Online simulations via nanoHUB: Nanomaterial Mechanics Explorer

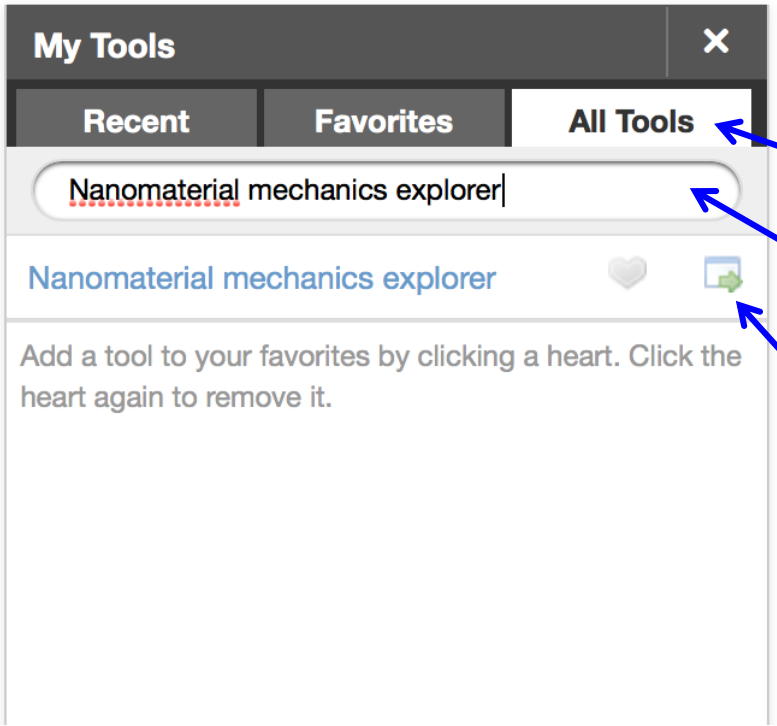
First-time User Guide

Ale Strachan (strachan@purdue.edu)
Kiettipong Banlusan, Sam Reeve, Mitch Wood

School of Materials Engineering & Birck Nanotechnology Center
Purdue University
West Lafayette, Indiana USA

1) Launch the Nanomaterial Mechanics Explorer Tool

- Log in to nanoHUB
- From My Tools on nanoHUB dashboard, search for “Nanomaterial mechanics explorer” and launch the tool, or go directly to the tool at https://nanohub.org/tools/nanomatmech/



My Tools on nanoHUB dashboard

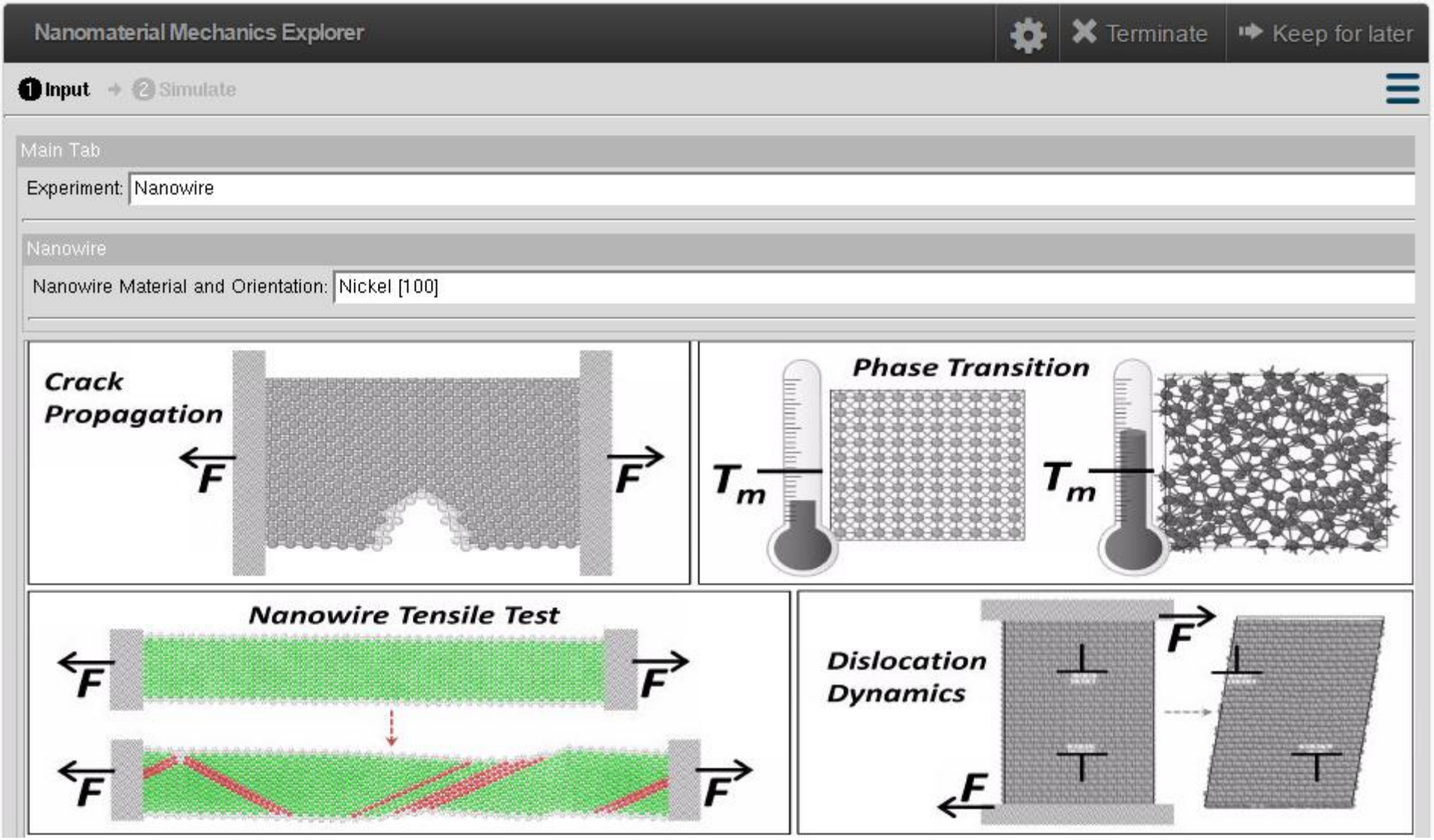
All Tools tab

Search for “Nanomaterial mechanics explorer”

