Instructions for Running First DFT Calculations on MSU High Performance Computing

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Goal

This tutorial is intended guide you through process of submitting density functional theory calculations to MSU high performance computing. The goal of this tutorial is to submit jobs with as few terminal commands as possible.

Most of the steps below are just part of setting up and you'll never need to do them again. Once you have completed the setup, submitting jobs will be as easy as uploading inputs and, logging into a compute node, and typing `submit.sh`.

Request access to HPC and software

Get a high performance computing (HPC) account by asking your advisor to submit a request at https://contact.icer.msu.edu/account).
Request access to Gaussian and ORCA at their respective links.
Log in to HPCC with ondemand.hpcc.msu.edu

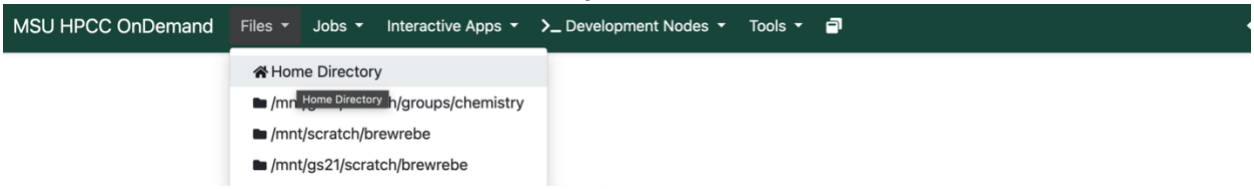
Download submission script and sample input files

Navigate here and download the files called

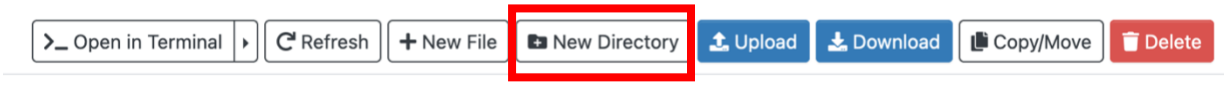
AcCl.gjf
submit.sh
water.inp
.bashrc

Upload the submission script to HPC

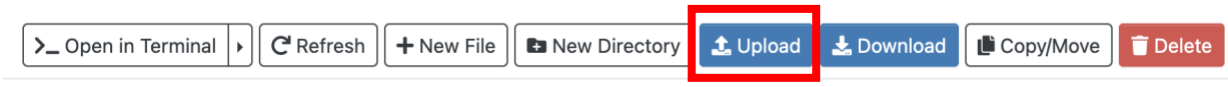
Click on “Files” and select “Home Directory”



Create a new directory in your Home Directory and name it “scripts”. Note that naming of files and directories is case sensitive, eg (“scripts” not “Scripts”)

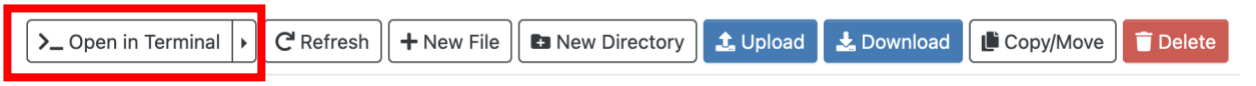


Click on your “scripts” directory so you’re working inside of it. Upload submit.sh to scripts directory

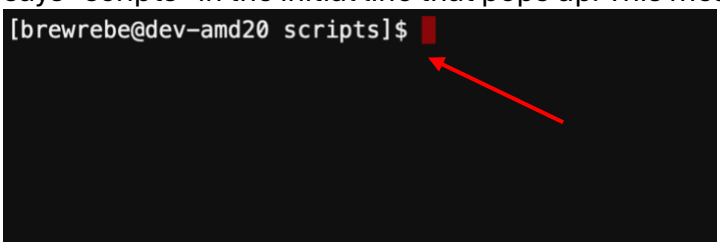


Enable execution permission on submission script

While in the scripts directory click on “Open in Terminal”

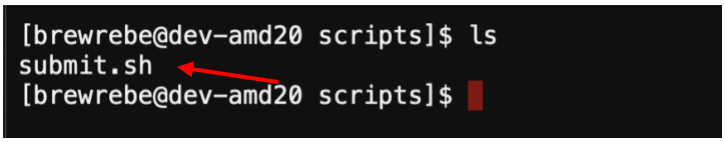


This opens an interface in which you’ll type all your commands – confirm that your interface says “scripts” in the initial line that pops up. This means you’re in the correct directory.



