Intermediate Level Introduction to Computing at CARC

1 hour version with Gaussian

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Version 0.1

Goals

- 1) SLURM scheduler literacy
- 2) Example Gaussian

- We wont cover file transfer, storage systems, module system, conda, PBS. (These are all covered in depth in the video tutorials)

Logging into Hopper

First login to the Linux **workstation** in front of you. Your CARC username is on the sign in sheet.

If you have logged in before use your existing password

Otherwise, your initial password is Welcome2CARC

This is an “important step” so don’t let me move on until you have logged in

Logging into Hopper


```
ssh vanilla@hopper.alliance.unm.edu
```

Should prompt you for a password…

Don’t let me move on until you are able to login.

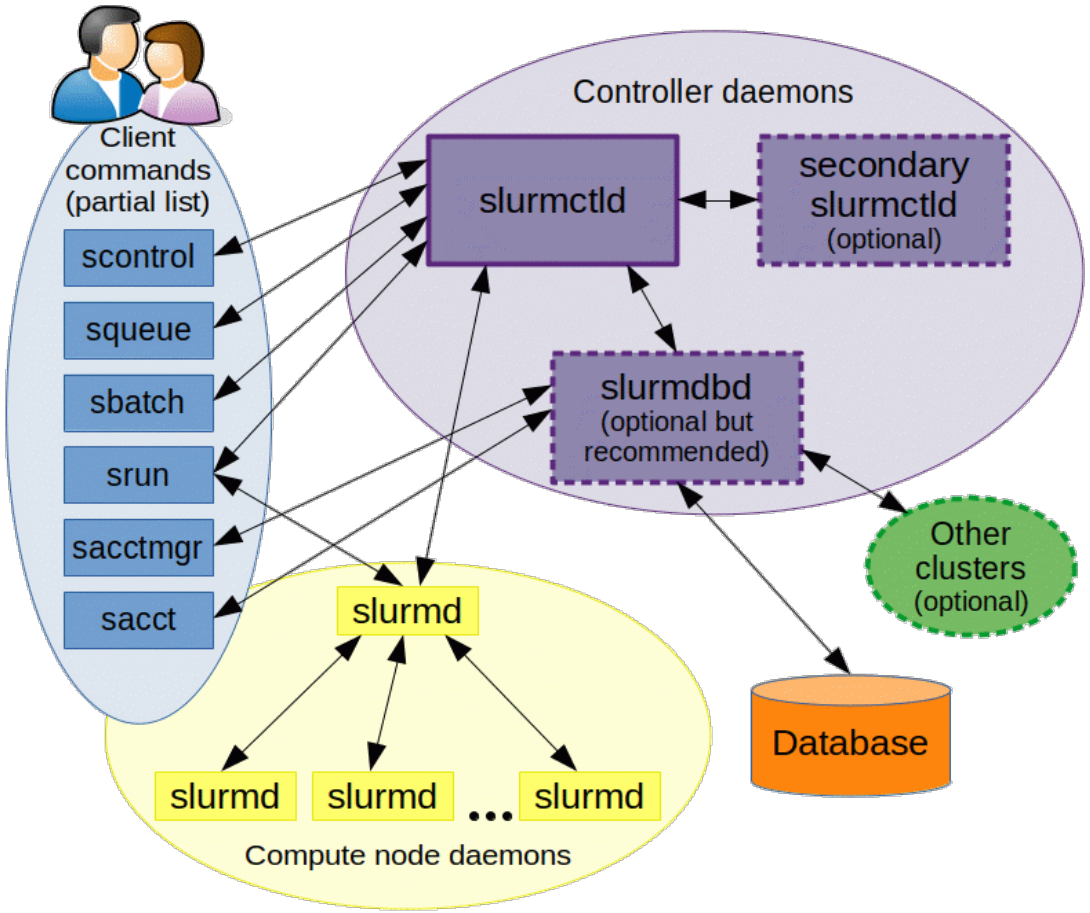
Replace vanilla with your name (unless your last name is Ice)

Logging into Hopper

```
Welcome to Hopper

  Be sure to review the "Acceptable Use" guidelines posted on the CARC website.

  For assistance using this system email help@carc.unm.edu.

  Tutorial videos can be accessed through the CARC website: Go to
    http://carc.unm.edu, select the "New Users" menu and then click
      "Introduction to Computing at CARC".

  Warning: By default home directories are world readable. Use the chmod command
    to restrict access.

  Don't forget to acknowledge CARC in publications, dissertations, theses and
    presentations that use CARC computational resources:

  "We would like to thank the UNM Center for Advanced Research Computing,
  supported in part by the National Science Foundation, for providing the
  research computing resources used in this work."

  Please send citations to publications@carc.unm.edu.

  There are three types of slurm partitions on Hopper:
  1) General - this partition is accessible by all CARC users.

  2) Condo - preemtable scavenger queue available to all condo users. Your job must use checkpointing to use this
queue or you will lose any work you have done if it is preempted by the partition's owner.

  3) Named partitions - these partitions are available to condo users working under the grant/lab/center that
purchased the associated hardware.

  Type "qgrok" to get the status of the partitions.
--------------------------------------------------------------------------------
Last login: Wed Jul 27 17:46:13 2022 from 129.24.246.68
mfricke@hopper:~ $
```

Simple Linux Utility for Resource Management

slurm
workload manager




ENJOY
Slurm
SODA
IT'S HIGHLY ADDICTIVE!
VOTED #1 SOFT DRINK OF THE 31ST CENTURY!

```
[vanilla@hopper ~]$ qgrok
queues      free   busy   offline  jobs   nodes  CPUs   GPUs   CPUs/node  GPUs/node  Memory/node  time_limit   CPU_limit
-----       -----  -----  -------  -----  -----  -----  -----  ---------  ---------  -----------  -----------  ---------
general     4      6      0        4      10     320    0      32         0          93G          2-00:00:00   64
debug       2      0      0        0      2      64     0      32         0          93G          4:00:00      8
condo       22     25     4        7      51     1632   28     32         2          93G-1.5T     2-00:00:00   192
bugs        2      0      0        0      2      64     0      32         0          93G          7-00:00:00
```

```
vanilla@hopper:~ $ qgrok
queues      free   busy   offline  jobs   nodes  CPUs   GPUs
-----       -----  -----  -----    -----  -----  -----  -----
general     1      9      0        7      10     320    0
debug       2      0      0        0      2      64     0
condo       18     19     1        7      38     1216   8
bugs        0      2      0        0      2      64     0
pcnc        1      1
pathogen    1      0
tc          5      5
gold        2      0
fishgen     0      1
neuro-hsc   8      6
cup-ecs     0      2
tid         0      1
biocomp     0      1
chakra      1      0
pna         0      0
totals:     19     28
```

Open partitions for use by everyone with a CARC account.

Purchased by the Office for the Vice President for Research.

```
vanilla@hopper:~ $ qgrok
queues      free   busy   offline  jobs   nodes  CPUs   GPUs
-----       -----  -----  -----    -----  -----  -----  -----
general     1      9      0        7      10     320    0
debug       2      0      0        0      2      64     0
condo       18     19     1        7      38     1216   8
bugs        0      2      0        0      2      64     0
pcnc        1      1      0        0      2      64     0
pathogen    1      0      0        0      1      32     0
tc          5      5      0        3      10     320    0
gold        2      0      0        0      2      64     0
fishgen     0      1      0        0      1      32     0
neuro-hsc   8      6      0        0      14     448    0
cup-ecs     0      2      0        2      2      64     4
tid         0      1      0        0      1      32     2
biocomp     0      1      0        0      1      32     1
chakra      1      0      0        0      1      32     1
pna         0      0      1        0      1      32     0
totals:     19     28     1        14     48     1536   8
```

```
vanilla@hopper:~ $ qgrok
queues      free   busy   offline  jobs   nodes  CPUs   GPUs
-----       -----  -----  -----    -----  -----  -----  -----
general     1      9      0        7      10     320    0
debug       2      0      0        0      2      64     0
condo       18     19     1        7      38     1216   8
bugs        0      2      0        0      2      64     0
pcnc        1      1
pathogen    1      0
tc          5      5
gold        2      0
fishgen     0      1
neuro-hsc   8      6
cup-ecs     0      2
tid         0      1
biocomp     0      1
chakra      1      0
pna         0      0
totals:     19     28
```

Private partitions

- Reserved for use by the purchaser.
- Request access by emailing support@carc.unm.edu and CC the partition owner.

```
mfricke@hopper:~ $ qgrok
queues      free   busy   offline  jobs   nodes  CPUs   GPUs
-----       -----  -----  -----    -----  -----  -----  -----
general     1      9      0        7      10     320    0
debug       2      0      0        0      2      64     0
condo       18     19     1        7      38     1216   8
bugs        0      2      0        0      2      64     0
pcnc        1      1
pathogen    1      0
tc          5      5
gold        2      0
fishgen     0      1
neuro-hsc   8      6
cup-ecs     0      2
tid         0      1
biocomp     0      1
chakra      1      0
pna         0      0
totals:     19     28
```

Condo "scavenger" partition

- Allows you to use compute nodes purchased by another group that are currently idle.
- May be interrupted at any time if the owners start to use it.

```
[vanilla@hopper ~]$ quotas
Home Directory (/users/vanilla):
quota: Cannot resolve mountpoint path /root/.spack: Permission denied
Disk quotas for user vanilla (uid 659):
     Filesystem   space   quota   limit   grace   files   quota   limit   grace
chama:/home/homes
                 1527M    100G    200G           14913   4295m   4295m
---------------------------
Centerwide user scratch (/carc/scratch/users/mfricke)

Quota information for storage pool Default (ID: 1):

      user/group     ||           size          ||    chunk files
     name     |  id  ||    used    |    hard    ||  used   |  hard
--------------|------||------------|------------||---------|---------
       mfricke|  1512||  592.71 GiB | 1024.00 GiB ||    32784|unlimited

Centerwide scratch quota for project mfricke2016174 (/carc/scratch/projects/mfricke2016174)

Quota information for storage pool Default (ID: 1):
      user/group     ||           size          ||    chunk files
     name     |  id  ||    used    |    hard    ||  used   |  hard
--------------|------||------------|------------||---------|---------
mfricke2016174|2016142||  190.97 GiB| 1024.00 GiB||    23704|unlimited
```

```
[vanilla@hopper ~]$ sinfo --partition debug
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
debug        up    4:00:00      2   idle hopper[011-012]
```

sinfo reports information about partitions

```
[vanilla@hopper ~]$ sinfo --partition debug
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
debug        up    4:00:00      2   idle hopper[011-012]
```

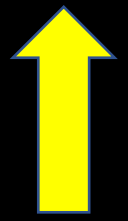
The debug queues are intended for testing your programs.

And for interactive jobs.

```
[vanilla@hopper ~]$ sinfo --partition debug
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
debug        up    4:00:00      2   idle hopper[011-012]
```

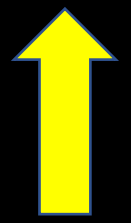
Name

```
[vanilla@hopper ~]$ sinfo --partition debug
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
debug        up    4:00:00      2   idle hopper[011-012]
```



You can run a “job” for up to 4 hrs.

```
[vanilla@hopper ~]$ sinfo --partition debug
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
debug        up    4:00:00      2   idle hopper[011-012]
```



There are two nodes in this partition.

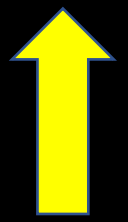
```
[vanilla@hopper ~]$ sinfo --partition debug
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
debug        up    4:00:00      2   idle hopper[011-012]
```

The names of the nodes in the partition

```
[vanilla@hopper ~]$ sinfo --partition debug
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
debug        up    4:00:00      2   idle hopper[011-012]
```

The names of the nodes in the partition

```
[vanilla@hopper ~]$ sinfo --partition general
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
general*     up 2-00:00:00      9  alloc hopper[001-009]
general*     up 2-00:00:00      1   idle hopper010
```



Hopper001 through 009 are running jobs.

Hopper010 is waiting to be used.

```
[vanilla@hopper ~]$ hostname
hopper
[vanilla@hopper ~]$
```

Running on the Head Node.

The head node’s name is “hopper”.

```
[vanilla@hopper ~]$ hostname
hopper
[vanilla@hopper ~]$ man hostname
```

```
[vanilla@hopper ~]$ hostname
hopper
[vanilla@hopper ~]$ man hostname
(‘q’ to quit)

[vanilla@hopper ~]$ man man
(‘q’ to quit)
```

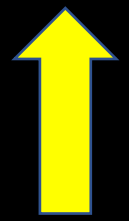
[vanilla@hopper ~]$ man sinfo

```
sinfo(1)                                    Slurm
Commands                                    sinfo(1)

NAME
       sinfo - View information about Slurm nodes and partitions.

SYNOPSIS
       sinfo [OPTIONS...]

DESCRIPTION
       sinfo is used to view partition and node information for a system running
Slurm

OPTIONS
       -a, --all
              Display  information  about  all partitions. This causes information
to be displayed about partitions that are configured as hidden and partitions
that are unavailable to the user's group.
```

[vanilla@hopper ~]$ sinfo --all

```
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
general*     up 2-00:00:00      9  alloc hopper[001-009]
general*     up 2-00:00:00      1   idle hopper010
debug        up    4:00:00      2   idle hopper[011-012]
condo        up 2-00:00:00      1  down* hopper045
condo        up 2-00:00:00      3    mix hopper[018-020]
condo        up 2-00:00:00     16  alloc hopper[013-015,028-036,049-052]
condo        up 2-00:00:00     18   idle hopper[016-017,021-027,037-044,053]
bugs         up 7-00:00:00      2  alloc hopper[013-014]
pcnc         up 7-00:00:00      1  alloc hopper015
pcnc         up 7-00:00:00      1   idle hopper016
pathogen     up 7-00:00:00      1   idle hopper017
tc           up 7-00:00:00      3    mix hopper[018-020]
tc           up 7-00:00:00      2  alloc hopper[029-030]
tc           up 7-00:00:00      5   idle hopper[021-025]
gold         up 7-00:00:00      2   idle hopper[026-027]
fishgen      up 7-00:00:00      1  alloc hopper028
neuro-hsc    up 7-00:00:00      6  alloc hopper[031-036]
neuro-hsc    up 7-00:00:00      8   idle hopper[037-044]
cup-ecs      up 7-00:00:00      2  alloc hopper[049-050]
tid          up 7-00:00:00      1  alloc hopper051
biocomp      up 7-00:00:00      1  alloc hopper052
chakra       up 7-00:00:00      1   idle hopper053
pna          up 7-00:00:00      1  down* hopper045
```

```
[vanilla@hopper ~]$ srun --partition debug hostname
```

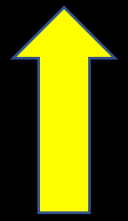


Tell slurm to run a program
on a compute node…

```
[vanilla@hopper ~]$ srun --partition debug hostname
```

Run the program on a compute node in the debug partition.

```
[vanilla@hopper ~]$ srun --partition debug hostname
```



The program to run.

```
[vanilla@hopper ~]$ srun --partition debug hostname
srun: Account not specified in script or
~/.default_slurm_account, using latest project
You have not been allocated GPUs. To request GPUs,
use the -G option in your submission script.
hopper011
```

```
[vanilla@hopper ~]$ squeue
```

```
[vanilla@hopper ~]$ squeue
 JOBID PARTITION     NAME     USER ST       TIM
 4314   general      PRE erowland PD      0:00
 4315   general      PRE erowland PD      0:00
 4317   general      PRE erowland PD      0:00
 4318   general      PRE erowland PD      0:00
```

PD means programs that are waiting their turn.

