591V Multiscale Materials Modeling

Computational Lab-1

Outline: Today's class

Outline:

Part A: Simulation tools (nanoHUB etc.)

Example: Deformation of nanowire

Part B: Visualization (VMD)

Examples: visualize the output file, make snapshots and movie.

Objectives:

1. Everyone has account on nanoHUB, logged in, reviewed tools
2. Basic idea of how to use nanoHUB
3. Everyone has VMD downloaded and installed and done some basic tests

PART A: nanoHUB website

Limited code development required

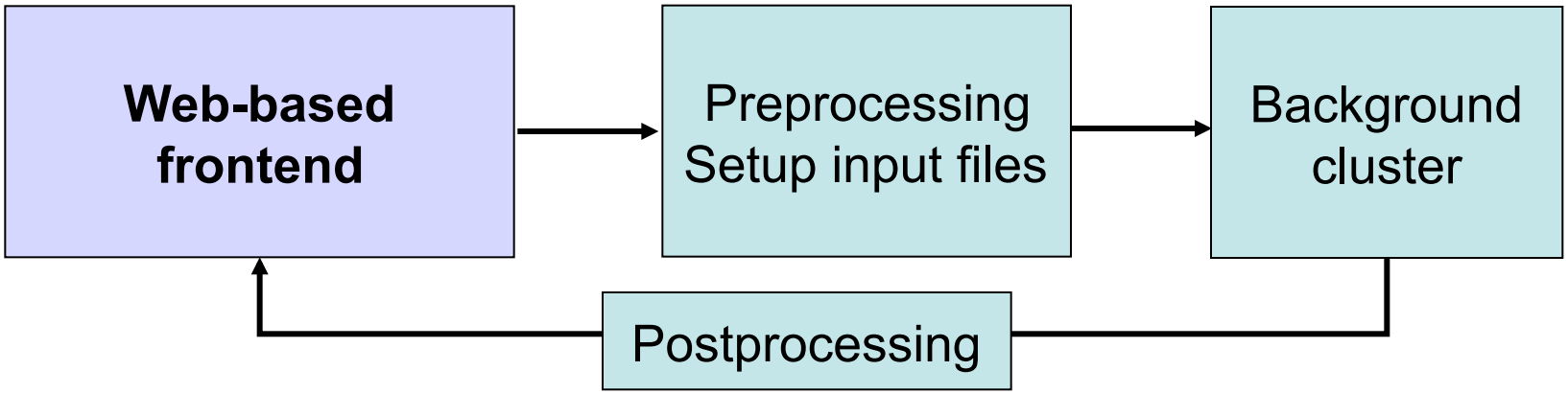
We will use a website-driven simulation framework
https://nanohub.org/

Web-enabled high performance computing

- Run complex code through simple web interface
- Submission of jobs to queuing system (background), notification per email when job is done

Benefits

- Avoid coding and complexities of particular codes
- Make complex simulation tools available to broad community



Supported by NSF

nanoHUB: https://nanohub.org

More than 330 tools:
https://nanohub.org/resources/tools

For new accounts

nanoHUB.org an NCN project — ONLINE SIMULATION AND MORE FOR NANOTECHNOLOGY

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You are here: Tools › Nanowire Tensile Deformation Lab › About

Nanowire Tensile Deformation Lab

By Markus Buehler[1], Justin Riley[1], Joo-Hyoung Lee[1], 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 1.2 - published on 15 Feb 2011

DOI: 10.254/nanohub-r9559.3 cite this

This tool is closed source.

View All Supporting Documents

8.5 RANKING

69 user(s), detailed usage

0 Citation(s)

0 questions (Ask a question)

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SEE ALSO

No results found.

RECOMMENDATIONS

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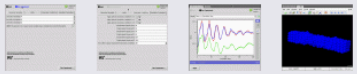
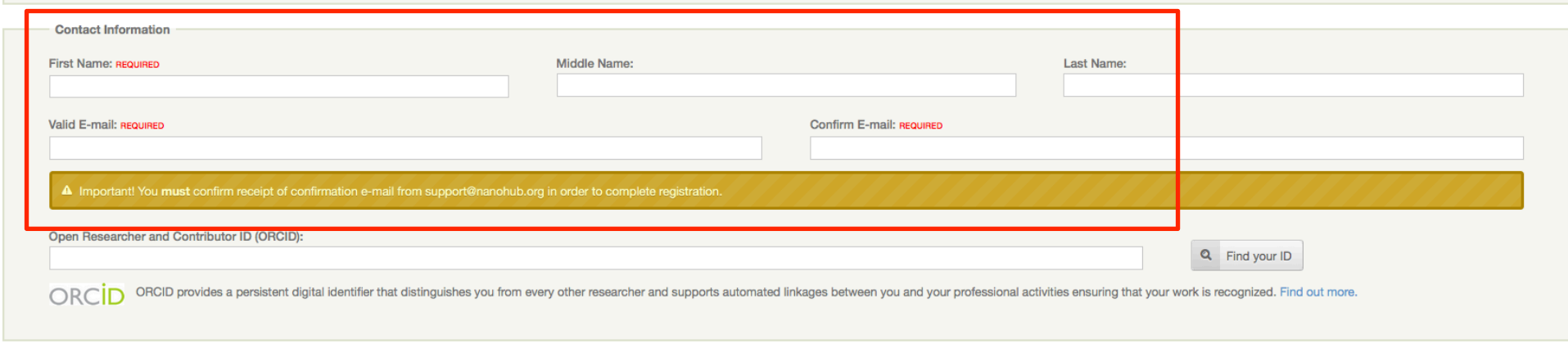