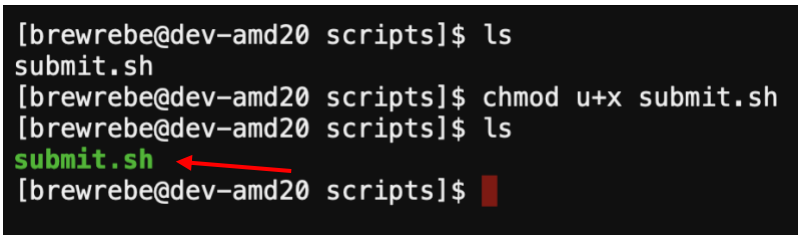
Into the terminal prompt type `ls` (to list the content of the directory) and press return.

The output of the terminal should show `submit.sh` in white (the white indicates execution permissions are not enabled yet)



Type `chmod u+x submit.sh` and press return.

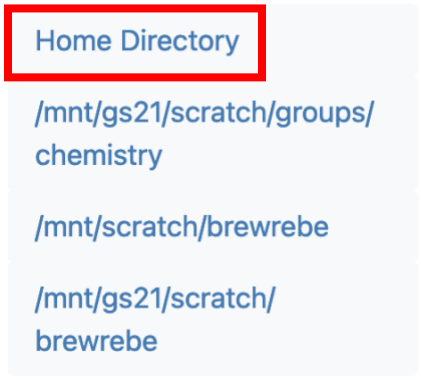
Type `ls` and hit return again. Now `submit.sh` should show up in green indicating that permissions are enabled.



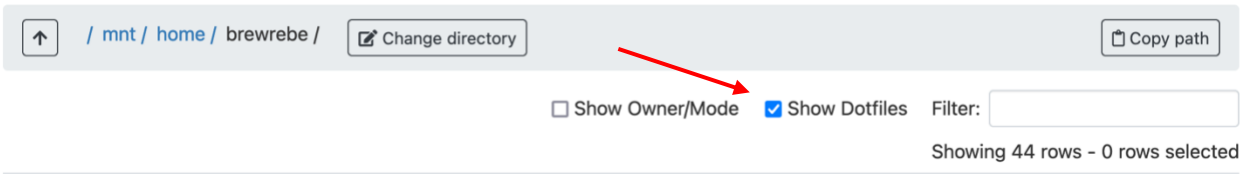
Close out of the terminal – you should be back in your scripts directory

Add scripts to your path

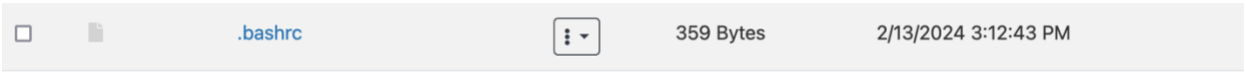
Return to Home Directory



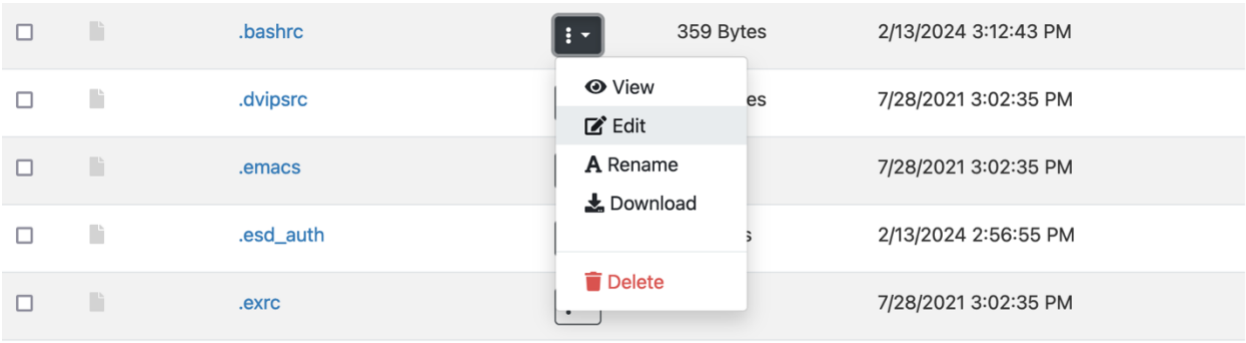
You should see a checkbox labeled “Show dot files”. Check that box.