Shows you what the slurm scheduler is doing right now.

Here we can see that user ’erowland’ has a lot of programs waiting to run.

```
2 (QOSMaxCpuPerUserLimit)
2 (QOSMaxCpuPerUserLimit)
2 (QOSMaxCpuPerUserLimit)
2 (QOSMaxCpuPerUserLimit)
2 (QOSMaxCpuPerUserLimit)
2 (QOSMaxCpuPerUserLimit)
2 (QOSMaxCpuPerUserLimit)
2 (QOSMaxCpuPerUserLimit)
2 (QOSMaxCpuPerUserLimit)
2 (QOSMaxCpuPerUserLimit)
2 (QOSMaxCpuPerUserLimit)
2 (QOSMaxCpuPerUserLimit)
2 (QOSMaxCpuPerUserLimit)
2 (QOSMaxCpuPerUserLimit)
2 (QOSMaxCpuPerUserLimit)
2 (QOSMaxCpuPerUserLimit)
2 (QOSMaxCpuPerUserLimit)
2 (QOSMaxCpuPerUserLimit)
2 (QOSMaxCpuPerUserLimit)
```

```
[vanilla@hopper ~]$ squeue
 JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
             4314   general      PRE erowland PD       0:00      2 (QOSMaxCpuPerUserLimit)
             4315   general      PRE erowland PD       0:00      2 (QOSMaxCpuPerUserLimit)
             4317   general      PRE erowland PD       0:00      2 (QOSMaxCpuPerUserLimit)
             4318   general      PRE erowland PD       0:00      2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
             4337   general      PRE erowland PD       0:00      2 (QOSMaxCpuPerUserLimit)
```

The reason these jobs are not running is that ‘erowland’ is already using the maximum number of CPUs they are allowed.

```
[vanilla@hopper ~]$ squeue -t R --all
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
              4405     condo    2ndMA  mfricke  R 1-07:48:30      6 hopper[031-036]
              5208     condo       NN      kgu  R    5:48:49      1 hopper015
              5210     condo       NN      kgu  R    6:30:13      1 hopper014
              5209     condo       NN      kgu  R    6:31:13      1 hopper013
              5206     condo       NN      kgu  R    6:32:13      1 hopper051
              5207     condo       NN      kgu  R    6:32:13      1 hopper052
              5205     condo       NN      kgu  R    6:32:43      1 hopper028
              4595   cup-ecs golConfi aalasand  R 2-06:51:59      1 hopper050
              4594   cup-ecs golConfi aalasand  R 2-06:52:03      1 hopper049
              5120   general jupyterh   jacobm  R   11:45:47      1 hopper007
              4313   general      PRE erowland  R    1:17:29      2 hopper[003-004]
              5111   general    1stMA  mfricke  R   11:15:28      2 hopper[005-006]
              5025   general      c2n    jxzuo  R       1:50      1 hopper001
              5024   general      c2n    jxzuo  R      31:28      1 hopper002
              5203   general       NN      kgu  R    6:37:50      1 hopper009
              5201   general       NN      kgu  R    6:38:14      1 hopper008
              4390        tc UCsTpCyd lepluart  R 2-15:18:18      3 hopper[018-020]
              5198        tc       NN      kgu  R    6:40:19      1 hopper030
              5196        tc       NN      kgu  R    6:40:31      1 hopper029
```

```
[vanilla@hopper ~]$ srun --partition debug --ntasks 2 hostname
srun: Account not specified in script or
~/.default_slurm_account, using latest project
You have not been allocated GPUs. To request GPUs, use the -G
option in your submission script.
hopper011
hopper011
```

```
[vanilla@hopper ~]$ srun --partition debug --ntasks 2 hostname
srun: Account not specified in script or
~/.default_slurm_account, using latest project
You have not been allocated GPUs. To request GPUs, use the -G
option in your submission script.
hopper011
hopper011
```

You ran two copies of your program.

ntasks is the number of copies to run.

```
[vanilla@hopper ~]$ srun --partition debug --ntasks 8 hostname
srun: Account not specified in script or
~/.default_slurm_account, using latest project
hopper011
hopper011
hopper011
You have not been allocated GPUs. To request GPUs, use the -G
option in your submission script.
hopper011
hopper011
hopper011
hopper011
hopper011
hopper011
```

You ran eight copies of your program.

ntasks is the number of copies to run.

```
[vanilla@hopper ~]$ srun --partition debug --ntasks 8 hostname
srun: Account not specified in script or
~/.default_slurm_account, using latest project
hopper011
hopper011
hopper011
You have not been allocated GPUs. To request GPUs, use the -G
option in your submission script.
hopper011
hopper011
hopper011
hopper011
hopper011
```

By default, each task (copy of your program) is allowed to use one CPU.

Many programs are able to use more than one CPU at a time.

```
[vanilla@hopper ~]$ srun --partition debug --ntasks 2 --cpus-per-task 2 hostname
srun: Account not specified in script or ~/.default_slurm_account, using latest project
You have not been allocated GPUs. To request GPUs, use the -G option in your submission
script.
hopper011
hopper011
```

Here we are telling SLURM to run 2 copies of our program and let each copy of our program use 2 CPUs.

```
[vanilla@hopper ~]$ srun --partition debug --nodes 2 -ntasks-per-node 4 hostname
srun: Account not specified in script or ~/.default_slurm_account, using
latest project
hopper012
You have not been allocated GPUs. To request GPUs, use the -G option in
your submission script.
hopper012
hopper011
hopper011
hopper012
hopper012
hopper011
hopper011
```

Here we are telling SLURM to run 4 copies of our program on 2 different compute nodes.

This is useful when our programs need a bigger share of the compute node.

```
[vanilla@hopper ~]$ srun --partition debug --nodes 2
--ntasks-per-node 2 --cpus-per-task 2 hostname
srun: Account not specified in script or
~/.default_slurm_account, using latest project
hopper011
You have not been allocated GPUs. To request GPUs, use
the -G option in your submission script.
hopper011
hopper012
hopper012
```

And we can combine all three.

```
[vanilla@hopper ~]$ srun --partition debug --mem 4G
--nodes 2 --ntasks-per-node 2 --cpus-per-task 2
hostname
srun: Account not specified in script or
~/.default_slurm
hopper012
hopper012
You have not be                                    se
the -G option i
hopper011
Hopper011
```

And we can specify how much memory we want.

--mem 4G means give me 4 gigabytes of memory per node.

```
[vanilla@hopper ~]$ srun --partition debug --mem 4G
--nodes 2 --ntasks-per-node 2 --cpus-per-task 2
hostname
srun: Account not specified in script or
~/.default_slurm
hopper012
hopper012
You have not be                                    se
the -G option i
hopper011
Hopper011
```

Why does all this matter?

The purpose of SLURM is to provide you the hardware your programs need.

So you have to understand what those requirements are really well.

```
[vanilla@hopper ~]$ srun --partition debug --mem 4G
--nodes 2 --ntasks-per-node 2 --cpus-per-task 2 hostname
srun: Account not specified in script or
~/.default_slurm_account, using latest project
hopper012
hopper012
You have not be                                    se
the -G option i
hopper011
Hopper011
```

1) **Can my program use multiple CPUs?**
2) **How much memory does my program need?**
3) **Can my program use multiple compute nodes (MPI*, GNU Parallel*)?**
4) **Can my program use GPUs?**

```
[vanilla@hopper ~]$ srun --partition debug --mem 4G
--nodes 2 --ntasks-per-node 2 --cpus-per-task 2 hostname
srun: Account not specified in script or
~/.default_slurm_account, using latest project
hopper012
hopper012
You have not been                                    se
the -G option in
hopper011
Hopper011
```

This command is getting pretty long.

We can use shell scripts to automate all this in batch mode.

Interactive vs Batch Mode

Interactive Mode

- Everything so far has been interactive. You request hardware, run your program, and get the output on your screen right away.

Batch Mode

- Most programs at an HPC center are run in “batch” mode.
- Batch mode means we write a shell script that the SLURM scheduler runs for us. The script requests hardware just like we did with salloc and then runs the commands in the script.
- Whatever would have been written to the screen is saved to a file instead.

```
[vanilla@hopper ~]$ git clone https://lobogit.unm.edu/CARC/workshops.git
Cloning into 'workshops'...
remote: Enumerating objects: 132, done.
remote: Counting objects: 100% (75/75), done.
remote: Compressing objects: 100% (43/43), done.
remote: Total 132 (delta 33), reused 74 (delta 32), pack-reused 57
Receiving objects: 100% (132/132), 57.58 KiB | 3.60 MiB/s, done.
Resolving deltas: 100% (51/51), done.
```

Rather than make you write shell scripts lets just download some we wrote for this workshop…

```
[vanilla@hopper intro_workshop]$ pwd
/users/vanilla/workshops/intro_workshop
[vanilla@hopper intro_workshop]$ cat slurm/workshop_example.sh
#!/bin/bash
#SBATCH --partition debug
#SBATCH --ntasks 4
#SBATCH --time 00:05:00
#SBATCH --job-name ws_example
#SBATCH --mail-user your_username@unm.edu
#SBATCH --mail-type ALL

hostname
```

Let's take a look at the workshop_example.sh script in the slurm directory…

```
[vanilla@hopper intro_workshop]$ sbatch slurm/workshop_example.sh
sbatch: Account not specified in script or ~/.default_slurm_account,
using latest project
Submitted batch job 5252
[vanilla@hopper intro_workshop]$
```

We submit our slurm shell script with the sbatch command.

```
[vanilla@hopper intro_workshop]$ sbatch slurm/workshop_example.sh
sbatch: Account not specified in script or ~/.default_slurm_account,
using latest project
Submitted batch job 5252
[vanilla@hopper intro_workshop]$
```

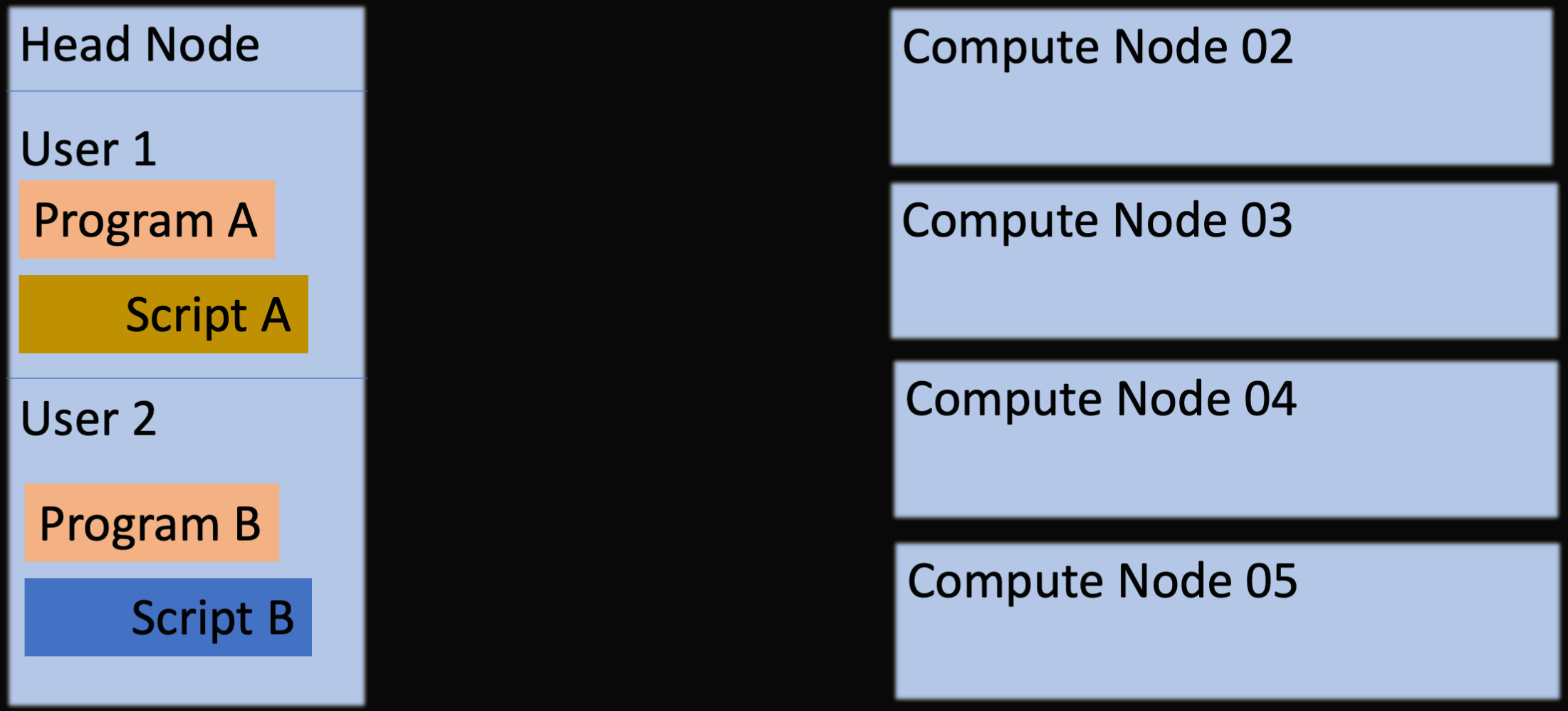
We submit our slurm shell script with the sbatch command.

