Online simulations via nanoHUB: Molecular dynamics simulation of melting

In this tutorial:

- Setup an MD simulation for bulk Aluminum
- Increase the system temperature with time to study melting
- Explore melting in an Al nanoparticle

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STEP 1: launch the nanoMATERIALS tool

From your *My HUB* page launch nanoMATERIALS

- From *All Tools* find: nano-Materials Simulation Toolkit

- Launch tool by clicking on:

STEP 2: setup the atomistic simulation cell

From the *Input Model* tab of the tool

- Start with an Al unit cell
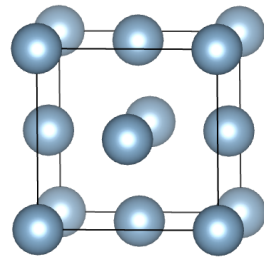 - 4-atom cubic fcc cell:

Cell vectors:
$a = a_0(1,0,0)$
$b = a_0(0,1,0)$
$c = a_0(0,0,1)$
With $a_0 = 0.402$ nm

Fractional atomic positions
(0,0,0)
(0.0, 0.25, 0.25)
(0.25, 0.0, 0.25)
(0.25, 0.25, 0.0)

- Replicate unit cell to create supercell
  - Replicate 5 times in each direction
  - Total number of atoms: 4x5x5x5 = 500

nano-Materials Simulation Toolkit

| Input Model | Energy Expression | Driver Specification | Advanced Op |

Input model: Al_unitcell.bgf

Create Supercell

a direction: 5
b direction: 5
c direction: 5

Simulation cell parameters

Modify simulation cell parameters: ● ▬ ☐ no

Fixed atomic coordinates: Cartesian

Length a: 5A
Length b: 5A
Length c: 5A

Translate atoms

X direction: 0A
Y direction: 0A
Z direction: 0A

Simulation cell will be infinitively periodic with no free surfaces
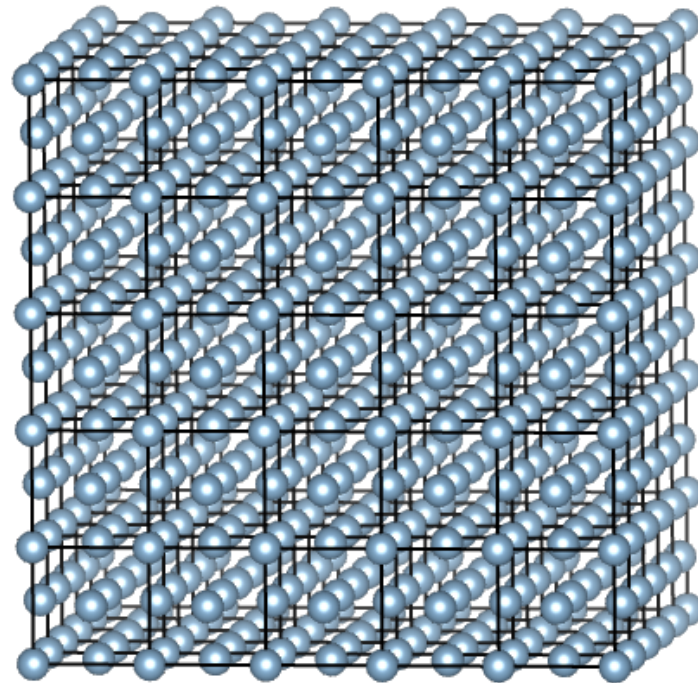
STEP 2: setup the atomistic simulation cell

