Lab: deformation of nanoscale materials

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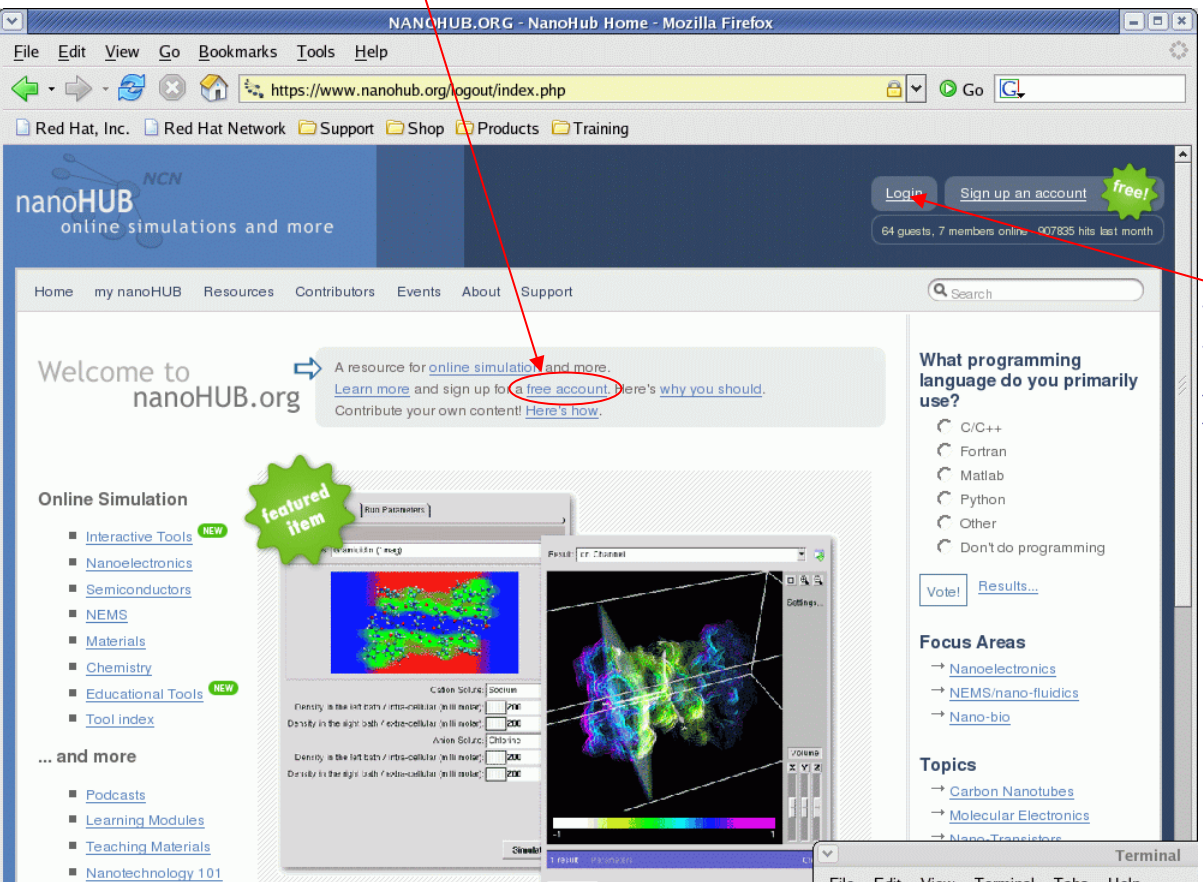
nanoMATERIALS simulations toolkit

In order to run the nanoMATERIALS simulations toolkit you need to register as a user of the nanoHUB:
Go to www.nanohub.org
and click on:



