1.021, 3.021, 10.333, 22.00 Introduction to Modeling and Simulation
Spring 2018

Recitation #2

nanoHUB and Visual Molecular Dynamics
Nanowire Tensile Deformation Lab

Recitation instructor: Francisco Martin-Martinez

email: fmartinm@mit.edu

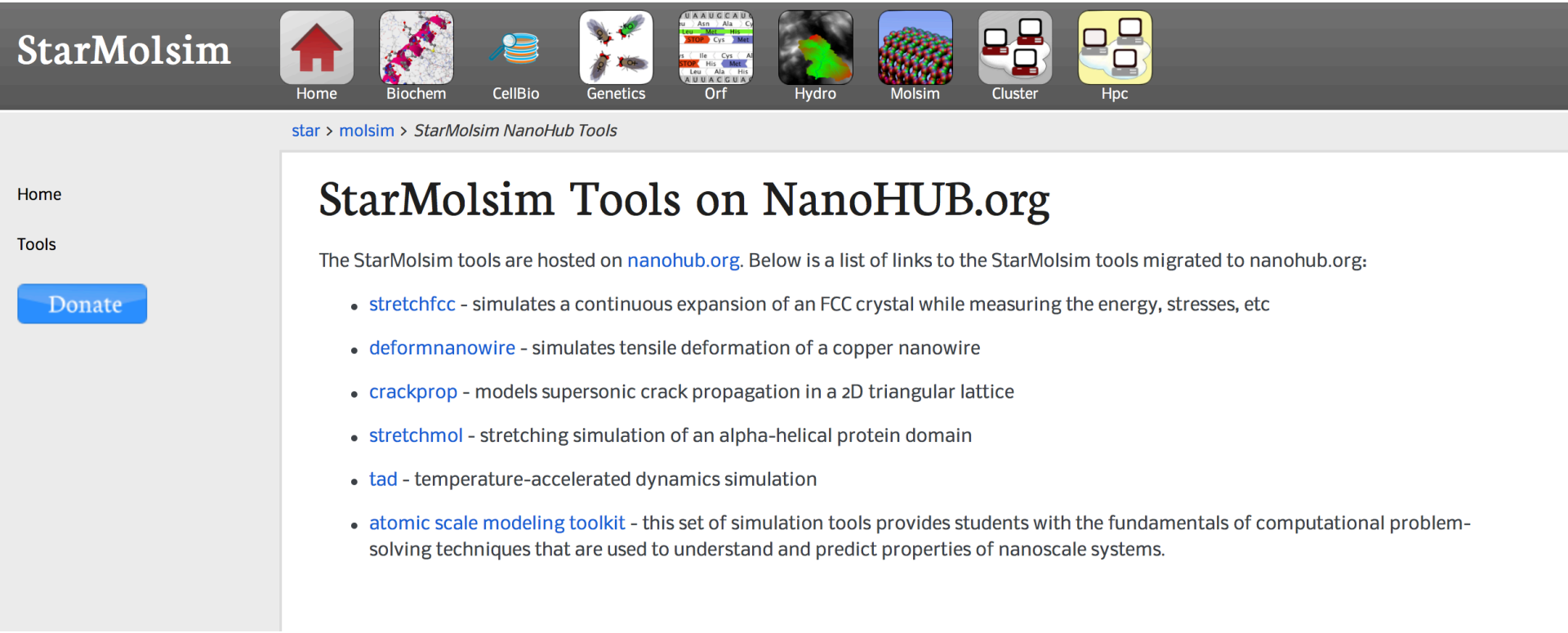
Massachusetts Institute of Technology

Review from last week

- Working groups for Psets
- Checking on VMD installation and nanoHUB configuration.
- Review on basics concepts on Molecular Dynamics
- QM vs MD simulations
- Questions?

Getting to work with nanoHUB and VMD: Nanowire Tensile Deformation Lab

Simulation index (MIT tools for IM/S):
http://star.mit.edu/molsim/nanohub/index.html



https://nanohub.org/tools/deformnanowire

Nanowire Tensile Deformation Lab

By Markus Buehler[1], Justin Riley[1], Joo-Hyoung Lee, Jeffrey C Grossman[2]

1. Massachusetts Institute of Technology (MIT) 2. Massachusetts Institute of Technology

Simulates tensile deformation of a copper nanowire

Launch Tool

Version 1.8 published on 03 Sep 2014

doi:10.4231/D3901ZG81 cite this

View All Supporting Documents

Tool Audience Unrated

36 users, detailed usage

0 Citation(s)

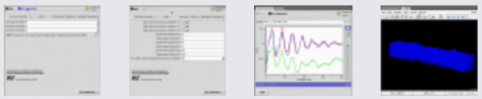
0 questions (Ask a question)

0 review(s) (Review this)

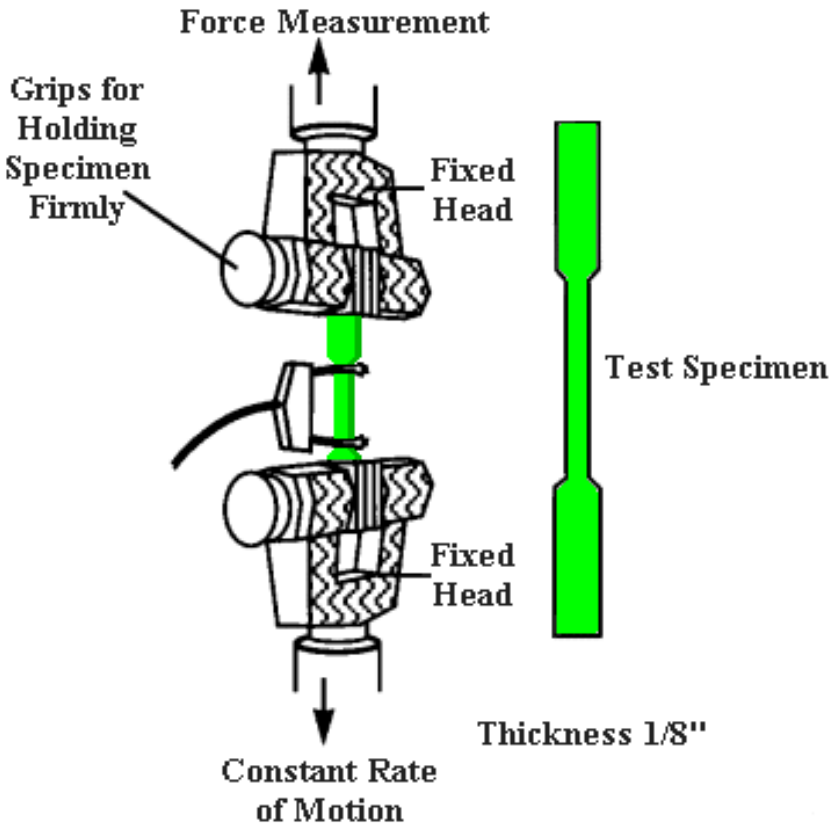
0 wish(es) (New Wish)

Share: ...

About | Usage | Citations | Questions | Reviews | Wishlist | Versions | Supporting Docs

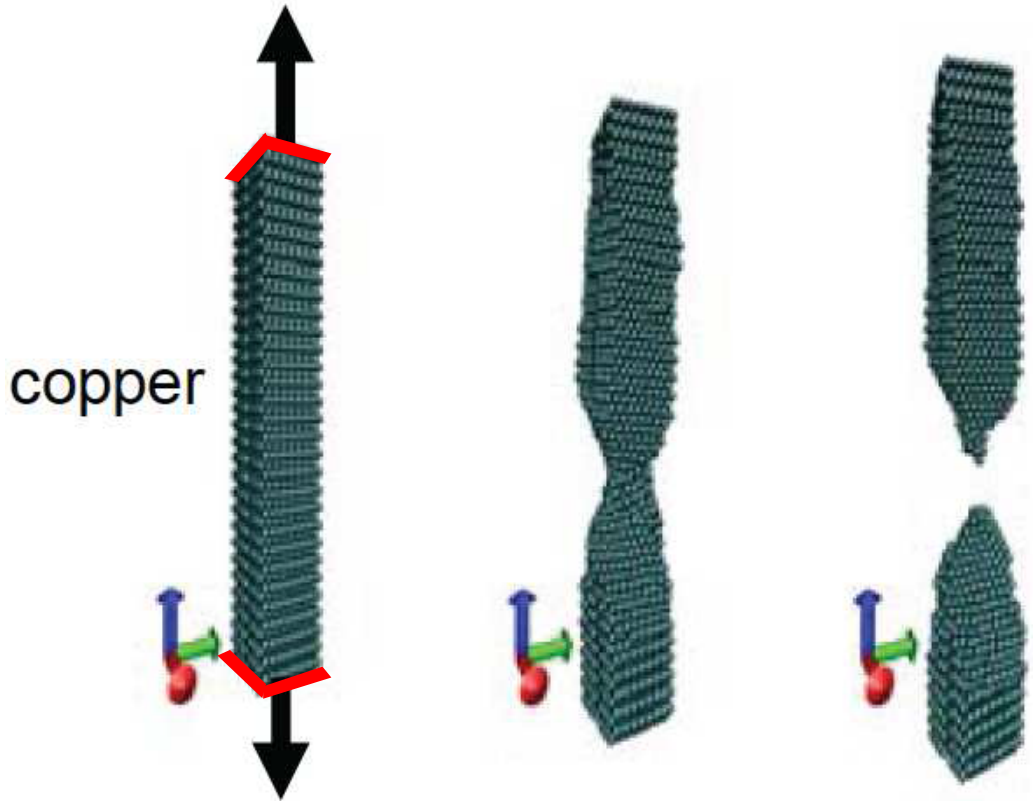


Real experiment



Our simulation

Some atoms at boundary clamped (move in a prescribed way)