- Al unit cell
  - 4-atom cubic fcc cell:
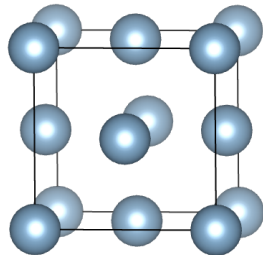
- Supercell:
  - Replicate 5 times in each direction
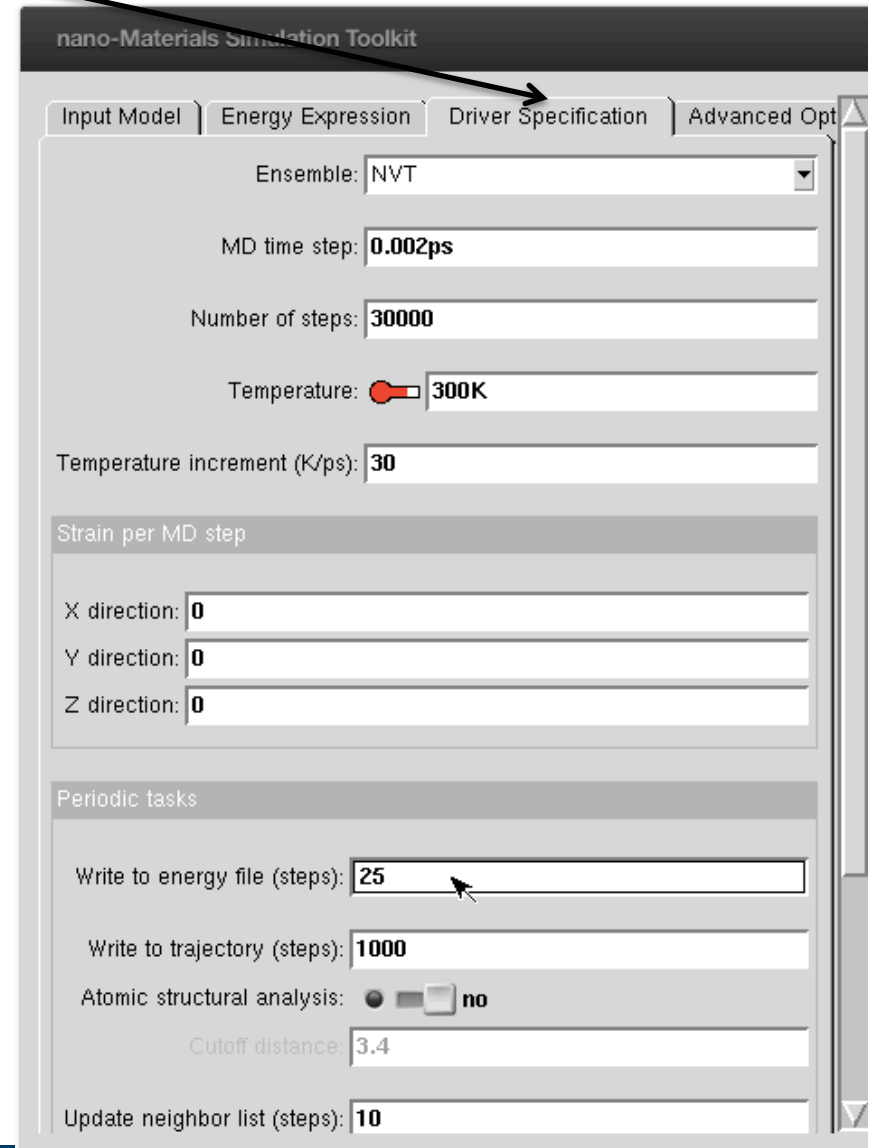 - Total number of atoms: 4x5x5x5 = 500

One large cell with 500 atoms
(no internal boundaries)

Simulation cell will be infinitively periodic with no free surfaces

STEP 3: setup the run parameters

From the *Driver Specification* tab of the tool

- NPT ensemble
  - Control temperature & pressure
- Timestep to solve equations of motion:
  0.002 ps (2 fs)
- Number of MD steps 30,000
  - Total simulation time:
    30,000x0.002ps=60 ps
- Temperature
  - Start simulation at room temp
- Temperature increment
  - 30 K/ps
  - Temperature increase during run:
    60ps x 30K/ps = 1800
  - Final temperature: 1200 K + 300 K =
    2100K

STEP 3 (cont.): setup the run parameters

From the *Driver Specification* tab of the tool

- Do not strain the simulation cell
  - Barostat will take care of thermal expansion and keep pressure at 1 atm.
- Periodic tasks:
  - Write thermodynamic info every 25 steps
  - Write atomic snapshot for viz. every 1000 steps
- Run the simulation
  - Simulation will take approximately 10 mins
  - Think about what you expect to obtain

