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:

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

```
./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/charmm-c36a6-xt4-mpi and ~cnrowley/bin/charmm-c36a6-xt4-remd

PBS script looks like this:

```bash
export MPICH_PTL_SEND_CREDITS=-1
export MPICH_MAX_SHORT_MSG_SIZE=8000
export MPICH_PTL_UNEX_EVENTS=80000
export MPICH_UNEX_BUFFER_SIZE=100M
aprun -n $NCPUS ~/bin/charmm-c36a6-xt4-remd < $JOBNAME.inp > $JOBNAME.out
```