Our quick note on units

In the molecular modeling code:

Reference **length** is l* = 1 A˚ = 1E-10 m

Reference **energy** is E* = 1 eV (Amount of energy gained by an electron moved across an electric potential difference of one volt)

Reference **mass** m* = 1 a.m.u. (1/12 the mass of an atom of carbon-12)

All input and output from the simulation code is expressed in these units.

e.g.,

$P^* = [\text{Force}]/[\text{Length}]^2 = [\text{Energy}]/[\text{Length}]/[\text{Length}]^2 = E^*/l^{*3} = \text{eV/A}^{\circ 3}$

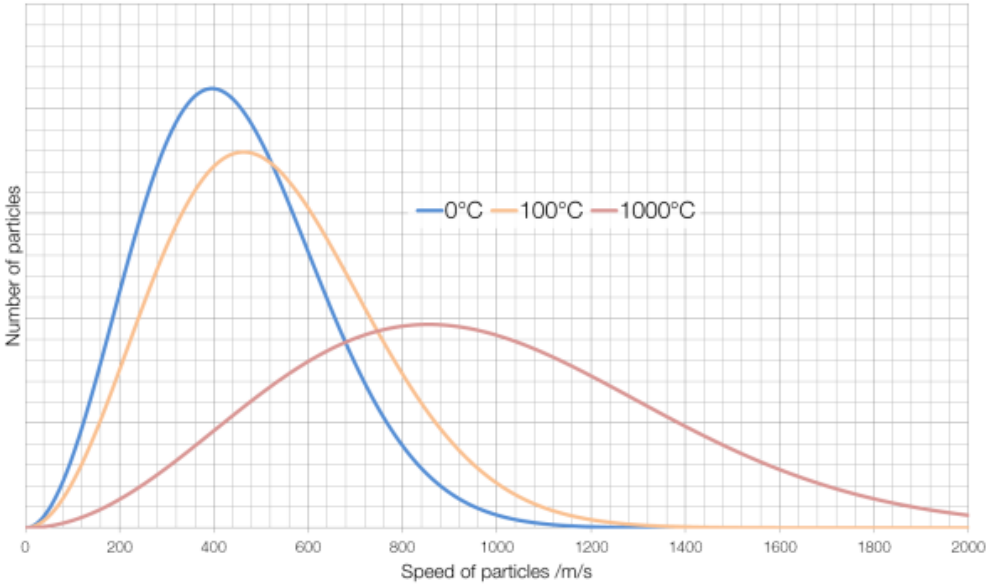
$1\ \text{eV/A}^{\circ 3} = 160.2\ \text{GPa}$

Units of Temperature

Temperature: average kinetic energy of all the particles in a system.

The velocities (kinetic energy) follow a Maxwell–Boltzmann distribution

We can use units of Energy for Temperature, if we know the relationship between them: the Boltzmann constant