STEP 4: explore the results interactively
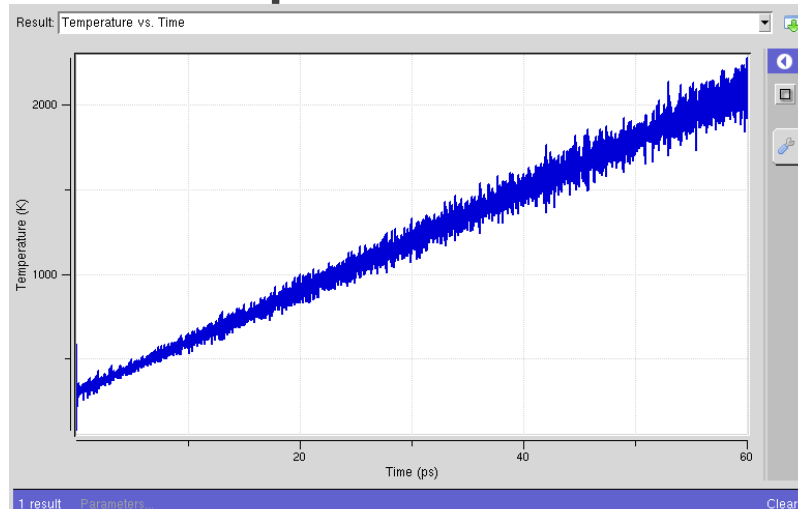
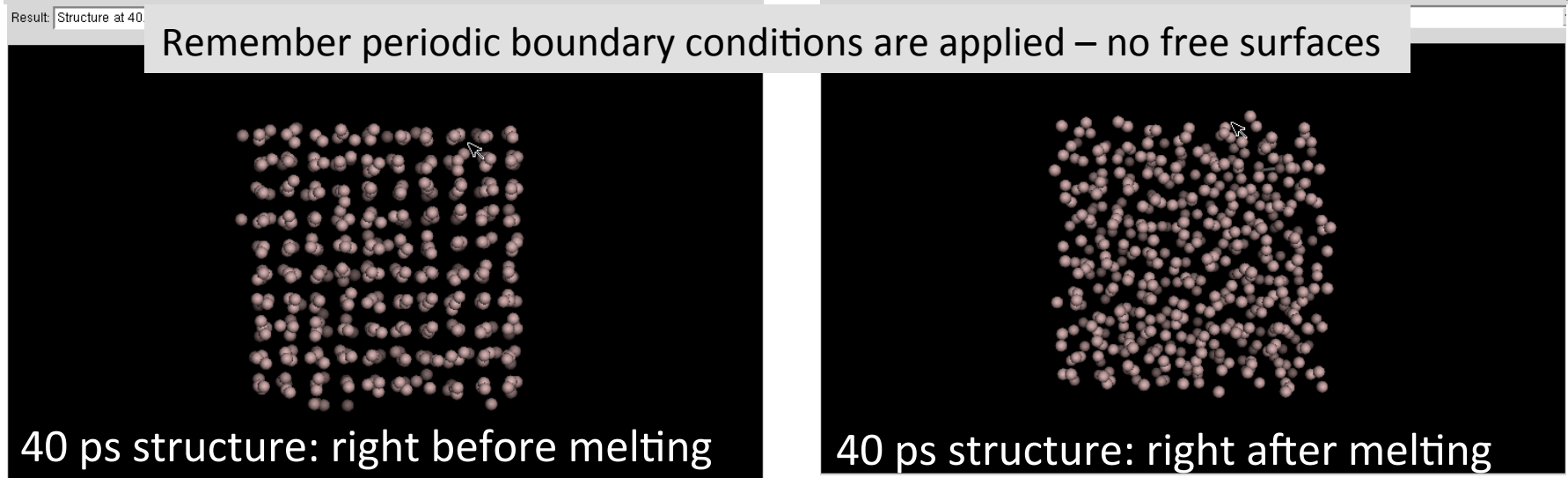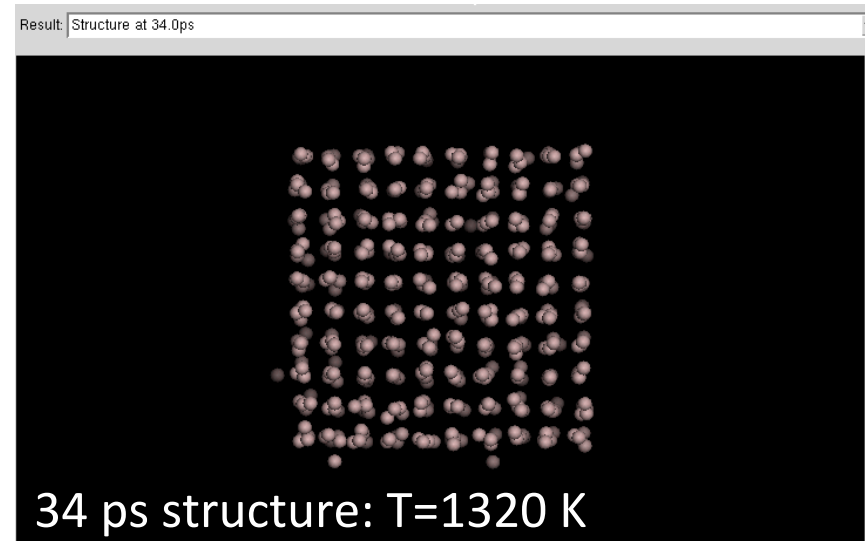Temperature vs. time shows expected increase

