# NEMD simulation of Ar thermal conductivity

# Initialization

units lj

dimension 3

newton on

boundary p p p

atom\_style atomic

neighbor 0.3 bin

neigh\_modify check yes

lattice fcc 0.844

region box block -4 4 -4 4 -4 4 units lattice

create\_box 1 box

create\_atoms 1 box

region hot block INF INF INF INF -0.5 0 units lattice

region cold block INF INF INF INF 3.5 4 units lattice

mass 1 1.0

velocity all create 0.71 458127641 mom yes rot yes dist gaussian units box

pair\_style lj/cut 2.8

pair\_coeff 1 1 1.0 1.0 # LJ parameters for Ar-Ar

fix temp all temp/berendsen 0.71 0.71 0.0466

fix nve all nve

compute ke all ke/atom

variable temp atom c\_ke/(1.5\*1.0)

fix temp\_profile all ave/spatial 1 100000 100000 z lower 0.5 v\_temp file temp.profile units lattice

compute hot\_temp all temp/region hot

compute cold\_temp all temp/region cold

variable delta\_temp equal c\_hot\_temp-c\_cold\_temp

fix delta\_out all ave/time 1 100000 100000 v\_delta\_temp file delta\_temp.dat # temperature gradient

thermo\_style custom step temp etotal vol

thermo\_modify lost warn

thermo 100

# Run

timestep 0.000466

run 100001

unfix temp

fix heat\_swap all thermal/conductivity 10 z 16

fix e\_exchange all ave/time 10 10000 100000 f\_heat\_swap file e\_exchange.dat #Energy exchanged

variable thermal\_conductivity equal f\_e\_exchange/(0.000466\*10.0\*2.0\*f\_delta\_out)\*1.3806504e-23/(3.405e-10\*3.405e-10)\*sqrt(1.67e-21/6.633e-26) #lj units to real units

fix thermal\_conductivity\_out all ave/time 100000 1 100000 v\_thermal\_conductivity file thermal\_conductivity.dat

# Run

run 10000000

Thermal\_conductivity results based on timesteps

Temp profile based on bins

Initial timesteps

Final timesteps

Heat flux

Delta Temp