Amber

Purpose: Molecular Dynamics
Latest version: 20
Licence: ⚠ Must be provided by the user.
Proprietary licence ext-link
Website: *http://ambermd.org/_ext-link*

Amber is a collection of programs for setting-up, running and analysing molecular dynamics simulations.

Amber refers both to a collection of about 50 programs for building, configuring and minimising molecular structures, setting up force fields, running simulations, analysing trajectories, and computing system properties, and to a force field for biomolecules implemented by the Amber programs.

SLURM Submit script example

More information about the submit script can be found using the ***Job Script Generator***.

Sbatch options:

The options shown in the example are detailed below. For more information and a more comprehensive list of available options, see the ***sbatch command page***.

- **-J**: Name for the job's allocation.
- **-e**: Name of the sterr redirection filename.
- **-o**: Name of the stdout redirection filename.
- **-p**: Name of the partition (queue) where the job will be submited.
- **-n**: Number of tasks.

amber_example.slm

```
#!/bin/bash
#SBATCH -J amber_example
#SBATCH -e amber_example.%j.err
#SBATCH -o amber_example.%j.out
#SBATCH -p std
#SBATCH -n 1
#SBATCH -t 0-02:00

module load apps/amber/18

##
#  Modify the input and output files!

cp -r ${SLURM_SUBMIT_DIR}/{*.inp,*.top,*.crd}
${SCRATCH}
cd ${SCRATCH}

srun pmemd.MPI -O \
               -i amber_example.inp \
               -p amber_example.top \
               -c amber_example.crd \
               -o amber_example.out

cp ./*.out ${SLURM_SUBMIT_DIR}
```

- **-t**: Set the job's time limit. If the job don't finish before the time runs out, it will be killed.

Software execution information:

The **pmemd** program is the comercial-high-performance version of **sander**, general purpose MD engine of Amber. Here is a summary of the command line options for them:

- **-O:** Overwrite output files if they exist.
- **-A:** Append output files if they exist.
- **-i:** Input file. Default input name: *mdin*.
  - Contains control data for the min /md run.
- **-p:** Input file. Default input name: *prmtop*.
  - Contains molecular topology, force field, periodic box type, atom and residue names.
- **-c:** Input file. Default input name: *inpcrd*.
  - Contains initial coordinates and (optionally) velocities and periodic box size.
- **-r:** Output structure file. Default input name: *restrt*.
  - Contains final coordinates, velocity, and box dimensions for restarting run.
- **-o:** Output energy file. Default input name: *mdout*.
  - Contains user readable state info and diagnostics.
  - ***-o stdout*** will send output to stdout (to the terminal) instead of to a file.
- **-x:** Output energy file. Default input name: *mdcrd*.
  - Contains coordinate sets saved over trajectory.
- **-e:** Output energy file. Default input name: *mden*.

    - Contains extensive energy data over trajectory (not synchronized with mdcrd or mdvel).

- **-inf:** Output energy file. Default input name: *mdinfo*.
    - Latest mdout-format energy info.