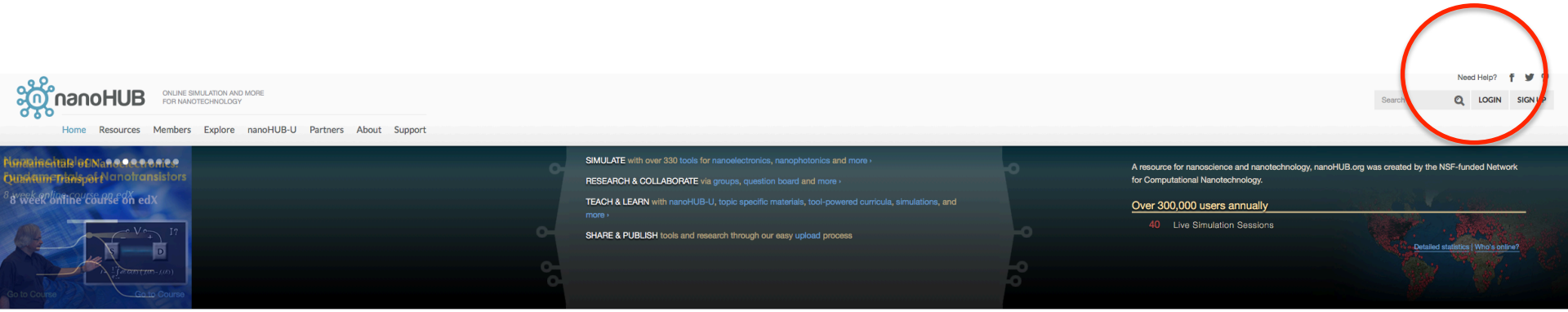
Description — This tool allows the user to simulate the effects of applying tensile stress at each end of a Copper nanowire.

Credits — Software Tools for Academics and Researchers Office of Educational Innovation and Technology Massachusetts Institute of Technology

Cite this work — Researchers should cite this work as follows:

Markus Buehler; Justin Riley; Joo-Hyoung Lee; Jeffrey C Grossman (2011), "Nanowire Tensile Deformation Lab," DOI: 10254/nanohub-r9559.3. (DOI: 10254/nanohub-r9559.3).


Contact Information
First Name: REQUIRED
Middle Name:
Last Name:
Valid E-mail: REQUIRED
Confirm E-mail: REQUIRED
Important! You must confirm receipt of confirmation e-mail from support@nanohub.org in order to complete registration.
Open Researcher and Contributor ID (ORCID):
Find your ID
ORCID provides a persistent digital identifier that distinguishes you from every other researcher and supports automated linkages between you and your professional activities ensuring that your work is recognized. Find out more.



POPULAR TOPICS | TRENDING TOPICS

- **Fermi-Dirac Statistics** *8 Presentations*
- **Newton's Law Basics** *10 Presentations*
- **CMOS Process Steps** *4 Course Lectures, 1 Learning Module, 1 Presentation, 1 Teaching Material, 1 Tutorial*
- **Thin Film Solar Cells** *4 Presentations, 3 Course Lectures, 1 Paper*
- **Charging Effects** *6 Course Lectures, 2 Teaching Materials*
- **Nanoscale Semiconductor Interfaces** *2 Presentations, 1 Learning Module, 1 Tutorial*
- **Schottky Diodes** *5 Presentations, 3 Course Lectures*
- **Atomic Force Microscopy** *6 Presentations, 1 Tutorial*
- **Density States** *7 Course Lectures, 2 Presentations, 1 Teaching Material*
- **Scanning Probe Microscopy** *4 Animations, 2 Tutorials, 1 Course Lecture, 1 Presentation*
- **Introduction To Bio-NEMS Bionanotechnology** *5 Tutorials*
- **Cyclic Peptide Nanotubes** *3 Course Lectures, 2 Presentations, 1 Research Seminar*

Contribute to a topic, or start a new one! Get started

FEATURED

nanoHUB-U : **Your source for cutting-edge topics distilled into short lectures with quizzes, homework, practice exams.**

NEEDS :The NSF-Funded Electronics Content Node.

nanoBIO :The NSF-Funded nanoBIO Content Node.

Carbon nanotube based fixed-fixed NEMS : Simulates pull-in behavior of Carbon nanotube based NEMS with fixed-fixed boundary conditions,... - in Tools

Theoretical Analysis of Gold Nanoparticles - in Teaching Materials

MSE 640 Lecture 12: Diffraction contrast imaging, Part 2 - in Online Presentations

ECE 495N Lecture 22: Density of States I - featured on iTunes U

evanscent modes considered?
- asked by Debanjan Basu, in Answers

I take courses on nanoHUB.org to understand the device semiconductor physics needed to design and prototype nano devices, and the courses on nanoHUB ...»

Jay Morreale, p-brane LLC (2012) - in Notable Quotes

NEW IN RESOURCES

Unified View of Electron and Phonon Transport
in Online Presentations, 10 Nov 2015

[Illinois] Translational Nanomedicine from Drug Discovery to Preclinical Studies
in Online Presentations, 10 Nov 2015

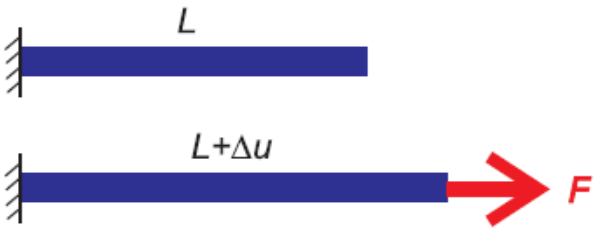
[Illinois] Biophysics 401 Lecture 19: Fluorescence Microscopy & Imaging
in Online Presentations, 10 Nov 2015

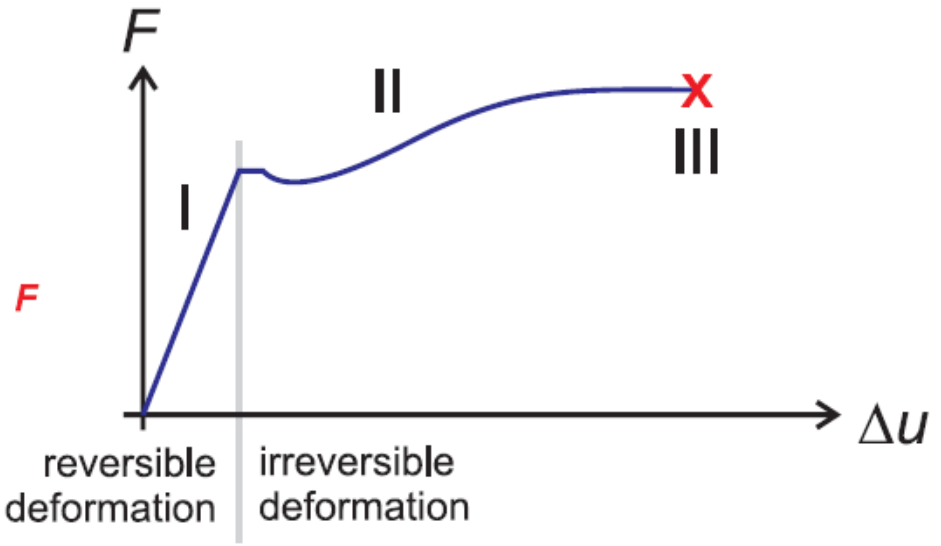
[Illinois] BioNanotechnology Summer Institute 2015
in Online Presentations, 10 Nov 2015

