body_orient.cpp
body_theta.cpp

- bo_xxx.dat
- theta_xxx.dat

- Original trajectory file
(dump_npt_o.1.lammpstrj)

reorder.cpp

- COM trajectory file
(dump_1_reorder.lammpstrj)

- com_1.xxx.dat

- hex_1_xxx.lammpstrj

theta.cpp

phicorre.cpp

- theta_1_all.txt

Decided theta value
paircorre.cpp

Note:

All the files whose name are marked in blue represent that they are created by LAMMPS.

All the files whose name are marked in black represent that they are created by the codes provided in relative folders.

- correlation.txt

- trans_1_all.txt

Black arrows: input of cpp files
Blue arrows: input of LAMMPS