Notice that the only output we get is a job id.

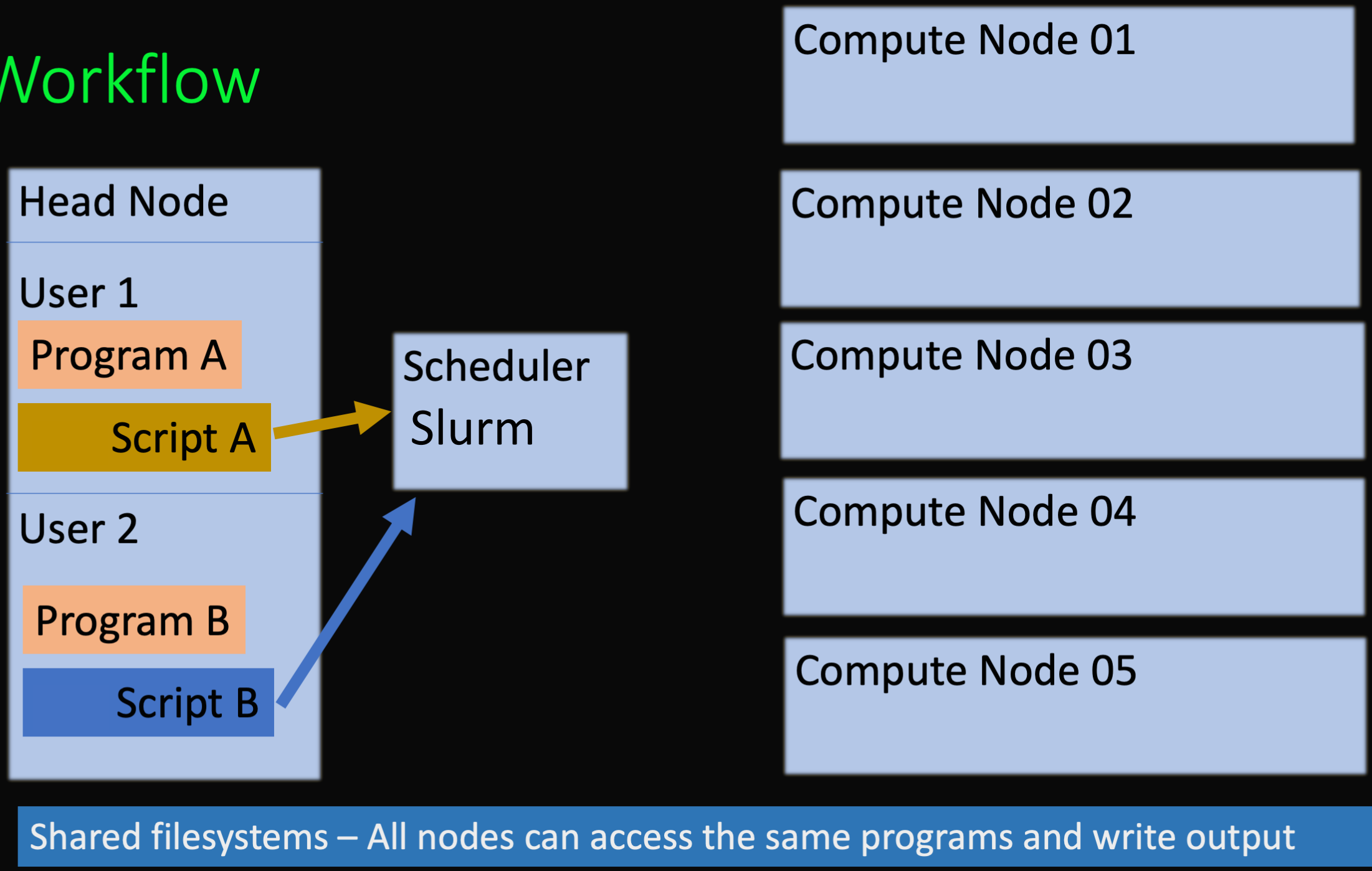
This indicates that the script was successfully sent to the scheduler.

The commands in the script will run as soon as the hardware requested is available.

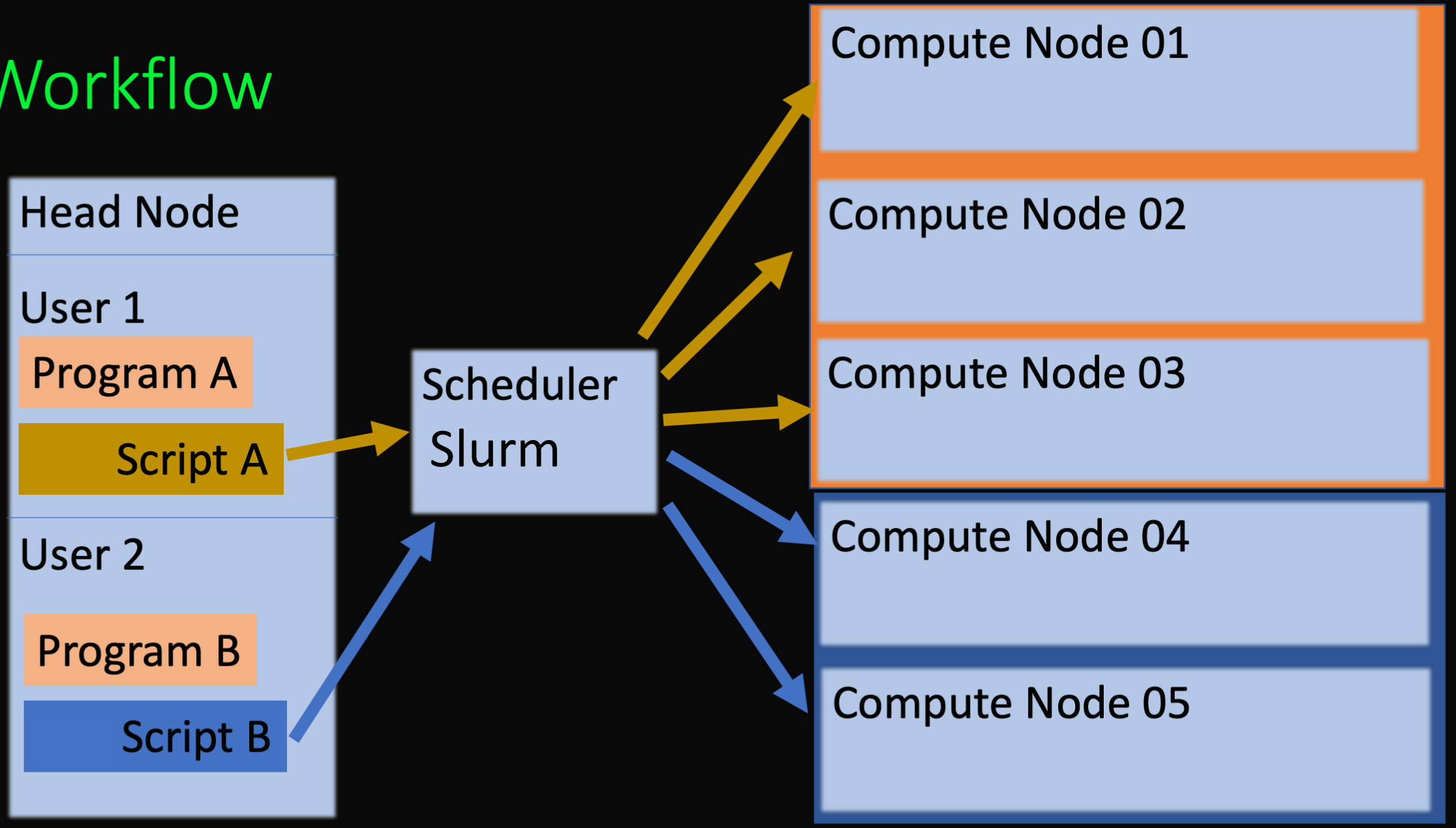
Workflow


Head Node
User 1
Program A
Script A
User 2
Program B
Script B
Compute Node 01
Compute Node 02
Compute Node 03
Compute Node 04
Compute Node 05
Shared filesystems – All nodes can access the same programs and write output

Workflow

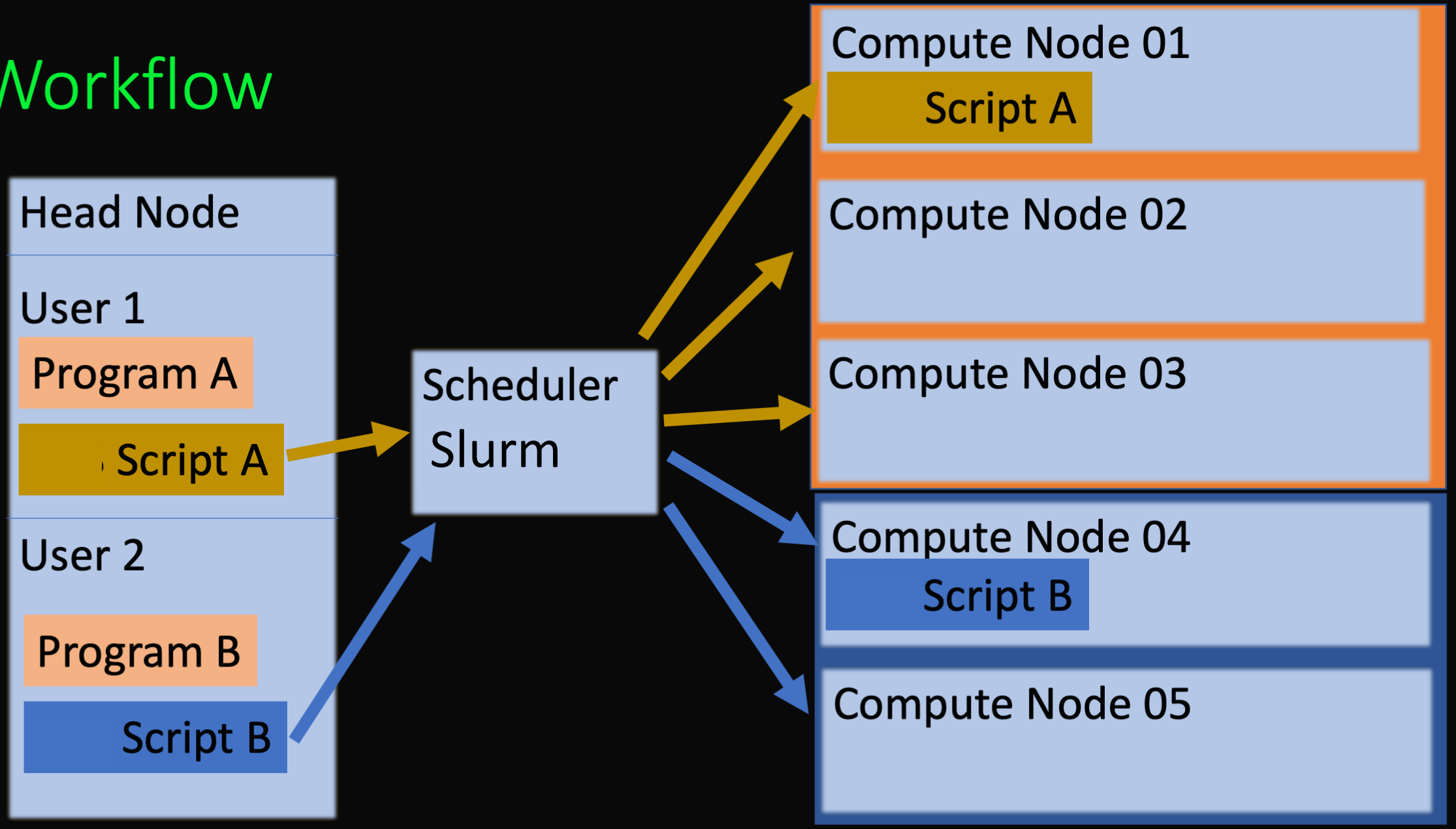

Head Node
User 1
Program A
Script A
User 2
Program B
Script B
Scheduler
Slurm
Compute Node 01
Compute Node 02
Compute Node 03
Compute Node 04
Compute Node 05
Shared filesystems – All nodes can access the same programs and write output