Molecular Dynamics Showcase Builder
in Tools, 09 Nov 2015

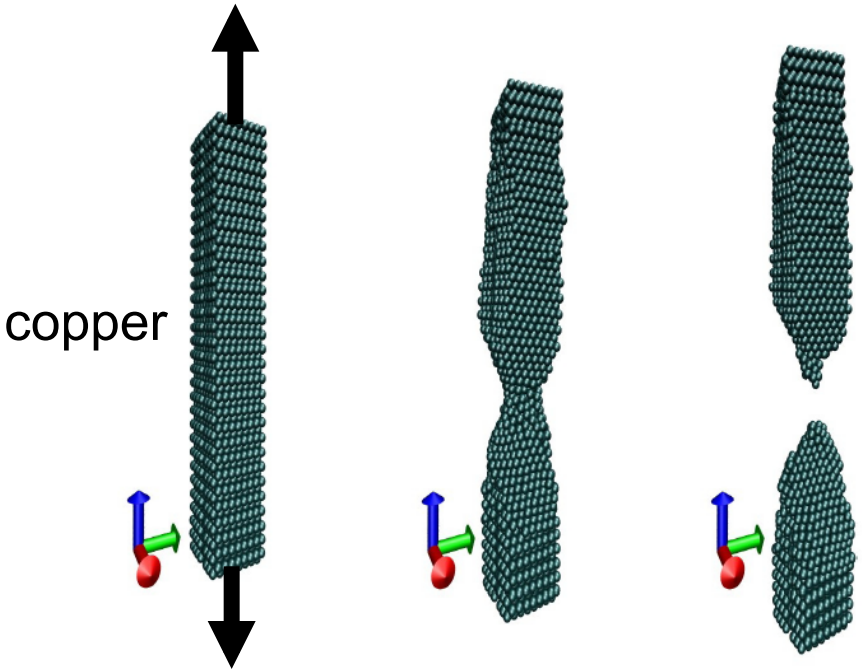
More new resources ›

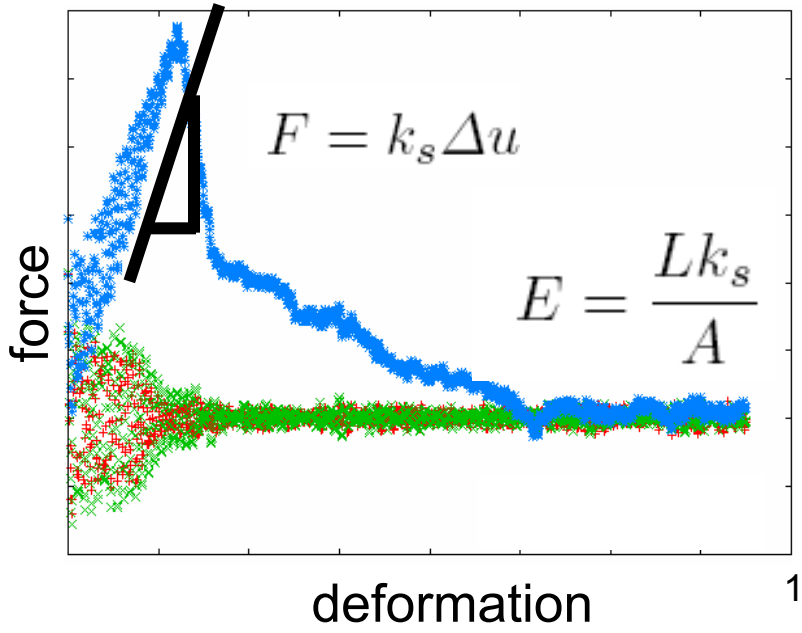
Example: Stretching nanowire

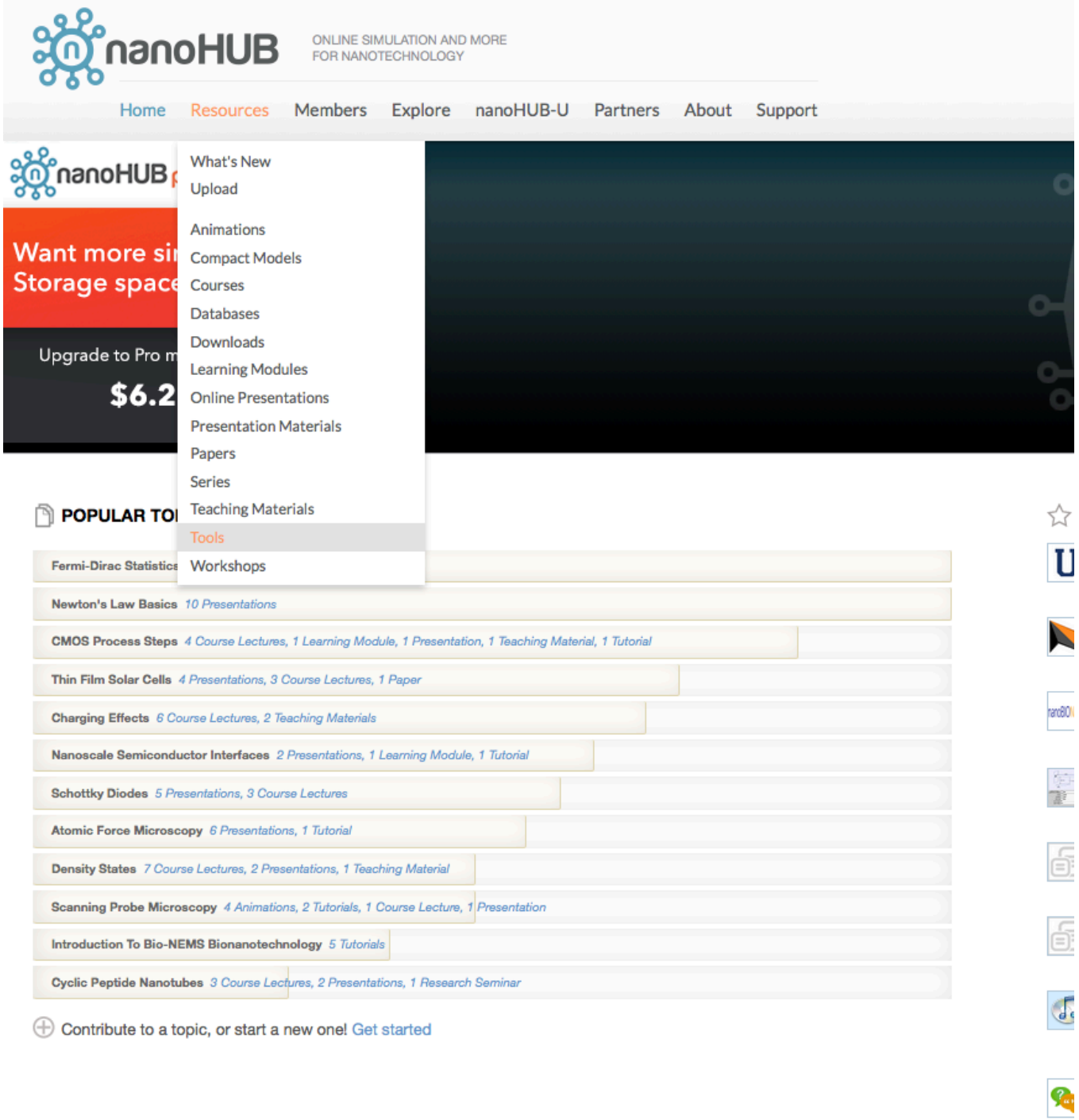




Boundary conditions:
Non-periodic in x,y,z
Atoms at both ends are fixed.



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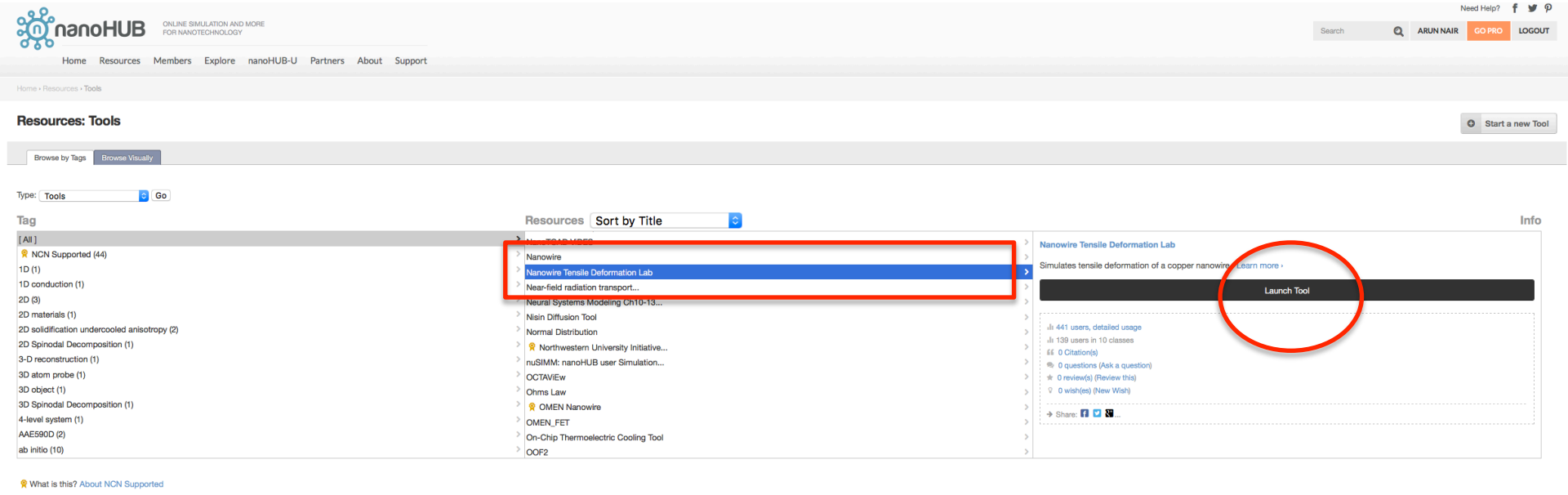
Upgrade to Pro m
$6.2
POPULAR TO
Fermi-Dirac Statistics
Newton's Law Basics 10 Presentations
CMOS Process Steps 4 Course Lectures, 1 Learning Module, 1 Presentation, 1 Teaching Material, 1 Tutorial
Thin Film Solar Cells 4 Presentations, 3 Course Lectures, 1 Paper
Charging Effects 6 Course Lectures, 2 Teaching Materials
Nanoscale Semiconductor Interfaces 2 Presentations, 1 Learning Module, 1 Tutorial
Schottky Diodes 5 Presentations, 3 Course Lectures
Atomic Force Microscopy 6 Presentations, 1 Tutorial
Density States 7 Course Lectures, 2 Presentations, 1 Teaching Material
Scanning Probe Microscopy 4 Animations, 2 Tutorials, 1 Course Lecture, 1 Presentation
Introduction To Bio-NEMS Bionanotechnology 5 Tutorials
Cyclic Peptide Nanotubes 3 Course Lectures, 2 Presentations, 1 Research Seminar
Contribute to a topic, or start a new one! Get started

Select Nanowire Tensile Deformation Lab



Nanowire Tensile Deformation Lab (9:15 am)

Terminate | Keep for later

1 Input → 2 Limits → 3 Boundary Conditions → 4 Simulation Parameters →

About this tool
Questions?

