# Documentation for StarCCM

Integration on Ganymede

# Table of Contents

Introduction	3
Installing VPN	3
Terminal Client	4
Ganymede Basics	5
Accessing Compute Node	7
Accessing StarCCM	7
Running Simulations Interactively	8
Running Batch Scripts	11
Commands TLDR	17

#### Introduction

Since everyone on the team is starting from a different place with respect to knowledge of Linux systems and specifically HPC systems, this documentation is written to provide a foundation for all members to learn and utilize the system. The goal is for this documentation to provide universal and reproducible results so anyone can start running simulations on Ganymede as efficiently as possible. This will correlate with the docs already written by CIRC while offering more details on Linux systems and using StarCCM in particular.

### **Installing the VPN**

Since CIRC already offers great documentation on connecting to Ganymede, this will mainly detail possible errors and ideas to keep in mind while following their docs, and I do not have a Mac to test on. First, you have to download and connect to the UTD VPN if you are not on Cometnet in order to connect to Ganymede. The Global Protect VPN is notorious for being buggy, so beware that it will probably not work the first install.

#### Linux

While Linux systems provide the easiest method to connect to Ganymede, it is recommended to use MacOS or Windows to download the VPN as at least on Fedora 36, Global Protect will not connect. CIRC does state that Linux is supported so your mileage may vary.

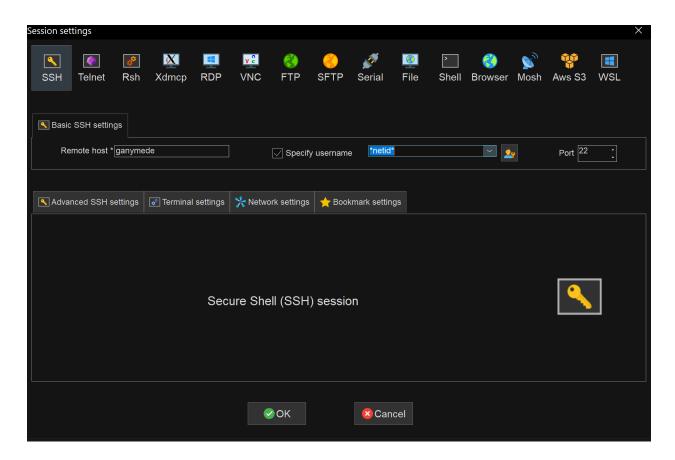
#### Windows

The Windows install for the VPN is much simpler, but may still cause issues when trying to connect. The first install on several systems tested, has returned a stale web request error when

signing in to the UTD SSO. This can normally be fixed by uninstalling and reinstalling. If the error persists, changing your default browser to google chrome seems to work consistently.

### **Terminal Client**

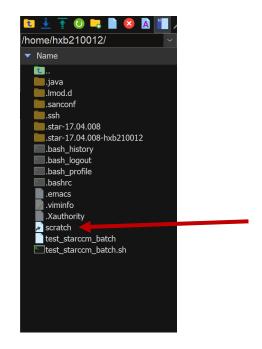
Ganymede requires either a terminal client to access it or a program such as X2Go which provides a virtual desktop over SSH. Both Linux and MacOS have their own built-in terminal so use using them will be easiest. For everyone else on Windows, MobaXTerm will be the easiest to quickly setup and access and share files with Ganymede. Assuming you are using MobaXTerm, you can right click on the left side under "User Sessions" then click "New Session". A window will appear where you will click on SSH at the top left.



In the "Remote host" box type <ganymede> as shown, then check the specify username and enter your netid in the box and click "OK" when done. This will allow you automatically

connect to Ganymede when you double click on the new session you created. After running the session for the first time, you will see a line asking for you to enter your password. Do note that Linux terminals will not show the characters you type. Once you type in your password and hit enter, a box will appear asking if you want to remember the password on this system. Clicking yes will save the password allowing you to connect to Ganymede by only double clicking the session.