Workflow



Shared filesystems – All nodes can access the same programs and write output

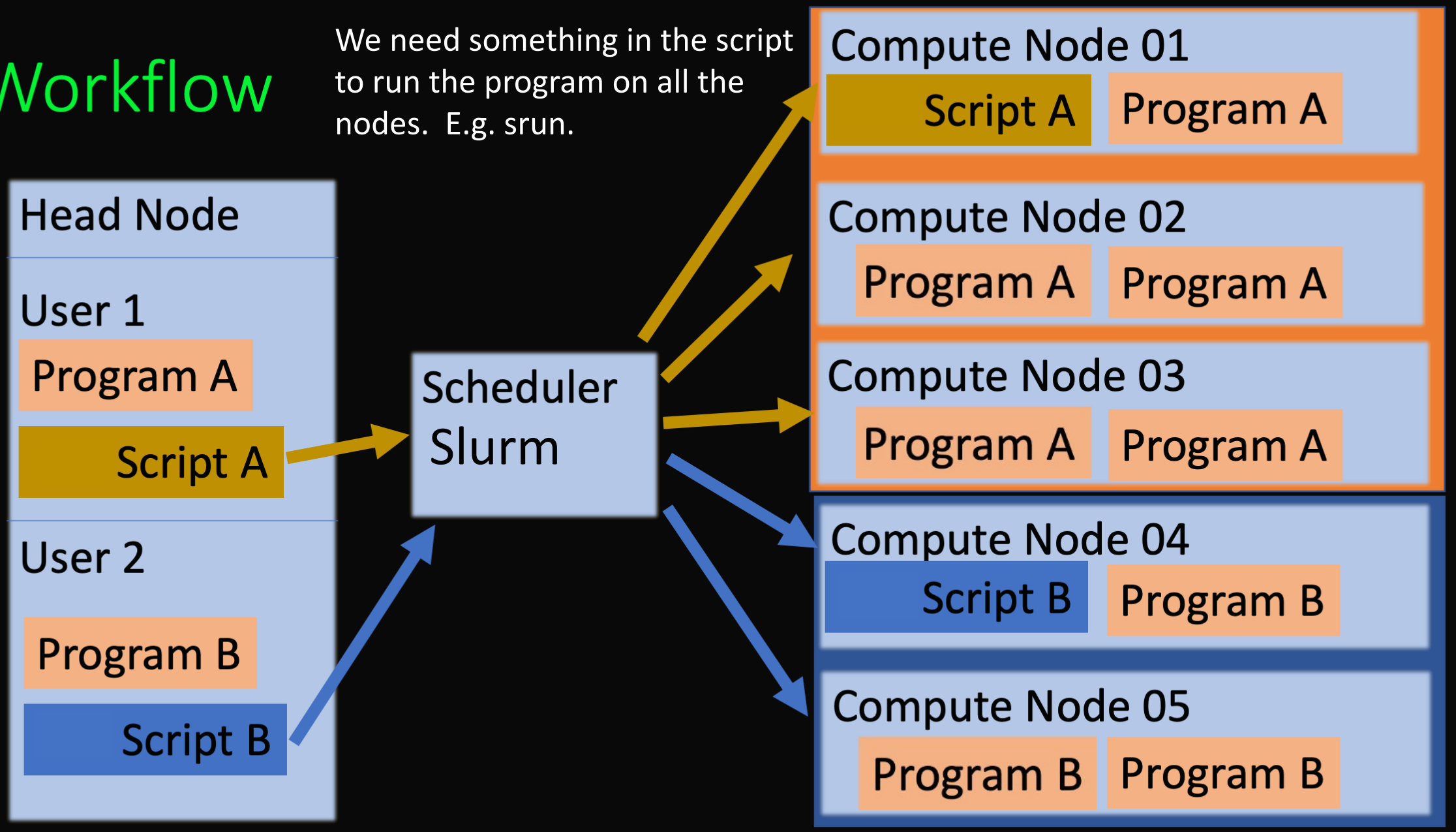
Workflow



Shared filesystems – All nodes can access the same programs and write output

Workflow

We need something in the script to run the program on all the nodes. E.g. srun.



Shared filesystems – All nodes can access the same programs and write output

```
[vanilla@hopper intro_workshop]$ ls
code  data  pbs  slurm  slurm-5252.out
```

The **hostname** command is very fast so everyone's job should finish in a few seconds.

When it is finished you will have a new file named slurm-{your job id}.out.

```
[vanilla@hopper intro_workshop]$ ls
code  data  pbs  slurm  slurm-5252.out
```

When it is finished you will have a new file named slurm-{your job id}.out.

```
[vanilla@hopper intro_workshop]$ cat slurm-5252.out
hopper011
```

```
[vanilla@hopper intro_workshop]$ ls
code  data  pbs  slurm  slurm-5252.out
```

When it is finished you will have a new file named slurm-{your job id}.out.

```
[vanilla@hopper intro_workshop]$ cat slurm-5252.out
hopper011
```

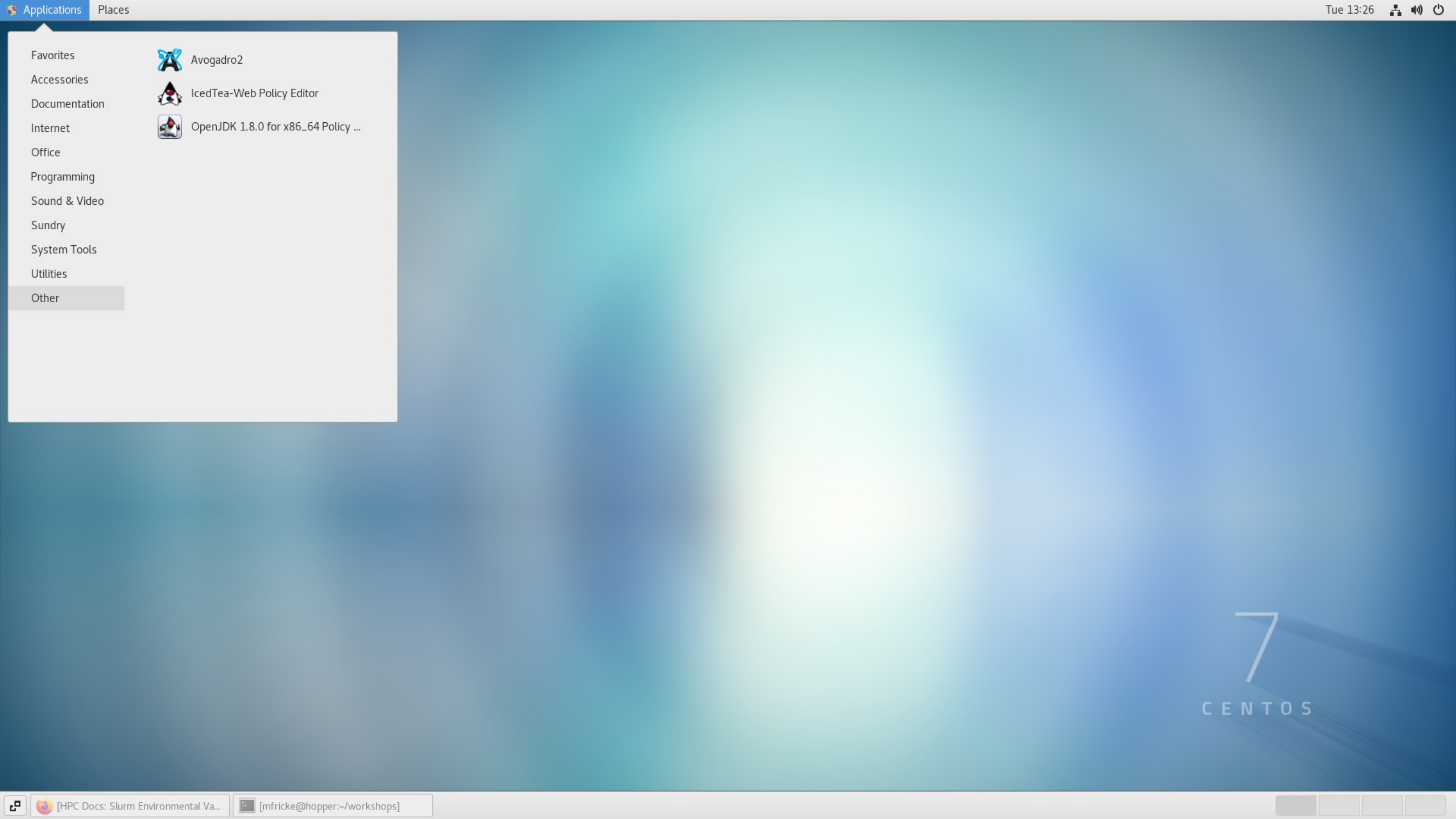
Why did it only run the program once instead of 4 times?

```
[vanilla@hopper intro_workshop]$ sbatch slurm/workshop_example1.sh
sbatch: Account not specified in script or ~/.default_slurm_account,
using latest project
Submitted batch job 5252
[vanilla@hopper intro_workshop]$
```

Take a look at the output file.

General Purpose Computational Chemistry Package

We will design a molecule using Avogadro and then optimize its geometry with Gaussian


Applications
Places
Tue 13:26
Favorites
Accessories
Documentation
Internet
Office
Programming
Sound & Video
Sundry
System Tools
Utilities
Other
Avogadro2
IcedTea-Web Policy Editor
OpenJDK 1.8.0 for x86_64 Policy ...
7
CENTOS
[HPC Docs: Slurm Environmental Va...
[mfricke@hopper:~/workshops]

Untitled - Avogadro 1.90.0

File Edit View Crystal Extensions Quantum Help

New Open Save Save As Molecule

Draw

Element: Carbon (6)

Bond Order: Automatic

Adjust Hydrogens

Display Types

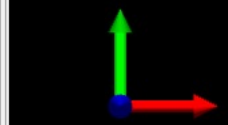
- Crystal Lattice
- Ball and Stick
- Licorice
- Van der Waals
- Wireframe
- Meshes
- Reference Axes Overlay
- Van der Waals (AO)

View Configuration | Display Types

Molecules

Untitled ()

Split Horizontal Split Vertical Close



Untitled* - Avogadro 1.90.0

File Edit View Crystal Extensions Quantum Help

New Open Save Save As Molecule

Draw

Element: Carbon (6)

Bond Order: Automatic

Adjust Hydrogens

Display Types

- [x] Crystal Lattice
- [x] Ball and Stick
- [ ] Licorice
- [ ] Van der Waals
- [ ] Wireframe
- [ ] Meshes
- [x] Reference Axes Overlay
- [ ] Van der Waals (AO)

View Configuration | Display Types

Molecules

Untitled (CH4)

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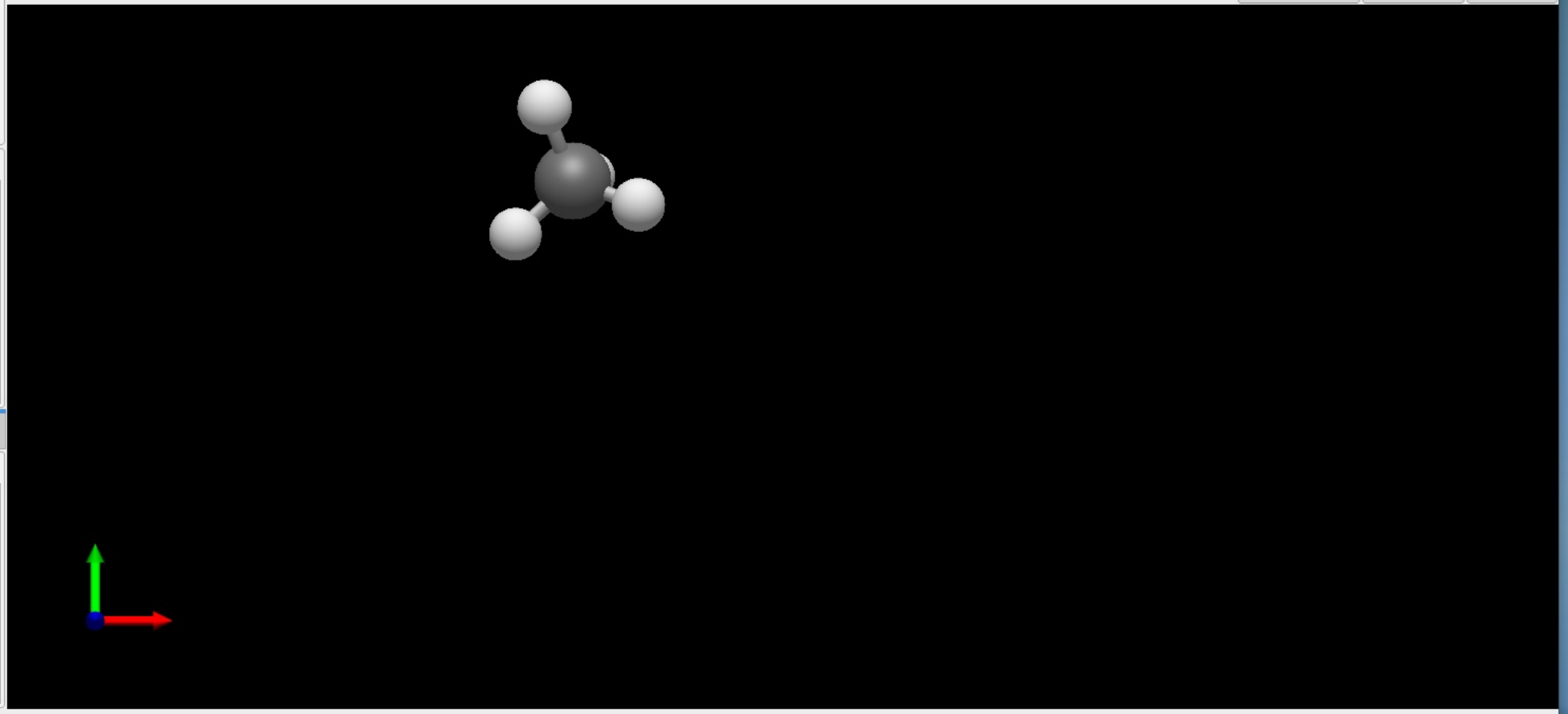
Split Horizontal Split Vertical Close



Applications Places Avogadro2

Untitled* - Avogadro 1.90.0

File Edit View Crystal Extensions Quantum Help

New Open Save Save As Molecule

Draw

Element: Carbon (6)

Bond Order: Automatic

Adjust Hydrogens

Display Types

- [x] Crystal Lattice
- [x] Ball and Stick
- [ ] Licorice
- [ ] Van der Waals
- [ ] Wireframe
- [ ] Meshes
- [x] Reference Axes Overlay
- [ ] Van der Waals (AO)

View Configuration | Display Types

Molecules

Untitled (C2H8)