Find the file that is labeled “.bashrc”



Click the three dot menu and select “edit”



This will pull up a file editor. Add a line to the bottom of the file that says `PATH=$PATH:~/scripts`

The file should now look like this:

```
test -f /etc/profile.dos && . /etc/profile.dos

# Some applications read the EDITOR variable to determine your favourite text
# editor. So uncomment the line below and enter the editor of your choice :-)
#export EDITOR=/usr/bin/vim
#export EDITOR=/usr/bin/mcedit

# add aliases if there is a .aliases file
test -s ~/.alias && . ~/.alias
PATH=$PATH:~/scripts

```

OPTIONAL: You can add another line that says

```
alias sq='squeue  --format="%.18i %.30j %.8u %.8T %.10M %.9l" --me'
```

This makes some stuff look prettier and easier to digest in your terminal view.

Your file should now look like this:

```
test -f /etc/profile.dos && . /etc/profile.dos

# Some applications read the EDITOR variable to determine your favourite text
# editor. So uncomment the line below and enter the editor of your choice :-)
#export EDITOR=/usr/bin/vim
#export EDITOR=/usr/bin/mcedit

# add aliases if there is a .aliases file
test -s ~/.alias && . ~/.alias
PATH=$PATH:~/scripts
alias sq='squeue  --format="%.18i %.30j %.8u %.8T %.10M %.9l" --me'

```

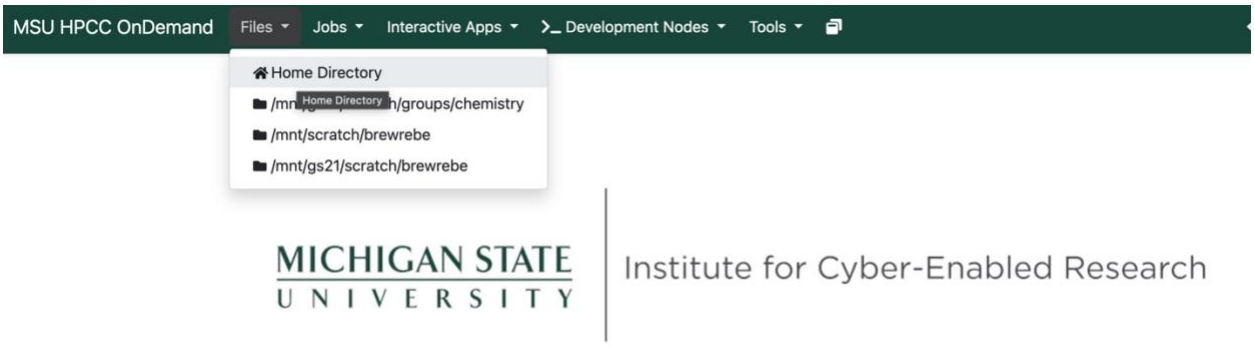
Hit save and exit out of the file editor tab.

Log out of your on-demand session and login again.

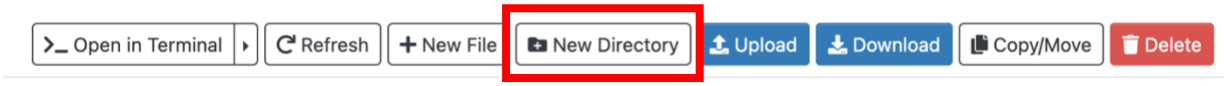
You can see a copy of my .bashrc file here.