Nanowire Geometry

Unit cells x-direction: 4 + −

Unit cells y-direction: 4 + −

Unit cells z-direction: 4 + −

change to 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

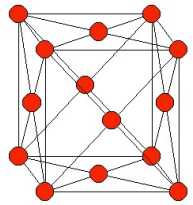
Equatorial radius (along y): 3

Polar radius (along z): 3

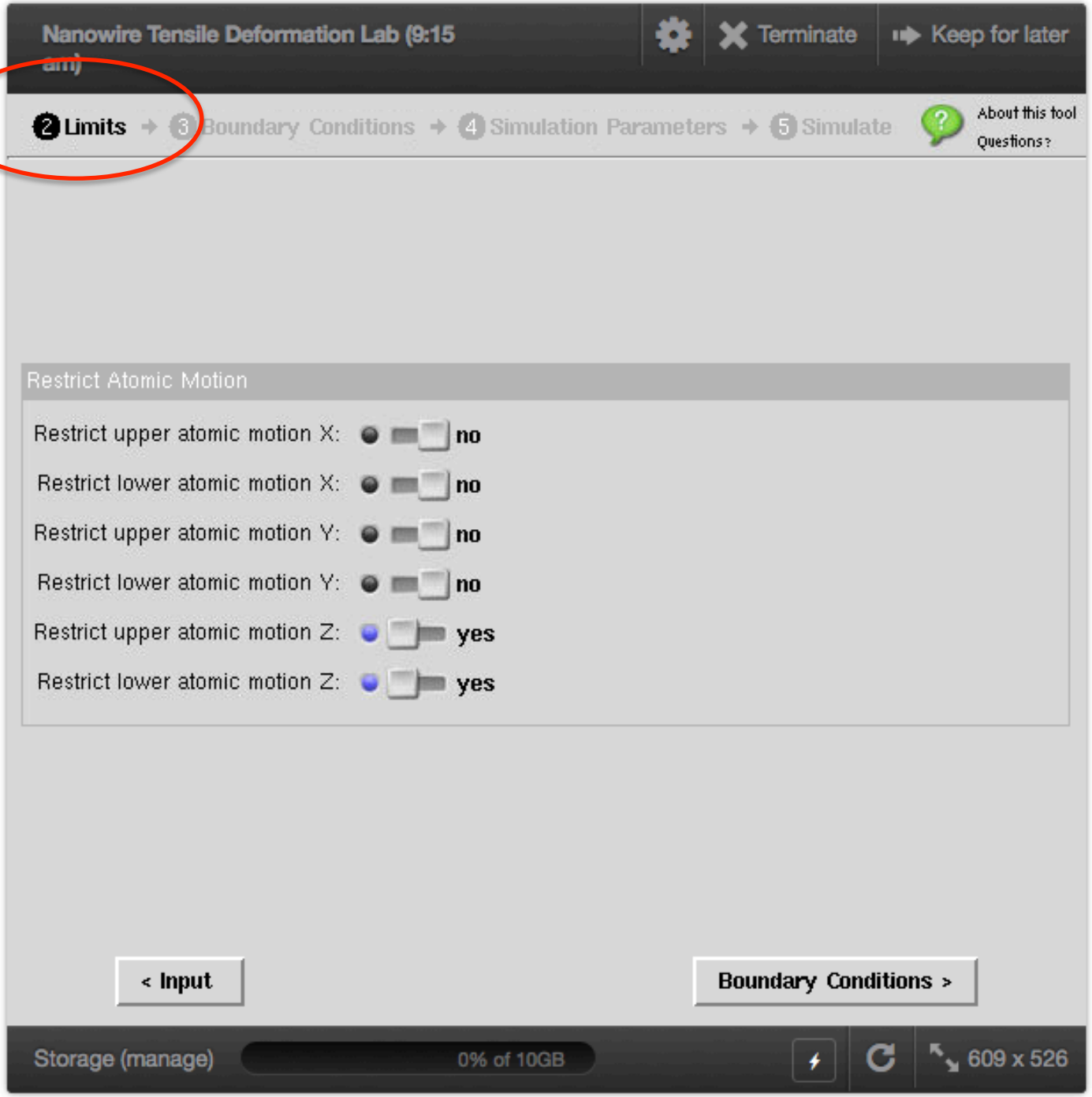
NOTE: This geometry is for a Copper nanowire modeled using an embedded atom model (EAM) potential.

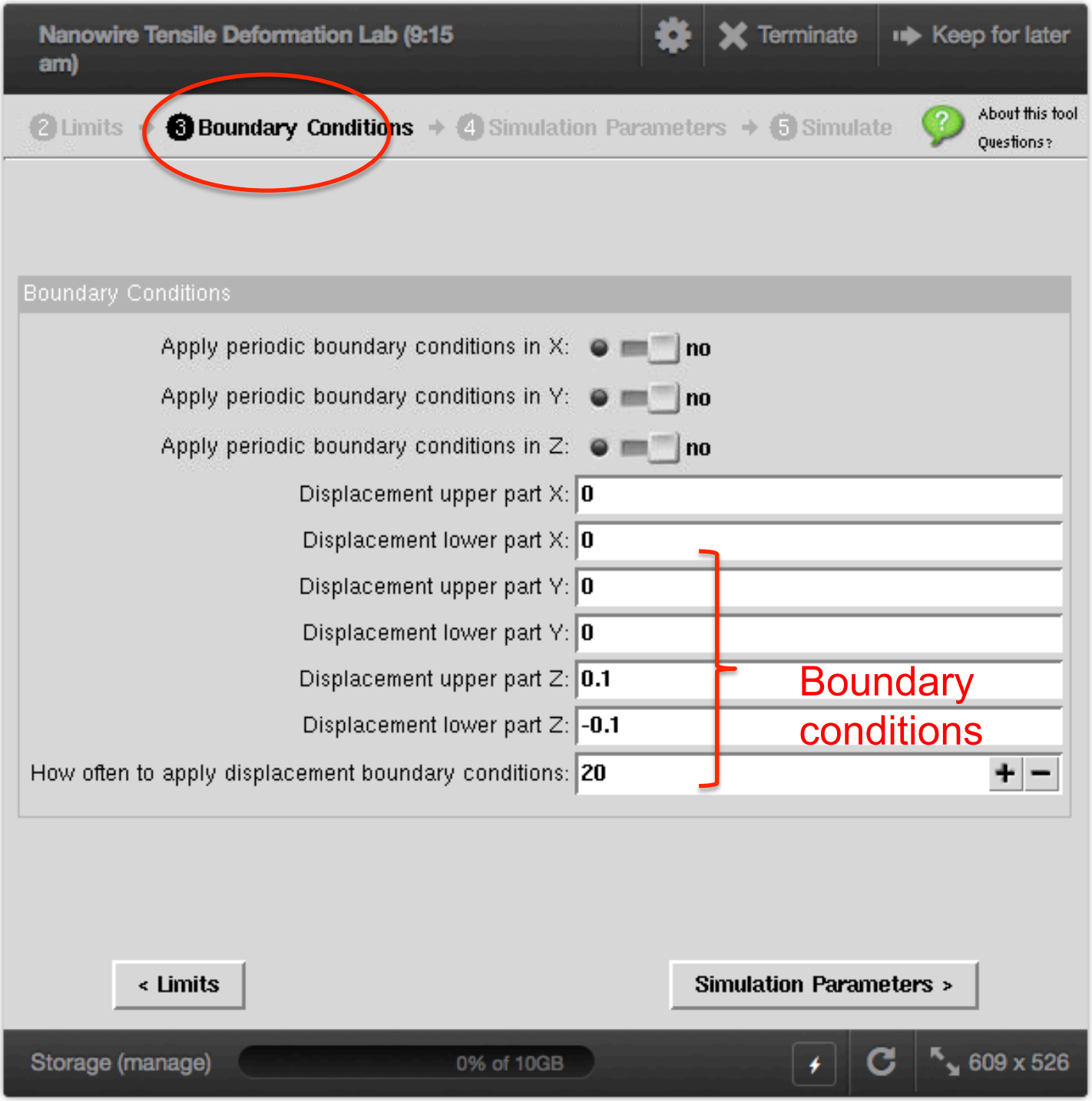
Limits »

