AMBER

AMBER 16 is available in the FGCI gird environment

Below is a sampe job description file for parallel amber job.

```
&
(executable=runamber.sh)
(jobname=amber-test)
(stdout=std.out)
(stderr=std.err)
(gmlog=gridlog_1)
(walltime=1h)
(memory=1000)
(disk=1000)
(count=8)
(inputfiles=
( "gbin" "gbin" )
( "md12.x" "md12.x" )
( "prmtop" "prmtop" )
)
(outputfiles=
   ( "output.tar" "output.tar" )
)
```

Sample command file (runamber.sh) corresponding the job description file above:

```
#!/bin/sh
echo "Hello Amber!"

module load AMBER

srun sander.MPI -O -p prmtop -i gbin -c md12.x -o mdout.dhfr_serial
ls -l
tar cf output.tar ./*
echo "Bye Amber!"
exit
```