Potential energy and volume jump up right after 40 ps (T~1500 K)
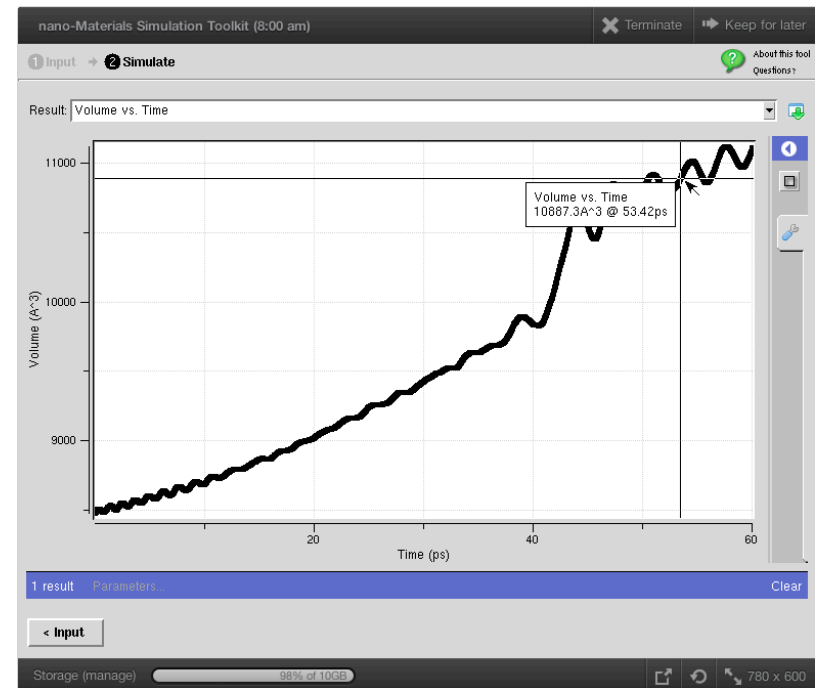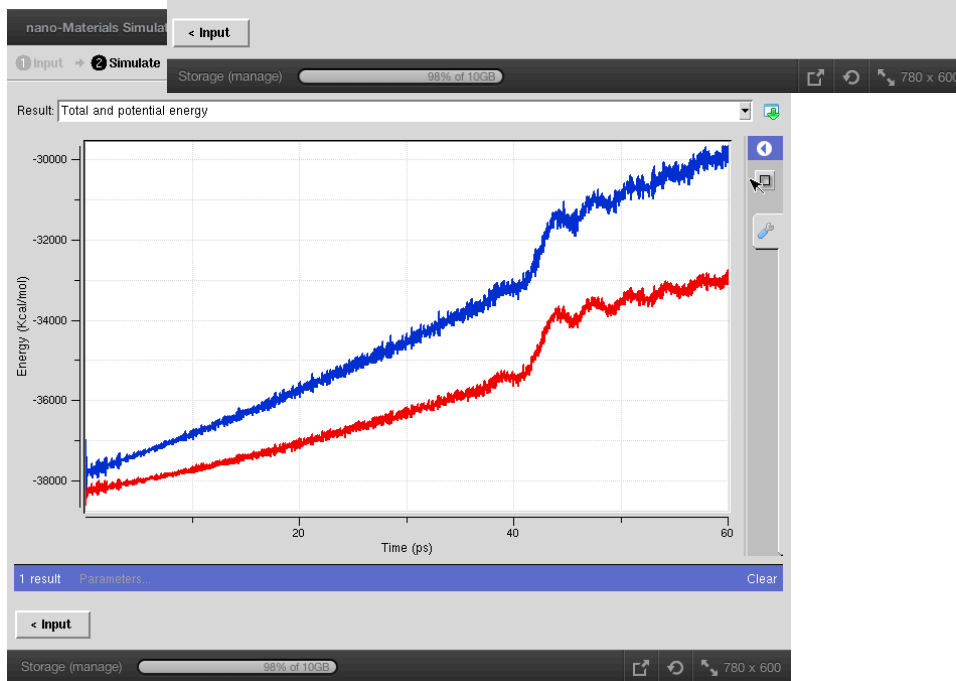
STEP 4: explore atomic configurations

Result: Structure at 2.0ps

2 ps structure: low temperature

Result: Structure at 34.0ps

34 ps structure: T=1320 K

Result: Structure at 40.

Remember periodic boundary conditions are applied – no free surfaces

40 ps structure: right before melting

40 ps structure: right after melting
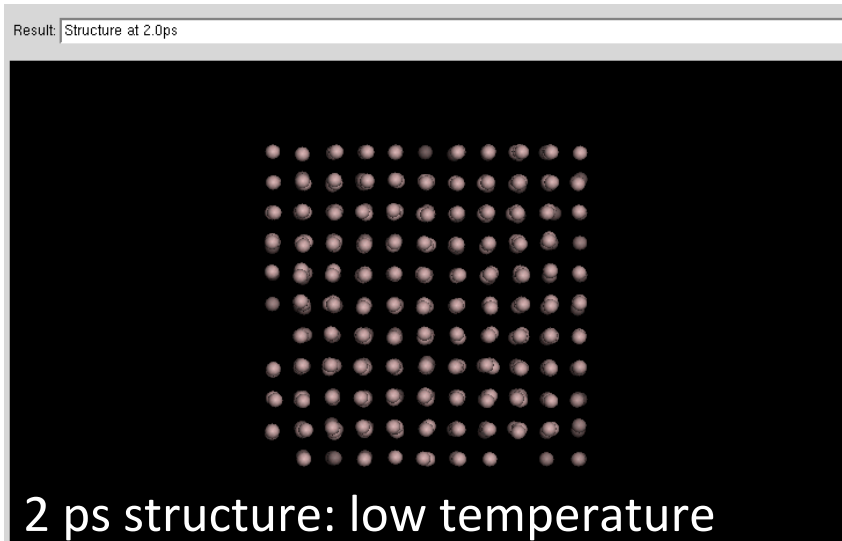
You can also visualize an animation of the trajectory

