

• Original trajectory file (dump\_npt\_h.1.2.lammpstrj) reorder\_tilt.cpp • COM trajectory file (dump\_1.2\_reorder.lammpstrj)

• com\_1.xxx.dat

theta\_tilt.cpp

• theta\_1.2\_all.txt

Decided theta value  
paircorre\_tilt.cpp

• trans\_1\_all.txt

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.