Launch the tool

2) Front page and the default runs

- *Four main options –tutorials for each simulation type coming soon*

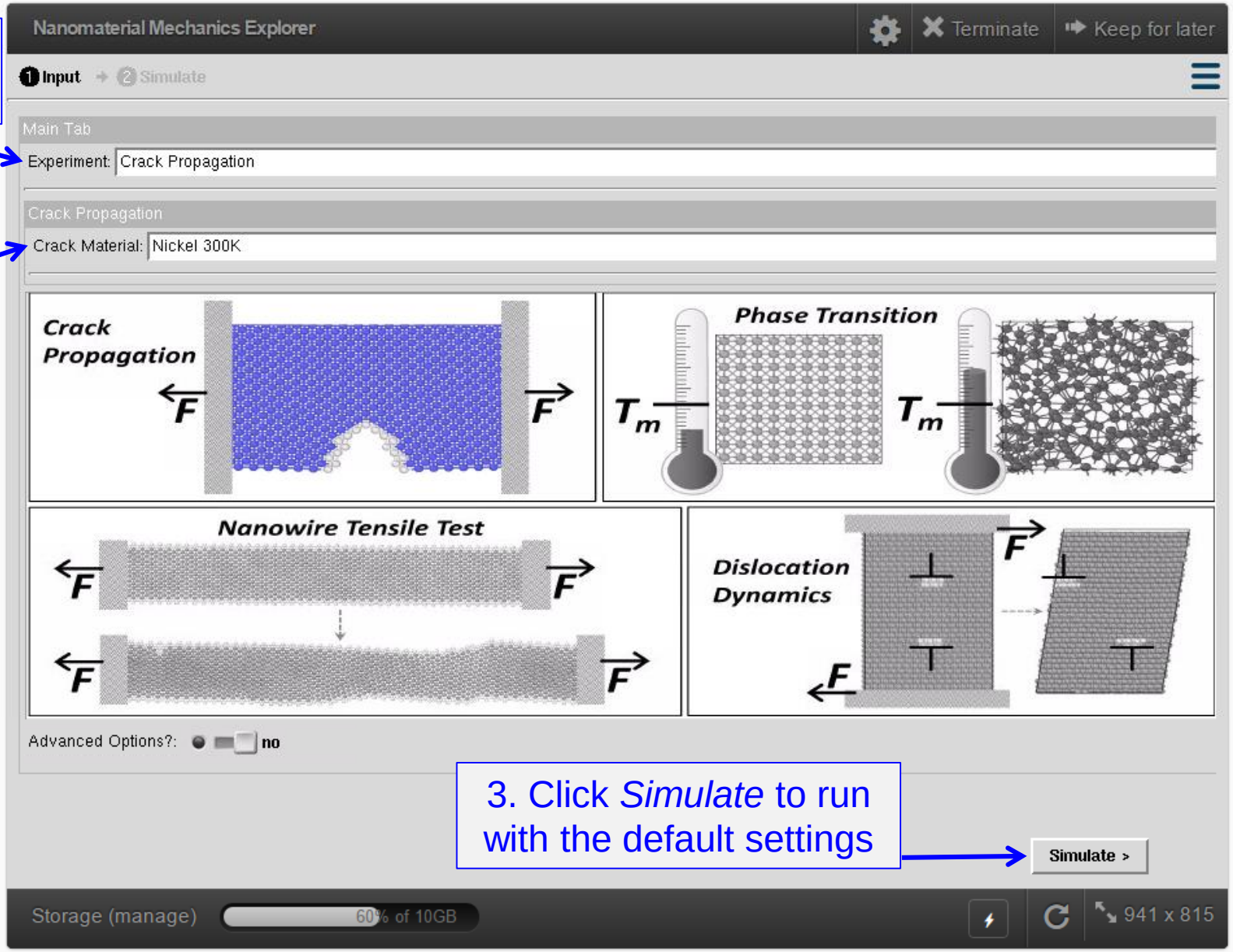


2) Run simulation

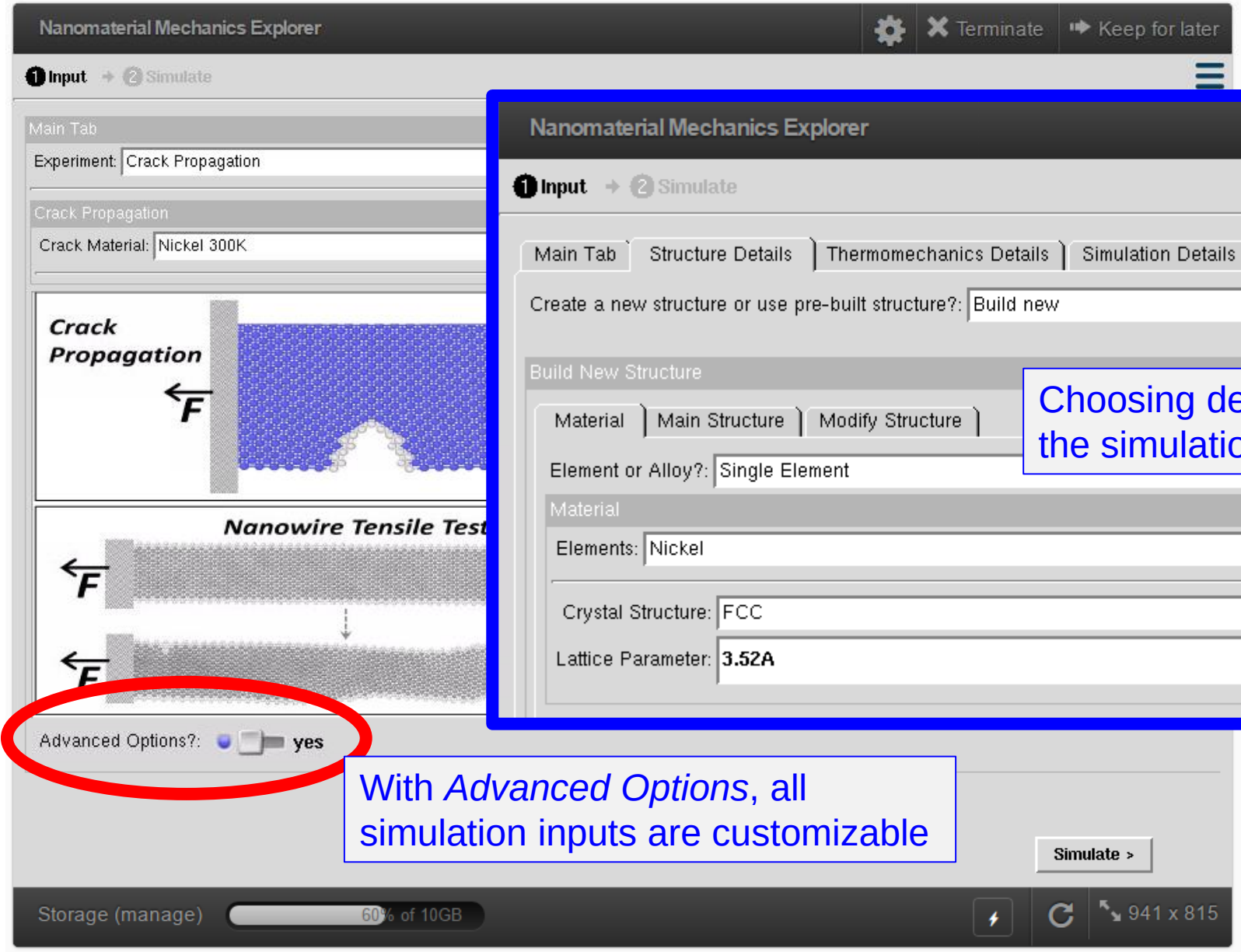
1. Select the test type:

2. Select provided example:

(The default runs will take 30 – 60 min)



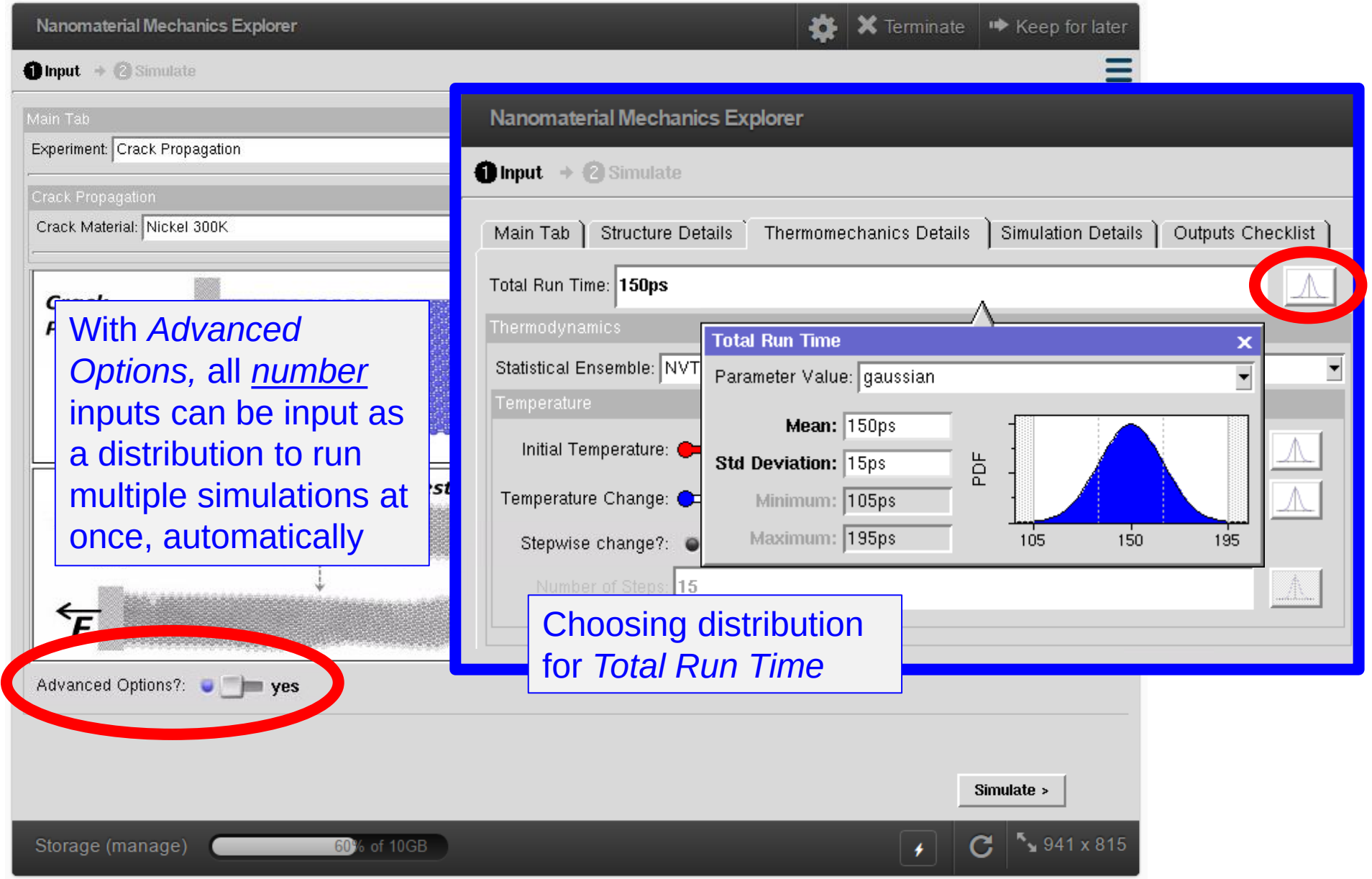
(*Advanced Options*)