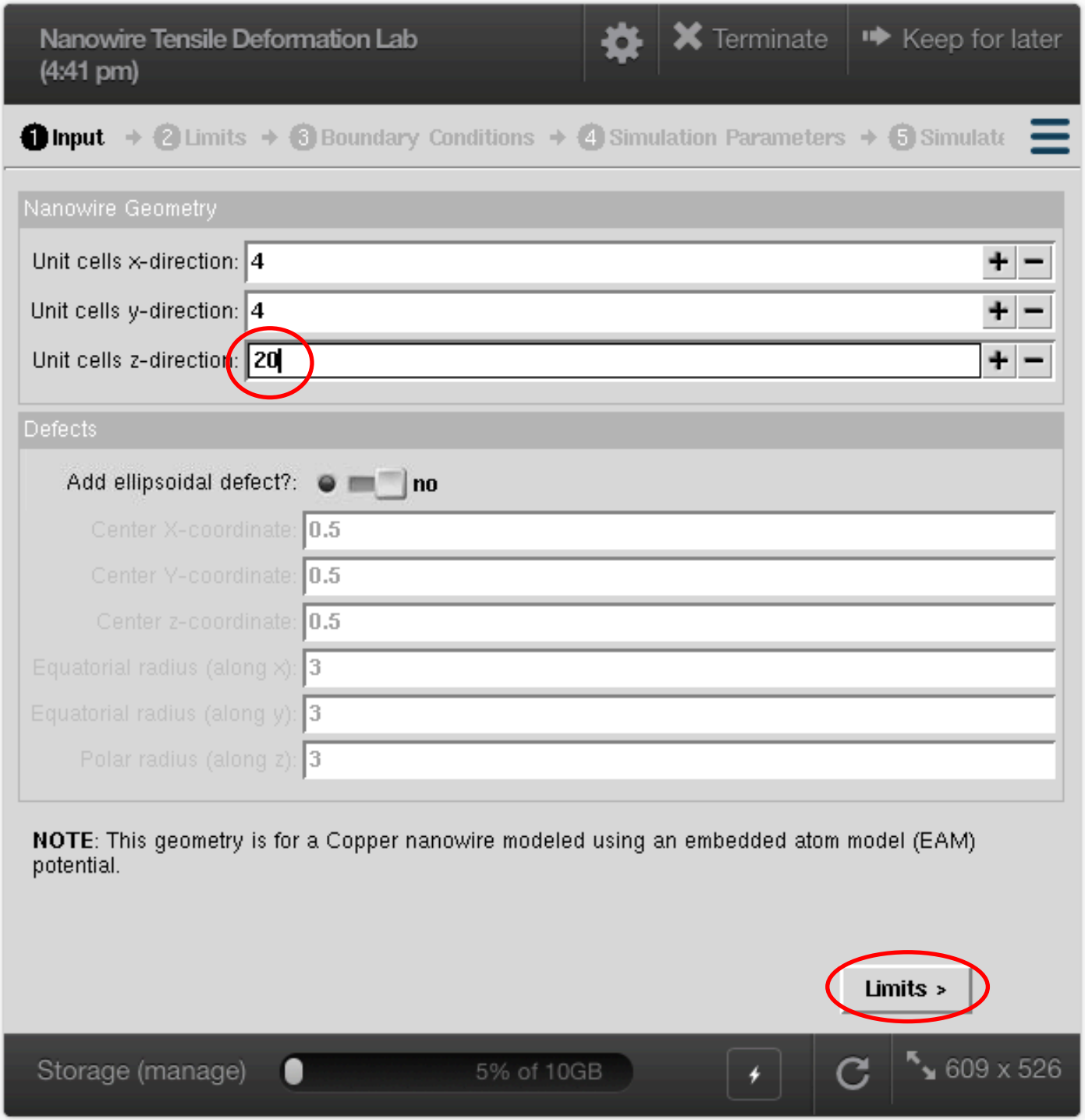


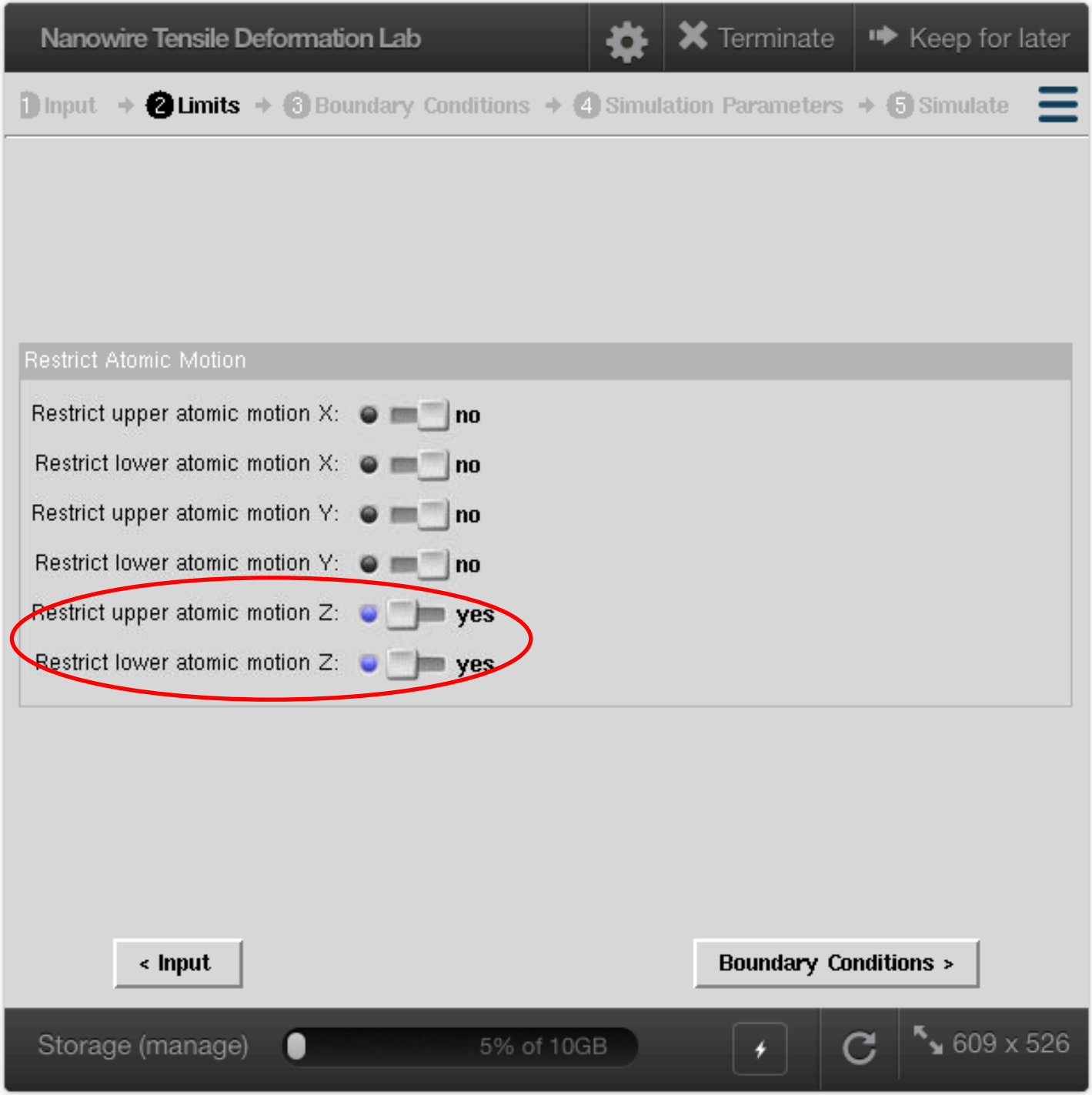
$$E = K_B T$$

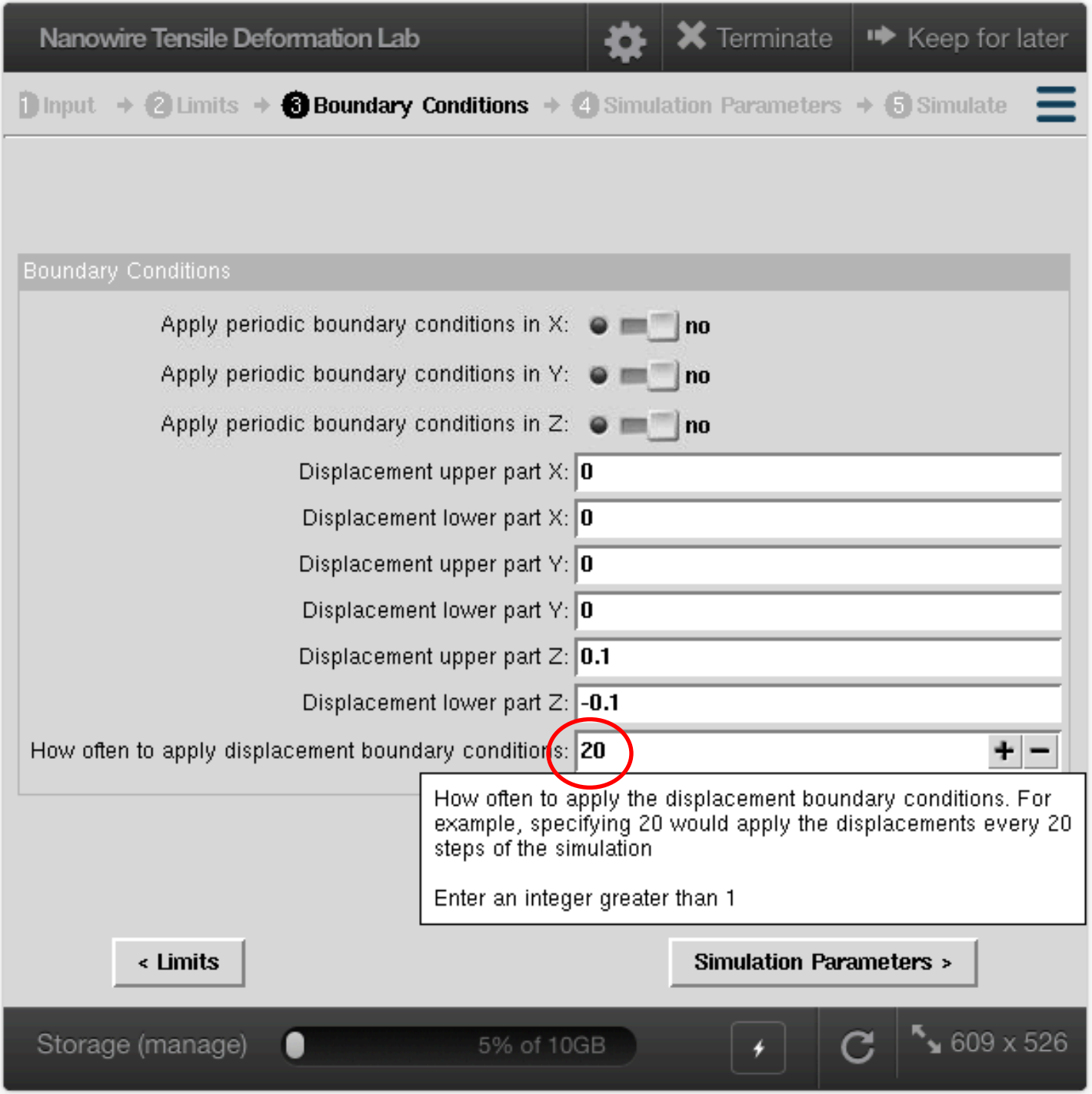
$K_B = 1.38064852 \times 10^{-23}$ J K^{-1}

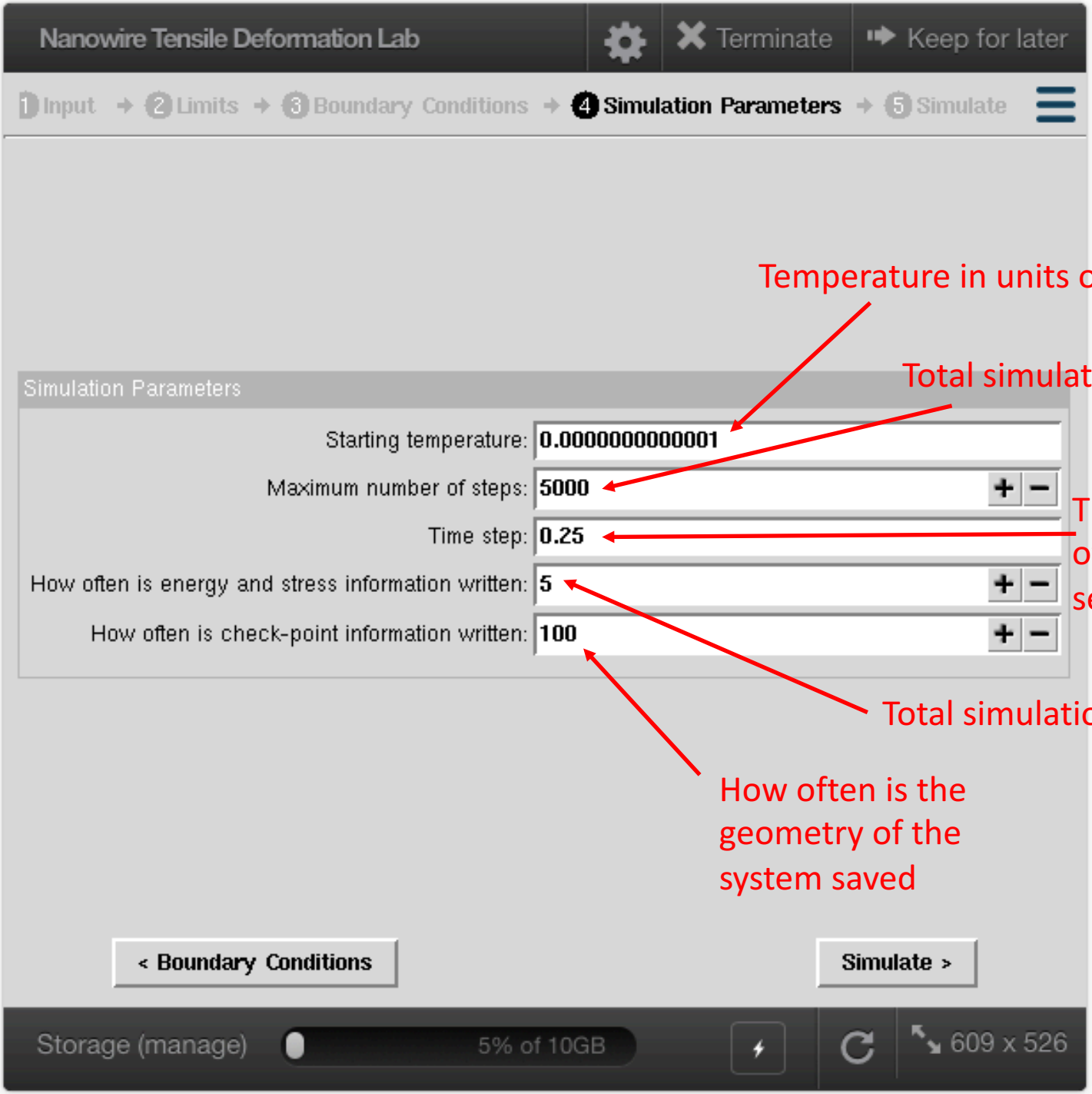
Our units of temperature are eV (based on a Maxwell–Boltzmann distribution).