# **Ganymede Basics**



For our purposes, Ganymede has two file systems that we have access to. The first is the home directory where you are in when you login. Each user only has 20GB allocated in here and has serious bandwidth limitations for larger scripts. Since each simulation we run will be multiple GBs in size and intensive, all files should be stored in the scratch directory. Every user has their own scratch directory and there are no limits on the size each user has. In addition to the different storage spaces, there are two different nodes we have access to. When we connect to Ganymede, we are connected to the login node which hands connections and works with Slurm, the job scheduler, to run jobs on a compute node; however, for every computational task we need to run it on a compute node. CIRC gives more details on exactly the specs of the systems and also gives examples for manipulating files from the command line, so go there first for any question not covered here. Because most of the users will be running MobaXTerm, this will give explain moving files using its GUI. The easiest way to upload files from your computer to your scratch directory is to click on the icon that says "scratch" on the left side of the screen. Once the scratch directory is listed, right click followed by "upload to current folder" which will bring up

a normal windows file explorer where you can search for the file you want to upload. You can also click third icon at the top of the directory to upload to the current directory.



To go back to the home directory view you can click on the drop down menu and click "/home/netid".

## **Accessing a Compute Node**

In order to run our simulations, we have to connect to a compute node. For the moment, we cannot use multiple nodes in parallel to run our jobs, but it is possible so this will be updated when that is available. We have two main methods to access a compute node, srun and salloc. Since Ganymede uses the job scheduler slurm, these commands will all start with a s. Srun is the easier to understand option and is invoked by typing this into the terminal.

Srun is the slurm command to ask for a compute node, -N 1 asks for 1 node, -n 16 gives us all 16 cores from that 1 node, -p normal allocates us the normal partition, and -pty /bin/bash is needed

to allocate the node properly for our use case. After hitting enter, a 1 node will be queued and allocated to you when available. You know you are in a compute node when you see @compute-x-x-xx.

```
[hxb210012@ganymede ~]$ srun -N 1 -n 16 -p normal --pty /bin/bash [hxb210012@compute-7-2-26 ~]$ ■
```

The second method is using salloc followed by squeue to access the node.

```
[hxb210012@ganymede ~]$ salloc -p normal -n 16 salloc: Granted job allocation 497649
Disk quotas for user hxb210012:
                           Usage
                                              Soft Limit
Disk
                                                                          Hard Limit
/home/hxb210012
                            1920K
                                              20000M
                                                                          30000M
[hxb210012@ganymede ~]$ squeue -u $USER
                                                USER ST
                                                                 TIME NODES NODELIST(REASON)
               JOBID PARTITION
                                      NAME
              497649
                                      bash hxb21001 R
                                                                 0:23
                                                                             1 compute-7-2-26
                         normal
Warning: Permanently added 'compute-7-2-26,10.247.129.63' (ECDSA) to the list of known hosts. [hxb210012@compute-7-2-26 ~]$ ■
```

Salloc -p normal -n 16 uses the same options as srun shown above. This allocates a compute node to the user. Squeue displays the compute node you are allocated with -u \$USER specifying your account. Then you can type ssh -X node name to connect into the compute node.

## **Accessing StarCCM+**

To change directory into where the executable of star is located, you type:

```
[hxb210012@compute-7-2-26 ~]$ cd /petastore/ganymede/home/SoftWare/List-Of-Software/START-CCM/17.04.008/STAR-CCM+17.04.008 [hxb210012@compute-7-2-26 STAR-CCM+17.04.008]$ cd star [hxb210012@compute-7-2-26 star]$ cd bin [hxb210012@compute-7-2-26 bin]$
```

Now that you have access to the executable you can start running simulations. To run star you type "./starccm+" at the start of the line. Typing "./starccm+ --help" displays the command proc and info and what each parameter does in star.