Choosing details for the simulation *Material*

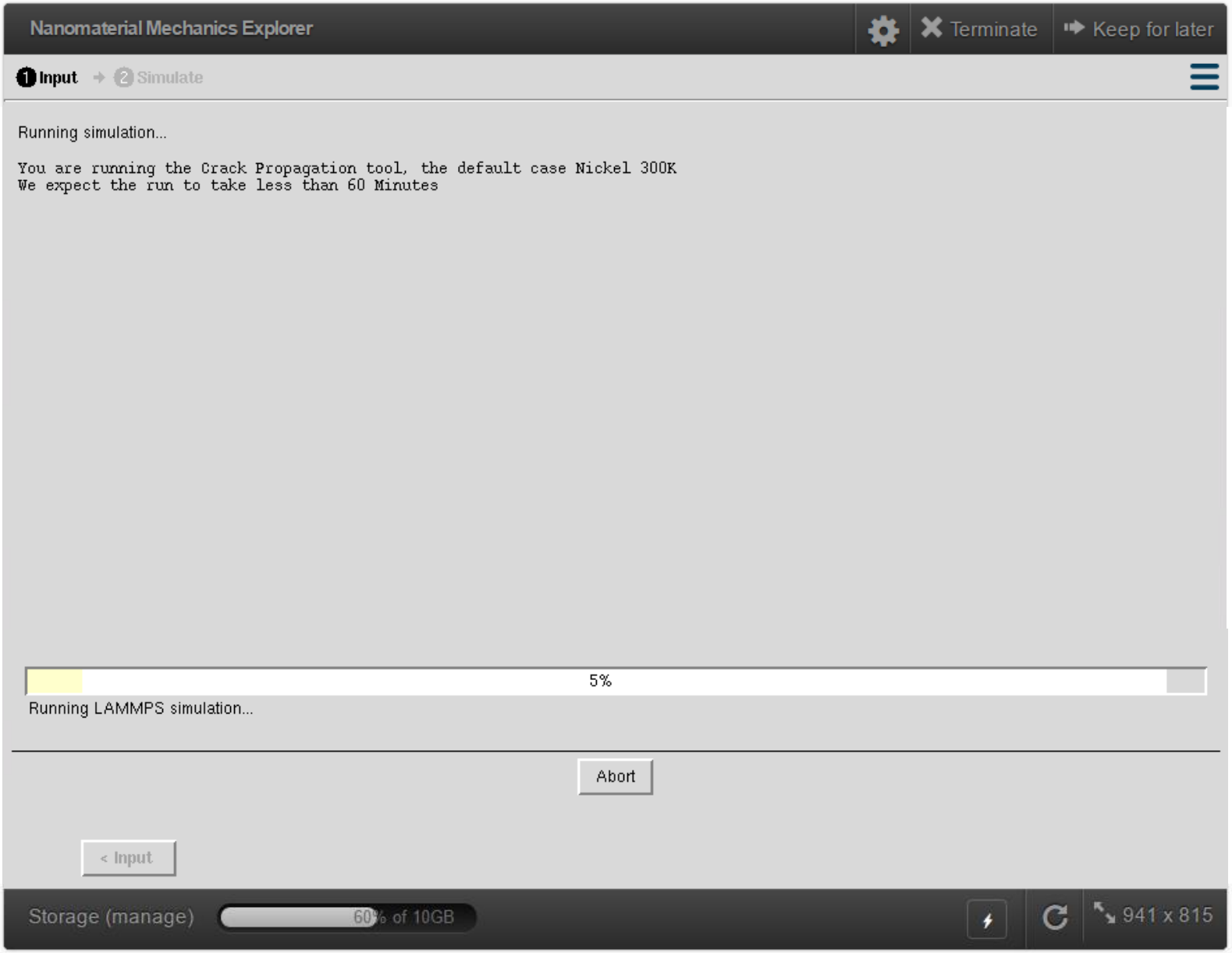
With *Advanced Options*, all simulation inputs are customizable

(Uncertainty Quantification with *Advanced Options*)



