Submitting RELION GPU jobs to Comet at SDSC

Michael Cianfrocco

Abstract

Below is a protocol for logging in and submitting a RELION GPU job to Comet GPU nodes at the San Diego Supercomputer Center.

Citation: Michael Cianfrocco Submitting RELION GPU jobs to Comet at SDSC. **protocols.io** dx.doi.org/10.17504/protocols.io.i3ecgje
Published: 21 Jul 2017

Protocol

Upload data to Comet

Step 1.

To move your data onto Comet, you can use globus.org for moving datasets easily from local machines / laptop to your Oasis storage directory.

Alternatively, you can always use scp or rsync from the command line.

Logging into Comet

Step 2.

To log onto Comet, ssh into Comet using Terminal on Mac OSX (Forget name for Windows):

$ ssh -X [username]@comet.sdsc.edu

-> You will use your xsede username & password

Step 3.

Navigate to your storage on Oasis & create a new project directory for your current dataset / sample:

$ cd /oasis/projects/nsf/[XSEDE allocation ID]/[username]

$ mkdir mysample

$ cd mysample

Prepare RELION job submission

Step 4.

From your project directory on Oasis, open the RELION GUI:

$ relion

Step 5.
Input parameters related to your job & select 'Print command'. Copy the output text after the command relion_refine or relion_refine_mpi.

Submit job to Comet

Step 6.
Create a new file (e.g. relion_gpu_submit.run)

Step 7.

Open file using 'vi' to include this template information:

```
#!/bin/bash

#SBATCH --job-name='reliongpu'

#SBATCH --output='reliongpu.%j.%N.out'

#SBATCH --partition=gpu

#SBATCH --nodes=1                    #For 1 node

#SBATCH --ntasks-per-node=24

#SBATCH --no-requeue

#SBATCH --gres=gpu:4

#SBATCH -t 2:00:00                   #Edit to give approx. time in hours here

#SBATCH --mail-type=begin,end

#SBATCH --mail-user=                 #Input email address here

#SBTACH --export=ALL

#SBATCH -A [ID]                      #Input XSEDE Project ID here

export MODULEPATH=/share/apps/compute/modulefiles/applications:$MODULEPATHmodule load relion/2.0.3dateibrun -np 5 --tpr 4 relion_refine_mpi [paste relion command here]
```

Step 8.

Click here for Cianfrocco Lab XSEDE Project ID number to include (need to be signed into UMich account & need permission to be able to view file)

Step 9.

Submit to Comet:

$ sbatch [filename]