Using EMAN2

On RHEL6 Machines

There is a manually compiled version with MPI available:

```
ssh -Y rhel6-64.slac.stanford.edu
```

you will need to load eman2 via:

```
export MODULEPATH=/afs/slac.stanford.edu/package/spack/share/spack/modules/linux-rhel6-x86_64:/usr/share/Modules
/modulefiles:/etc/modulefiles

module load eman2-master-gcc-4.9.4-tmcs6g7
```

then the programs for eman2 should available via command line.

In order to submit jobs into the batch system, you will need to create a script (using "vi bsub-mpi-example.sh" or similar)

```
#!/bin/bash
#
#BSUB -a mympi                          # set parallel operating environment
#BSUB -P cyroem                         # project code
#BSUB -J eman2-test                    # job name
#BSUB -n 64                             # request one slot for this job
#BSUB -W 72:00                          # Job wall clock limit hh:mm
#BSUB -q bulletmpi                      # queue
#BSUB -e errors-%J.log                  # error file name in which %J is replaced by the job ID
#BSUB -o output-%J.log                  # output file name in which %J is replaced by the job ID
#BSUB -B

# get necessary bins and libs in place
export MODULEPATH=/afs/slac.stanford.edu/package/spack/share/spack/modules/linux-rhel6-x86_64:/usr/share/Modules
/modulefiles:/etc/modulefiles

module load eman2-master-gcc-4.9.4-tmcs6g7


<<<eman2 command line here>>>
```

you can then submit the job via:

```
bsub < bsub-mpi-example.sh
```

please note that you will need to tune the number of nodes (-n) and the wall clock times (-W) to suit the command line arguments for eman2.

you can then monitor the progress of your job via the `bjobs` command. you can also monitor the continuous live output from your job using the `bpeek` command.

On GPU nodes

NB the GPU capabilities of EMAN2 are considered beta (my words). please use with caution

The version of EMAN2 on the ocio-gpu nodes are NOT MPI enabled. They have been compiled with the expectation that only simple local computation is required.

```
ssh -Y ocio-gpu01.slac.stanford.edu
```

There is a bunch of modules that are required to be loaded prior to a functional EMAN2 instance:

```
module load eman2-master-gcc-4.8.5-pri5spm
```

(i'll find a way of auto loading the others in the future)

As long as you ssh in with the -Y option (and you have a x server running on your local machine) you should be able to bring up the relevant GUIs.

Spack Notes

GPU:

```
spack -k install -v   eman2+cuda % gcc ^fftw+openmp~mpi  ^cmake ~doc+ncurses+openssl+ownlibs~qt
^ncurses+symlinks ^hdf5~mpi ^qt@4.8.6%gcc@4.8.5+dbus~examples~gtk~krellpatch+opengl+phonon~webkit
^mesa+llvm+swrender ^mesa-glu+mesa
```

Non-GPU + MPI

```
spack install --keep-stage  -v  eman2+mpi %gcc@4.9.4 ^fftw+openmp+mpi ^openmpi@1.10.3~cuda~java+disable-dlopen
schedulers=lsf ^boost@1.58.0  ^cmake ~doc+ncurses+openssl+ownlibs~qt  ^ncurses+symlinks ^hdf5+mpi ^qt@4.8.6
+dbus+opengl+phonon^mesa+swrender
```