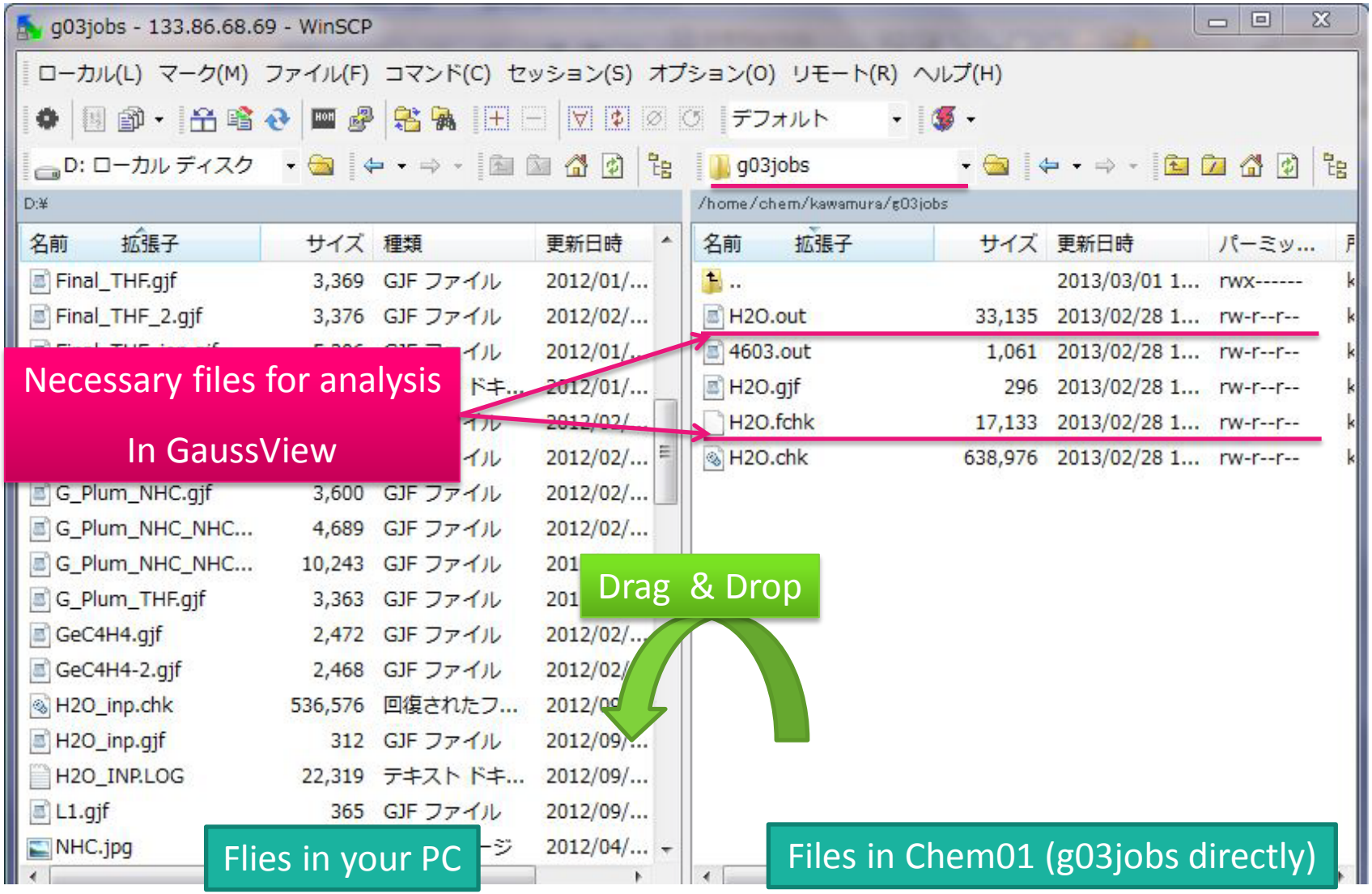
**H2O.fchk : formatted checkpoint file**

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



# 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 | **3.47** | **12** | **2** | **96** |
| chem02 | **3.47** | **12** | **3** | **96** |
| chem03 | **2.67** | **4** | **1** | **6** |
| chem04 | **2.33** | **8** | **2** | **16** |
| chem05 | **3.00** | **8** | **2** | **16** |

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 chem01because 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
8th building room 571（internal tel: 3582）
Theoretical / computational chemistry laboratory