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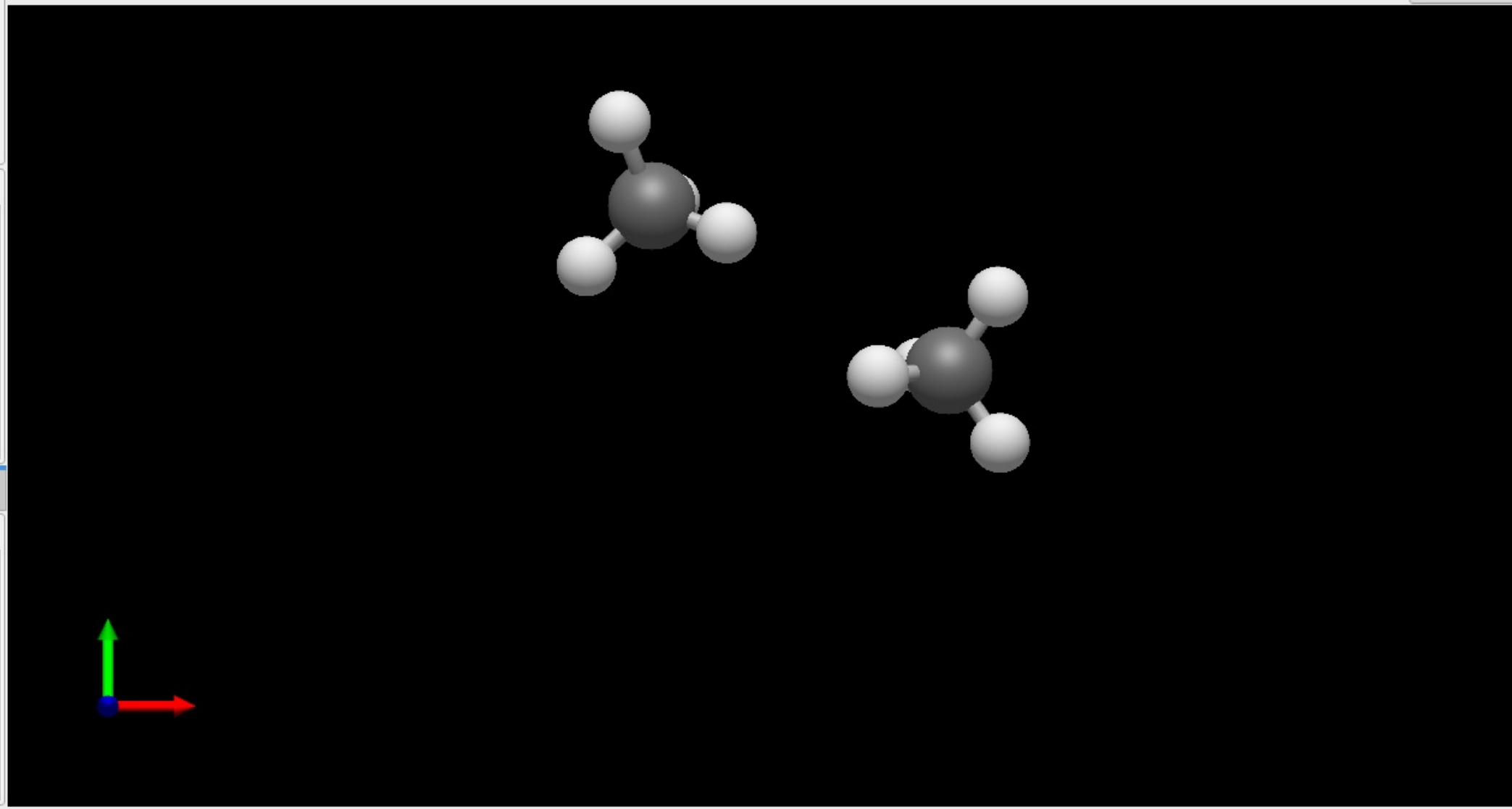

Untitled* - Avogadro 1.90.0

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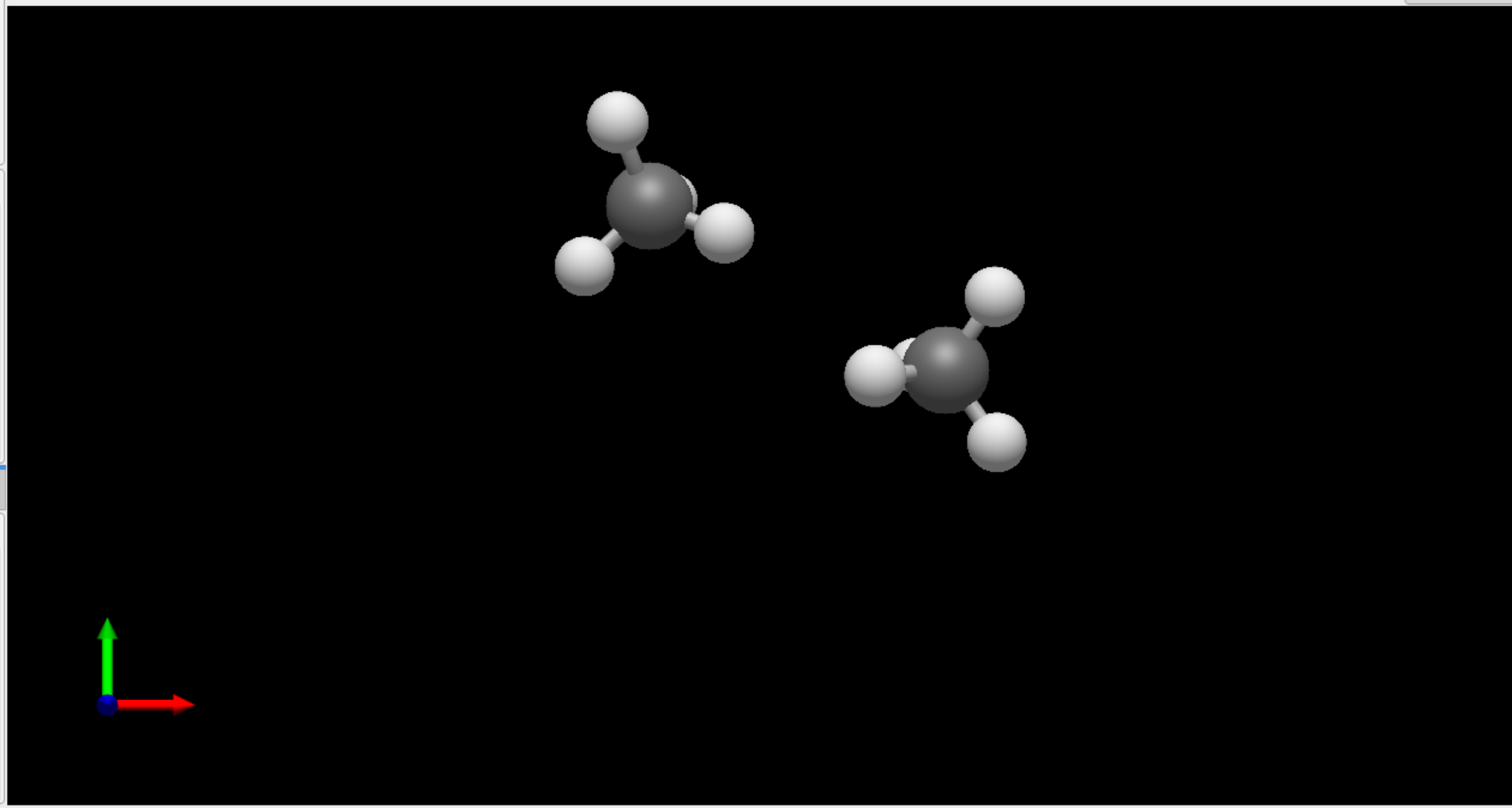
(C2H8)



Untitled* - Avogadro 1.90.0

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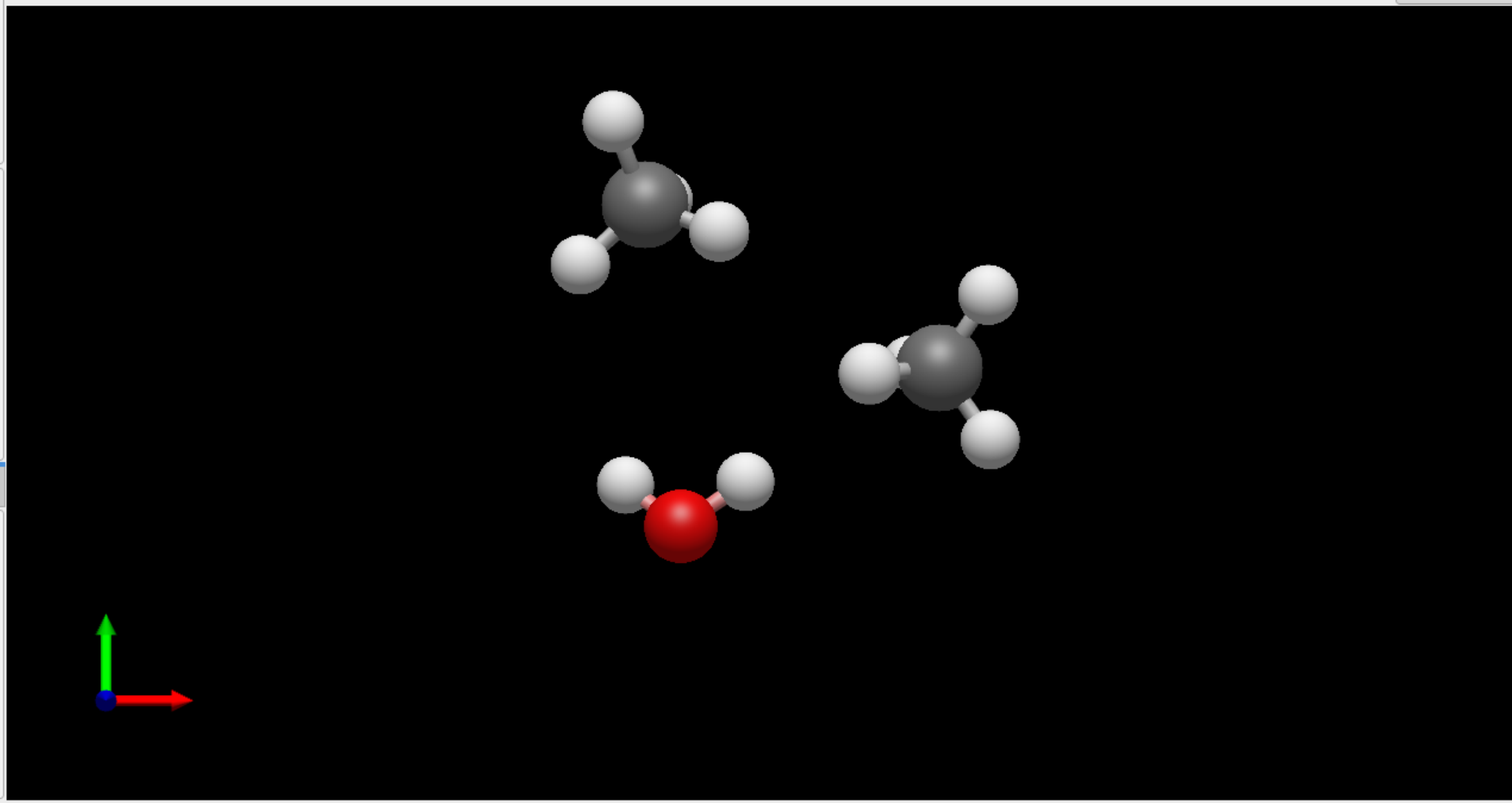

Untitled* - Avogadro 1.90.0

View Crystal Extensions Quantum Help

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Adjust Hydrogens

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C2H11OCl)

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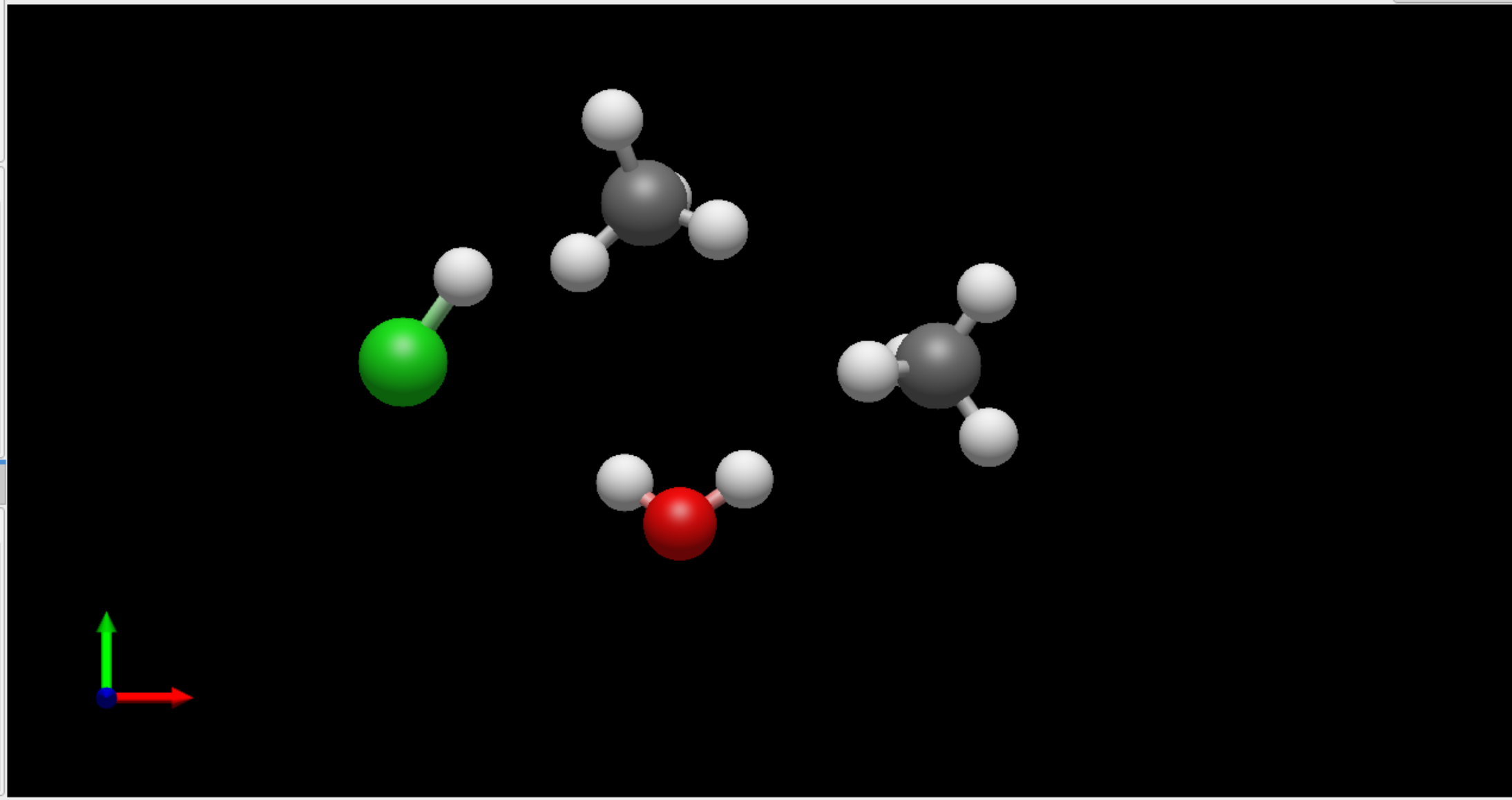
Split Horizonta