2) Wait for simulation results

Notes about the simulation are shown while it runs

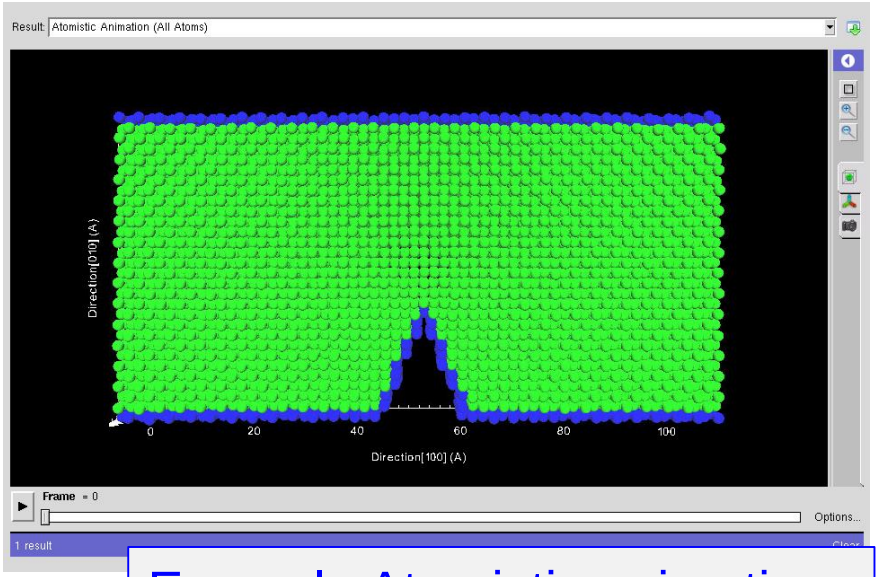


3) Explore simulation results

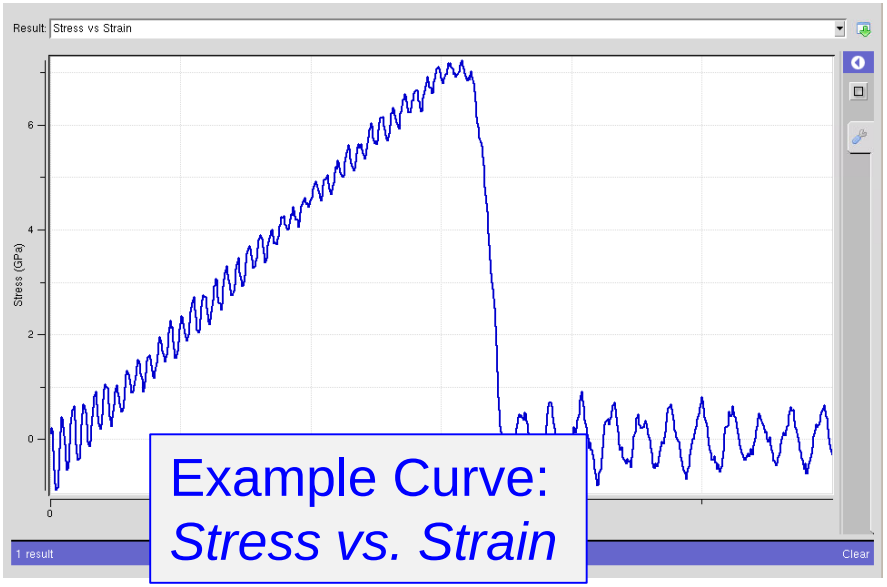
A. Atomistic animations

B. Curves

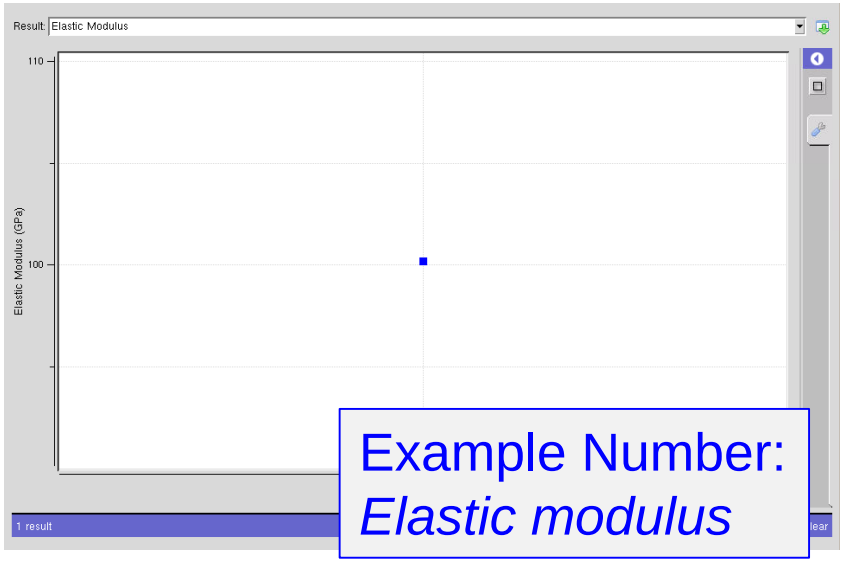
C. Numbers



Example Atomistic animation:
All atoms

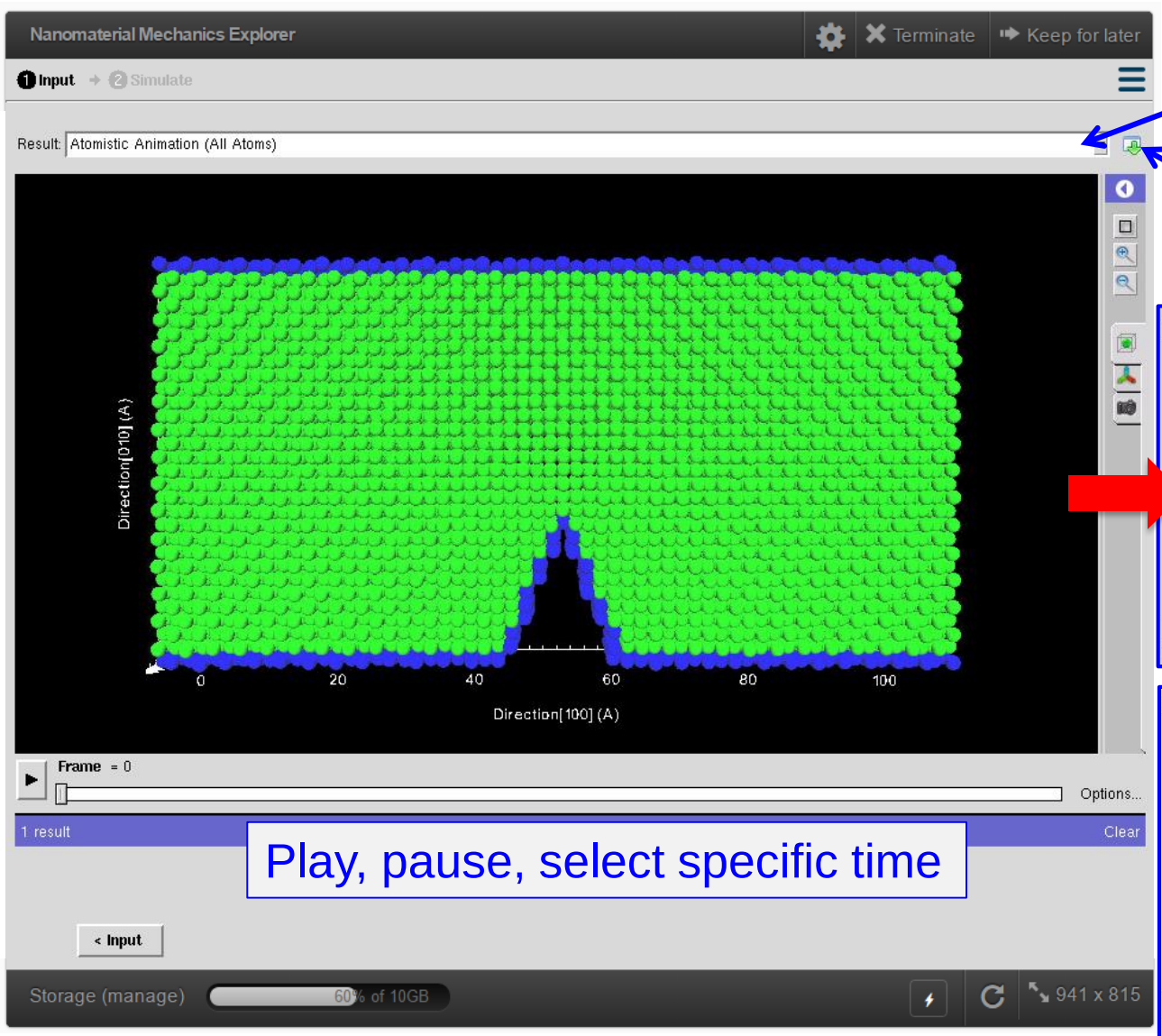


Example Curve:
Stress vs. Strain



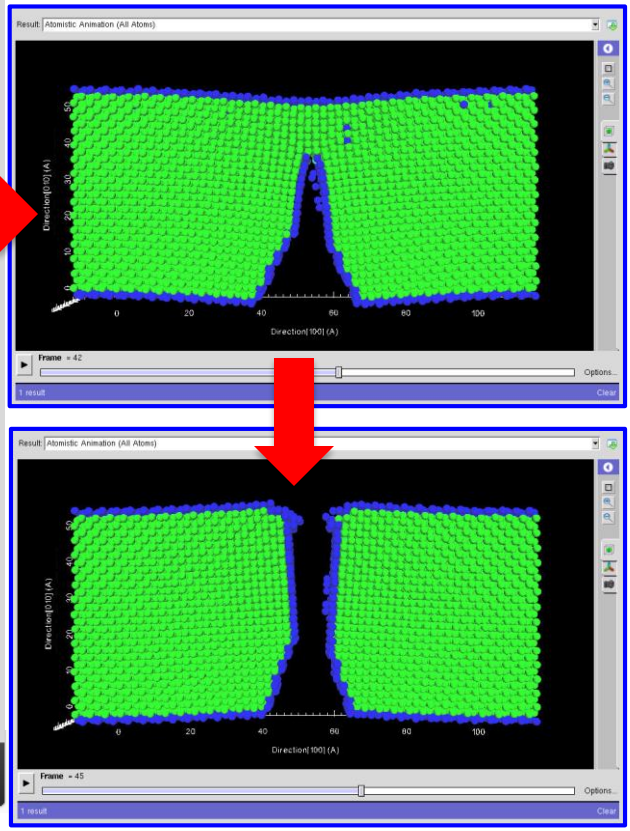
Example Number:
Elastic modulus

3A) Atomistic Animation (*All Atoms*)



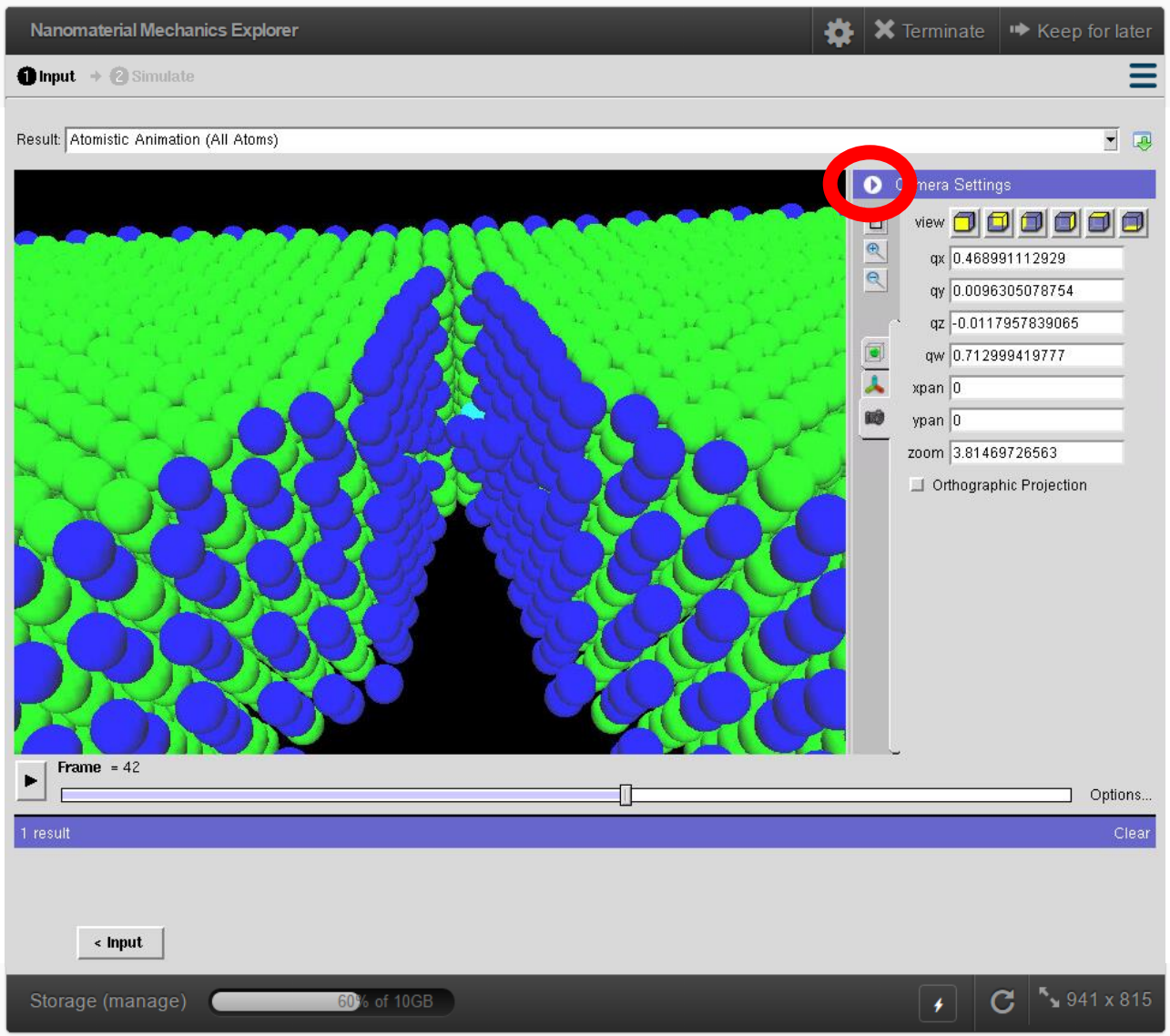
Select result with drop-down menu

Download the current result



Play, pause, select specific time

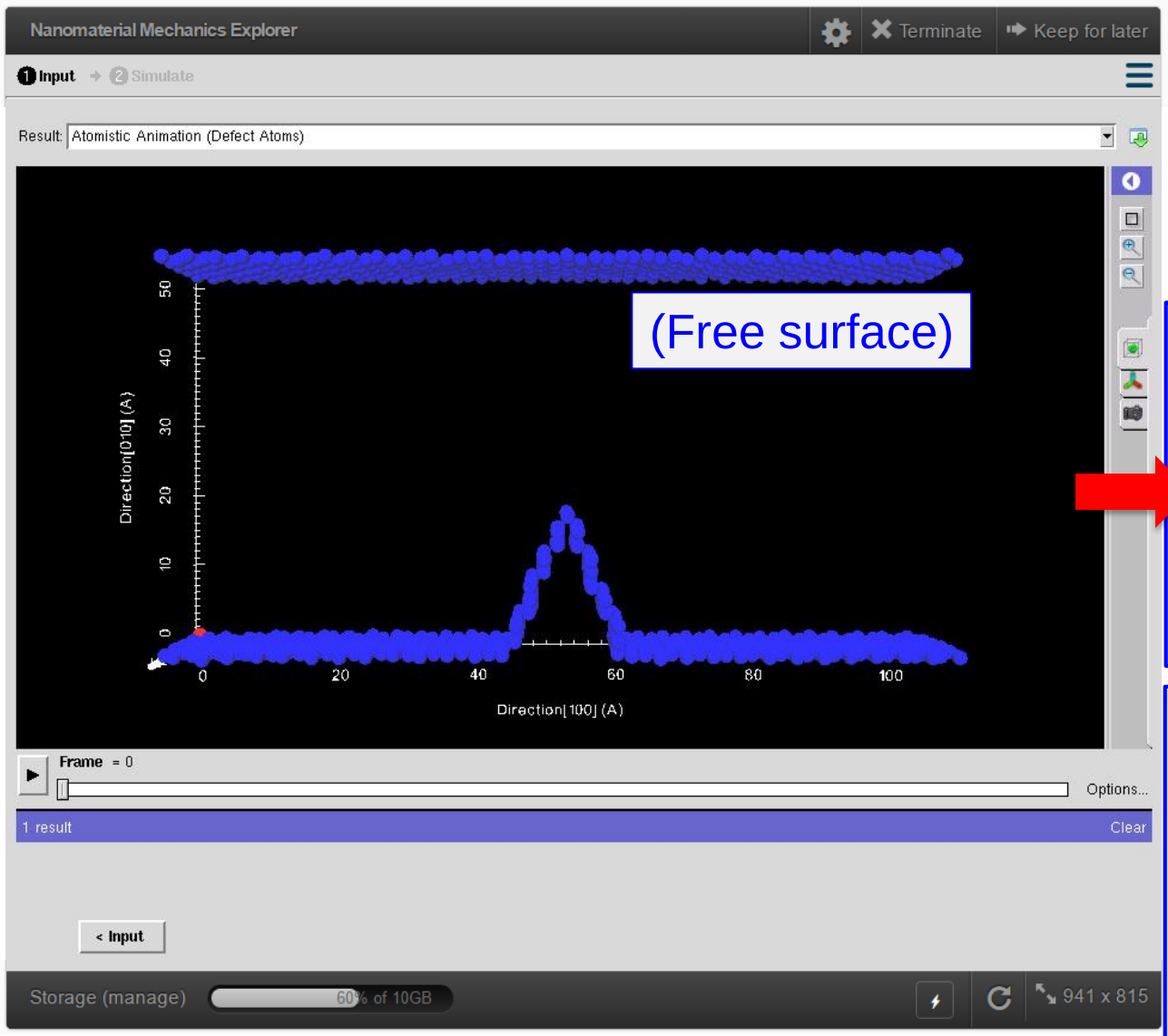
3A) Atomistic Animation (*All Atoms*)