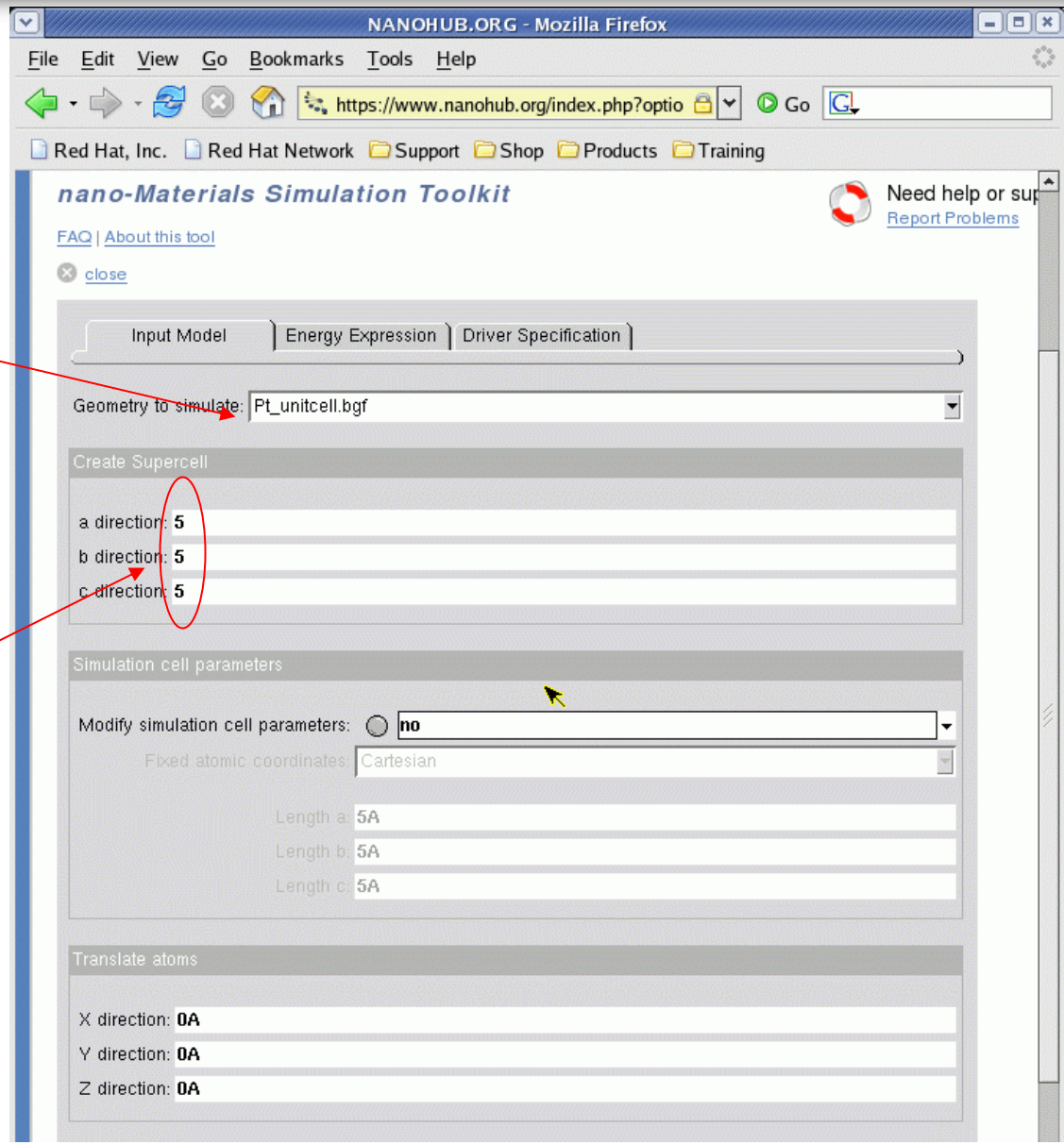
Login and then click select nanoMATERIALS tool

A simple MD runs with nanoMATERIALS

Determine initial model for simulation

Select a model (Pt_nanowire)

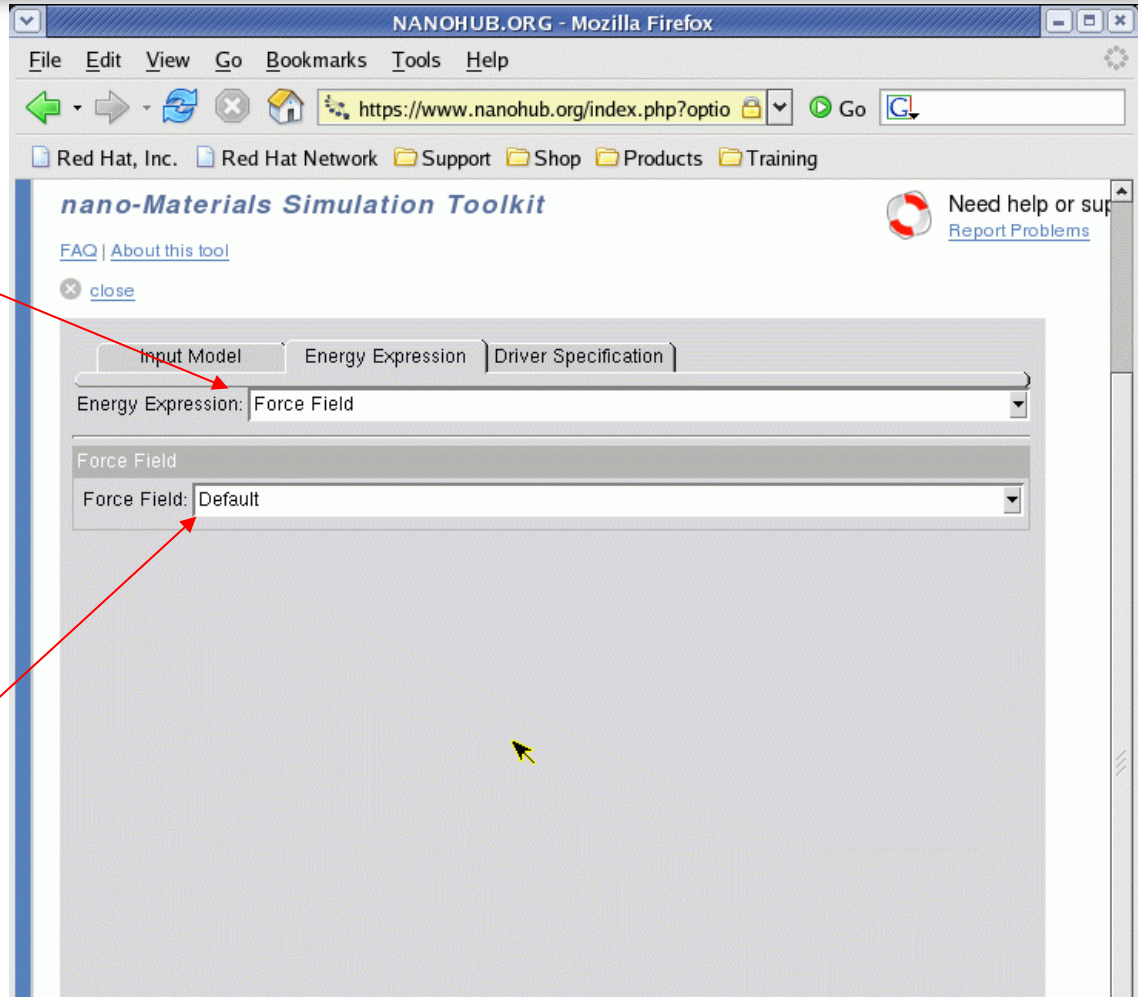
Make a 5 5 5 supercell



A simple MD runs with nanoMATERIALS

Energy expression

Select how the energy (and derived quantities) of the system will be determined



We will let the program pick the force field for us (a many body Sutton Chen force field)