## **Running Simulations**

There are many different options and methods to running simulations, but this will detail the easiest method until I have time to test them and update here. Simplest method is to type "./starccm+ -batch run -np 16 <location and name of .sim file> -tokensonly -licpath 1999@ganymede".

```
./starccm+ - batch \ run \ -np \ 16 \ /petastore/ganymede/home/hxb210012/MasterSimulationv1.sim \ -tokensonly \ -licpath \ 1999@ganymede
```

Once the simulation starts you should see something like this

### Breakdown of the command:

- "./starccm+"
  - o Starts the executable for star
- "-batch run"
  - o Batch opens star without the GUI
  - o -run tells the solver to run until the stopping criteria is met

- "-np 16"
  - o -np 16 runs star using 16 cores
    - 16 is chosen since it is the max per the one node we are using, but fewer can be used
- "/petastore/ganymede/home/<netid>/MasterSimulationv1.sim"
  - o Represents the absolute file path to the simulation file we are trying to use
- "-tokensonly"
  - Specifies to only use DOEtoken licenses
- "-licpath 1999@ganymede"
  - o Specifies to use the license of Star: 1999@ganymede

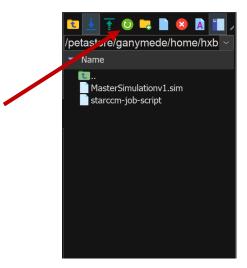
# **Running Batch Scripts**

While the method above is fine for running a single short simulation with only one node, we will not always have the time to wait for resources to become available, so we can use batch scripts to queue and run our simulations automatically.

To start, download the .java file, .sh batch file from box under Baseline Simulation/HPC Baseline, and use any .sim file you want. Then go to MobaXTerm (or any other terminal client but this is for Moba specifically), click on your scratch directory and right-click to create new directory. Finally, right click or follow the directions earlier to upload the .java file and the .sim file to this folder. It should look something like this: (note /simtest is just the name of the directory I created yours will be different)



Next go back into the scratch directory and upload the .sh file there. You will have to click on the green circle shown below to refresh in order to view the batch file.



Once you see the batch file, double click on it to open the file. You should see this:

Before doing anything else, change anywhere you see hxb210012 to your own netid otherwise this will not work.

A break down of what each command does:

- "#!/bin/bash"
  - Just tells it to run using the bash shell, for our purposes just means the command line
- "#SBATCH"
  - o Specifies to use Slum batch settings
  - o "—partition=normal"
    - Requests resources from the normal partition on Ganymede
  - o "---nodes=1"
    - Requests for 1 node
  - o "---ntasks=16"
    - Requests for 16 cores to be used
  - o "-time=01:00:00"
    - Sets a time limit of 1 hour for the simulation
      - hh:mm:ss up to 96 hours
  - o "—mail-type=All" and "mail-user=<netid>"
    - Are you used to email you when the system begins and finishes running the simulation
    - optional

- o "—output=/home/netid/scratch/simtest/file.output"
  - Outputs a file with details about the simulation
  - It is optional but good for debugging
- o "export CDLMD\_LICENSE\_FILE=1999@ganymede.utdallas.edu"
  - Grabs a license to run the software
- o "cd

/petastore/ganymede/home/SoftWare/List-Of-Software/START-CCM/17.04.008"

- Navigates to where star is located
- o "STAR-CCM+17.04.008/star/bin/starccm+"
  - Navigates to and runs star
- o "-batch/home/netid/scratch/simtest/RescalePostProc.java,run"
  - Runs without the GUI
  - First starts the .java macro file
  - Then runs until the stopping criteria is met
- o "-np 16"
  - Requests for all 16 cores of our 1 node to be used
- o "/home/netid/scratch/simtest/file.sim"
  - Is the location of the sim file located in the directory you put it in earlier
- o "-tokensonly"
  - Specifies to only use DOEtoken licenses

Again, make sure to change it to your own netid for this to work. While you don't have to place the sim file and java file in their own directory, depending on the simulation you run, it will help to contain all the scenes and files in one place for each simulation. Then save and exit the file.