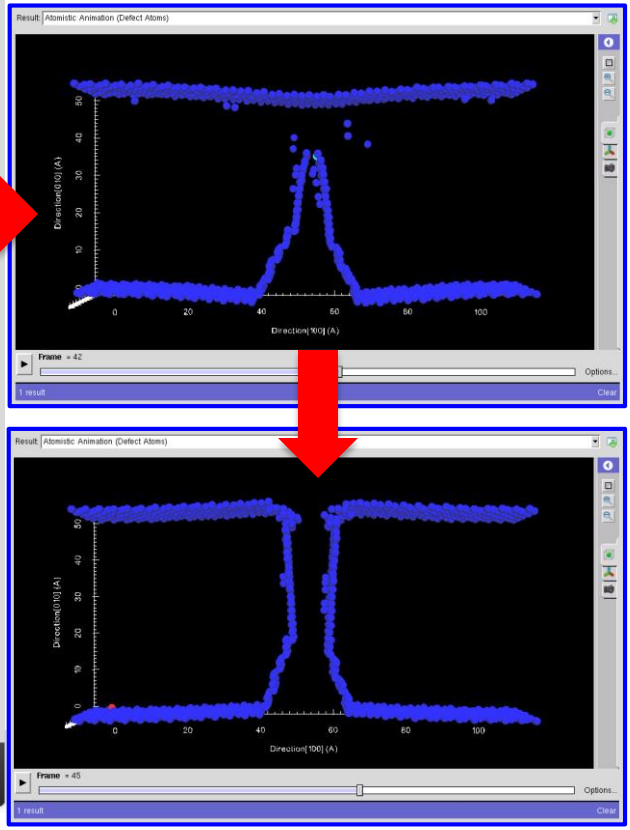
Can rotate, zoom, and move with mouse

Side-bar allows changing all animation settings

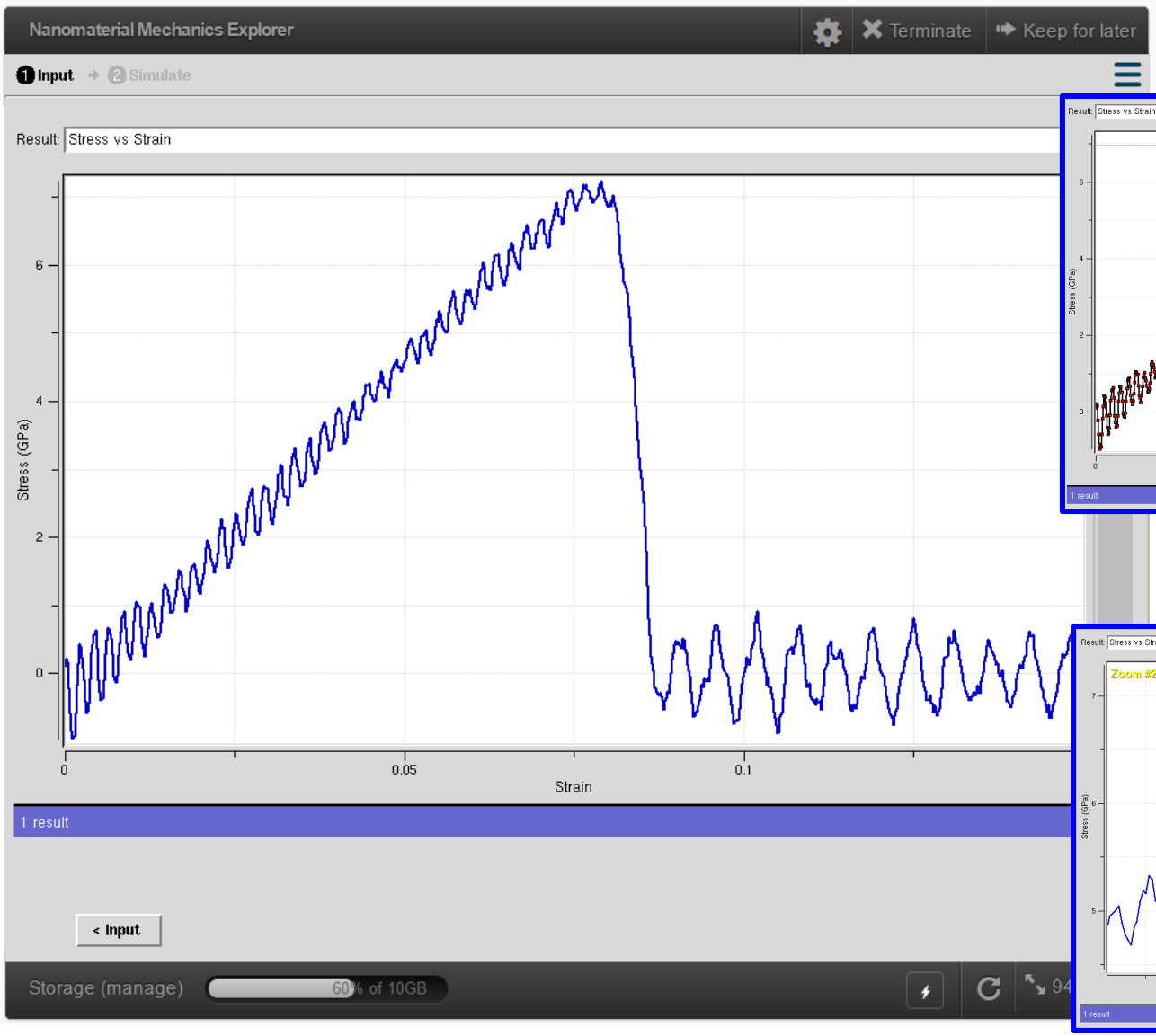
3A) Atomistic Animation (*Defect Atoms*)



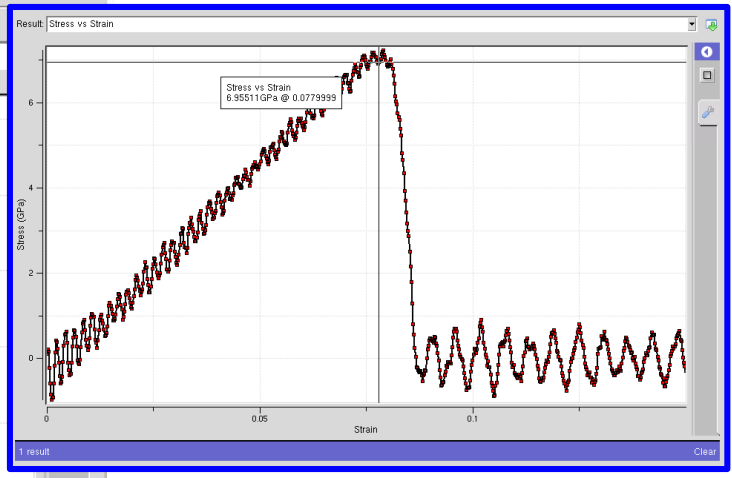
Similar to *All Atoms* output, but only shows atoms of a different crystal structure than the bulk material



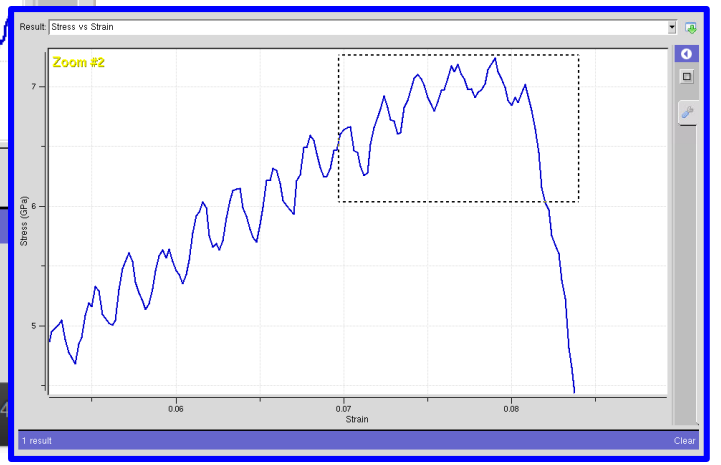
3B) Curve (*Stress vs Strain*)