A simple MD runs with nanoMATERIALS

Driver options

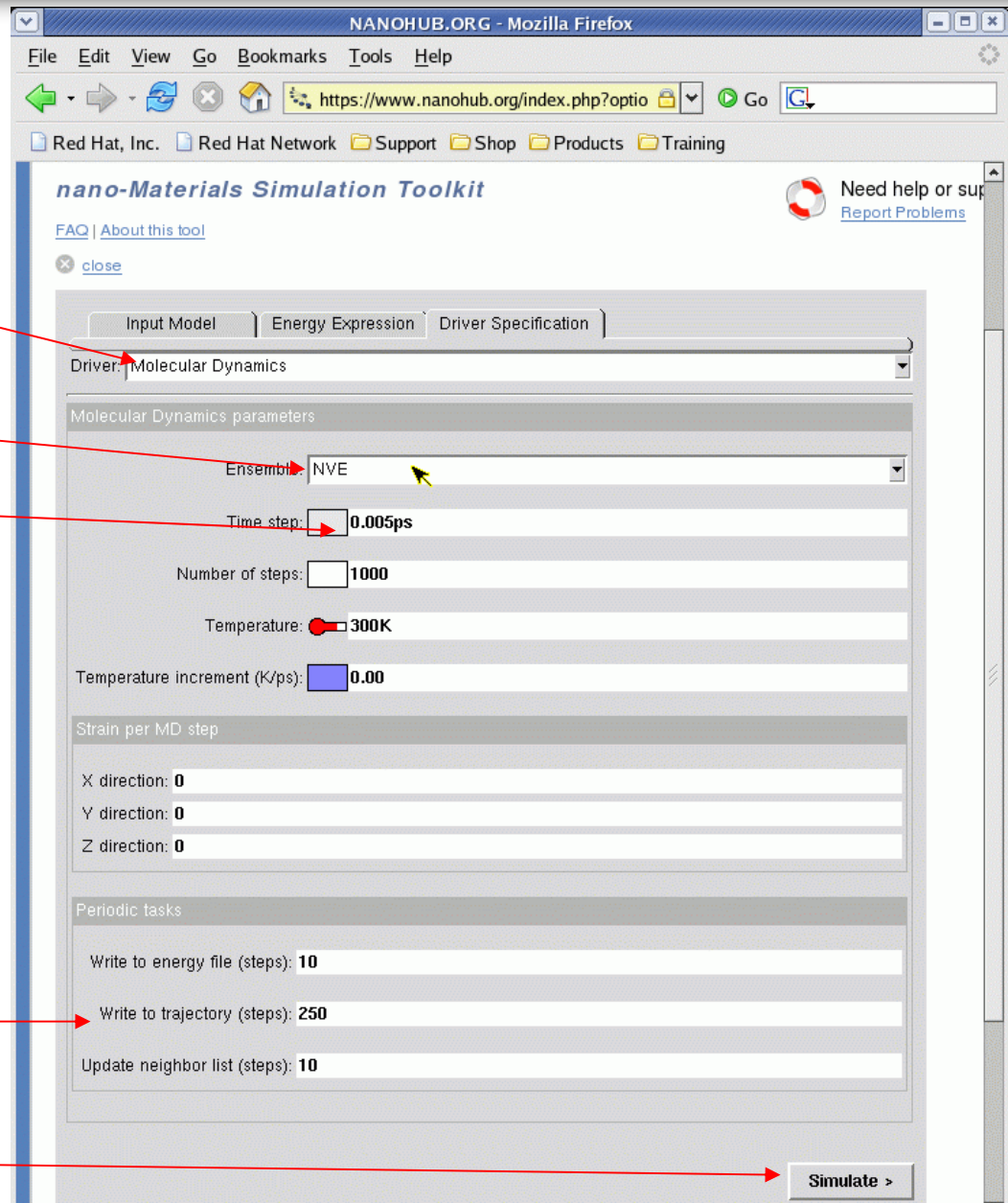
What type of simulation?

Ensemble (NVE)

Time-step (5 fs)