$T^* = [\text{Energy}]/K_B = E^*/K_B = \text{eV}/K_B = 1.6022\times10\text{-}19 \text{ J}/(1.3806\times10\text{-}23 \text{ J/K}) = 11605\text{K}$

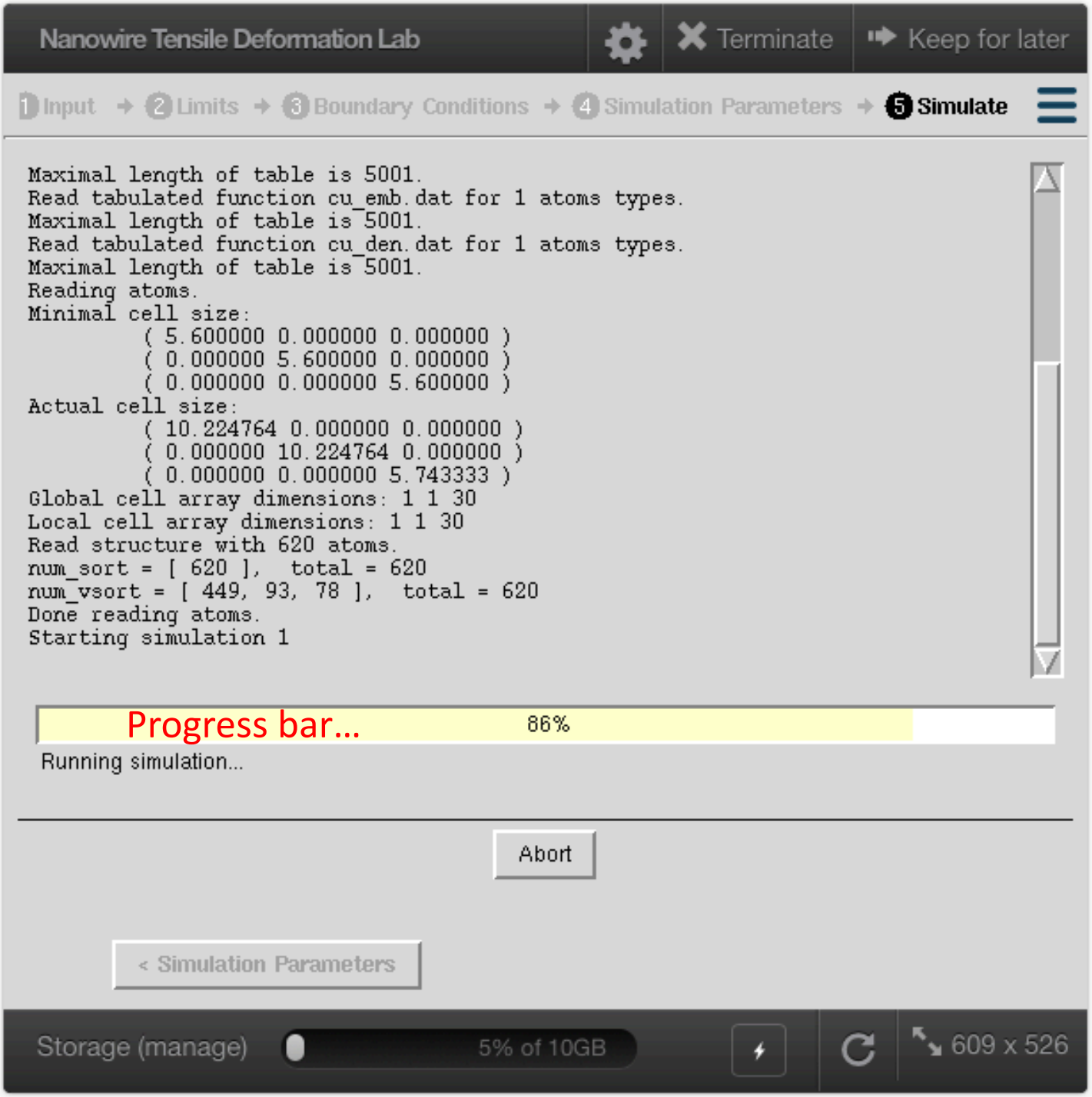

Nanowire Tensile Deformation Lab
(4:41 pm)
Terminate
Keep for later
1 Input
2 Limits
3 Boundary Conditions
4 Simulation Parameters
5 Simulate
Nanowire Geometry
Unit cells x-direction: 4
Unit cells y-direction: 4
Unit cells z-direction: 20
Defects
Add ellipsoidal defect?: no
Center X-coordinate: 0.5
Center Y-coordinate: 0.5
Center z-coordinate: 0.5
Equatorial radius (along x): 3
Equatorial radius (along y): 3
Polar radius (along z): 3
NOTE: This geometry is for a Copper nanowire modeled using an embedded atom model (EAM) potential.
Limits »
Storage (manage)
5% of 10GB
609 x 526

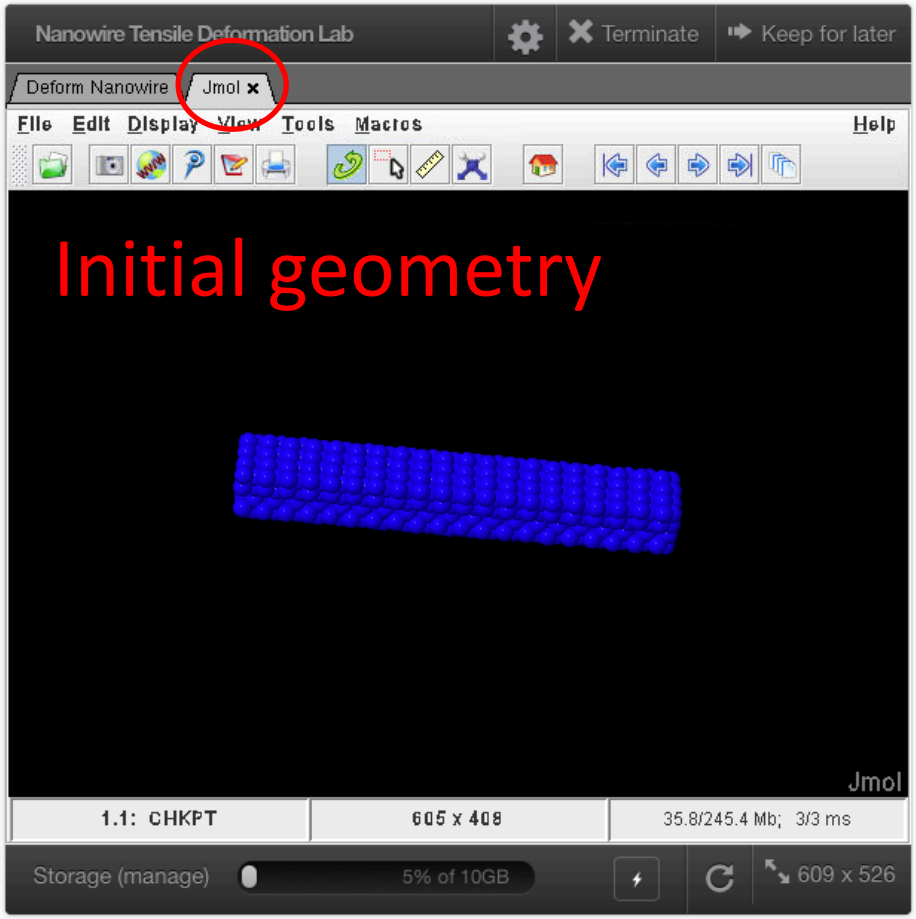

Nanowire Tensile Deformation Lab
Terminate
Keep for later
1 Input
2 Limits
3 Boundary Conditions
4 Simulation Parameters
5 Simulate
Restrict Atomic Motion
Restrict upper atomic motion X: no
Restrict lower atomic motion X: no
Restrict upper atomic motion Y: no
Restrict lower atomic motion Y: no
Restrict upper atomic motion Z: yes
Restrict lower atomic motion Z: yes
< Input
Boundary Conditions >
Storage (manage)
5% of 10GB
609 x 526

