CHARMM

Basic Commands:

- module available charmm To check versions of CHARMM currently loaded on Beagle2
- module load charmm to have the binaries of charmm added to your path (all files will be called charmm)

Write to beagle-support@lists.uchicago.edu if you have problems with this version or you require a different one.

We now have parallel CHARMM and parallel/parallel replica exchange CHARMM running on Beagle2. Our group will test the executables over the next few days. The performance is underwhelming in comparison to Kraken on a small job (116 processors), so we may need to do further optimization. Thanks to everyone for their suggestions with this.

The source used is Wei’s patched c36a6 code: /home/cnrowley/programs/charmm/c36a6_patch

The compile instructions are:

export XTPE_LINK_TYPE=dynamic
module purge
module load PrgEnv-gnu
module load cray-mpich2
module list

Currently Loaded Modulefiles:
1) python/2.7.1(default) 4) cblas/3.0(default) 7) swig/2.0.2(default) 10)
   PrgEnv-gnu/3.1.49A
2) fftw/3.2.2.1(default) 5) metis/4.0.1(default) 8) numpy/python2.7/1.5.1 11) cray-
   mpich2/5.6.1(default) 
3) acml/4.4.0(default) 6) SuiteSparse/3.6.0(default) 9) xtpe-network-gemini

./install.com xt4 xlarge M MPICH X86_64 +CMPI +REPDSTR +GENCOMM +ASYNC_PME /* REMD charmm */
./install.com xt4 xlarge M MPICH +CMPI
/* parallel charmm */

The executables are available on Beagle2 at: ~/cnrowley/bin/charm-c36a6-xt4-mpi and ~/cnrowley/bin/charm-c36a6-xt4-remd

PBS script looks like this:

export MPICH_PTL_SEND_CREDITS=-1
export MPICH_MAX_SHORT_MSG_SIZE=8000
export MPICH_PTL_UNEX_EVENTS=800000
export MPICH_UNEX_BUFFER_SIZE=100M

aprun -n $NPUS ~/bin/charm-c36a6-xt4-remd < $JOBNAME.inp > $JOBNAME.out