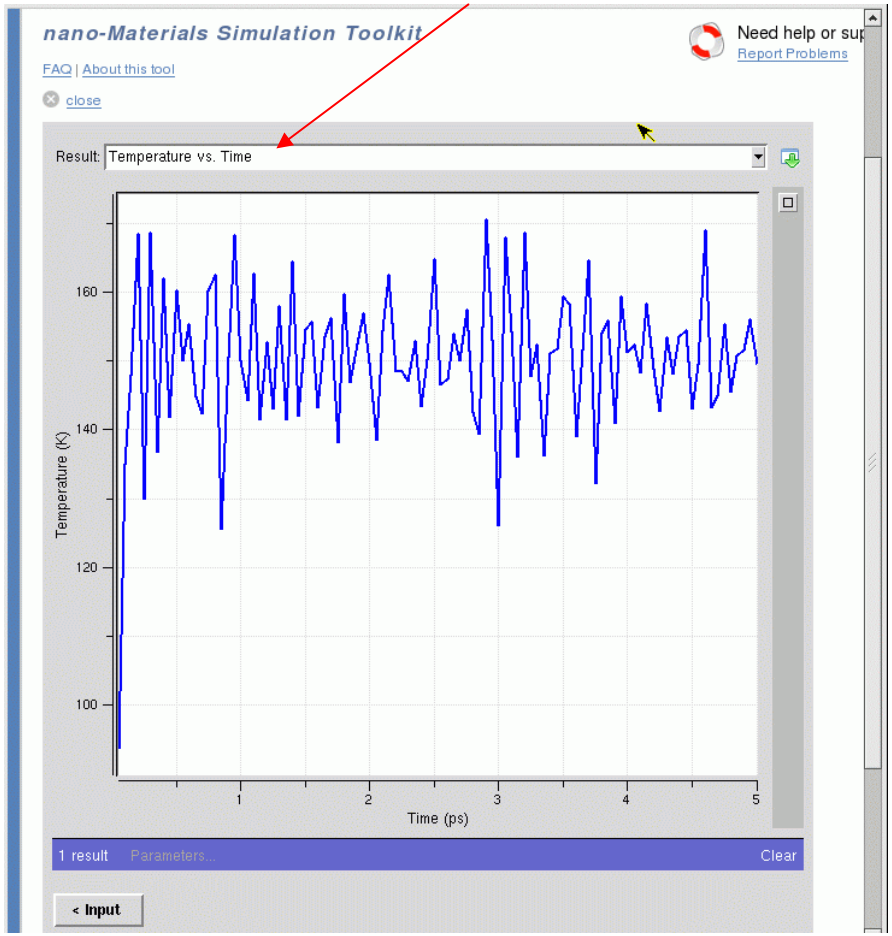
Write a frame in the trajectory every 250 MD steps

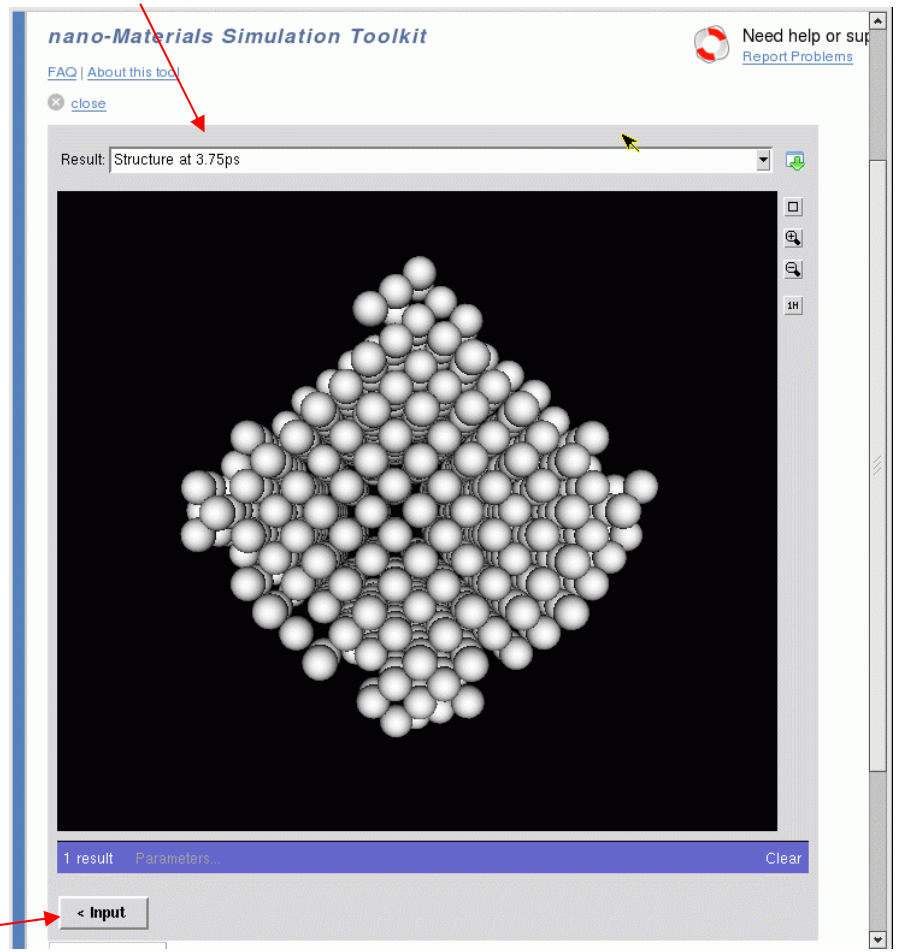
Run simulation



nanoMATERIALS: simulation results

Select the output to visualize (plots or snapshots)



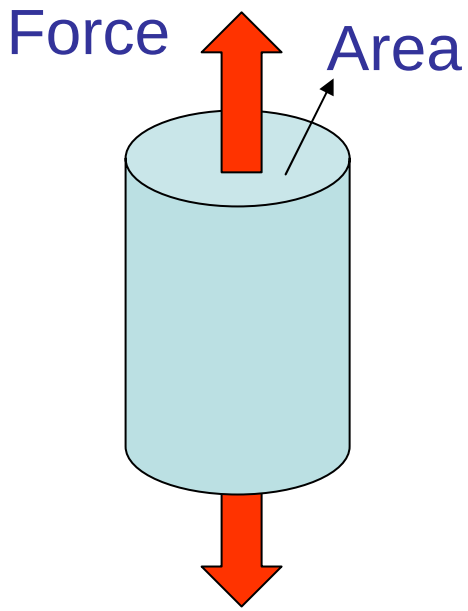


Back to input panels

Q: Why is the temperature about half of the input value?