Discussion and assignment – Part 1

- Melting is marked by an abrupt increase in potential and total energy (this is due to the latent heat of fusion)

- Estimate the temperature at which the system melts and compare it with the experimental melting temperature of Al (930 K)

- Discuss possible origins for any discrepancy you find
  - Think about equilibrium melting temperature and the temperature at materials melt and solidify

- Now we will study the melting of an Al nanoparticle
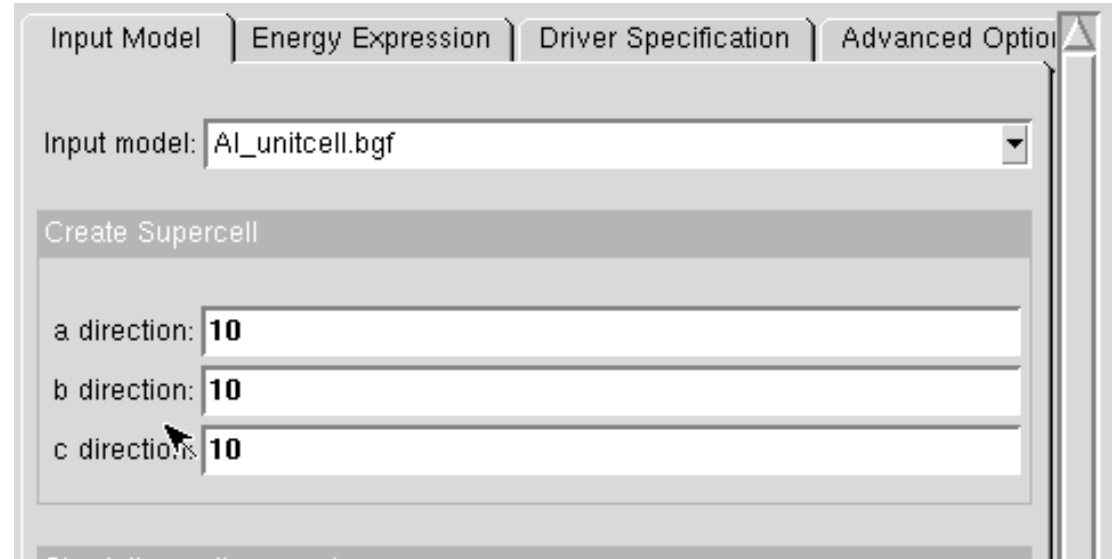
STEP 5: create a spherical nanoparticle