Untitled* - Avogadro 1.90.0

File Edit View Crystal Extensions Quantum Help

New Open Save Save As Molecule

Draw

Element: Chlorine (17)

Bond Order: Automatic

Adjust Hydrogens

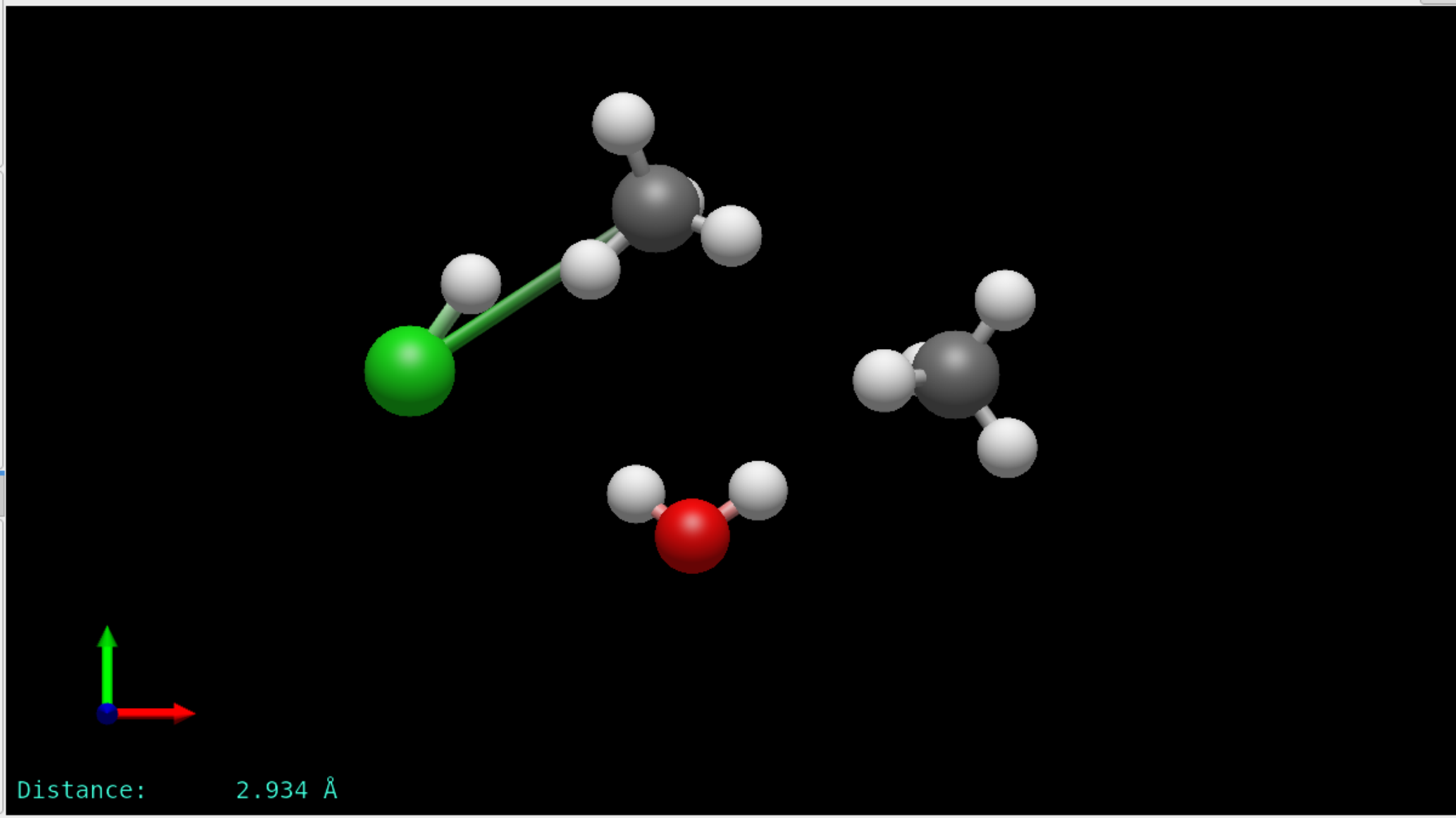
Display Types

- Crystal Lattice
- Ball and Stick
- Licorice
- Van der Waals
- Wireframe
- Meshes
- Reference Axes Overlay
- Van der Waals (AO)

View Configuration | Display Types

Molecules

Untitled (C2H11OCl)

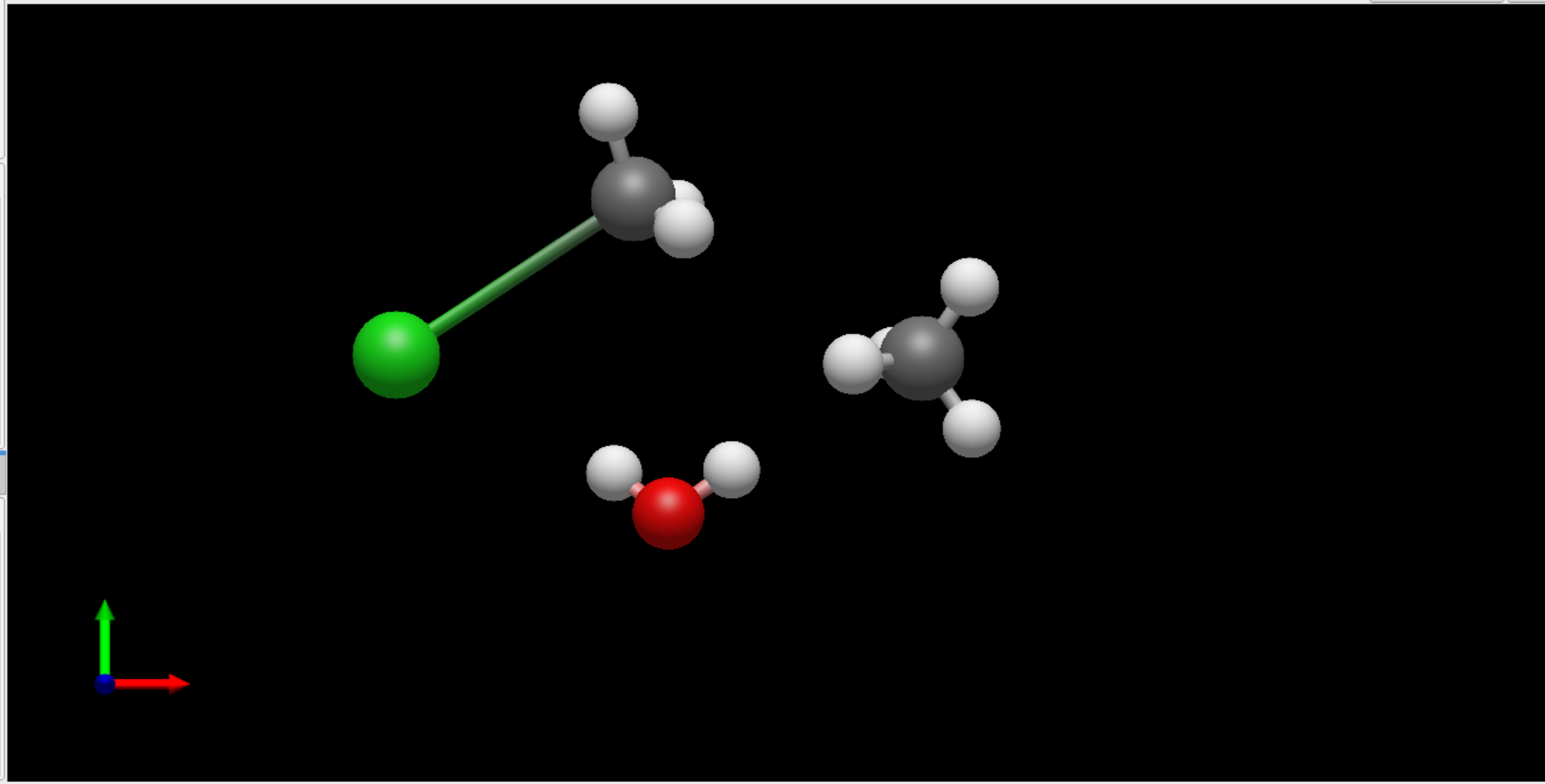


Untitled* - Avogadro 1.90.0

Crystal Extensions Quantum Help

Open Save Save As Molecule

Split Horizontal Spli



Applications Places Avogadro2

Untitled* - Avogadro 1.90.0

File Edit View Crystal Extensions Quantum Help

New Open Save Save As Molecule

Draw

Element: Chlorine (17)

Bond Order: Double

Adjust Hydrogens

Display Types

- [x] Crystal Lattice
- [x] Ball and Stick
- [ ] Licorice
- [ ] Van der Waals
- [ ] Wireframe
- [ ] Meshes
- [x] Reference Axes Overlay
- [ ] Van der Waals (AO)

View Configuration | Display Types

Molecules

Untitled (C2H5OCl)

*

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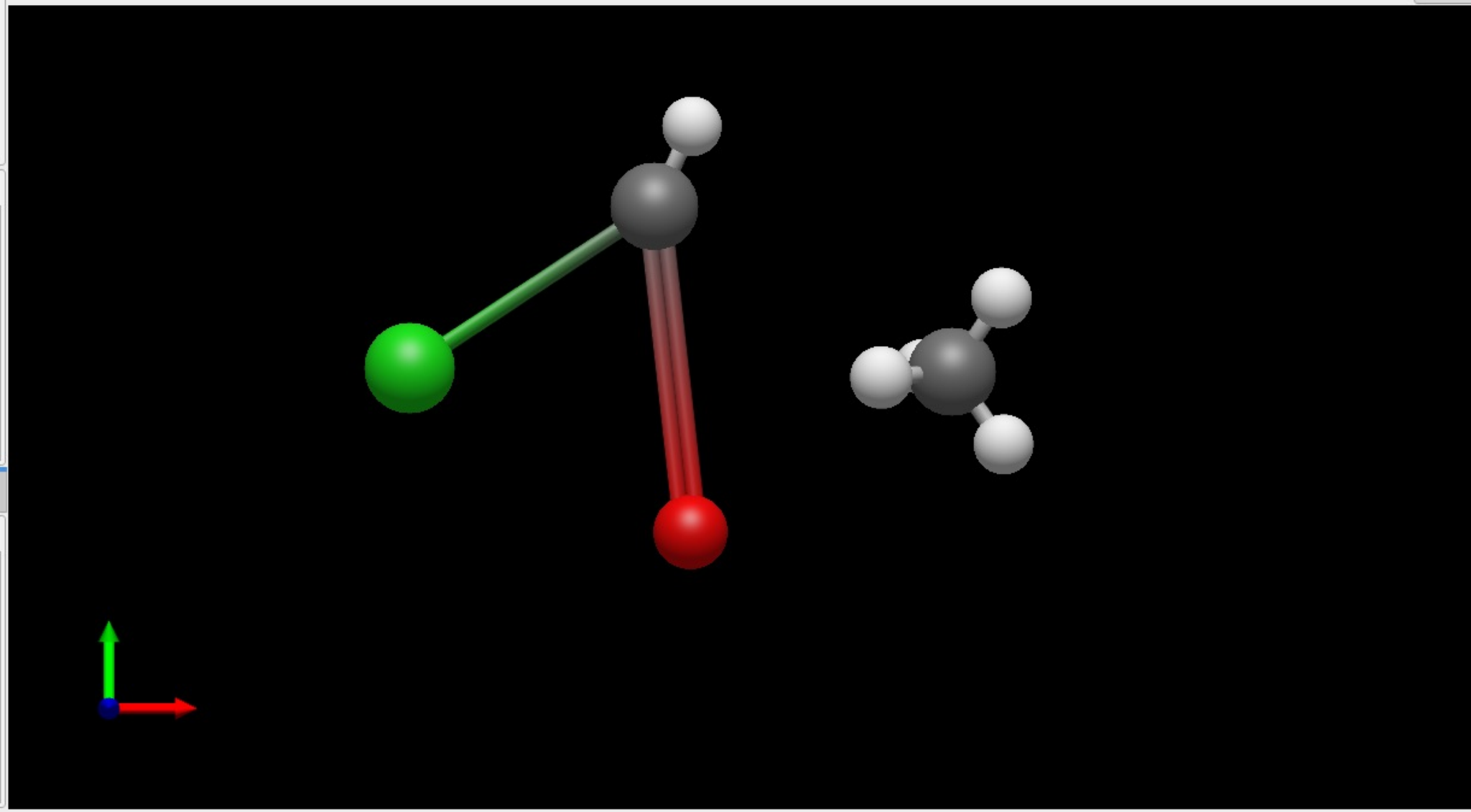

Untitled* - Avogadro 1.90.0

le Edit View Crystal Extensions Quantum Help

New Open Save Save As Molecule

raw

Element: Chlorine (17)

ond Order: Single

Adjust Hydrogens

isplay Types

Crystal Lattice
Ball and Stick
Licorice
Van der Waals
Wireframe
Meshes
Reference Axes Overlay
Van der Waals (AO)

View Configuration | Display Types

olecules

ntitled (C2OCl)