Create a directory and upload input files into it

Click on “Files” and select “Home Directory”

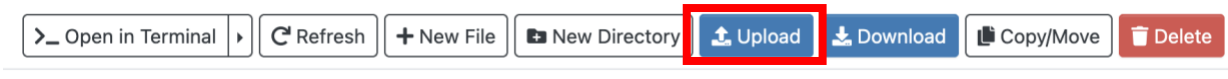


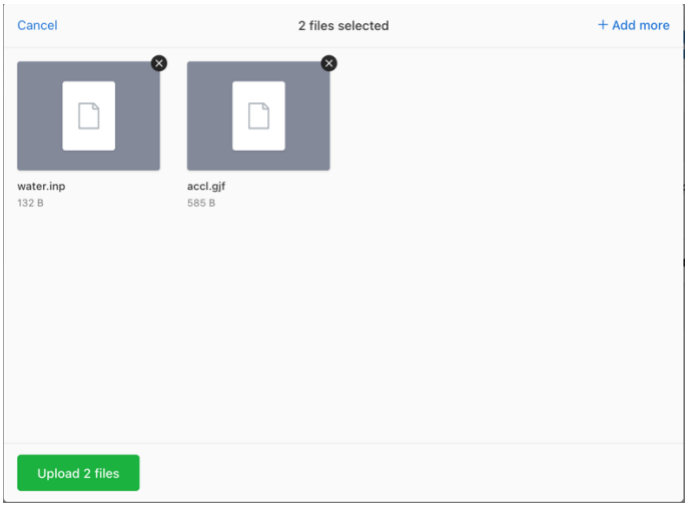
Click New Directory while in your Home Directory – label this “my_first_calcs”



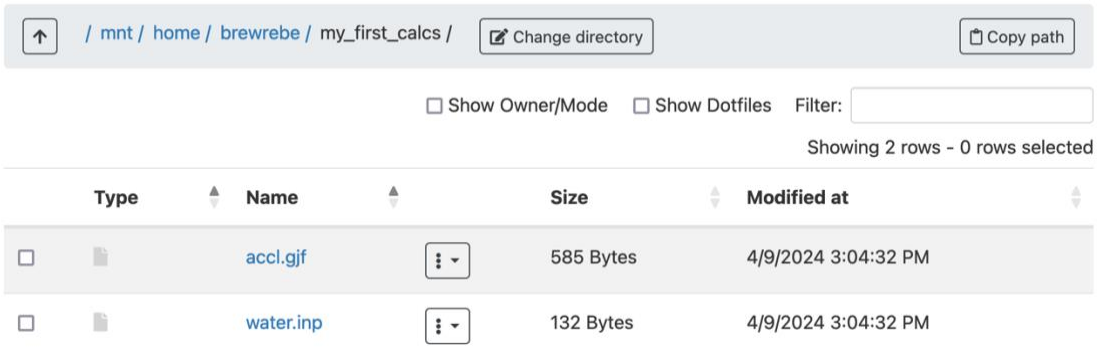
Click into your “my_first_calcs” directory

Now upload the input vials that you downloaded (water.inp and AcCl.gjf) into “my_first_calcs” folder.



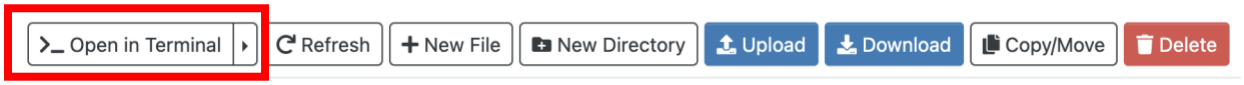


You should now see these two files in your “my_first_calcs” directory

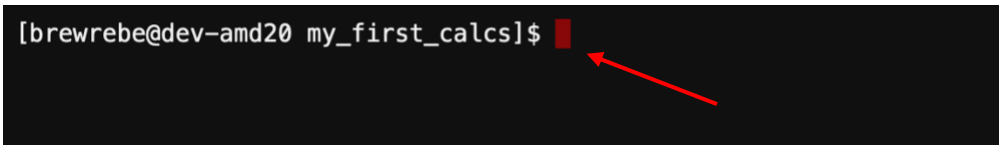


Submit your jobs

While in “my_first_calcs” directory, click “open in terminal”



Confirm that your interface says “my_first_calcs” in the initial line that pops up. This means you’re in the correct directory.