Elements of Deformation & Failure

- Elastic deformation
  - Recoverable (if load is removed material goes back to original length)
  - Strain is proportional to strain
- Plastic deformation
  - Permanent shape change even after load is deformed
  - Material changed – atomic level rearrangement of neighbors
- Failure
  - Material separates in two
  - It usually follows “necking”



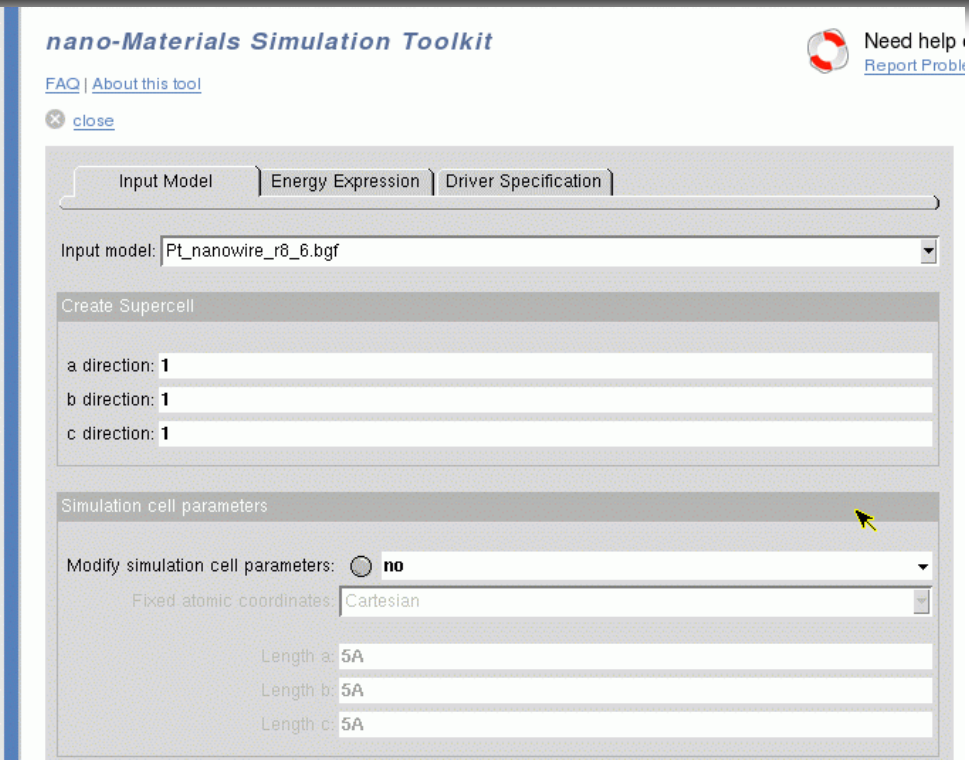
$$\text{Stress} = \frac{\text{Force}}{\text{Area}}$$

