```
### DEFINE SIMULATION BOX GEOMETRY ###
lattice sc …
region box block 0 15 0 15 0 15
create_box 1 box
create_atoms 1 box

### DEFINE PHYSICAL PROPERTIES OF ATOMS ###
mass 1 1.0
pair_style lj/cut/opt 3.0
pair_coeff 1 1 1.0 1.0
neighbor 2.0 bin

### SPECIFY THE REQUIRED THERMODYNAMIC STATE ###
variable T equal ...
variable timestep equal ...

### ASSIGN ATOMIC VELOCITIES ###
velocity all create ${T} 12345 dist gaussian rot yes mom yes

### SPECIFY ENSEMBLE ###
timestep ${timestep}
fix nve all nve

### THERMODYNAMIC OUTPUT CONTROL ###
thermo_style custom time etotal temp press vol
thermo 10

### RECORD TRAJECTORY ###
dump traj all custom 1000 output-1 id x y z

### SPECIFY TIMESTEP ###

### RUN SIMULATION TO MELT CRYSTAL ###
run 10000
unfix nve
reset_timestep 0

### BRING SYSTEM TO REQUIRED STATE ###
variable tdamp equal ${timestep}*100
variable pdamp equal ${timestep}*1000
fix nvt all nvt temp ${T} ${T} ${tdamp}

run 10000
fix nve all nve
unfix nvt
reset_timestep 0

### MEASURE SYSTEM STATE ###
thermo_style custom step etotal temp press density
variable dens equal density
variable dens2 equal density*density
variable etotal equal etotal
```

```
variable temp equal temp
variable temp2 equal temp*temp
variable press equal press
variable press2 equal press*press
variable etotal2 equal etotal*etotal
variable numatoms2 equal atoms*atoms
fix aves all ave/time 100 1000 100000 v_dens v_temp v_press v_dens2 v_temp2
v_press2 v_etotal2 v_etotal v_vol
run 100000

variable avedens equal f_aves[1]
variable avetemp equal f_aves[2]
variable avepress equal f_aves[3]
variable errdens equal sqrt(f_aves[4]-f_aves[1]*f_aves[1])
variable errtemp equal sqrt(f_aves[5]-f_aves[2]*f_aves[2])
variable errpress equal sqrt(f_aves[6]-f_aves[3]*f_aves[3])
variable aveetotal2 equal f_aves[7]
variable aveetotal equal f_aves[8]
variable avevol equal f_aves[9]

variable heatcap equal
${numatoms2}*(${aveetotal2}-${aveetotal}*${aveetotal})/
(${avetemp}*${avetemp})

variable Coverv equal ${heatcap}/${avevol}

print "Averages"
print "--------"
print "Density: ${avedens}"
print "Stderr: ${errdens}"
print "Temperature: ${avetemp}"
print "Stderr: ${errtemp}"
print "Pressure: ${avepress}"
print "Stderr: ${errpress}"
print “Heat Capacity over Volume”: ${Coverv}
```