Type ssh dev-amd20-v100 and press return.
Type submit.sh and press return.

You should receive a “Submitted batch job” and a string of numbers – this means you submitted your job successfully! Good job!

```
[brewrebe@dev-amd20 my_first_calcs]$ submit.sh
Submitted batch job 33659858
```

Type sq and hit return to receive a report of the jobs you have in the queue
Pending – the job is waiting to start
Running – lists the amount of time the job has been running

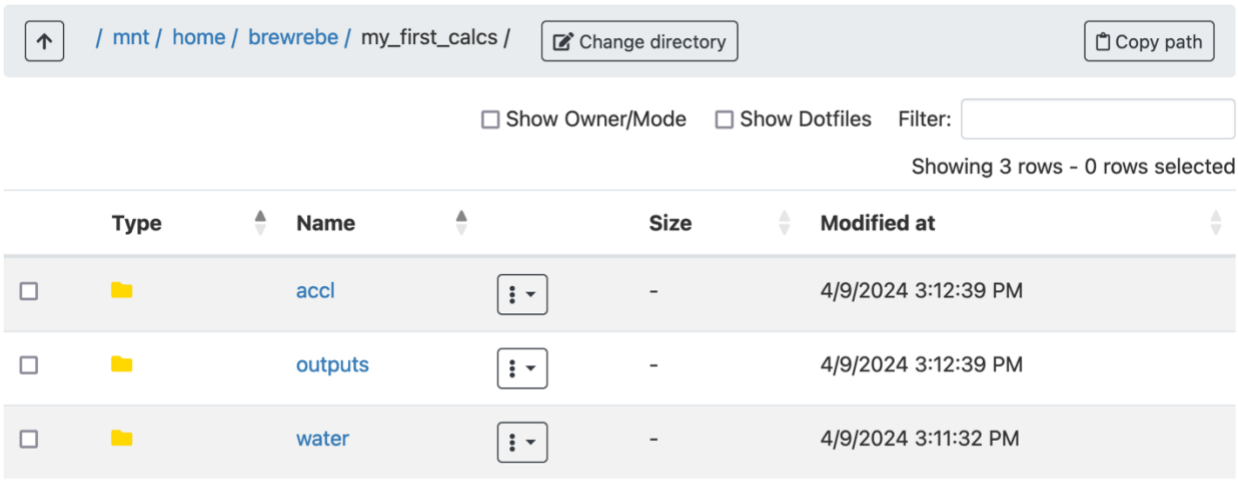
```
[brewrebe@dev-amd20 my_first_calcs]$ sq
Tue Apr 09 15:12:19 2024
             JOBID PARTITION     NAME     USER    STATE       TIME TIME_LIMI  NODES NODELIST(REASON)
          33659858 general-s     accl brewrebe  RUNNING       0:34   4:00:00      1 lac-021
Checking the Queue
  Total     1 Jobs in the queue for brewrebe
            1 Jobs Running
            0 Jobs Pending
            0 Jobs Completed
[brewrebe@dev-amd20 my_first_calcs]$
```

Check ouputs

To find your completed job, close out of the terminal – you should still be in "my_first_calcs" folder

There should be three new folders here – they should be called "water", "AcCl", and "outputs"

Most of what we need will be in "outputs"



Within a few minutes the jobs will complete and you can find them in your outputs folder.

Once the output files are in the output folder, you can open them to view the job results and confirm they ran normally.

Scroll all the way to the bottom of the file to confirm that the job finished successfully.