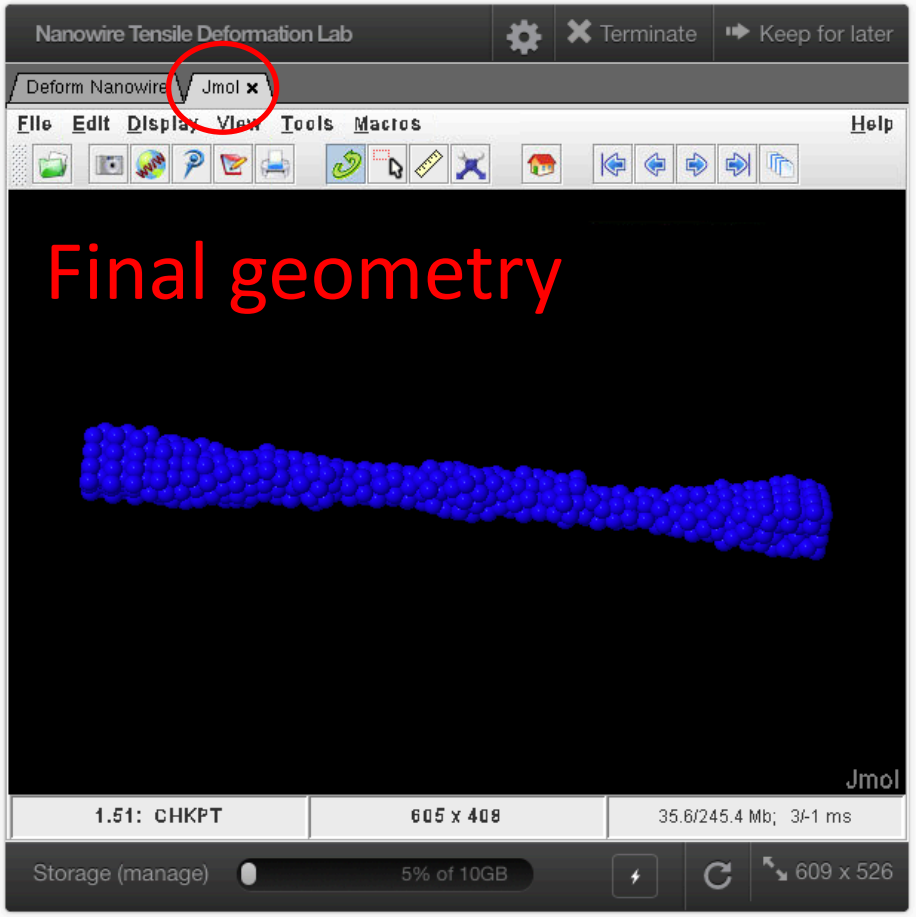

Nanowire Tensile Deformation Lab
Terminate
Keep for later
1 Input
2 Limits
3 Boundary Conditions
4 Simulation Parameters
5 Simulate
Boundary Conditions
Apply periodic boundary conditions in X: no
Apply periodic boundary conditions in Y: no
Apply periodic boundary conditions in Z: no
Displacement upper part X: 0
Displacement lower part X: 0
Displacement upper part Y: 0
Displacement lower part Y: 0
Displacement upper part Z: 0.1
Displacement lower part Z: -0.1
How often to apply displacement boundary conditions: 20
How often to apply the displacement boundary conditions. For example, specifying 20 would apply the displacements every 20 steps of the simulation
Enter an integer greater than 1
< Limits
Simulation Parameters >
Storage (manage)
5% of 10GB
609 x 526

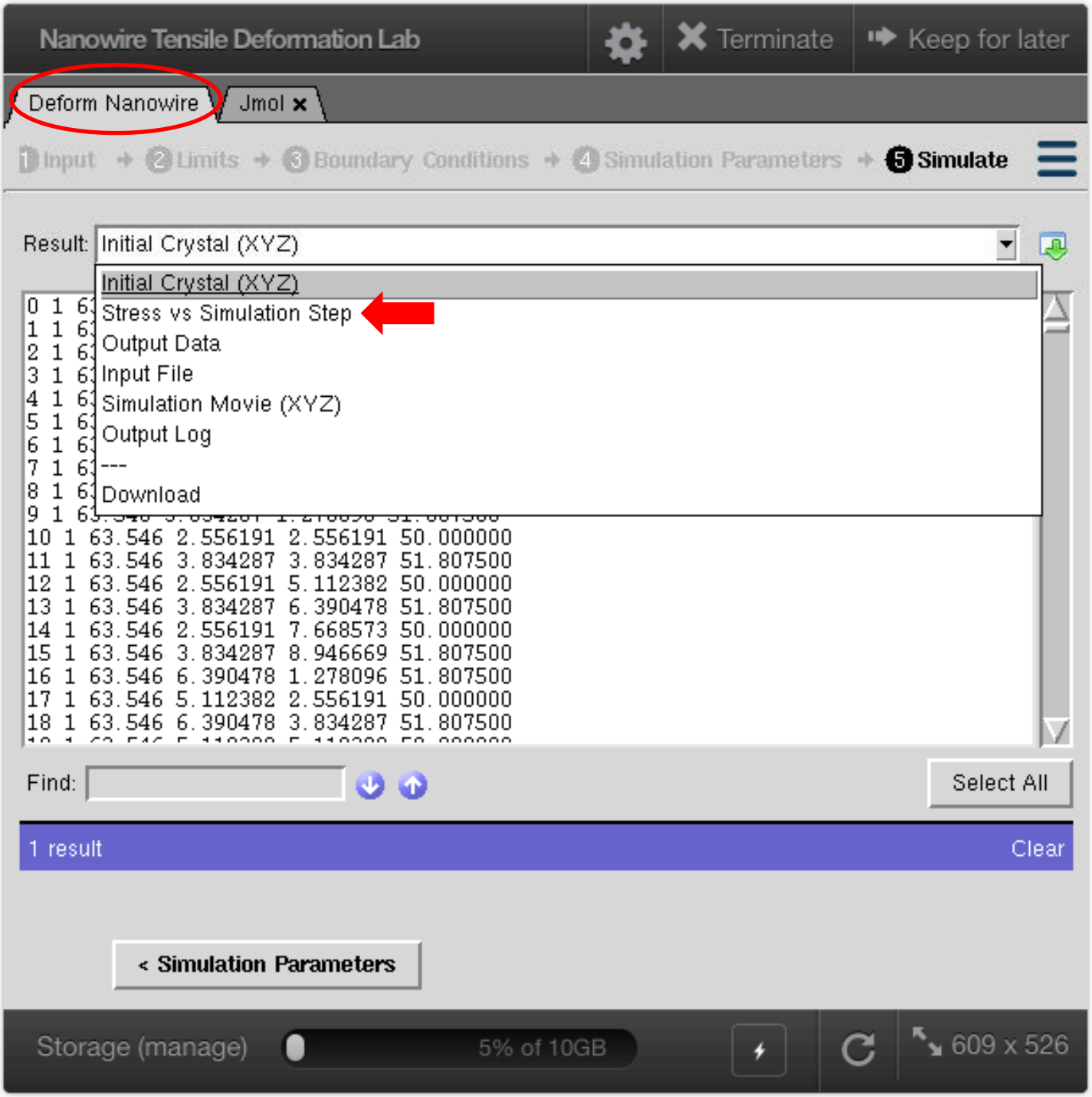

Nanowire Tensile Deformation Lab
Terminate
Keep for later
1 Input
2 Limits
3 Boundary Conditions
4 Simulation Parameters
5 Simulate
Simulation Parameters
Starting temperature: 0.0000000000001
Maximum number of steps: 5000
Time step: 0.25
How often is energy and stress information written: 5
How often is check-point information written: 100
< Boundary Conditions
Simulate >
Storage (manage)
5% of 10GB
609 x 526
Temperature in units of 11600K
Total simulations steps
Time in units of 1.014E-14 seconds
Total simulations steps
How often is the geometry of the system saved

Code output


Nanowire Tensile Deformation Lab
Terminate
Keep for later
1 Input
2 Limits
3 Boundary Conditions
4 Simulation Parameters
5 Simulate
Maximal length of table is 5001.
Read tabulated function cu_emb.dat for 1 atoms types.
Maximal length of table is 5001.
Read tabulated function cu_den.dat for 1 atoms types.
Maximal length of table is 5001.
Reading atoms.
Minimal cell size:
(5.600000 0.000000 0.000000)
(0.000000 5.600000 0.000000)
(0.000000 0.000000 5.600000)
Actual cell size:
(10.224764 0.000000 0.000000)
(0.000000 10.224764 0.000000)
(0.000000 0.000000 5.743333)
Global cell array dimensions: 1 1 30
Local cell array dimensions: 1 1 30
Read structure with 620 atoms.
num_sort = [620], total = 620
num_vsort = [449, 93, 78], total = 620
Done reading atoms.
Starting simulation 1
Progress bar...
86%
Running simulation...
Abort
< Simulation Parameters
Storage (manage)
5% of 10GB
609 x 526