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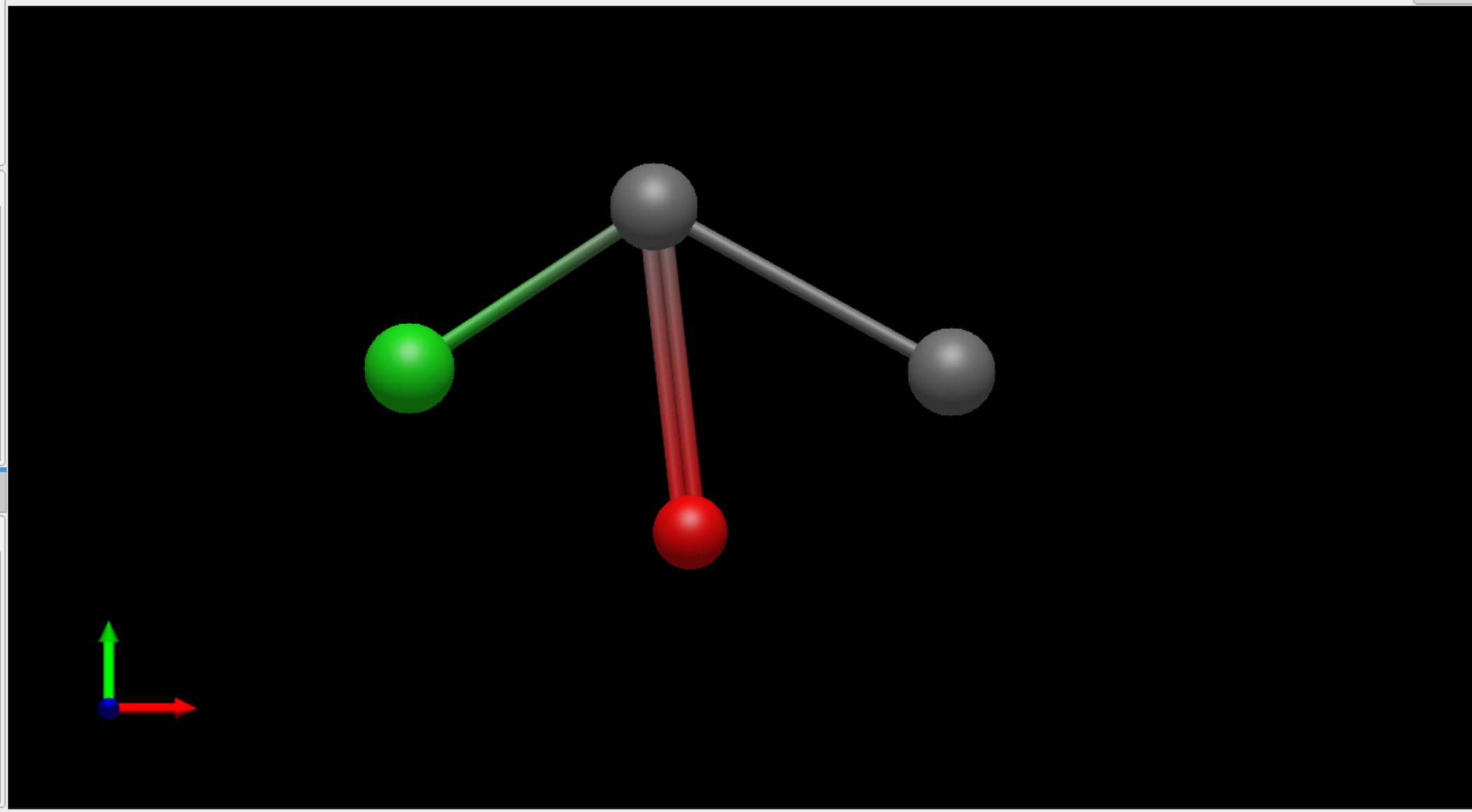

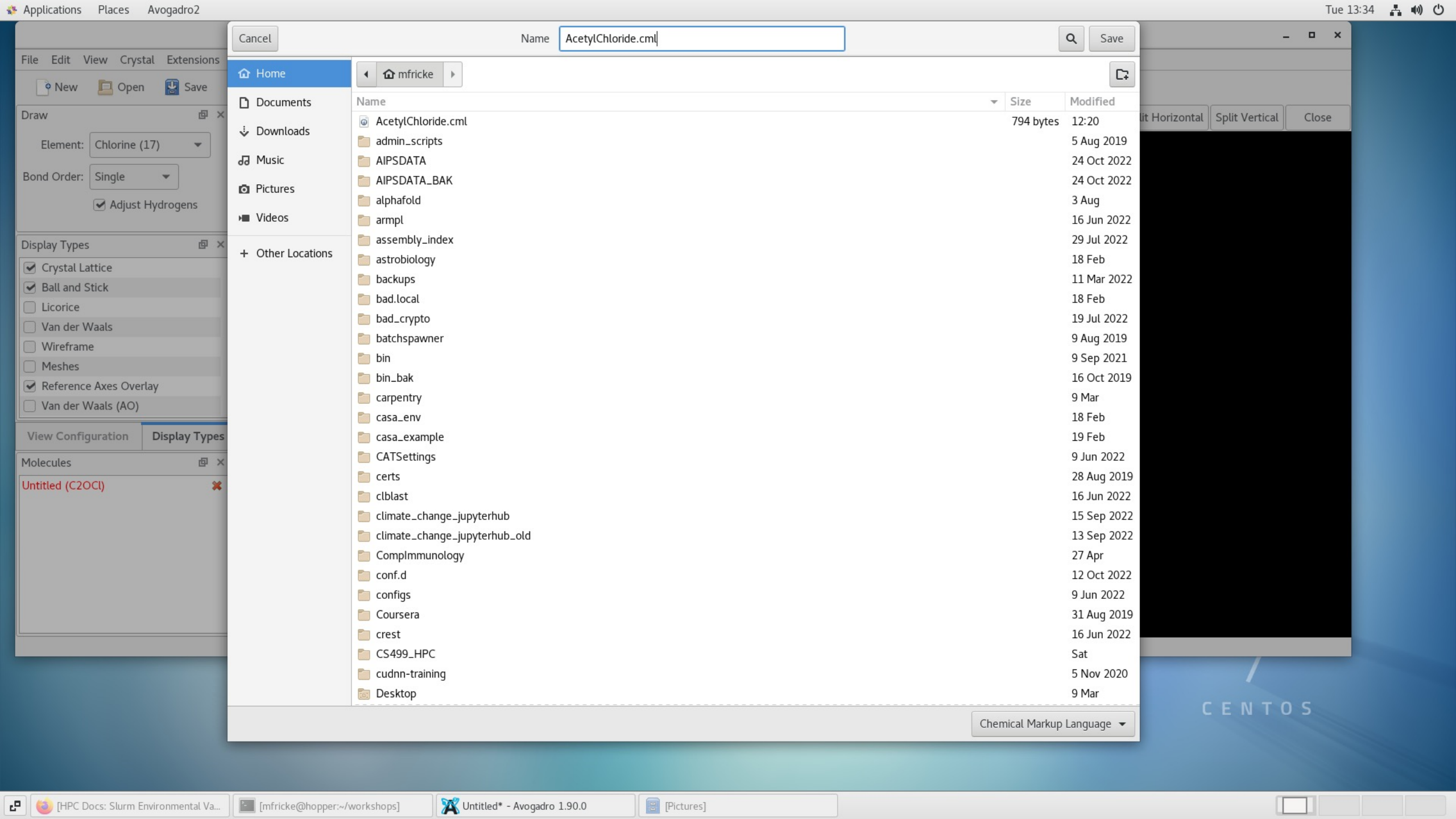
Applications
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Avogadro2
Tue 13:34
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Save
Draw
Element:
Chlorine (17)
Bond Order:
Single
Adjust Hydrogens
Display Types
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Ball and Stick
Licorice
Van der Waals
Wireframe
Meshes
Reference Axes Overlay
Van der Waals (AO)
View Configuration
Display Types
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Videos
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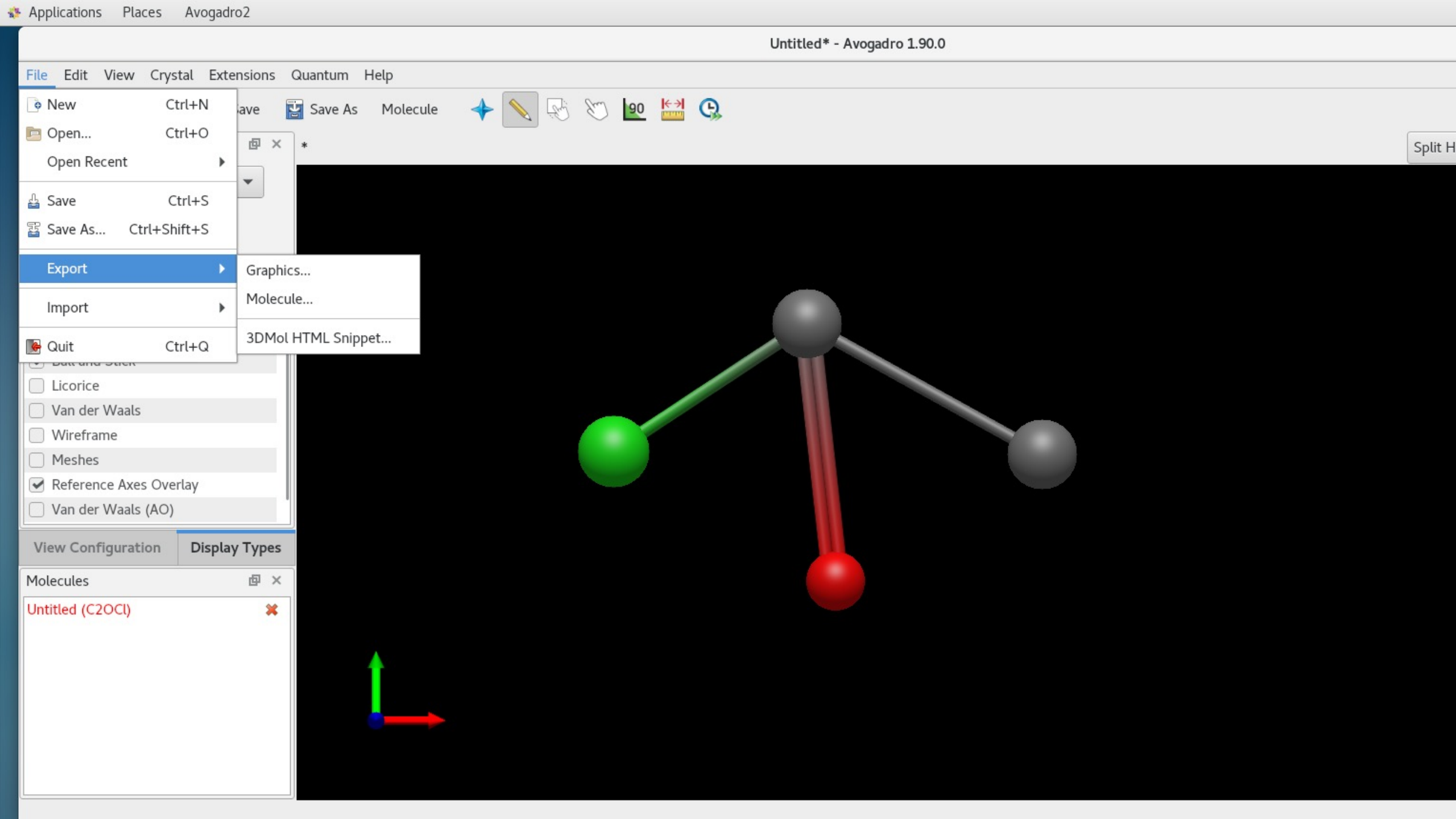
Modified
AcetylChloride.cml 794 bytes 12:20
admin_scripts 5 Aug 2019
AIPSDATA 24 Oct 2022
AIPSDATA_BAK 24 Oct 2022
alphafold 3 Aug
armpl 16 Jun 2022
assembly_index 29 Jul 2022
astrobiology 18 Feb
backups 11 Mar 2022
bad.local 18 Feb
bad_crypto 19 Jul 2022
batchspawner 9 Aug 2019
bin 9 Sep 2021
bin_bak 16 Oct 2019
carpentry 9 Mar
casa_env 18 Feb
casa_example 19 Feb
CATSettings 9 Jun 2022
certs 28 Aug 2019
clblast 16 Jun 2022
climate_change_jupyterhub 15 Sep 2022
climate_change_jupyterhub_old 13 Sep 2022
ComplImmunology 27 Apr
conf.d 12 Oct 2022
configs 9 Jun 2022
Coursera 31 Aug 2019
crest 16 Jun 2022
CS499_HPC Sat
cudnn-training 5 Nov 2020
Desktop 9 Mar
Chemical Markup Language
CENTOS
[HPC Docs: Slurm Environmental Va...
[mfricke@hopper:~/workshops]
Untitled* - Avogadro 1.90.0
[Pictures]