Length

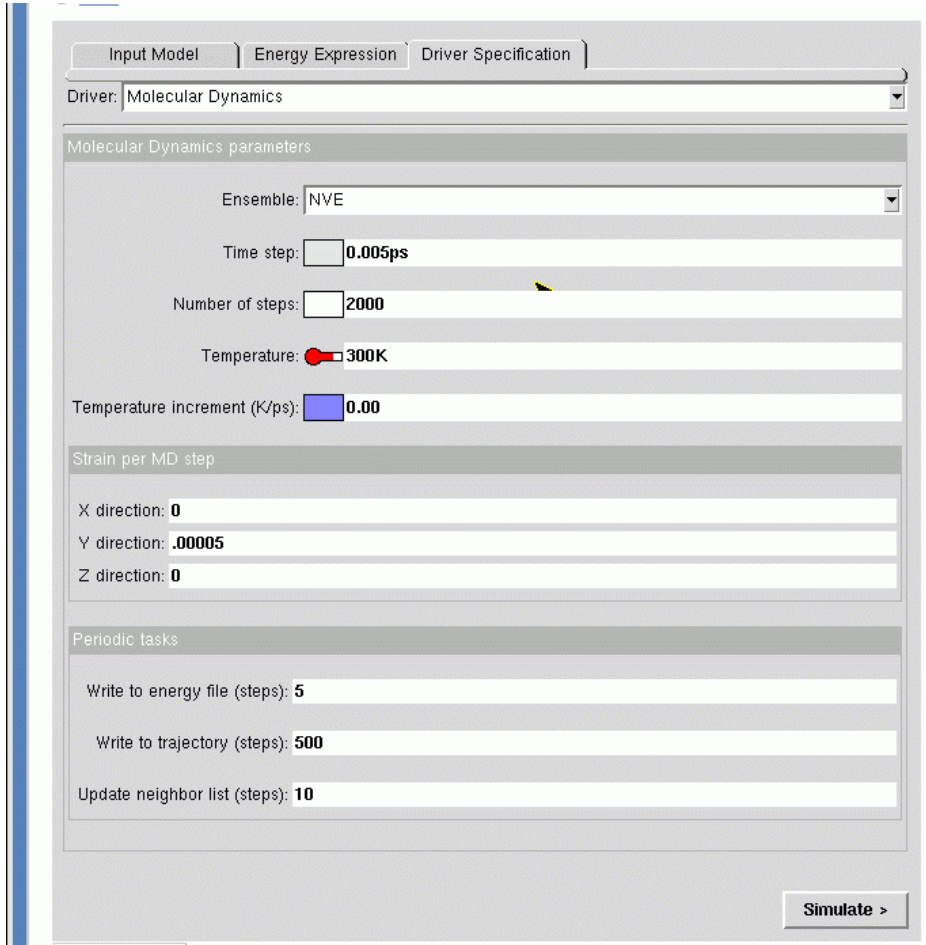
Original length

$$\text{Strain} = \frac{L - L_0}{L_0}$$

Non-equilibrium MD: deforming a material



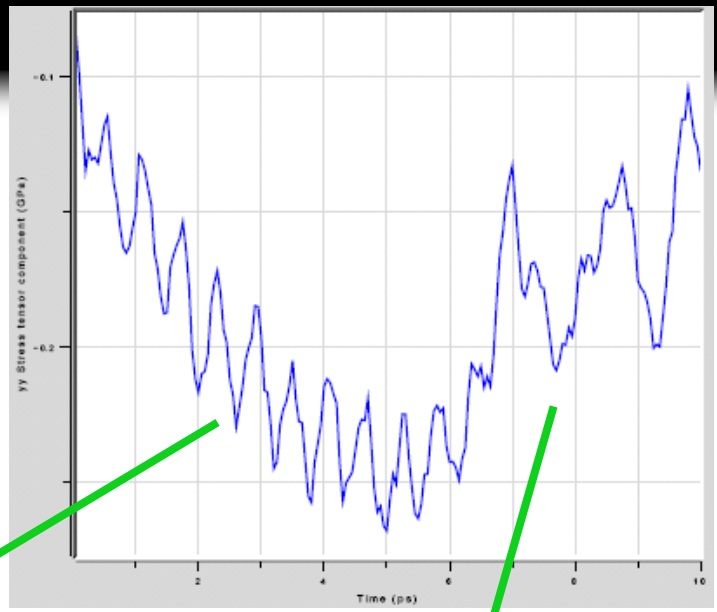
- Select model Pt_nanowire_r8_6
- NO SUPERCELL (1 1 1)

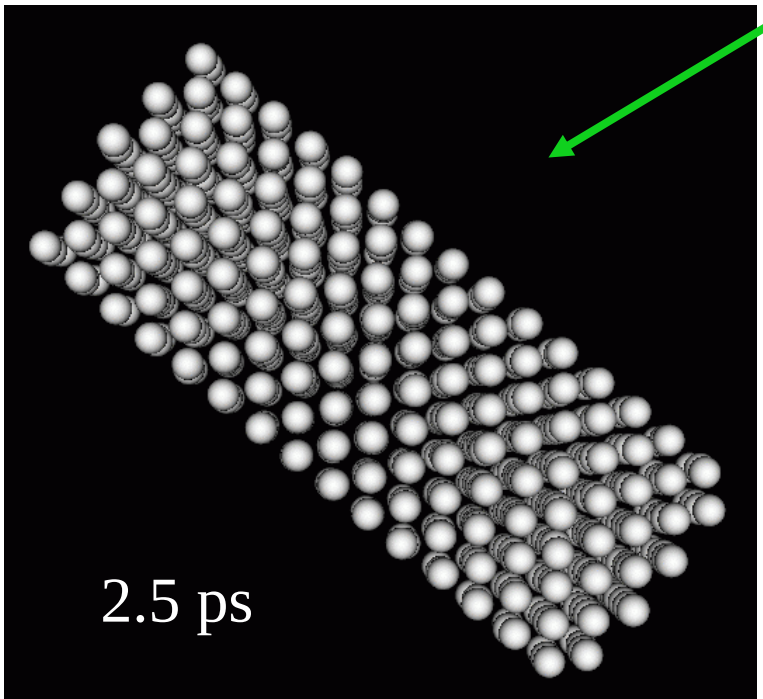


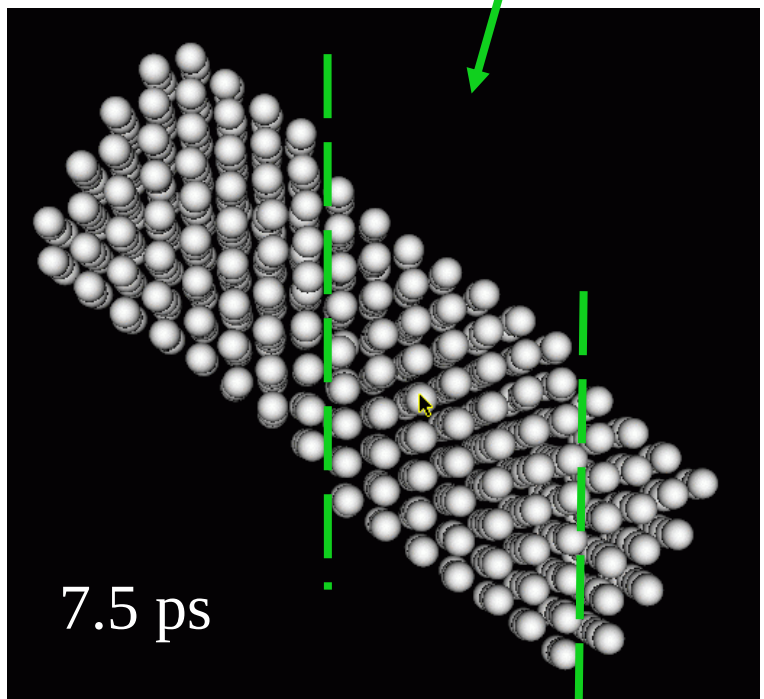
- Set to NVE
- Strain along the axis of the wire: 0.00005 (per step)