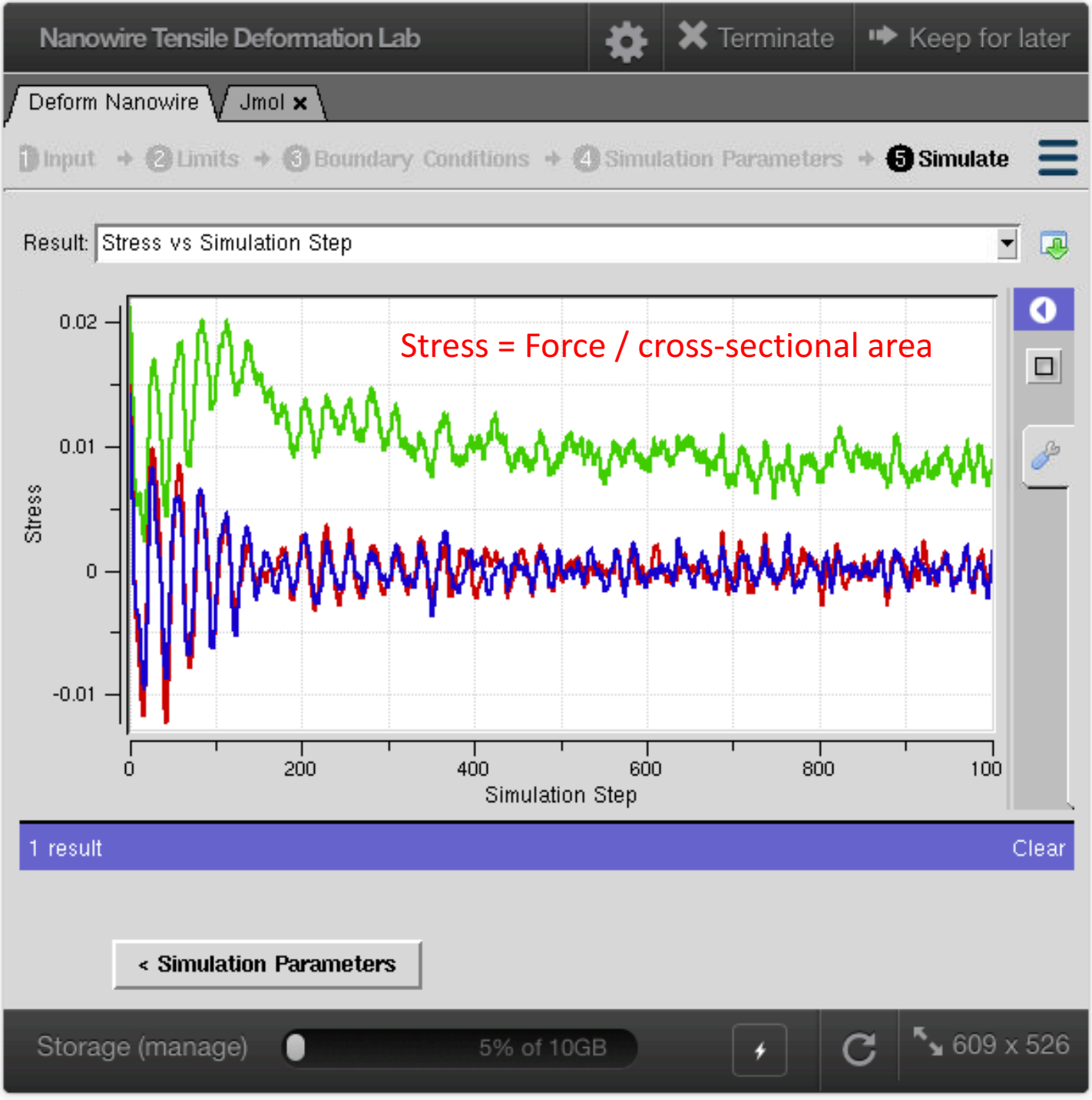

Nanowire Tensile Deformation Lab
Terminate
Keep for later
Deform Nanowire
Jmol
File Edit Display View Tools Macros Help
Initial geometry
Jmol
1.1: CHKPT
605 x 408
35.8/245.4 Mb; 3/3 ms
Storage (manage)
5% of 10GB
609 x 526

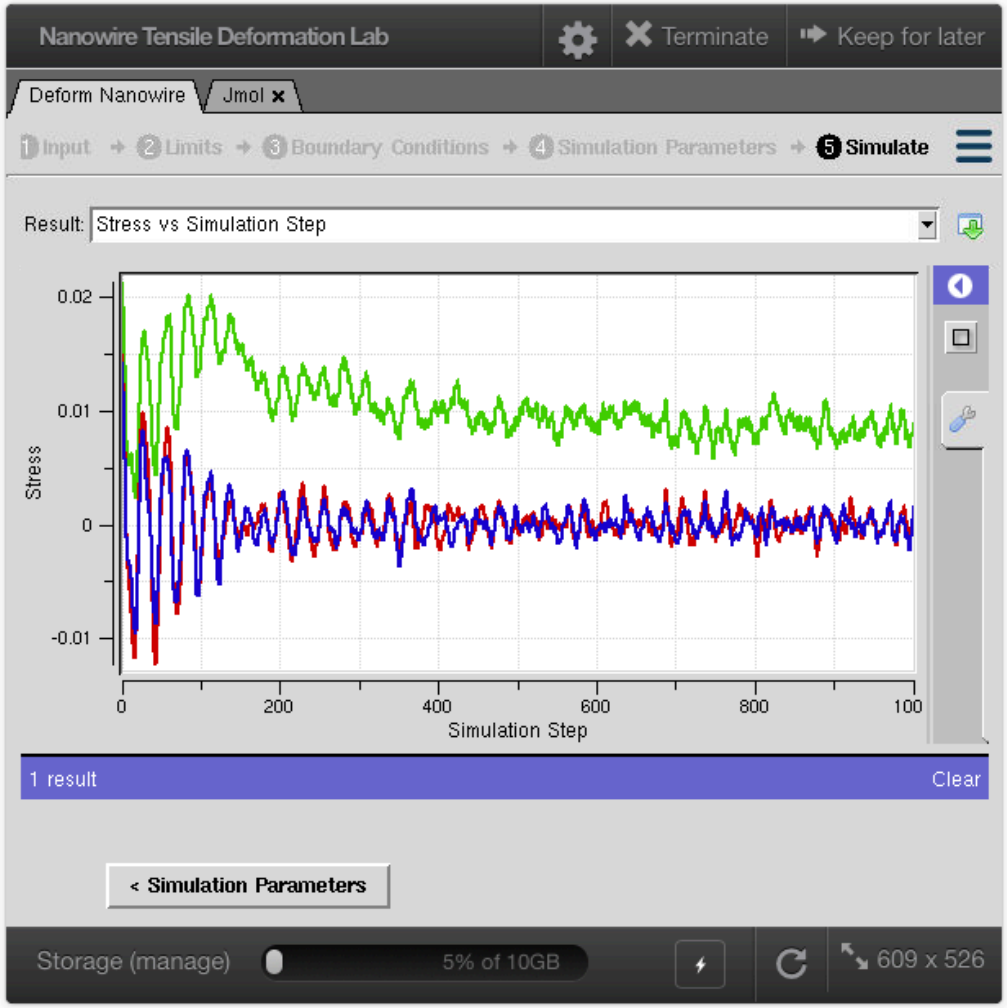

Nanowire Tensile Deformation Lab
Terminate
Keep for later
Deform Nanowire
Jmol
File Edit Display View Tools Macros Help
Final geometry
Jmol
1.51: CHKPT
605 x 408
35.6/245.4 Mb; 3/-1 ms
Storage (manage)
5% of 10GB
609 x 526

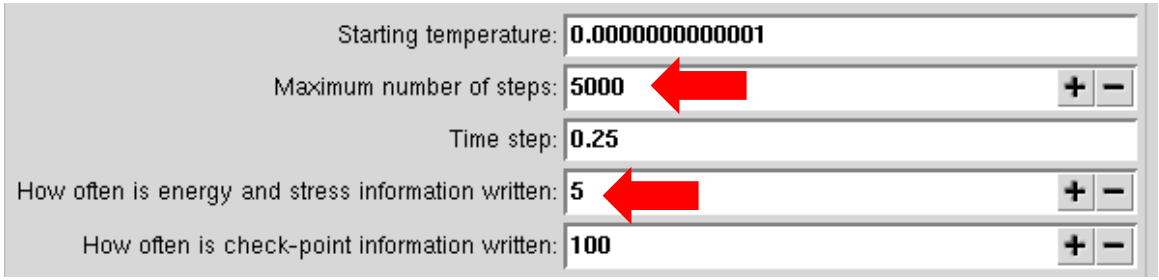

Nanowire Tensile Deformation Lab
Terminate
Keep for later
Deform Nanowire
Jmol
1 Input
2 Limits
3 Boundary Conditions
4 Simulation Parameters
5 Simulate
Result:
Initial Crystal (XYZ)
Initial Crystal (XYZ)
Stress vs Simulation Step
Output Data
Input File
Simulation Movie (XYZ)
Output Log

Download
10 1 63.546 2.556191 2.556191 50.000000
11 1 63.546 3.834287 3.834287 51.807500
12 1 63.546 2.556191 5.112382 50.000000
13 1 63.546 3.834287 6.390478 51.807500
14 1 63.546 2.556191 7.668573 50.000000
15 1 63.546 3.834287 8.946669 51.807500
16 1 63.546 6.390478 1.278096 51.807500
17 1 63.546 5.112382 2.556191 50.000000
18 1 63.546 6.390478 3.834287 51.807500
Find:
Select All
1 result
Clear
< Simulation Parameters
Storage (manage)
5% of 10GB
609 x 526