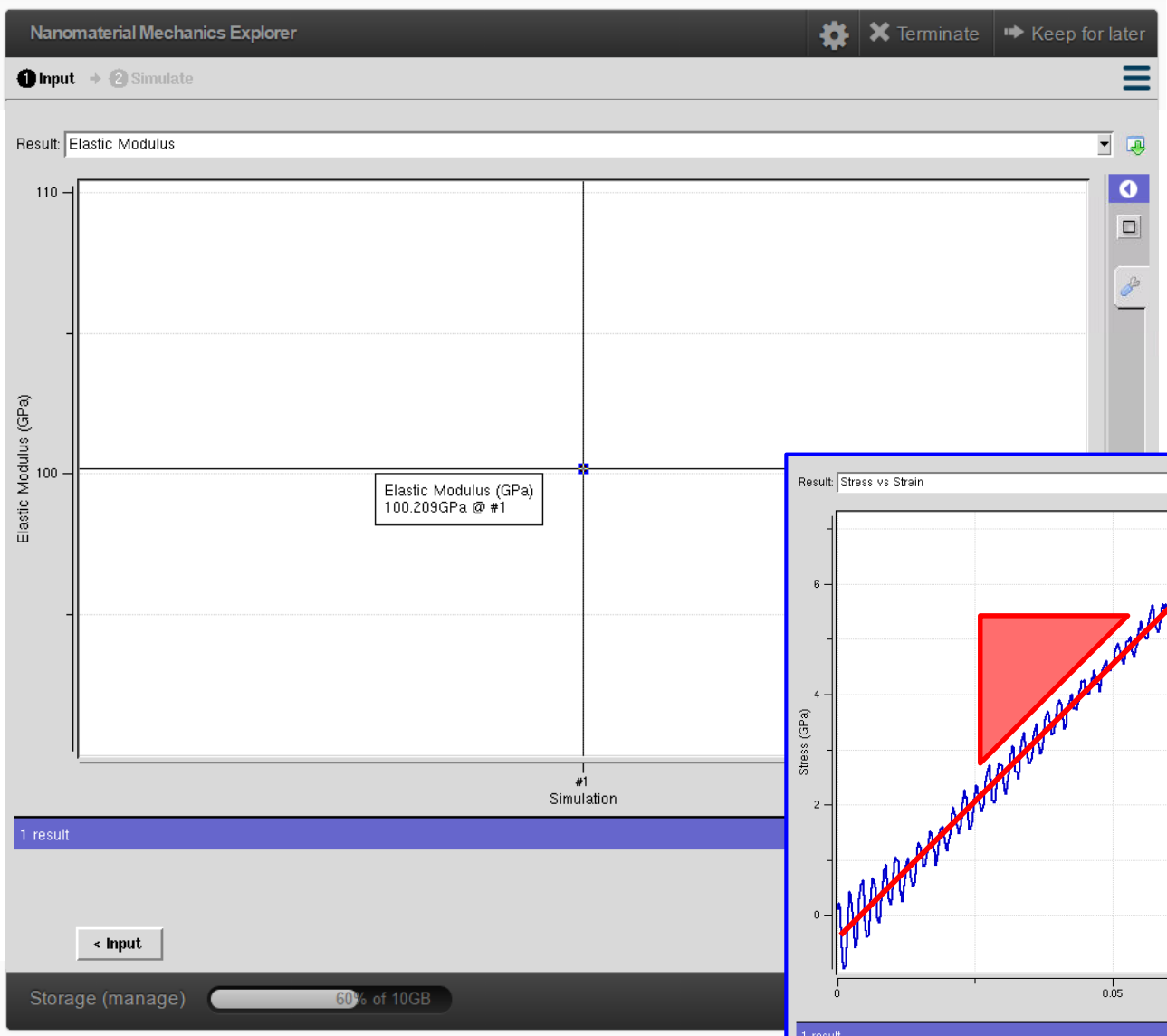
Mouse-over values



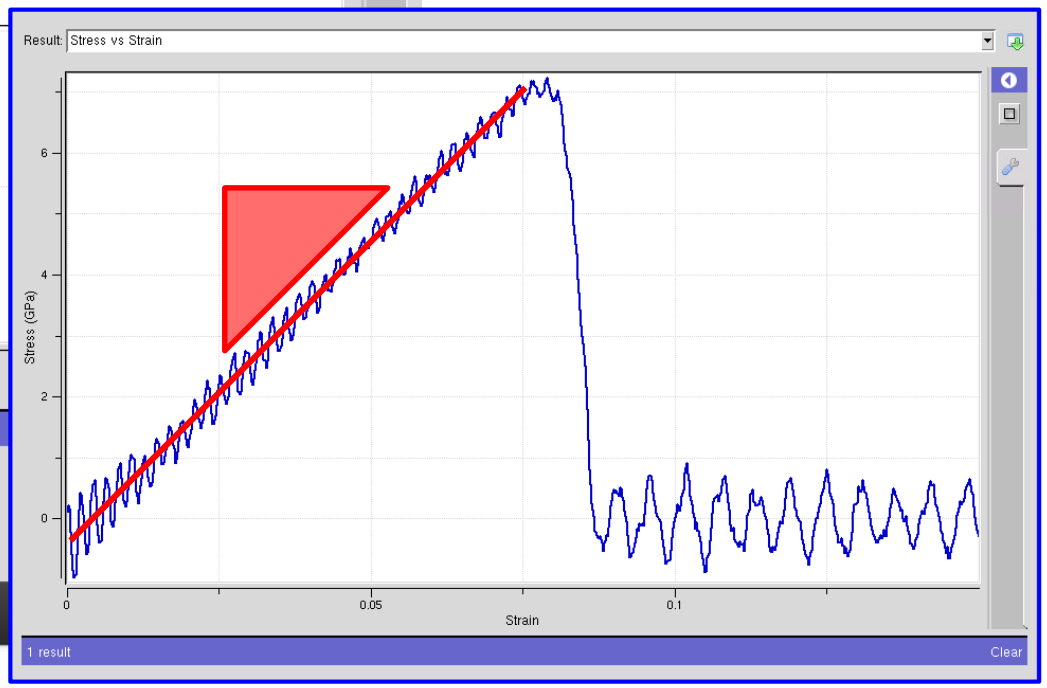
Zoom



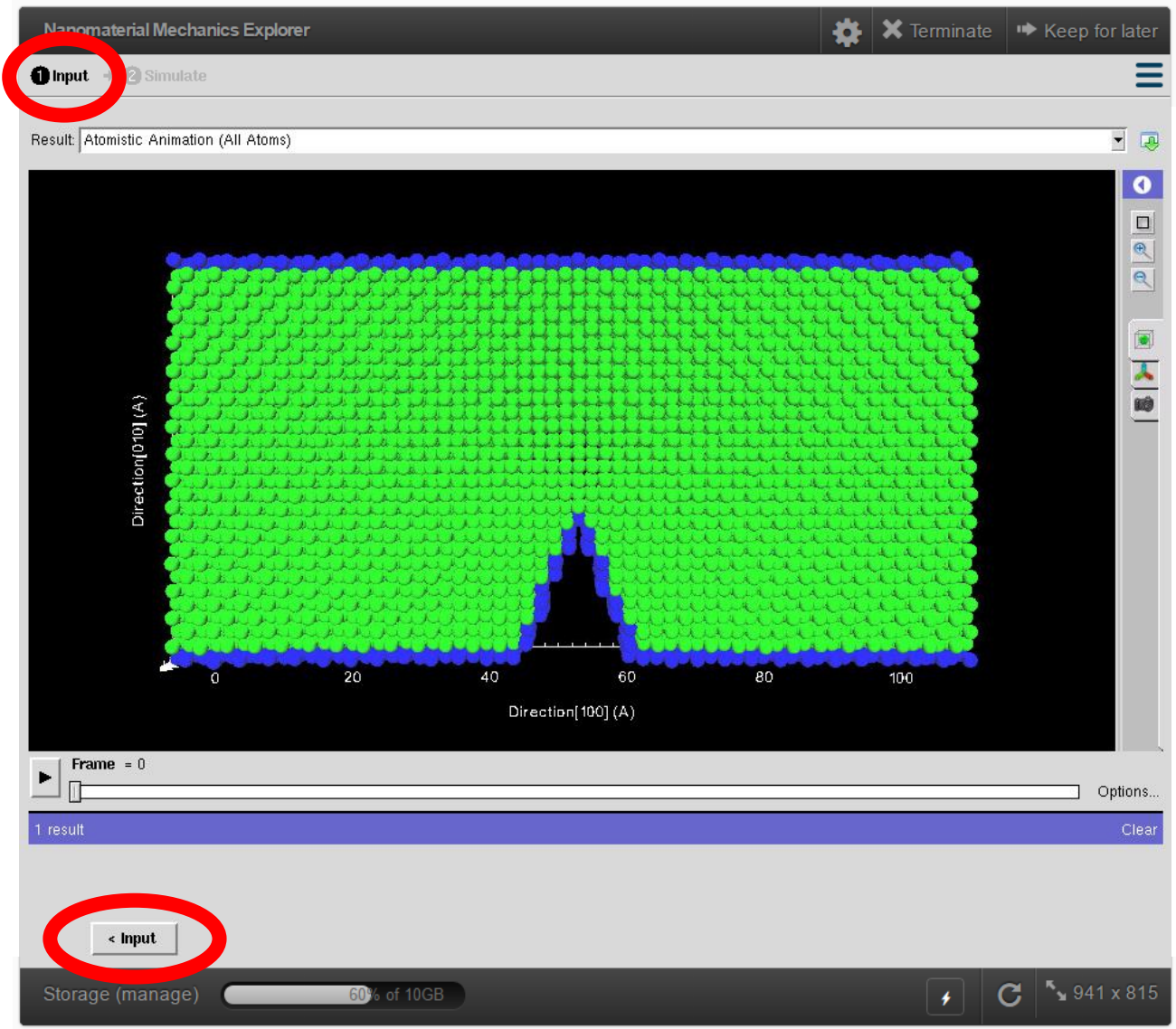
3C) Numbers (*Elastic Modulus*)