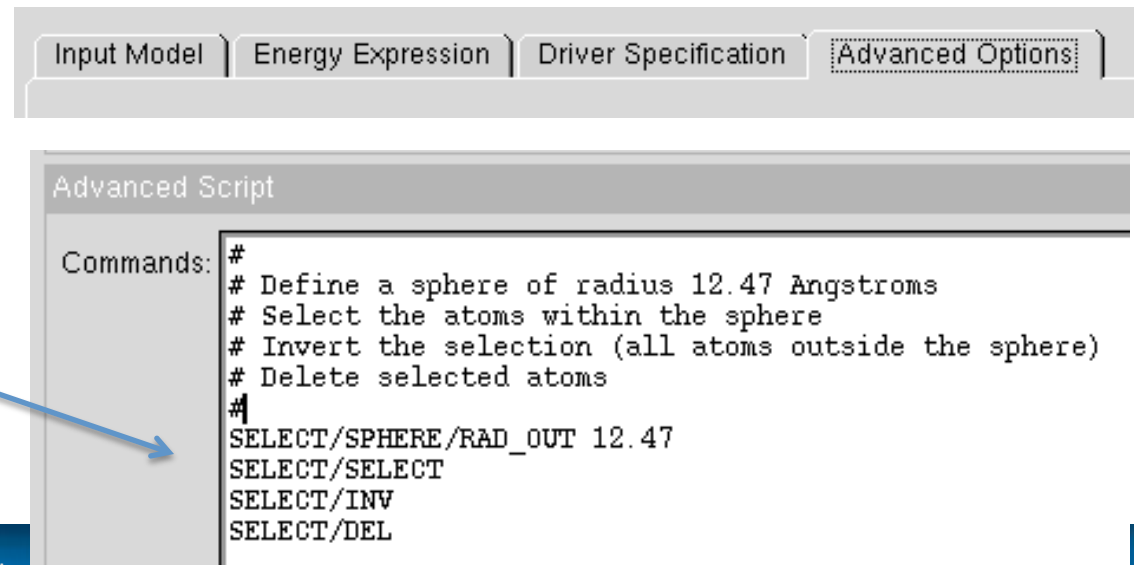We will *carve* a sphere out of a larger simulation cell
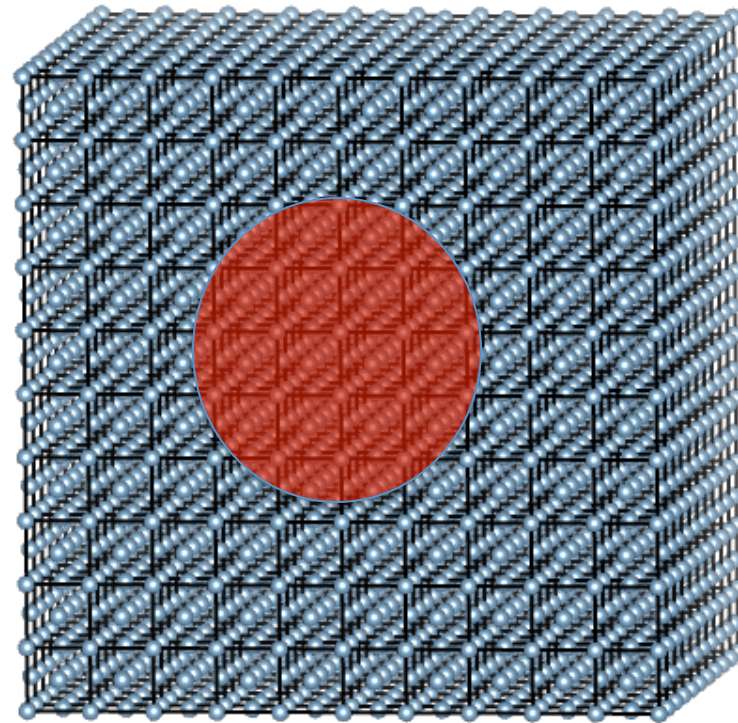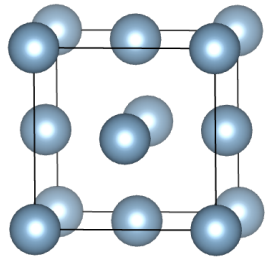
- Previous simulation volume: $(4.02 \times 5 \text{ Å})^3$
- Sphere radius (equivalent volume): 12.47 Å