Stress – Deformation data

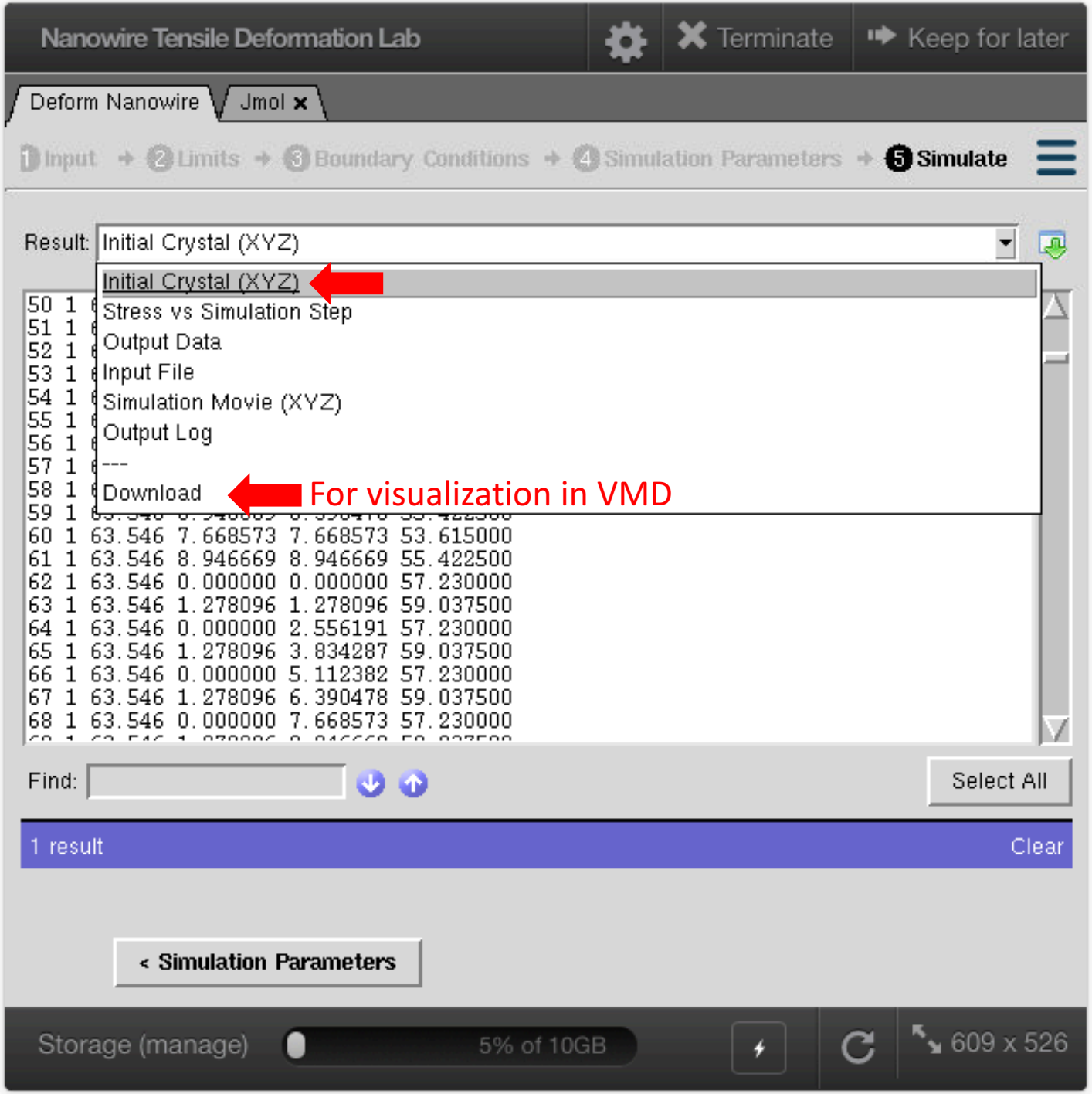




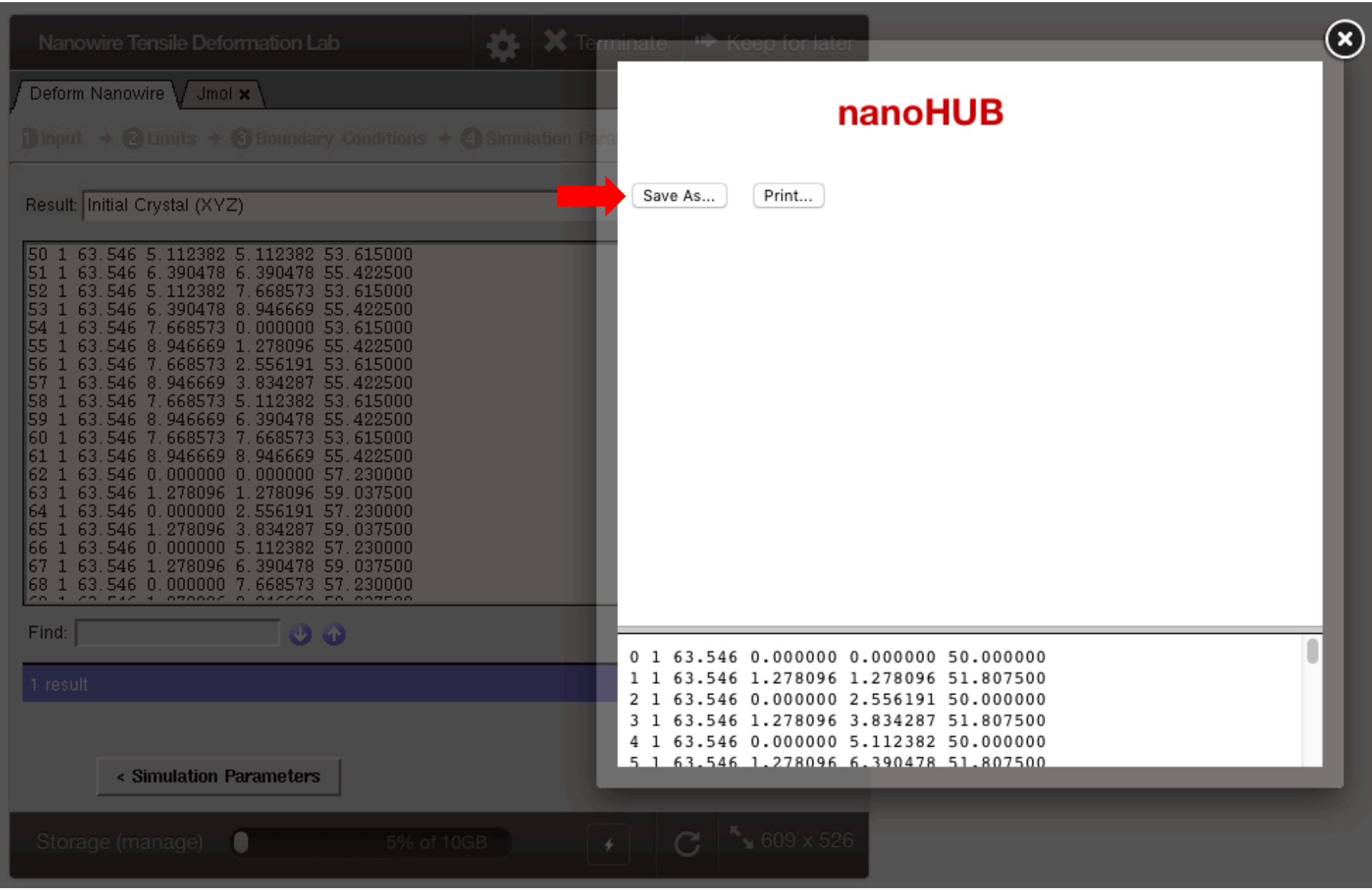


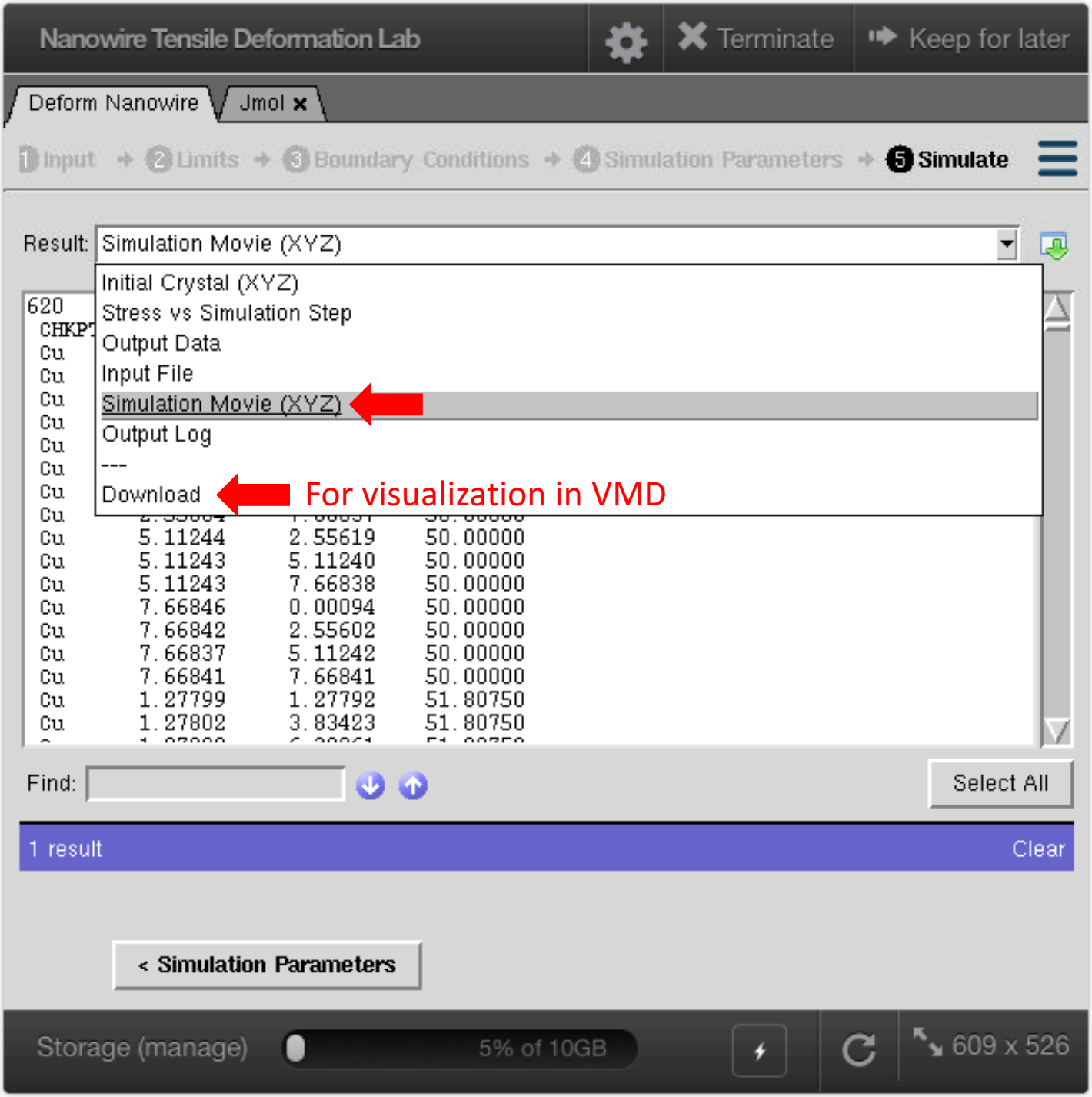
Simulation step = # of iterations written