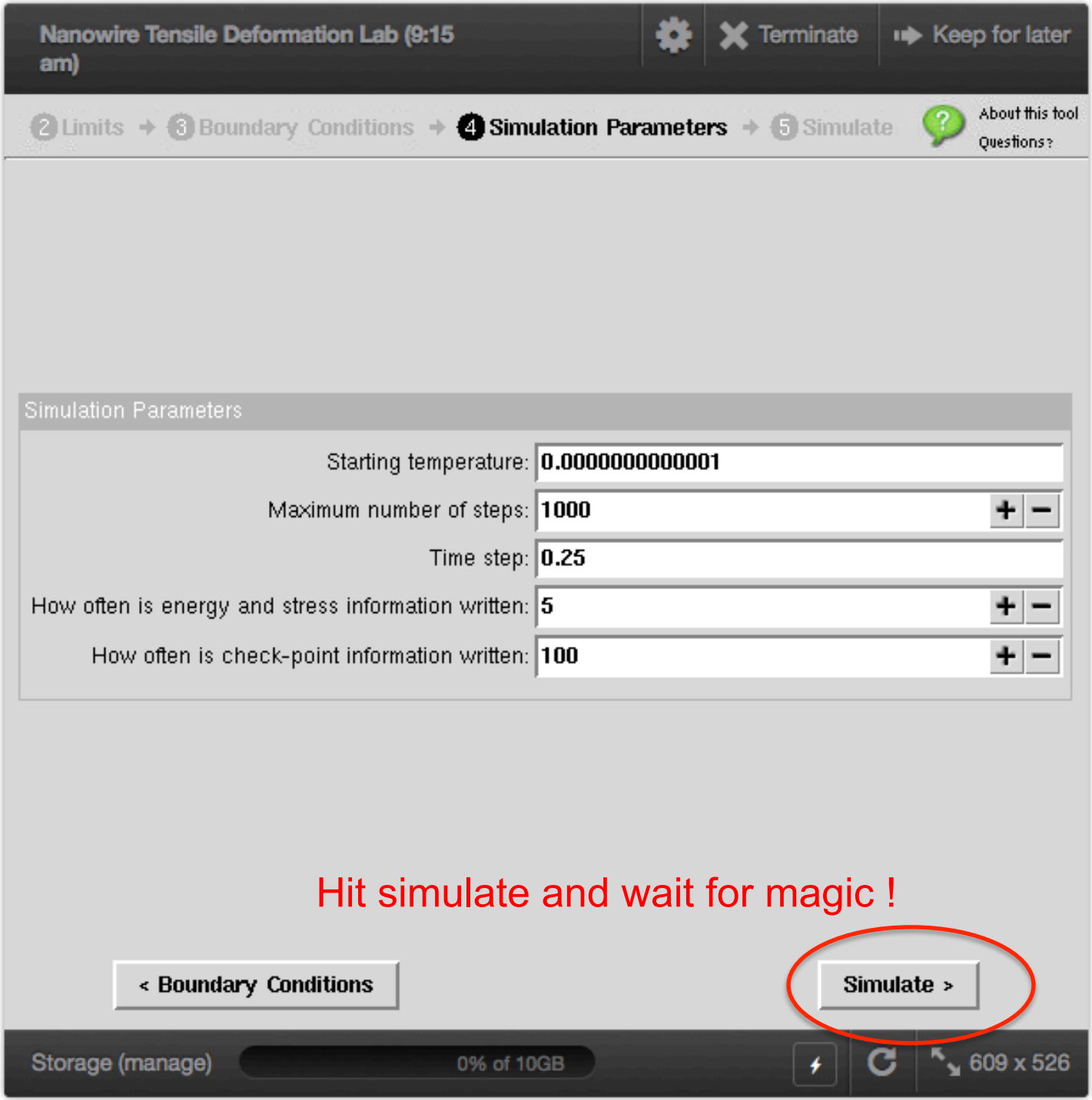
Storage (manage) 0% of 10GB 609 x 526

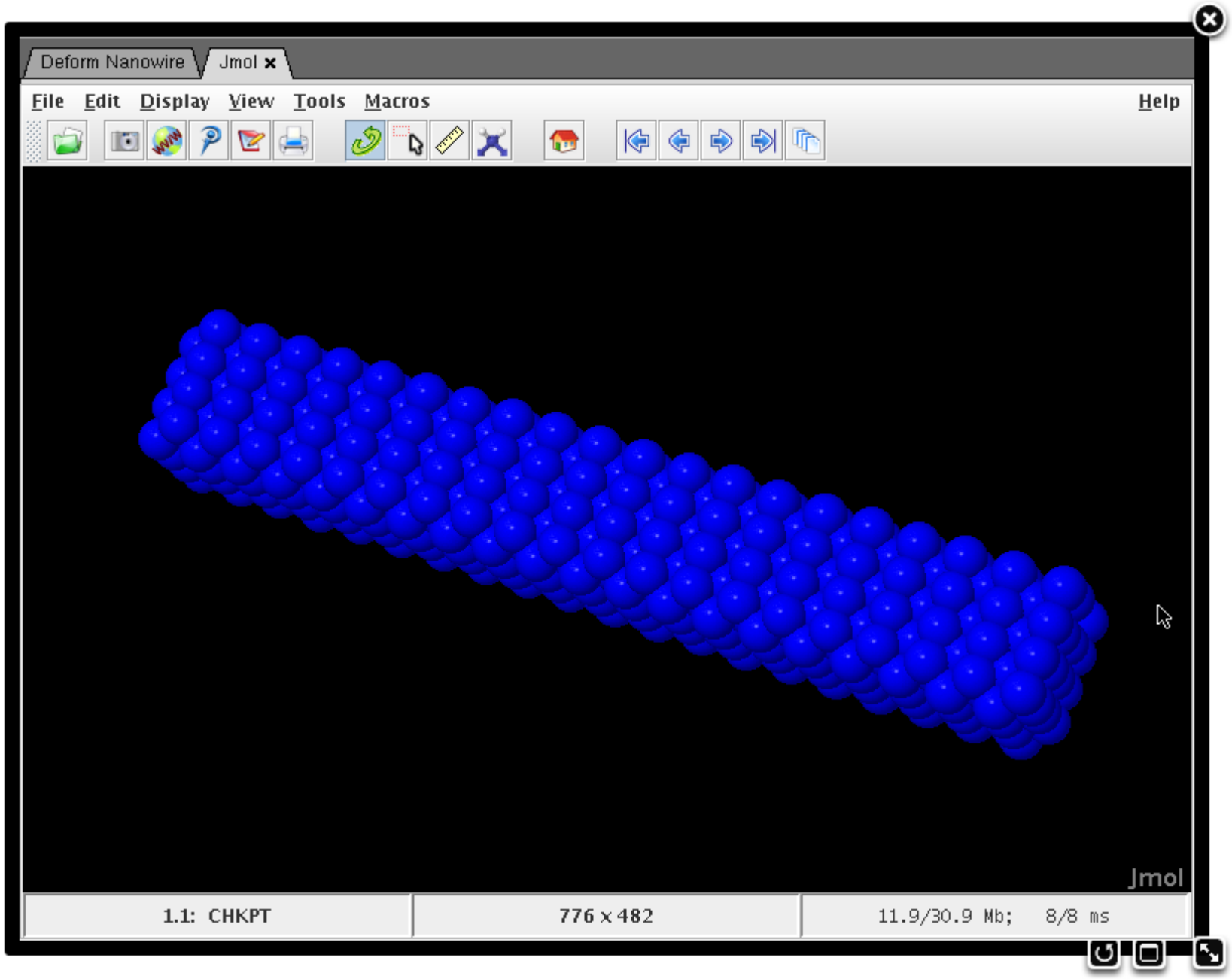


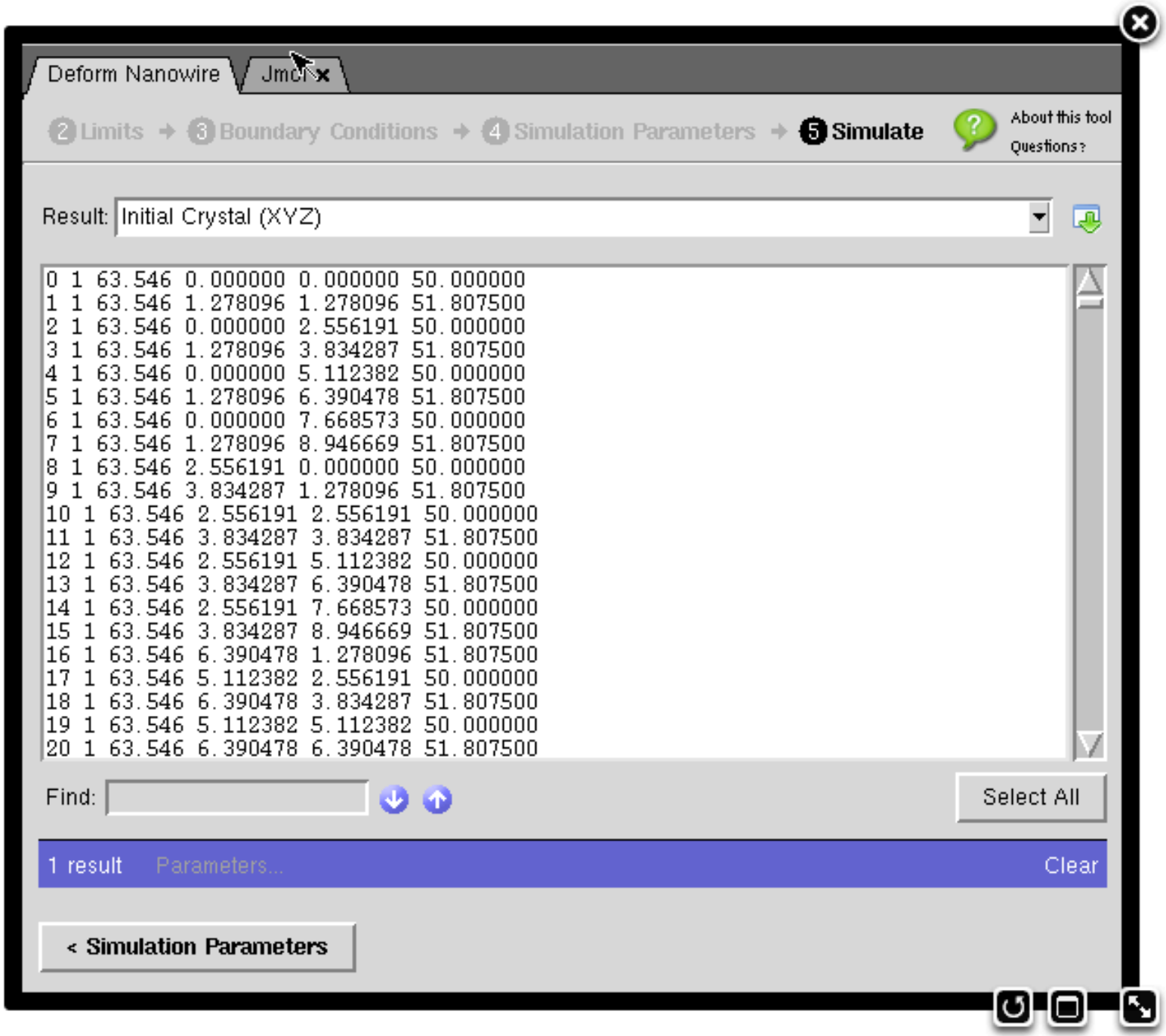
FCC lattice has 4 atoms per unit cell

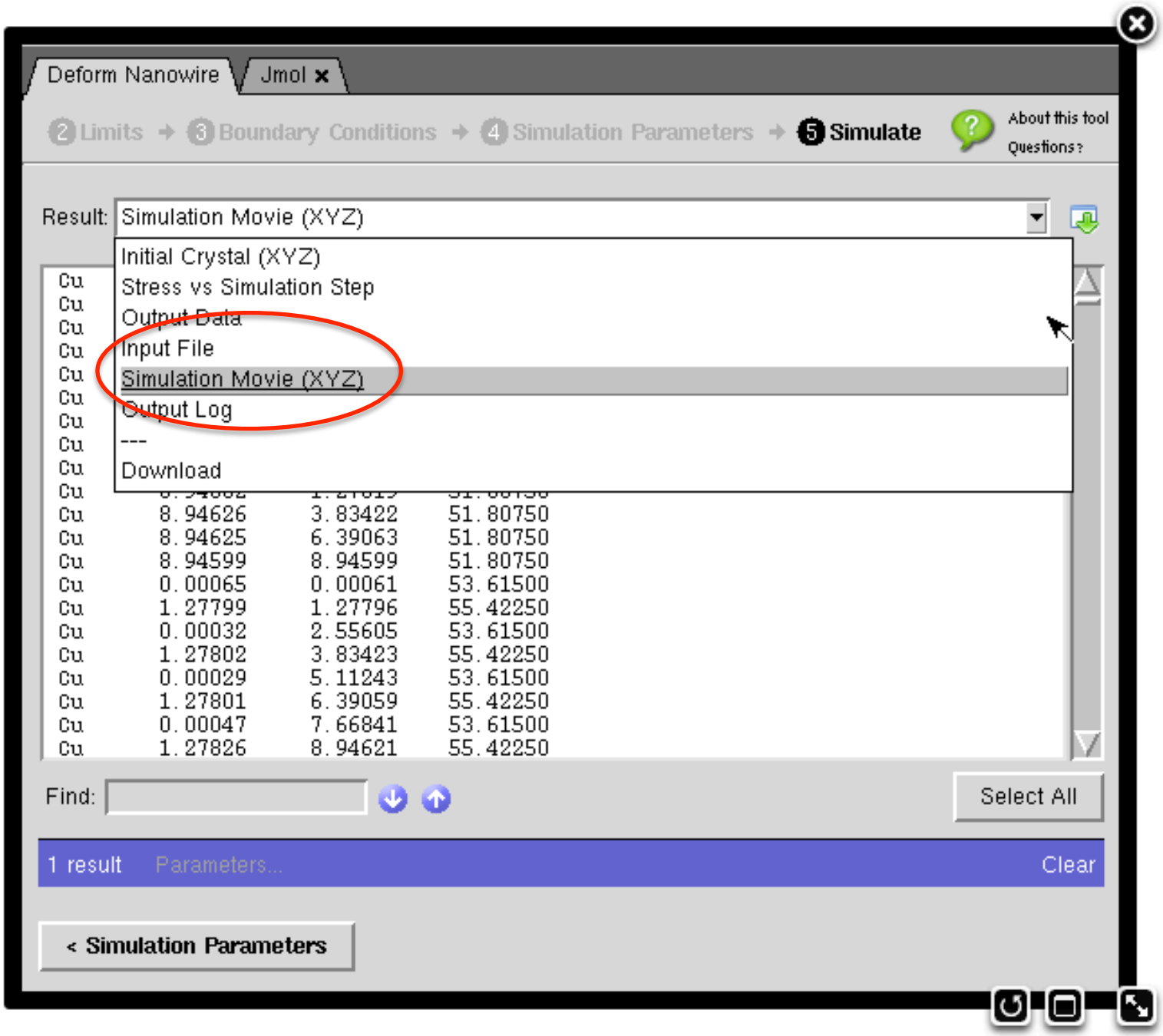

Nanowire Tensile Deformation Lab (9:15 am)
Terminate
Keep for later
2 Limits
3 Boundary Conditions
4 Simulation Parameters
5 Simulate
About this tool
Questions?
Restrict Atomic Motion
Restrict upper atomic motion X: no
Restrict lower atomic motion X: no
Restrict upper atomic motion Y: no
Restrict lower atomic motion Y: no
Restrict upper atomic motion Z: yes
Restrict lower atomic motion Z: yes
< Input
Boundary Conditions >
Storage (manage)
0% of 10GB
609 x 526


Nanowire Tensile Deformation Lab (9:15 am)
Terminate
Keep for later