STEP 5: create a spherical nanoparticle

Input Model Tab
Start with 10x10x10 supercell

Advanced Options Tab
Add the following to
Advanced Script text box

STEP 5: create a spherical nanoparticle

- Run is the same as before except for:
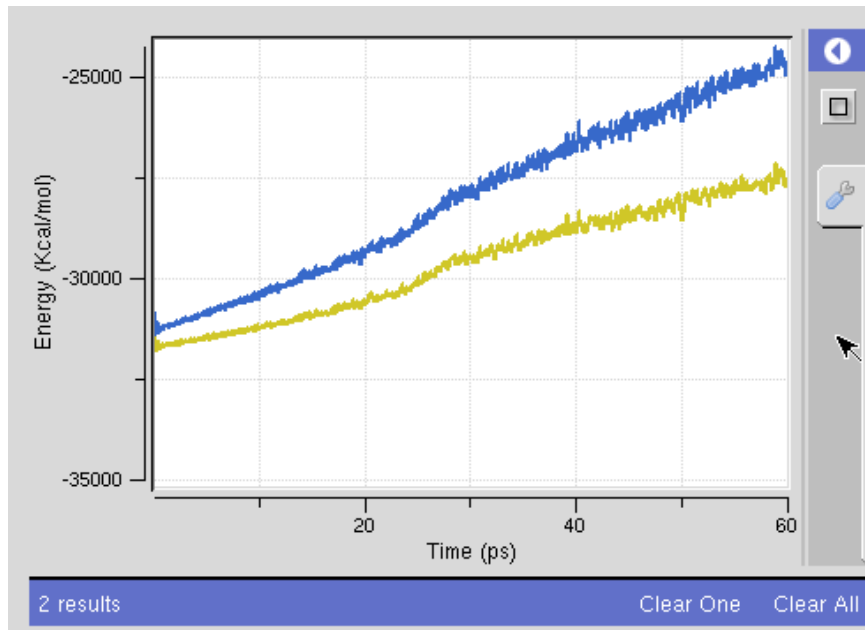 - The simulation cell volume will be kept constant
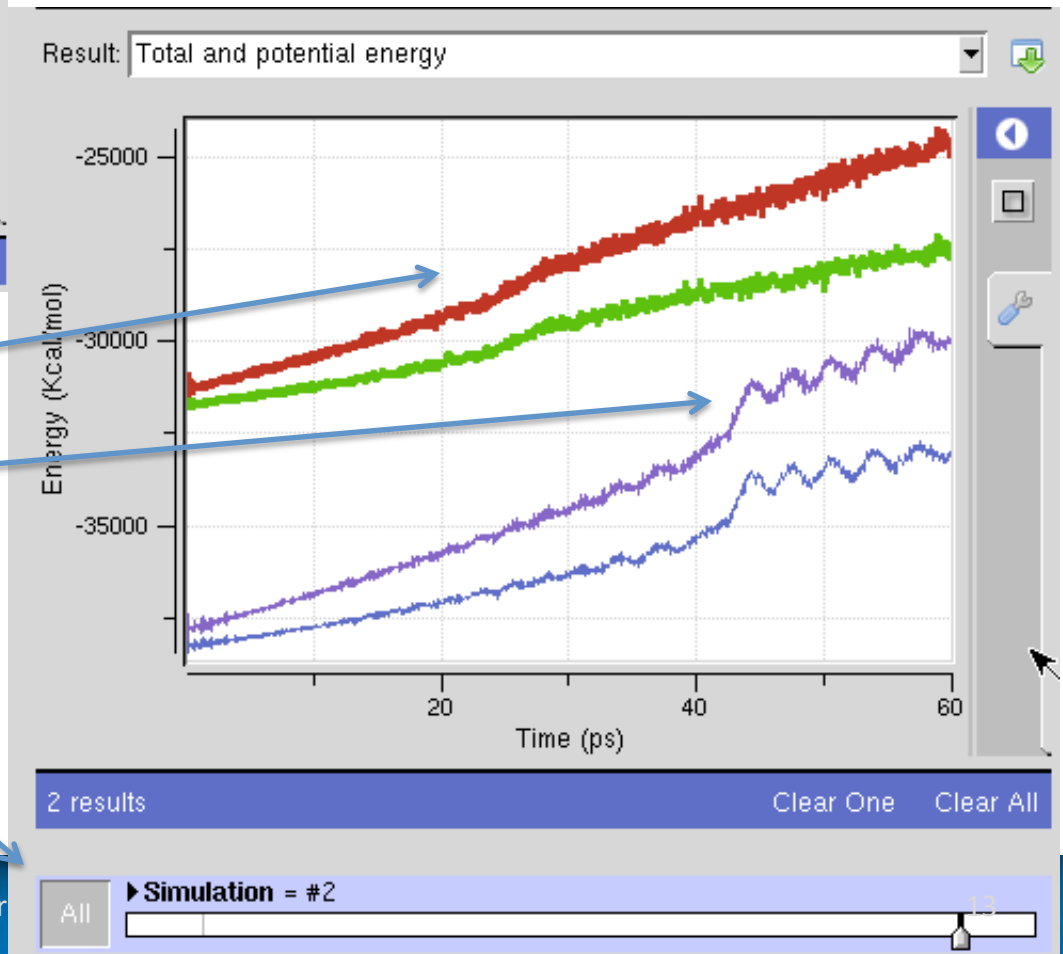 - Select NVT in Ensemble

- We have a sphere inside a large simulation box
- The size (volume) of the simulation box will be constant
- The sphere can expand inside the box