Finally, to run this batch file you only need two commands, cd scratch, and sbatch file.sh.

```
[hxb210012@ganymede ~]$ cd scratch
[hxb210012@ganymede scratch]$ sbatch starccm-job-script.sh
Submitted batch job 497771
```

Your batch file will now be submitted and queued by Slurm. If you opted for the email command before, you should receive emails before and after about the job; otherwise, you can just come back later and refresh the folder until you see the scenes and output file. There is also <u>squeue</u> to view information about the current running jobs.

Example Folder after running the master simulation. (will depend on the simulation file)

□ Coefficients Plot.jpg
□ Fluid Domain Mesh.sce
□ Front Wing Streamlines Isometric.jpg
□ Front Wing Streamlines Isometric.sce
□ Front Wing Streamlines Side View.sce
□ Front Wing Streamlines Side View.sce
□ Front Wing Streamlines Top View.jpg
□ Front Wing Streamlines Top View.jpg
□ Front Wing Streamlines Top View.sce
□ Front Wing Streamlines Top View.sce
□ Mass Flow of Radiator Monitor Plot.jpg
□ MasterSimulationv1\_outputtest Report.csv
□ MasterSimulationv1\_outputtest@00057.sim
□ MasterSimulationv1\_outputtest@00058.sim
□ Mesh Scene 1.sce
□ Overall Force Numbers.jpg
□ Pressure Coefficient Front Wing Bottom View.jpg
□ Pressure Coefficient Front Wing Bottom View.jpg
□ Pressure Coefficient Front Wing Side View.sce
□ Pressure Coefficient Front Wing Side View.sce
□ Pressure Coefficient Front Wing Side View.sce
□ Pressure Coefficient Rear Wing Bottom View.jpg
□ Pressure Coefficient Rear Wing Bottom View.jpg
□ Pressure Coefficient Rear Wing Bottom View.jpg
□ Pressure Coefficient Rear Wing Bottom View.sce
□ Pressure Coefficient Rear Wing Bottom View.sce
□ Pressure Coefficient Rear Wing Side View.sce
□ Pressure Coefficient Rear Wing Side View.jpg
□ Pressure Coefficient Rear Wing Top View.sce
□ Pressure Coefficient Rear Wing Top View.sce
□ Pressure Coefficient Rear Wing Top View.sce
□ Pressure Coefficient Side View.jpg
□ Pressure Coefficient Side View.jpg
□ Pressure Coefficient Top View.jpg
□ Pressure Coefficient Top View.sce
□ Pressure Coefficient Top View.sce
□ Pressure Coefficient Top View.sce
□ Radiator Streamlines Side View.sce
□ Radiator Streamlines Side View.sce
□ Radiator Streamlines Top View.sce
□ Radiator Streamlines Side View.sce
□ Radiator Streamlines Top View.sce
□ Radiator Streamlines Side View.sce
□ Radiator Streamlines Side View.sce
□ Radiator Streamlines

### **Commands TLDR:**

- Interactive
  - Srun -N 1 -np 16 -p normal –pty/bin/bash
  - ./starccm+ -batch run -np 16 <location and name of .sim file> -tokensonly -licpath
     1999@ganymede
  - ./starccm+ -batch macro.java,run -np 16 <location and name of .sim file> tokensonly -licpath 1999@ganymede
    - Uses a .java file in addition to normal
- Batch
  - o Note Last 3 lines should be only on one, may not matter though

```
#!/bin/bash
#SBATCH
            --partition=normal
#SBATCH
            --nodes=1
            --ntasks=16
#SBATCH
#SBATCH
            --time=01:00:00
#SBATCH
            --mail-type=ALL
#SBATCH
            --mail-user=netid
#SBATCH
            --output=/home/netid/scratch/scalarsim.output
export CDLMD_LICENSE_FILE=1999@ganymede.utdallas.edu
cd
/petastore/ganymede/home/SoftWare/List-Of-Software/START-CCM/17.04.008
STAR-CCM+17.04.008/star/bin/starccm+ -batch
/home/netid/scratch/RescalePostProc.java,run -np 16
/home/netid/scratch/MasterSimulationv1 outputtest.sim -tokensonly
```

Sbatch starcem-job-script.sh