Using gibbs_multireplica on LAMMPS

Compiling LAMMPS

- Download **lammps-22Aug18** from the following link: https://lammps.sandia.gov/tars/
- Inflate on OCS cluster in whichever directory you prefer.
- Once inflated go to: >lammps-22Aug18/src and type the following:

```
make clean-all
make yes-misc
make yes-user-misc
make yes-user-meamc
make yes-mc
make yes-replica
make yes-manybody
make package-update
make mpi
```

- After this compiles (takes 20-30 mins)
  >cd src/USER-MISC
- Copy gibbs_multireplica.ccp and gibbs_multireplica.h into this directory
- Go back to lammps-22Aug18/src/ directory
- recompile

```
make package-update
make mpi
```

- you should have an excecutable named **lmp_mpi**

EXAMPLE INPUT FILE (Binary Pt-Au)

```
## This file is called: in.gibbs_PtAu_fcc

#define variables
variable        tt equal 400.0      # target temperature
variable        pp equal 0.0      # target pressure

variable        temper_T world ${tt} ${tt}
variable        rep world 0 1
variable        each equal 100
variable        dach equal v_each*10
variable        ncycles equal 2000


# Create atoms or read from a file ( SEE EXAMPLE INPUT FILES)

# Read POTENTIALS

pair_style      eam/alloy
pair_coeff      * *   PtAu.eam.alloy Pt Au

# Run either NPT or NVT

fix    myfix all npt temp ${temper_T} ${temper_T} 1.0 iso ${pp} ${pp} 2.0 tchain 5 pchain 5
#fix   myfix all nvt temp ${temper_T} ${temper_T} 1.0 tchain 5

dump            1 all custom ${dach} dump.${rep} id type x y z

# Run multireplica MC moves

gibbs/multireplica 10000000  ${each}  ${ncycles} ${temper_T} myfix 123 888 types 1 2 fudge 0.50
#gibbs/multireplica 10000000  ${each}  ${ncycles} ${temper_T} myfix 123 888 types 1 1 fudge 0.50
```

Running the code

- Go to a directory to run test cases.
  For example have a directory called WORKDIR/MC2_AuPt
- Once inside, the code can be runned as follows:

```
rm -f log* dump* screen* file* *txt;
cp  /lammps-22Aug18/src/lmp_mpi .
mpirun -np 2 ./lmp_mpi partition 2x1 -in in.gibbs_PtAu_fcc
```

The partition flag reads as :
(num of worlds) x (num of processor per world)

Output

- log.lammps: output file for the whole job
  1. step
  2. mcflag
  3. intra_swap_acc
  4. inter_swap_acc
  5. flip_acc
  6. exchange_acc
  7. volume_acc
  8. Num atoms of species 1 in the universe
  9. Num atoms of species 2 in the universe
  10. Sum of previous two columns
  11. molar fraction of phase-α
  12. molar fraction of phase-β
  13. molar energy: $f^{\alpha} G^{\alpha} + f^{\beta} G^{\beta}$
  14. Max. number of particles to flip

Output

- log.lammps.*: output file for each phase
  This is the output of thermo_style inside the input file
  1. step
  2. temp
  3. Energy of a pair: epair
  4. volume
  5. Total Energy: etotal
  6. press
  7. density
  8. Number of Pt atoms: v_cPt
  9. Nubmer of Au atoms: v_cAu

Output

- chempot_prc*.txt: output due to Widom test
  1. step where test occurred
  2. chemical potential estimate (one value for binary)
  3. Running average of chemical potential (using last five estimates)
  4. average molar fraction phase-α
  5. average molar fraction phase-β