Applications
Places
Avogadro2
Untitled* - Avogadro 1.90.0
File
Edit
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Extensions
Quantum
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Open... Ctrl+O
Open Recent
Save Ctrl+S
Save As... Ctrl+Shift+S
Export
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Quit Ctrl+Q
Graphics...
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Save As
Molecule
Split H
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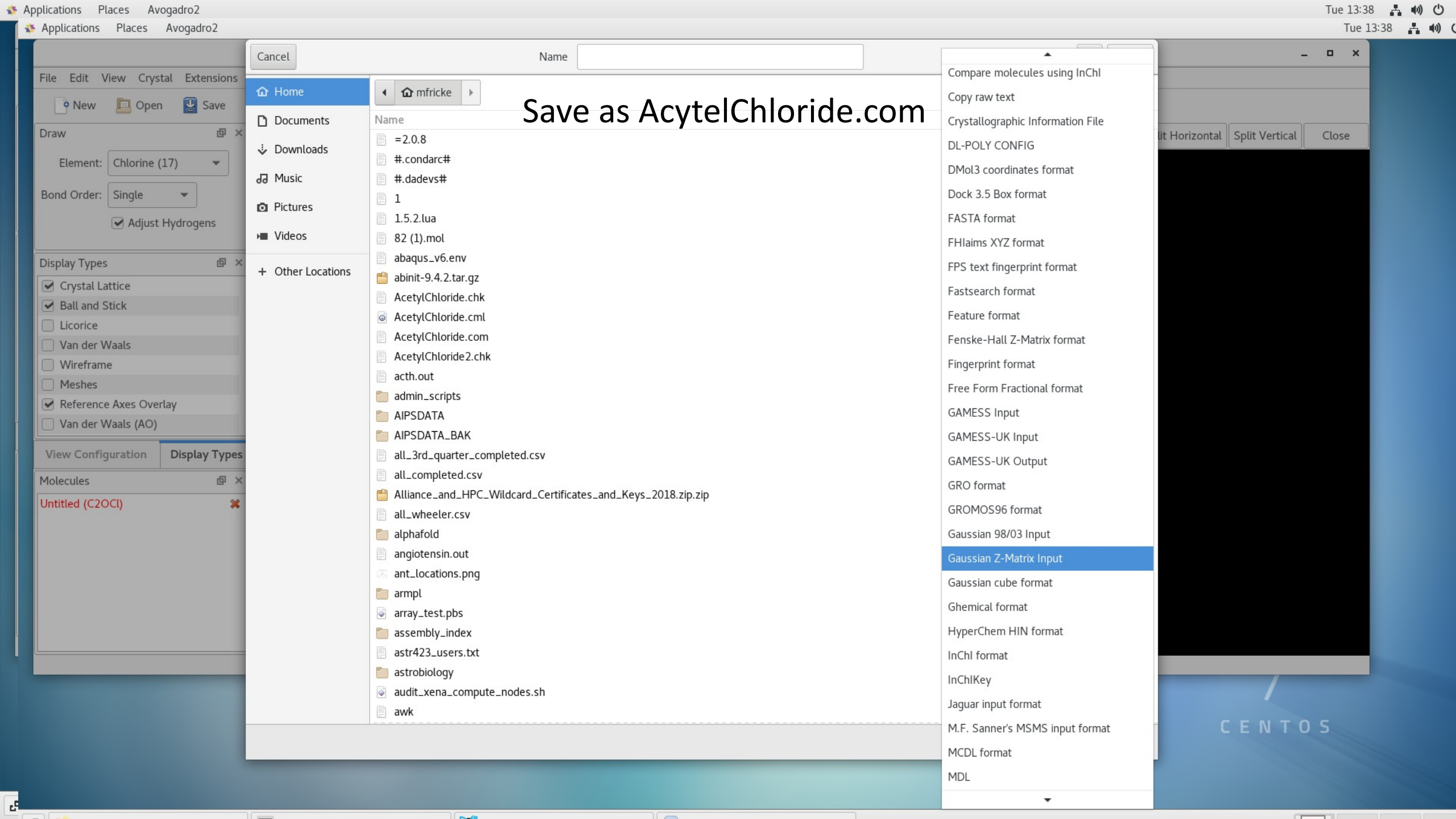
Meshes
Reference Axes Overlay
Van der Waals (AO)
View Configuration
Display Types
Molecules
Untitled (C2OCl)


Applications Places Avogadro2
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Element: Chlorine (17)
Bond Order: Single
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Crystal Lattice
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Van der Waals (AO)
View Configuration
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Molecules
Untitled (C2OCl)
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Name
=2.0.8
#.condarc#
#.dadevs#
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1.5.2.lua
82 (1).mol
abaqus_v6.env
abinit-9.4.2.tar.gz
AcetylChloride.chk
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AcetylChloride2.chk
acth.out
admin_scripts
AIPSDATA
AIPSDATA_BAK
all_3rd_quarter_completed.csv
all_completed.csv
Alliance_and_HPC_Wildcard_Certificates_and_Keys_2018.zip.zip
all_wheeler.csv
alphafold
angiotensin.out
ant_locations.png
armpl
array_test.pbs
assembly_index
astr423_users.txt
astrobiology
audit_xena_compute_nodes.sh
awk
Compare molecules using InChI
Copy raw text
Crystallographic Information File
DL-POLY CONFIG
DMol3 coordinates format
Dock 3.5 Box format
FASTA format
FHIaims XYZ format
FPS text fingerprint format
Fastsearch format
Feature format
Fenske-Hall Z-Matrix format
Fingerprint format
Free Form Fractional format
GAMESS Input
GAMESS-UK Input
GAMESS-UK Output
GRO format
GROMOS96 format
Gaussian 98/03 Input
Gaussian Z-Matrix Input
Gaussian cube format
Ghemical format
HyperChem HIN format
InChI format
InChIKey
Jaguar input format
M.F. Sanner's MSMS input format
MCDL format
MDL
CENTOS

```
scp AcetylChloride.com vanilla@hopper.alliance.unm.edu:~
AcetylChloride.com                    100%  269   114.7KB/s   00:00
```

ssh vanilla@hopper.alliance.unm.edu:~

```
--------------------------------------------------------------------------------
  Welcome to Hopper

  Be sure to review the "Acceptable Use" guidelines posted on the CARC website.

  For assistance using this system email help@carc.unm.edu.

  Tutorial videos can be accessed through the CARC website: Go to
    http://carc.unm.edu, select the "New Users" menu and then click
      "Introduction to Computing at CARC".

  vanilla@hopper:~ $
```

cd workshops/gaussian/
ls -l

```
total 1192
-rw-r--r-- 1 mfricke users     500 Sep 12 13:22 AcetylChloride.com
-rw-r-xr-- 1 mfricke users     795 Sep 12 14:15 gaussian16_linda_acetylchloride.sh
```

cd workshops/gaussian/

ls -l

```
total 1192
-rw-r--r-- 1 mfricke users     500 Sep 12 13:22 AcetylChloride.com
-rw-r-xr-- 1 mfricke users     795 Sep 12 14:15 gaussian16_linda_acetylchloride.sh
```

sbatch gaussian16_linda_acetylchloride.sh

```
sbatch: Using account 2016199 from ~/.default_slurm_account
Submitted batch job 2047647
```

cd workshops/gaussian/

ls -l

```
total 1192
-rw-r--r-- 1 mfricke users     500 Sep 12 13:22 AcetylChloride.com
-rw-r-xr-- 1 mfricke users     795 Sep 12 14:15 gaussian16_linda_acetylchloride.sh
```

cat gaussian16_linda_acetylchloride.sh

```
#!/bin/bash
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=4
#SBATCH --time=00:10:00
#SBATCH --job-name=g16_acetylchloride
#SBATCH --mail-user yourusername@unm.edu

module load gaussian/g16

# To make linda print verbose messages
export GAUSS_LFLAGS="-v"

INPUT_MOLECULE=$SLURM_SUBMIT_DIR/AcetylChloride.com
OUTPUT_FILE=$SLURM_SUBMIT_DIR/AcetylChloride.log

# Reformat the SLURM provided list of compute nodes to a format Gaussian can understand
# i.e. remove duplicates and replace newlines with commas
export GAUSS_WDEF=$(cat $CARC_NODEFILE | uniq | sed -z 's/\n/,/g;s/,$/\n/')

# Tell Linda to use as many nodes as requested by the user
export GAUSS_PDEF=$SLURM_CPUS_PER_TASK
echo "Parallelizing $GAUSS_PDEF processes across $GAUSS_WDEF nodes."

# Set the memory Gaussian variable
export GAUSS_MDEF=4GB

# Run Gaussian
g16 $INPUT_MOLECULE $OUTPUT_FILE
```

Gaussian uses a helper program called Linda to run multiple copies on multiple nodes. Linda does not understand SLURM so we have to spend some time converting SLURM information into a format Linda understand. That's most of this script.

watch squeue --me

```
Every 2.0s: squeue --me                                    hopper: Tue
Sep 12 14:37:13 2023

             JOBID PARTITION     NAME     USER ST TIME  NODES NODELIST(REASON)
           2047652   general g16_acet  mfricke  R 1:05   2 hopper[003-004]
```

Output will be written to AcetylChloride.log and slurm-<jobid>.out

matthew — mfricke@hopper:~/workshops/gaussian — ssh hopper — 185×58

```
  4[                                                                                                    0.0%]   20[                                                                                                    0.0%]
  5[||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||94.7%]   21[                                                                                                    0.0%]
  6[                                                                                                    0.0%]   22[                                                                                                    0.0%]
  7[|||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||89.4%]   23[                                                                                                    0.0%]
  8[|                                                                                                   0.7%]   24[                                                                                                    0.0%]
  9[                                                                                                    0.0%]   25[                                                                                                    0.0%]
  10[                                                                                                   0.0%]   26[                                                                                                    0.0%]
  11[                                                                                                   0.0%]   27[                                                                                                    0.0%]
  12[                                                                                                   0.0%]   28[                                                                                                    0.0%]
  13[                                                                                                   0.0%]   29[                                                                                                    0.0%]
  14[                                                                                                   0.0%]   30[                                                                                                    0.0%]
  15[                                                                                                   0.0%]   31[                                                                                                    0.0%]
  16[                                                                                                   0.0%]   32[                                                                                                    0.0%]
  Mem[|||||||||||||||||||||||||                                                                 13.7G/92.9G]   Tasks: 40, 75 thr, 435 kthr; 5 running
  Swp[||                                                                                        82.9M/85.2G]   Load average: 1.11 2.26 3.43
                                                                                                               Uptime: 20 days, 04:42:48

    PID USER       PRI  NI  VIRT   RES   SHR S  CPU%▽MEM%   TIME+  Command
 240218 mfricke     20   0 6020M  265M 23148 R 371.0  0.3   1:22.65 /opt/local/gaussian/g16/C.01/avx2/g16/linda-exe/l508.exel 536870912 AcetylChloride.chk 1 /carc/scratch/users/mfricke/G
 240306 mfricke     20   0 6020M  265M 23148 R  94.9  0.3   0:21.05 /opt/local/gaussian/g16/C.01/avx2/g16/linda-exe/l508.exel 536870912 AcetylChloride.chk 1 /carc/scratch/users/mfricke/G
 240305 mfricke     20   0 6020M  265M 23148 R  94.2  0.3   0:20.96 /opt/local/gaussian/g16/C.01/avx2/g16/linda-exe/l508.exel 536870912 AcetylChloride.chk 1 /carc/scratch/users/mfricke/G
 240304 mfricke     20   0 6020M  265M 23148 R  93.6  0.3   0:20.86 /opt/local/gaussian/g16/C.01/avx2/g16/linda-exe/l508.exel 536870912 AcetylChloride.chk 1 /carc/scratch/users/mfricke/G
 240353 mfricke     20   0 36220  5036  3244 R   1.3  0.0   0:00.10 htop
      1 root       20   0  232M 11176  8608 S   0.0  0.0   0:16.95 /sbin/init
    506 root       20   0  695M  6364  4740 S   0.0  0.0   1:17.53 /warewulf/bin/wwclient
    509 root       20   0  695M  6364  4740 S   0.0  0.0   0:01.80 /warewulf/bin/wwclient
    511 root       20   0  695M  6364  4740 S   0.0  0.0   0:03.08 /warewulf/bin/wwclient
    512 root       20   0  695M  6364  4740 S   0.0  0.0   0:03.20 /warewulf/bin/wwclient
    513 root       20   0  695M  6364  4740 S   0.0  0.0   0:03.33 /warewulf/bin/wwclient
    547 root       20   0  103M 23496 23044 S   0.0  0.0   0:02.61 /usr/lib/systemd/systemd-journald
    600 root       20   0 97888  7384  6992 S   0.0  0.0   0:01.34 /usr/lib/systemd/systemd-udevd
    792 rpc        20   0 67252  5092  4940 S   0.0  0.0   0:03.51 /usr/bin/rpcbind -w -f
    805 root       20   0  235M 11356 10844 S   0.0  0.0   0:19.76 /usr/sbin/rsyslogd -n
    806 dbus       20   0 76736  5212  4692 S   0.0  0.0   0:01.12 /usr/bin/dbus-daemon --system --address=systemd: --nofork --nopidfile --systemd-activation --syslog-only
    809 root       20   0  235M 11356 10844 S   0.0  0.0   0:19.39 /usr/sbin/rsyslogd -n
    810 root       20   0  235M 11356 10844 S   0.0  0.0   0:00.32 /usr/sbin/rsyslogd -n
    822 root       20   0  499M 33752 30424 S   0.0  0.0 23:02.61 /usr/libexec/platform-python -Es /usr/sbin/tuned -l -P
    827 root       20   0  109M  3264  3228 S   0.0  0.0   0:00.00 /usr/sbin/gssproxy -D
    828 root       20   0  109M  3264  3228 S   0.0  0.0   0:00.00 /usr/sbin/gssproxy -D
    829 root       20   0  109M  3264  3228 S   0.0  0.0   0:00.00 /usr/sbin/gssproxy -D
    830 root       20   0  109M  3264  3228 S   0.0  0.0   0:00.00 /usr/sbin/gssproxy -D
    831 root       20   0  109M  3264  3228 S   0.0  0.0   0:00.00 /usr/sbin/gssproxy -D
    832 root       20   0  109M  3264  3228 S   0.0  0.0   0:00.00 /usr/sbin/gssproxy -D
    835 munge      20   0  253M  6228  4784 S   0.0  0.0   1:44.83 /usr/sbin/munged
    837 munge      20   0  253M  6228  4784 S   0.0  0.0   1:42.73 /usr/sbin/munged
    838 munge      20   0  253M  6228  4784 S   0.0  0.0   0:00.78 /usr/sbin/munged
    839 munge      20   0  253M  6228  4784 S   0.0  0.0   0:00.77 /usr/sbin/munged
    889 root       20   0  499M 33752 30424 S   0.0  0.0 10:33.69 /usr/libexec/platform-python -Es /usr/sbin/tuned -l -P
    891 polkitd    20   0 1981M 18832 18284 S   0.0  0.0   0:00.42 /usr/lib/polkit-1/polkitd --no-debug
    897 polkitd    20   0 1981M 18832 18284 S   0.0  0.0   0:00.00 /usr/lib/polkit-1/polkitd --no-debug
```

ssh hopper<number>

htop

You have learned

- how to run programs using the SLURM scheduler
- the difference between interactive and batch jobs
- how to check the status of your jobs
- how to select debug vs general SLURM partitions
- how to ask for the hardware resources you need
- you ran the Gaussian code using SLURM