  Run the simulation with the new setup

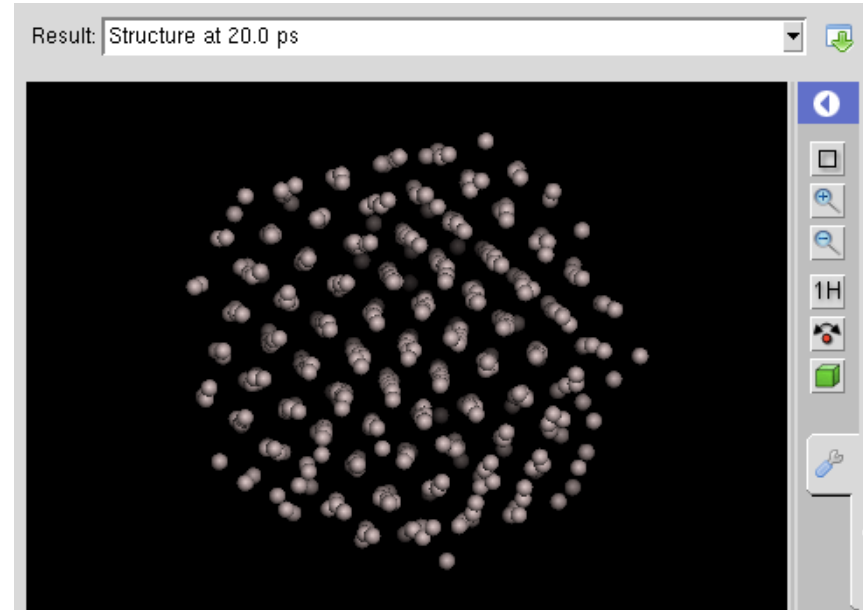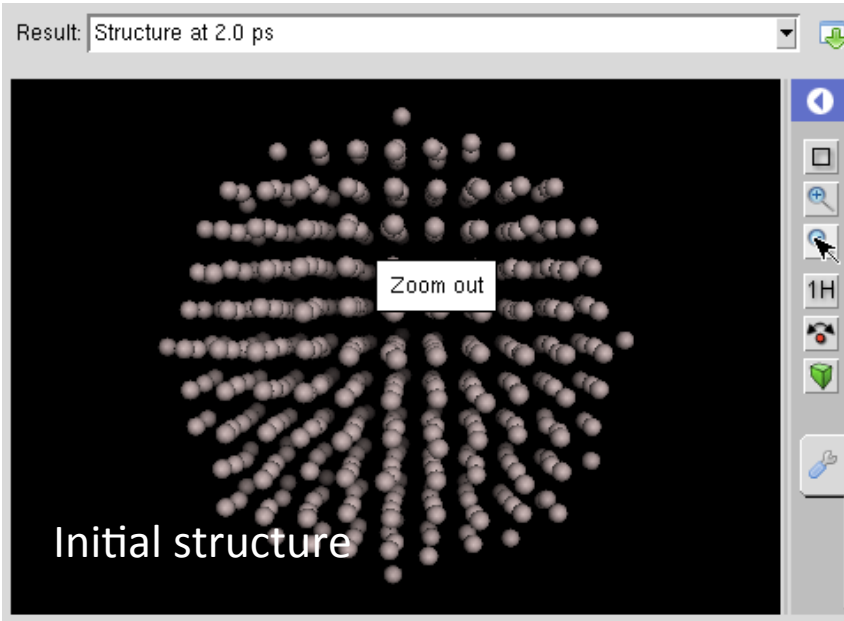# STEP 6: analyze nano particle melting

Potential energy and total energy during heating

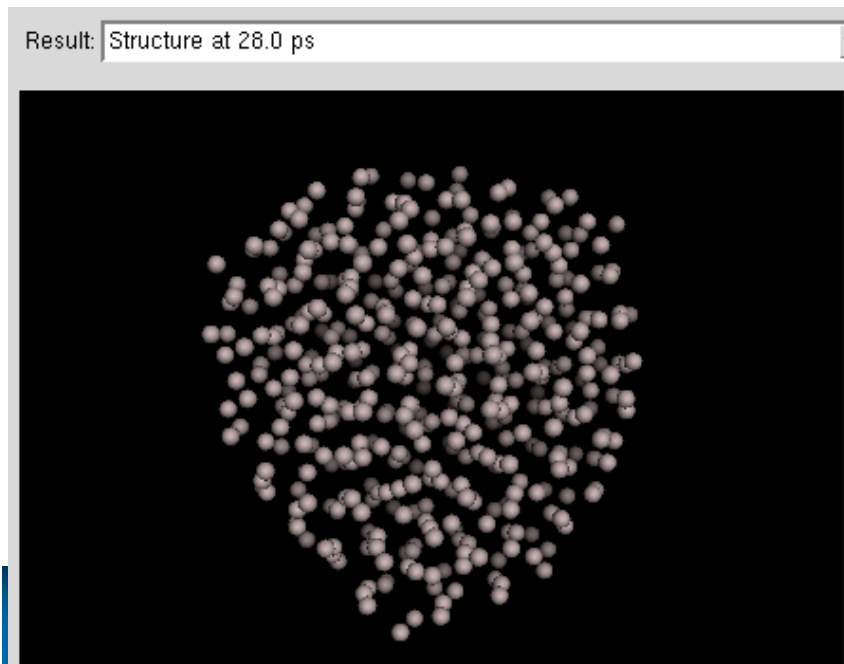Again, jumps in energies denote melting

You can compare the nano particle results with the original bulk samples by clicking All

STEP 6: melting of a nano particle

Result: Structure at 2.0 ps

Zoom out

Initial structure

Result: Structure at 20.0 ps

Result: Structure at 28.0 ps

- 20 ps - 300 K + 30 K/ps x 20ps = 900 K
- Still solid – but it has transformed in shape
- Facetted shape

- 28 ps - 300 K + 30 K/ps x 28ps = 1140 K
- Particle has melted

Discussion and assignment – Part 2

- At what temperature does the nano particle melt?

- Compare the melting of the nanoparticle with the bulk. Explain any differences.

- Why does the nanoparticle transform in shape before melting

- Open question: Does the decrease of melting temperature in nanoparticles have practical implications? Think about sintering

With the tool you can create models for other materials and geometries and study their melting