HERE: 5000 steps, written every 5 steps, a total of 1000 iterations written


Nanowire Tensile Deformation Lab
Terminate
Keep for later
Deform Nanowire
Jmol
1 Input
2 Limits
3 Boundary Conditions
4 Simulation Parameters
5 Simulate
Result:
Initial Crystal (XYZ)
Initial Crystal (XYZ)
Stress vs Simulation Step
Output Data
Input File
Simulation Movie (XYZ)
Output Log

Download
For visualization in VMD
50 1 6
51 1 6
52 1 6
53 1 6
54 1 6
55 1 6
56 1 6
57 1 6
58 1 6
59 1
60 1 63.546 7.668573 7.668573 53.615000
61 1 63.546 8.946669 8.946669 55.422500
62 1 63.546 0.000000 0.000000 57.230000
63 1 63.546 1.278096 1.278096 59.037500
64 1 63.546 0.000000 2.556191 57.230000
65 1 63.546 1.278096 3.834287 59.037500
66 1 63.546 0.000000 5.112382 57.230000
67 1 63.546 1.278096 6.390478 59.037500
68 1 63.546 0.000000 7.668573 57.230000
Find:
Select All
1 result
Clear
< Simulation Parameters
Storage (manage)
5% of 10GB
609 x 526


Nanowire Tensile Deformation Lab
Terminate
Keep for later
Deform Nanowire
Jmol
1 Input
2 Limits
3 Boundary Conditions
4 Simulation Para
Result:
Initial Crystal (XYZ)
50 1 63.546 5.112382 5.112382 53.615000
51 1 63.546 6.390478 6.390478 55.422500
52 1 63.546 5.112382 7.668573 53.615000
53 1 63.546 6.390478 8.946669 55.422500
54 1 63.546 7.668573 0.000000 53.615000
55 1 63.546 8.946669 1.278096 55.422500
56 1 63.546 7.668573 2.556191 53.615000
57 1 63.546 8.946669 3.834287 55.422500
58 1 63.546 7.668573 5.112382 53.615000
59 1 63.546 8.946669 6.390478 55.422500
60 1 63.546 7.668573 7.668573 53.615000
61 1 63.546 8.946669 8.946669 55.422500
62 1 63.546 0.000000 0.000000 57.230000
63 1 63.546 1.278096 1.278096 59.037500
64 1 63.546 0.000000 2.556191 57.230000
65 1 63.546 1.278096 3.834287 59.037500
66 1 63.546 0.000000 5.112382 57.230000
67 1 63.546 1.278096 6.390478 59.037500
68 1 63.546 0.000000 7.668573 57.230000
Find:
1 result
< Simulation Parameters
Storage (manage)
5% of 10GB
609 x 526
nanoHUB
Save As...
Print...
0 1 63.546 0.000000 0.000000 50.000000
1 1 63.546 1.278096 1.278096 51.807500
2 1 63.546 0.000000 2.556191 50.000000
3 1 63.546 1.278096 3.834287 51.807500
4 1 63.546 0.000000 5.112382 50.000000
5 1 63.546 1.278096 6.390478 51.807500


Nanowire Tensile Deformation Lab
Terminate
Keep for later
Deform Nanowire
Jmol
1 Input
2 Limits
3 Boundary Conditions
4 Simulation Parameters
5 Simulate
Result:
Simulation Movie (XYZ)
Initial Crystal (XYZ)
Stress vs Simulation Step
Output Data
Input File
Simulation Movie (XYZ)
Output Log

Download
For visualization in VMD
620
CHKPT
Cu 5.11244 2.55619 50.00000
Cu 5.11243 5.11240 50.00000
Cu 5.11243 7.66838 50.00000
Cu 7.66846 0.00094 50.00000
Cu 7.66842 2.55602 50.00000
Cu 7.66837 5.11242 50.00000
Cu 7.66841 7.66841 50.00000
Cu 1.27799 1.27792 51.80750
Cu 1.27802 3.83423 51.80750
Find:
Select All
1 result
Clear
< Simulation Parameters
Storage (manage)
5% of 10GB
609 x 526

Initial crystal

```
0 1 63.546 0.000000 0.000000 50.000000
1 1 63.546 1.278096 1.278096 51.807500
2 1 63.546 0.000000 2.556191 50.000000
3 1 63.546 1.278096 3.834287 51.807500
4 1 63.546 0.000000 5.112382 50.000000
5 1 63.546 1.278096 6.390478 51.807500
6 1 63.546 0.000000 7.668573 50.000000
7 1 63.546 1.278096 8.946669 51.807500
8 1 63.546 2.556191 0.000000 50.000000
9 1 63.546 3.834287 1.278096 51.807500
10 1 63.546 2.556191 2.556191 50.000000
11 1 63.546 3.834287 3.834287 51.807500
12 1 63.546 2.556191 5.112382 50.000000
13 1 63.546 3.834287 6.390478 51.807500
14 1 63.546 2.556191 7.668573 50.000000
15 1 63.546 3.834287 8.946669 51.807500
16 1 63.546 6.390478 1.278096 51.807500
17 1 63.546 5.112382 2.556191 50.000000
18 1 63.546 6.390478 3.834287 51.807500
19 1 63.546 5.112382 5.112382 50.000000
20 1 63.546 6.390478 6.390478 51.807500
21 1 63.546 5.112382 7.668573 50.000000
22 1 63.546 6.390478 8.946669 51.807500
23 1 63.546 7.668573 0.000000 50.000000
24 1 63.546 8.946669 1.278096 51.807500
25 1 63.546 7.668573 2.556191 50.000000
26 1 63.546 8.946669 3.834287 51.807500
27 1 63.546 7.668573 5.112382 50.000000
28 1 63.546 8.946669 6.390478 51.807500
29 1 63.546 7.668573 7.668573 50.000000
30 1 63.546 8.946669 8.946669 51.807500
31 1 63.546 0.000000 0.000000 53.615000
32 1 63.546 1.278096 1.278096 55.422500
33 1 63.546 0.000000 2.556191 53.615000
34 1 63.546 1.278096 3.834287 55.422500
35 1 63.546 0.000000 5.112382 53.615000
36 1 63.546 1.278096 6.390478 55.422500
37 1 63.546 0.000000 7.668573 53.615000
38 1 63.546 1.278096 8.946669 55.422500
39 1 63.546 2.556191 0.000000 53.615000
40 1 63.546 3.834287 1.278096 55.422500
41 1 63.546 2.556191 2.556191 53.615000
```

Movie

```
620
 CHKPT
 Cu       0.00084     0.00077     50.00000
 Cu       0.00054     2.55599     50.00000
 Cu       0.00051     5.11247     50.00000
 Cu       0.00067     7.66815     50.00000
 Cu       2.55570     0.00071     50.00000
 Cu       2.55601     2.55608     50.00000
 Cu       2.55607     5.11243     50.00000
 Cu       2.55604     7.66837     50.00000
 Cu       5.11244     2.55619     50.00000
 Cu       5.11243     5.11240     50.00000
 Cu       5.11243     7.66838     50.00000
 Cu       7.66846     0.00094     50.00000
 Cu       7.66842     2.55602     50.00000
 Cu       7.66837     5.11242     50.00000
 Cu       7.66841     7.66841     50.00000
 Cu       1.27799     1.27792     51.80750
 Cu       1.27802     3.83423     51.80750
 Cu       1.27800     6.39061     51.80750
 Cu       1.27824     8.94609     51.80750
 Cu       3.83418     1.27812     51.80750
 Cu       3.83425     3.83423     51.80750
 Cu       3.83424     6.39059     51.80750
 Cu       3.83424     8.94627     51.80750
 Cu       6.39070     1.27808     51.80750
 Cu       6.39058     3.83422     51.80750
 Cu       6.39059     6.39059     51.80750
 Cu       6.39063     8.94625     51.80750
 Cu       8.94602     1.27819     51.80750
 Cu       8.94626     3.83422     51.80750
 Cu       8.94625     6.39063     51.80750
 Cu       8.94599     8.94599     51.80750
 Cu       0.00065     0.00061     53.61500
 Cu       1.27799     1.27796     55.42250
 Cu       0.00032     2.55605     53.61500
 Cu       1.27802     3.83423     55.42250
 Cu       0.00029     5.11243     53.61500
 Cu       1.27801     6.39059     55.42250
 Cu       0.00047     7.66841     53.61500
 Cu       1.27826     8.94621     55.42250
```

To do in class: visualize the MD simulation with VMD. Create a picture and a movie

If you have time: simulate this…