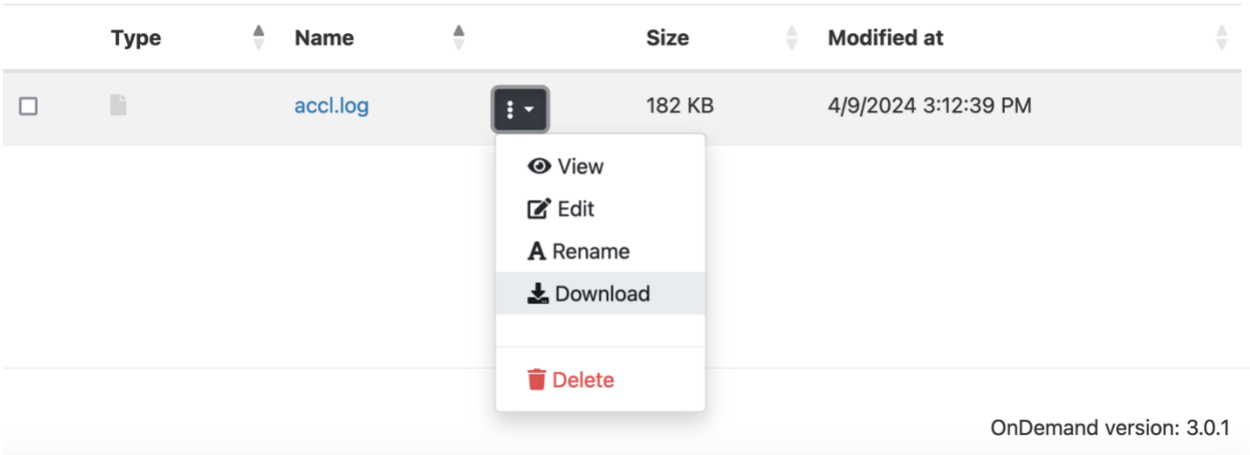
```
AND THIS OUR LIFE, EXEMPT FROM PUBLIC HAUNT,
FINDS TONGUES IN TREES, BOOKS IN THE RUNNING BROOKS,
SERMONS IN STONES, AND GOOD IN EVERYTHING.
I WOULD NOT CHANGE IT. -- W. SHAKESPEARE
AS YOU LIKE IT, ACT II, SCENE 1.
Job cpu time:       0 days  0 hours  3 minutes 20.6 seconds.
Elapsed time:       0 days  0 hours  0 minutes 14.1 seconds.
File lengths (MBytes):  RWF=    272 Int=      0 D2E=      0 Chk=     32 Scr=     32
Normal termination of Gaussian 16 at Tue Apr  9 15:12:39 2024.
```

```
Timings for individual modules:

Sum of individual times         ...       41.675 sec (=   0.695 min)
GTO integral calculation        ...       11.007 sec (=   0.183 min)  26.4 %
SCF iterations                  ...       13.153 sec (=   0.219 min)  31.6 %
SCF Gradient evaluation         ...       10.427 sec (=   0.174 min)  25.0 %
Geometry relaxation             ...        0.933 sec (=   0.016 min)   2.2 %
Analytical frequency calculation...        6.154 sec (=   0.103 min)  14.8 %

                    ****ORCA TERMINATED NORMALLY****
TOTAL RUN TIME: 0 days 0 hours 0 minutes 50 seconds 10 msec
```

Download the output files to your computer.



Once you have the output files downloaded, you can analyze them locally using Chimera X. This link provides step by step instruction on how to use Chimera X to analyze output files.

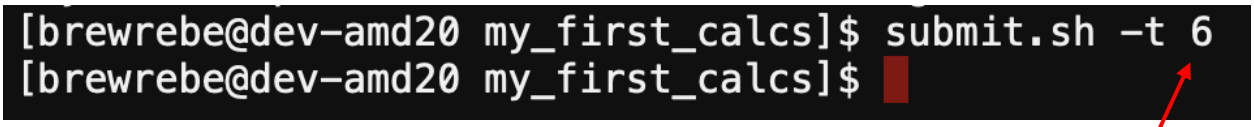
Notes

Typing `submit.sh -h` returns some options for submission script usage.

```
[brewrebe@dev-amd20 my_first_calcs]$ submit.sh -h
-p flag will ask for prompts for calculation parameters on each input
-c flag allows for specification of default number of cpus
-t flag allows for default specification of number of hours (4h or less is fastest)
Any files specified will be run. No arguments will run all in cwd)
[brewrebe@dev-amd20 my_first_calcs]$
```

The default is set at 4 hours (any time less than or equal to 4 hrs gives the job priority and it runs faster).

If you are running a more complicated job and need to change the default to run longer, type "submit.sh -t" and then the number of hours you want to edit the runtime to. As an example, I changed mine to 6 hours.



Now you can submit your job as you normally would, as directed previously in this document.