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# LAMMPS version: 17 Nov 2016
# This in-file simulates startup shear with Kremer-Grest model (DPD thermostat)
# Note: this in-file needs the chain coordinate file
#
# If find any bugs, questions or suggestions
# email to yjruan@ciac.ac.cn

#==================Basic variable====================
variable        Rate        equal 0.00005           #Shear rate

variable        Tstrain     equal 3.0               #total strain
variable        Nstrain     equal 1.0               #How many steps to dump config coordinate
variable        Npress      equal 0.2               #How many steps to dump thermo data et al

variable        Rcut        equal 2^(1.0/6.0)       #Rcut in LJ potential
variable        deltaT      equal 0.005             #step length
variable        Seed        equal 22046             #random seed

#==================Dump variable====================
variable        Nevery      equal 2000
variable        Nstep       equal round(v_Npress/v_Rate/v_deltaT)

variable        Noutput     equal round(v_Nstrain/v_Rate/v_deltaT)
variable        Ntotal      equal v_Noutput*v_Tstrain/v_Nstrain          #total timestep

#================Basic information=================
units           lj
atom_style      angle
special_bonds   fene
comm_modify     vel yes                             #This is important for ghost particles in DPD

#================Read chain configuration==========
read_data       data.chain

#=====================Force field==================
pair_style      hybrid/overlay lj/cut ${Rcut} dpd/tstat 1.0 1.0 ${Rcut} ${Seed}
pair_coeff      * * lj/cut 1.0 1.0
pair_modify     shift yes
pair_coeff      * * dpd/tstat 0.5

bond_style      fene
bond_coeff      * 30.0 1.5 1.0 1.0

angle_style     cosine
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angle_coeff       * 2.0
#====================Neighbourlist====================
neighbor          0.4 bin
neigh_modify      delay 0 every 1 check yes

#=====================Output=========================
compute           molChunk all chunk/atom molecule
compute           molRg       all gyration/chunk molChunk tensor    #calculate Rg of each Chunk

variable          Rg_x      equal ave(c_molRg[1])
variable          Rg_y      equal ave(c_molRg[2])
variable          Rg_z      equal ave(c_molRg[3])
variable          Rg          equal (v_Rg_x+v_Rg_y+v_Rg_z)

fix               1 all nve
fix               2 all deform 1 xy erate ${Rate} units box remap v

fix               3 all ave/time 1 ${Nevery} ${Nstep} c_thermo_press &
                   file "PRESS.DAT" mode vector format "%10.6f"

dump              1 all custom ${Noutput} dump.RE-POSITION_* id xu yu zu
dump_modify       1 sort id format line "%7d %21.14f %21.14f %21.14f"

dump              2 all custom ${Noutput} dump.VELOCITY_* id vx vy vz
dump_modify       2 sort id format line "%7d %21.14f %21.14f %21.14f"

thermo            ${Nstep}
thermo_style      custom step temp v_Rg_x v_Rg_y v_Rg_z v_Rg

#====================Other set=======================

timestep          ${deltaT}

run               ${Ntotal}
```