(Calculated from *Stress vs Strain* curve elastic regime)



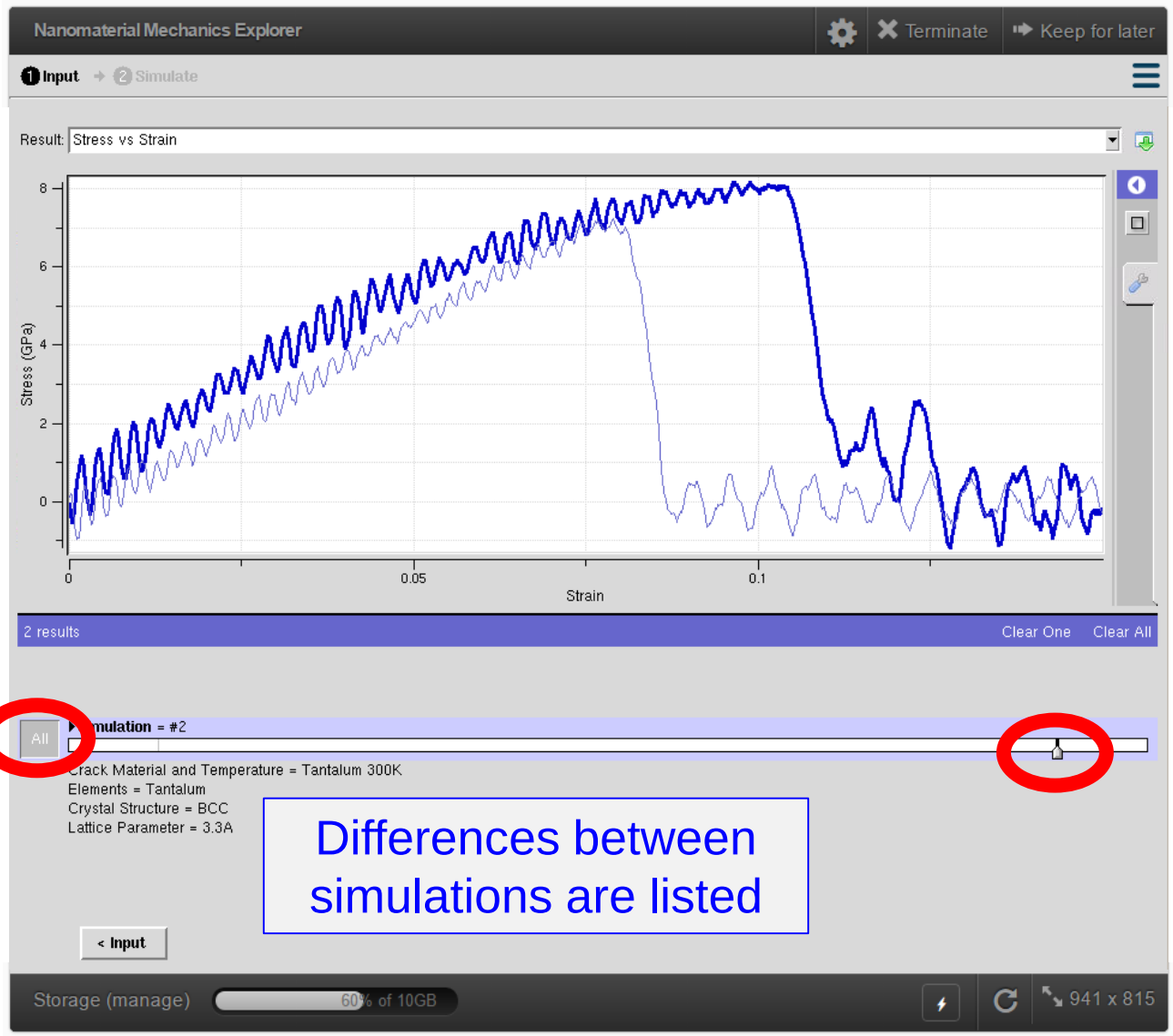
4) Run another!



Run another simulation to compare to the current results

Choose another default run or change *Advanced Options*

4) Compare results (Default Ni & Ta runs)



Outputs can be compared by selecting *"All"*, or examined individually

The selector bar chooses the primary result

Differences between simulations are listed

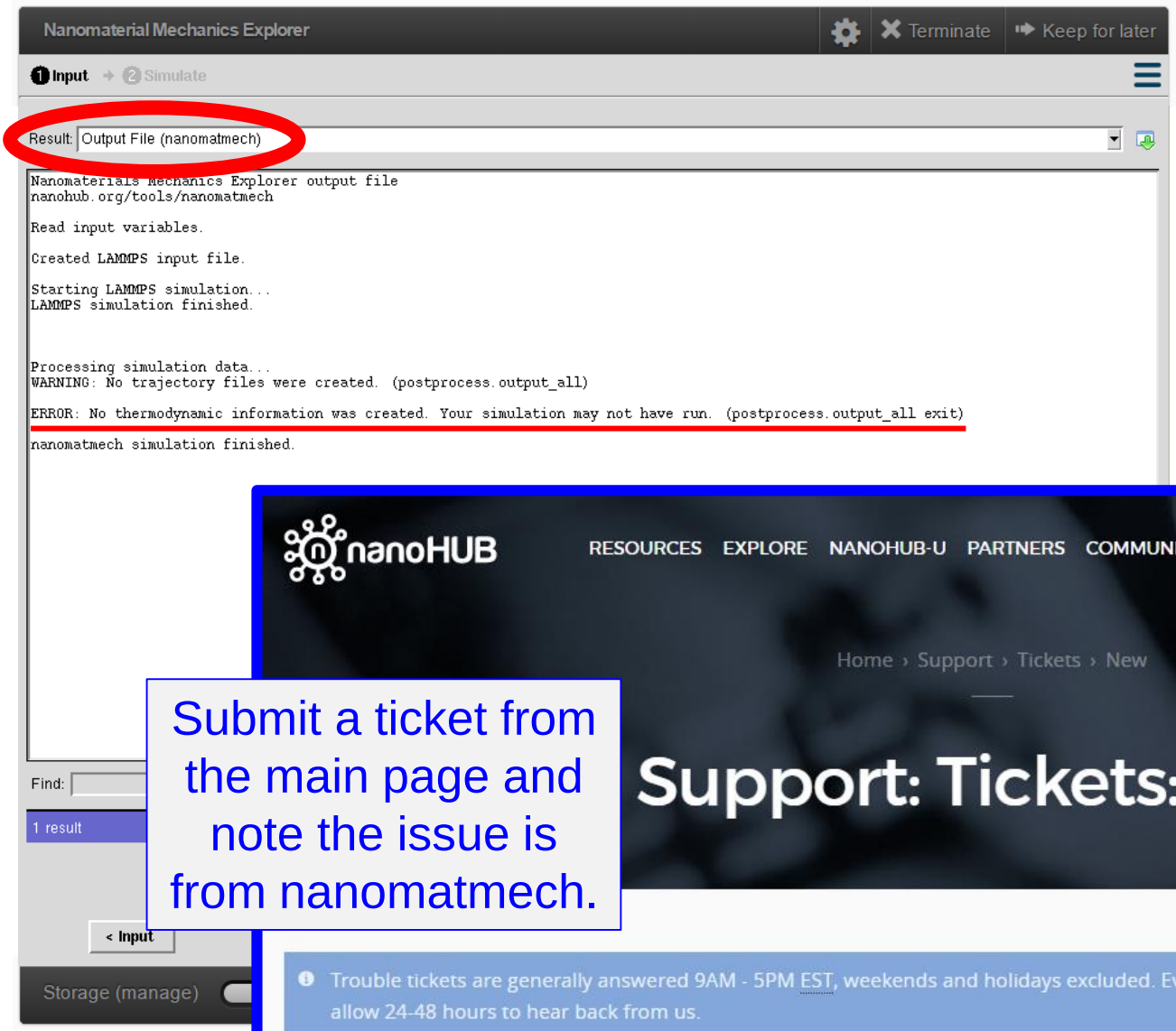
Online simulations via nanoHUB: Nanomaterial Mechanics Explorer

First-time User Guide: Extra tips

School of Materials Engineering & Birck Nanotechnology Center
Purdue University
West Lafayette, Indiana USA