Results

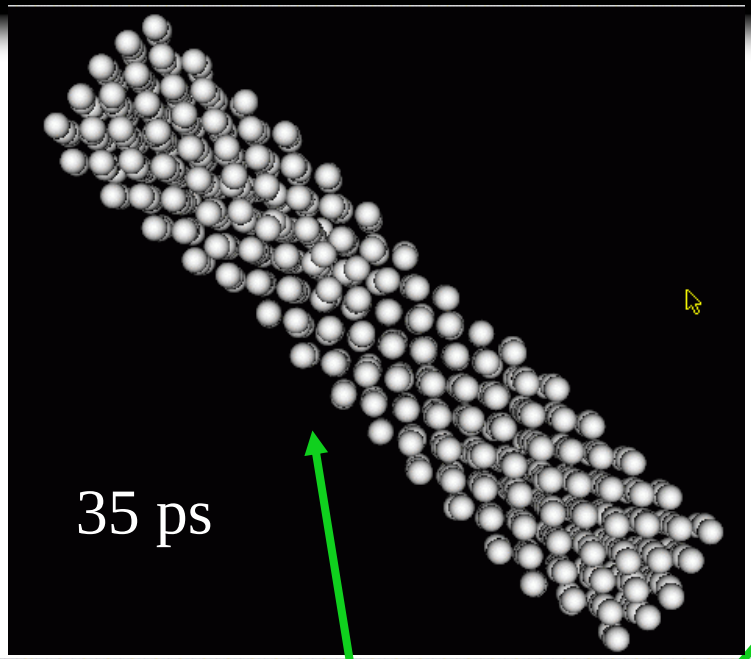
Elastic region up to about 5 ps
Plastic deformation leads to significant stress relaxation

