Amber Installs

NOTE: Each Amber directory contains scripts that you can source for setting up your environment:

- amber.sh (bash)
- amber.csh (csh)

Any additional requirements (such as scripts to source for MPI libraries or modules to load) will be listed in specific entries.

CHPC

XSEDE

Blue Waters

CHPC

/uufs/chpc.utah.edu/common/home/u0827715/Amber/GIT

- All MPI programs of Amber installs on CHPC resources require use of modules (default **mvapich2**, lonepeak **impi**).
- All python programs now require the **python/2.7.3** module.
- The default minimum CUDA for Amber is now 7.5: **/usr/local/cuda-7.5** (kepler is the current exception)

Ember (Intel)

amber-ember

Intel compilers

MPI: module load mvapich2

CUDA 7.5
export CUDA_HOME=/usr/local/cuda-7.5
export LD_LIBRARY_PATH=$CUDA_HOME/lib64:$LD_LIBRARY_PATH

Ember (Gnu)

amber-ember-gpu

GNU compilers

MPI:
module swap intel gcc
module load mvapich2

CUDA 7.5
export CUDA_HOME=/usr/local/cuda-7.5
export LD_LIBRARY_PATH=$CUDA_HOME/lib64:$LD_LIBRARY_PATH

Kingspeak

amber-kingspeak

Intel compilers

MPI: module load mvapich2

Tangent

Note: Unlike other CHPC resources, tangent does not appear to load the intel module by default.

amber-tangent

Intel compilers: module load intel

MPI: module load mvapich2

Kepler (GPU)

NOTE: Kepler does NOT use a queuing system. Before running on Kepler ensure no one else is running using the 'top' command.

amber-kepler

GNU compilers

CUDA 5.0: /usr/local/cuda-5.0

No MPI

Lonepeak

amber-lonepeak

Intel compilers

MPI: module load impi

Use 'mpirun', not 'mpiexec'

Bash Tricks

To ensure I'm always running the correct amber install on CHPC resources I add this line to my ~/.bashrc file:

```
source ~/.local_bashrc
```

This is where I keep all of my customizations. Then in my ~/.local_bashrc:

```
# Amber - machine-specific
if [[ ! -z `hostname | grep lonepeak` ]] ; then
  export AMBERHOME=/uufs/chpc.utah.edu/common/home/u0827715/Amber/GIT/amber-lonepeak
elif [[ ! -z `hostname | grep tangent` ]] ; then
  export AMBERHOME=/uufs/chpc.utah.edu/common/home/u0827715/Amber/GIT/amber-tangent
else
  export AMBERHOME=/uufs/chpc.utah.edu/common/home/u0827715/Amber/GIT/amber
fi
if [[ -f $AMBERHOME/amber.sh ]] ; then
  source $AMBERHOME/amber.sh
fi
```

XSEDE

Stampede

/work/00301/tg455746/GIT/amber-stampede

Intel compilers

Modules for GPU runs (default cuda, currently 6.5):
module load netcdf
module load cuda

Modules for CPU runs:
module load netcdf

Comet (still needs testing)

/oasis/projects/nsf/slc216/droe/GIT

amber (CPU only)

Intel compilers

Default system NetCDF: "module load netcdf"

amber-gpu (Serial GPU only)

GNU compilers (system default, NOT gnu 4.9.2)

CUDA 6.5: "module load cuda/6.5"

The compiler set up is not compatible with cuda 6.5; comet staff are working on building an mvapich2 for the system default gnu compiler, 4.4.7. Until then no pmemd.cuda.MPI.

Blue Waters

/projects/sciteam/gk4

All compiles on BW should load appropriate modules just to be safe (full static linking on BW has proven to be tricky at best). CUDA 5.0 is no longer supported on BW since the last SW upgrade.

amber-cpu (CPU only)

```
source /opt/modules/default/init/bash
module unload PrgEnv-cray
module load PrgEnv-pgi
module load netcdf
```

amber-gpu (GPU only, default CUDA)

```
source /opt/modules/default/init/bash
module unload PrgEnv-cray
module load PrgEnv-gnu
module load netcdf
module load cudatoolkit
```