AMBER

AMBER is a highly parallized suite of biomolecular simulation programs which use MPI and OpenMP on CPUs or CUDA (in combination with MPI) to run on GPUs.

Amber is distributed in two parts: AmberTools and Amber. Amber is a package of molecular simulation programs, AmberTools contains a collection of useful software to analyze and modify MD data. You can find a comprehensive manual here.

Short-Info

AMBER	
Category	MD-Simulations
Usage	CPU or GPU
Module-Versions	
AMBER12-18	

Examples

AmberTools on CPU with MPI: MMPBSA.py.MPI

The following example runs MMPBSA.py.MPI on 20 identical CPUs. Each of the called Sander jobs (used for surface and energy calculation) may take up to 4G of RAM - for bigger systems this has to be adjusted. The code below runs a 'stability calculation' for a single system. For a comprehensive overview the the AMBER18 manual.

Keep in mind, that MMPBSA calculations are more demanding in terms of memory than MMGBSA jobs.

MMPBSA_py_MPI.pbs

```
#!/bin/bash

#PBS -l walltime=XX:YY:ZZ
#PBS -l select=20:ncpus=1:mpiprocs=1:mem=4G
#PBS -l place=group=arch
#PBS -r n
#PBS -N Job Name
#PBS -A Project Name

# input files
INFILE=MMPBSA.infile
EOFILE=Output.dat
PRMTOP=Topology.prmtop
TRAJ=Trajectory.nc


# load Amber
module load Amber/18

# go to work dir
cd $PBS_O_WORKDIR

# def executable
MPI_EXE=`which MMPBSA.py.MPI`

# generate log file
LOGFILE=$PBS_O_WORKDIR/$PBS_JOBNAME"."$PBS_JOBID".log"
echo "$PBS_JOBID ($PBS_JOBNAME) @ `hostname` at `date` in "$PBS_O_WORKDIR"
START" > $LOGFILE
echo "`date +"%d.%m.%Y-%T"`" >> $LOGFILE
echo >> $LOGFILE
echo "GLOBAL PARAMETERS">> $LOGFILE
echo "---------------------------" >> $LOGFILE
echo "Node       : "$HOSTNAME >> $LOGFILE
echo "Arch       : "$ARCH >> $LOGFILE
echo "---------------------------" >> $LOGFILE
echo "RunDir     : "$PBS_O_WORKDIR >> $LOGFILE

#
MPICPUS=$(cat $PBS_NODEFILE | wc -l)
echo "# MPI CPUs: ${MPICPUS}" >> $LOGFILE

mpirun $MPI_EXE -i $INFILE -eo $EOFILE -cp $PRMTOP -y $TRAJ  >>$LOGFILE

qstat -f $PBS_JOBID >> $LOGFILE
echo "$PBS_JOBID ($PBS_JOBNAME) @ `hostname` at `date` in "$RUNDIR" END"
>> $LOGFILE
echo "`date +"%d.%m.%Y-%T"`" >> $LOGFILE
```