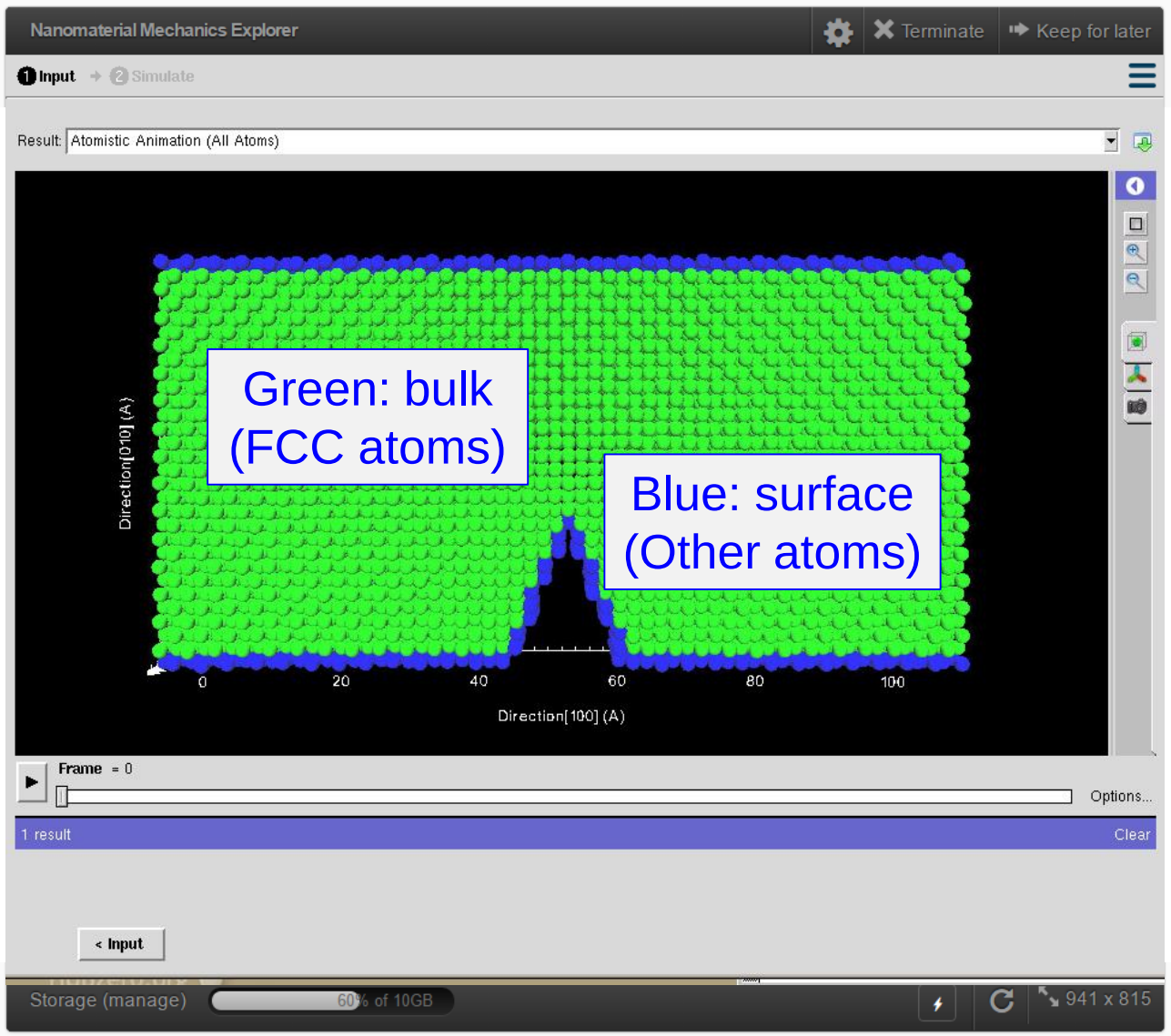
Errors!

The simulations may not always work! Note the error in the tool, in the nanomatmech Output File, or Thermodynamic Output File.



Submit a ticket from the main page and note the issue is from nanomatmech.

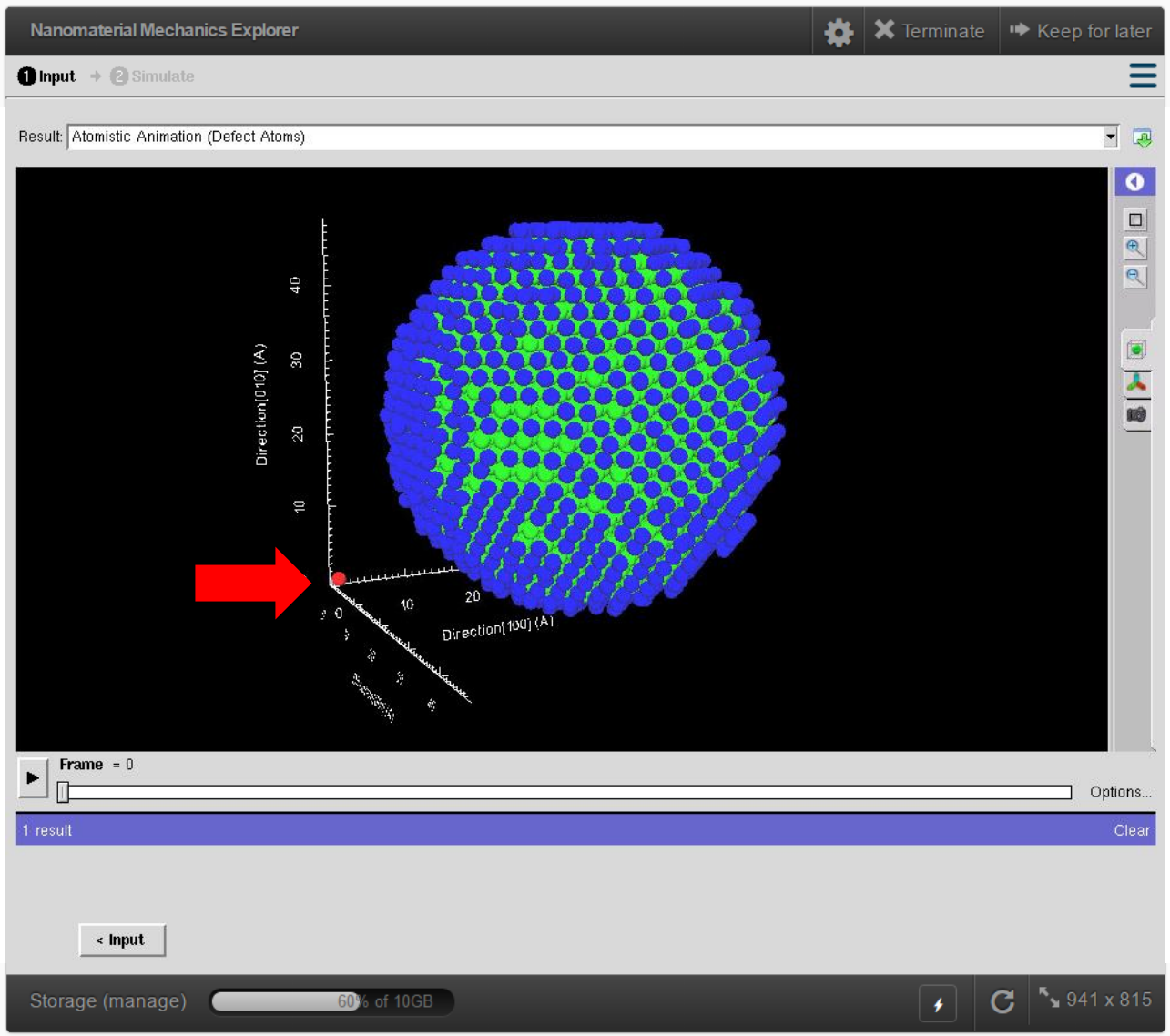
Atom colors



All atoms are colored by their local coordination (not by atom type)

- FCC atoms
- BCC atoms
- HCP atoms
- Other atoms

Origin marker



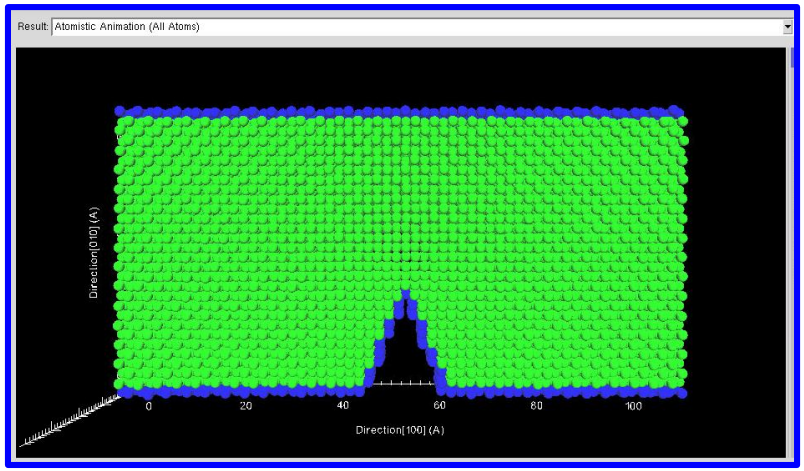
A single red "atom" marks the origin, but is not part of the simulation

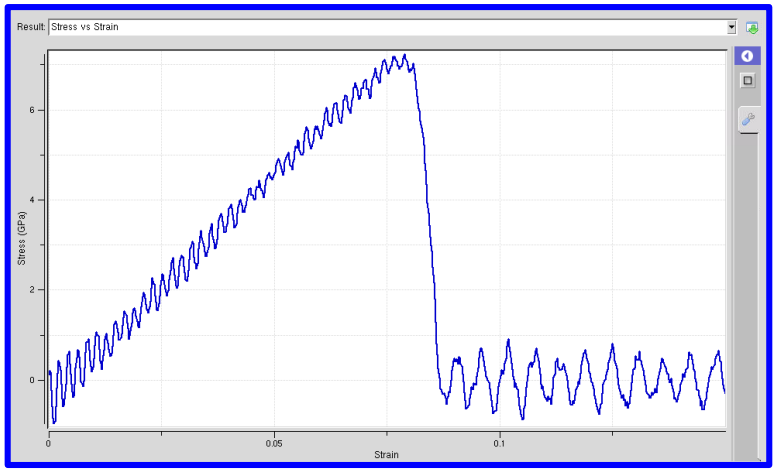
Multiple simulations

Multiple simulations may show some strange animation views to accommodate each

Multiple simulations may output different results, leading to some blank pages

Crack propagation





Nanoparticle melting