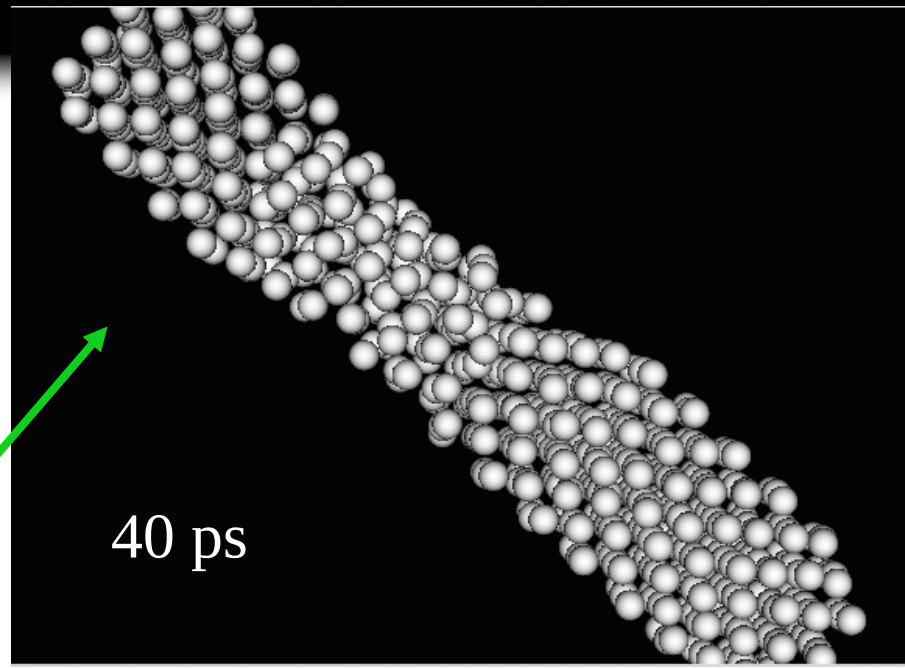


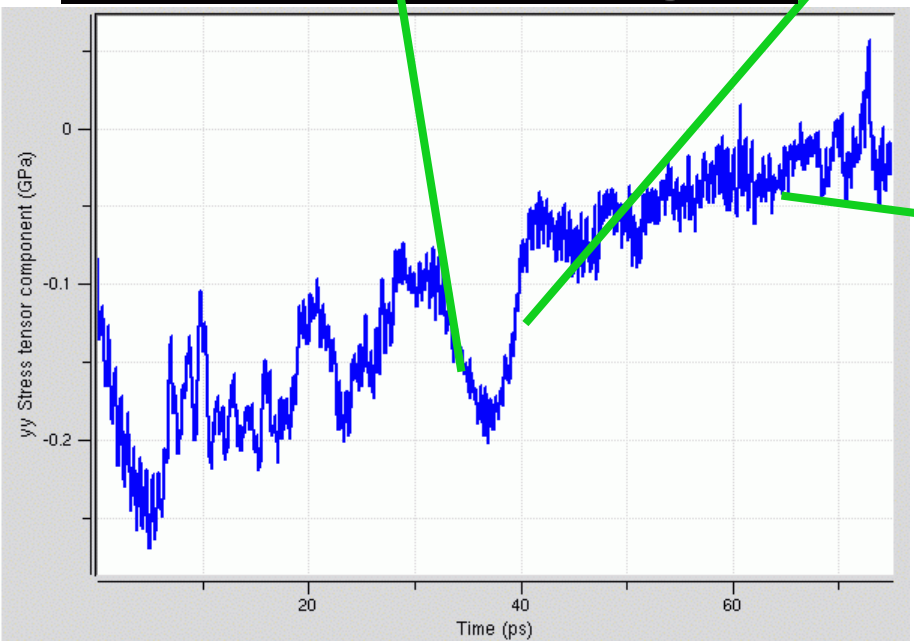


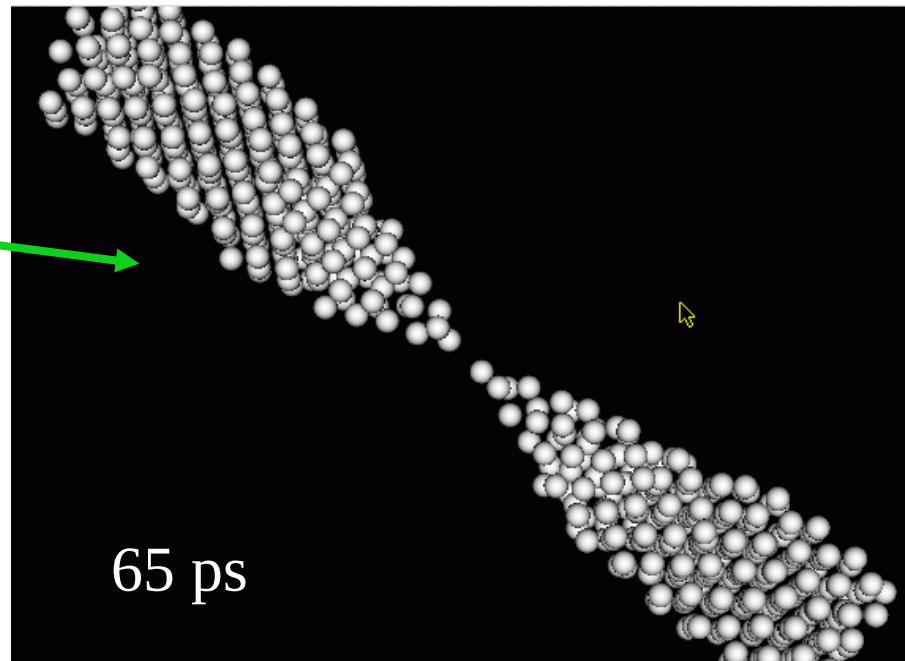


Results

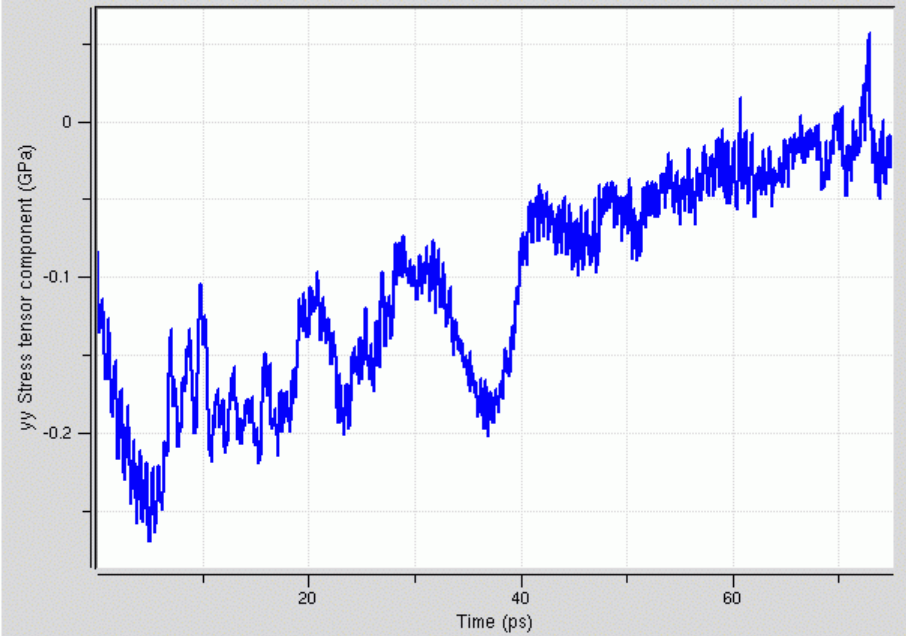

35 ps


40 ps


yy Stress tensor component (GPa)
0
-0.1
-0.2
20
40
60
Time (ps)


65 ps

Results



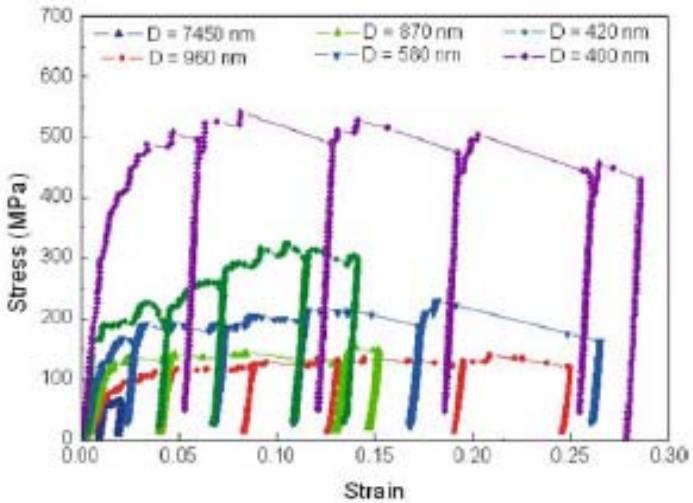


FIGURE 3 Stress–strain behavior of {001}-oriented pillars produced with a FIB: flow stresses increase significantly for pillars with the diameter of 500 nm or less

Gold nano-rods
Nix and collaborators, 2005

Suggested additional exercises

- What is the role of strain rate?
  - Half the strain per step and double the number of MD steps
  - Compare yield stress & maximum elongation
- Repeat for nano-wires with different sizes
  - Wires with radius 10.8 and 13 Å
  - Compare yield stress and maximum elongation

Note: there is a maximum allocated time and size for the simulations