2 Limits
3 Boundary Conditions
4 Simulation Parameters
5 Simulate
About this tool
Questions?
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
Boundary conditions
< Limits
Simulation Parameters >
Storage (manage)
0% of 10GB
609 x 526


Nanowire Tensile Deformation Lab (9:15 am)
Terminate
Keep for later
2 Limits
3 Boundary Conditions
4 Simulation Parameters
5 Simulate
About this tool
Questions?
Simulation Parameters
Starting temperature: 0.0000000000001
Maximum number of steps: 1000
Time step: 0.25
How often is energy and stress information written: 5
How often is check-point information written: 100
Hit simulate and wait for magic !
< Boundary Conditions
Simulate >
Storage (manage)
0% of 10GB
609 x 526


Deform Nanowire
Jmol
File Edit Display View Tools Macros Help
Jmol
1.1: CHKPT
776 x 482
11.9/30.9 Mb; 8/8 ms


Deform Nanowire
Jmol
2 Limits → 3 Boundary Conditions → 4 Simulation Parameters → 5 Simulate
About this tool
Questions?
Result: Initial Crystal (XYZ)
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
Find:
Select All
1 result
Parameters...
Clear
< Simulation Parameters


Deform Nanowire
Jmol
2 Limits
3 Boundary Conditions
4 Simulation Parameters
5 Simulate
About this tool
Questions?
Result:
Simulation Movie (XYZ)
Initial Crystal (XYZ)
Stress vs Simulation Step
Output Data
Input File
Simulation Movie (XYZ)
Output Log

Download
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
Find:
Select All
1 result
Parameters...
Clear
< Simulation Parameters

PART B: Visualization

Visualization of results

http://www.ks.uiuc.edu/Research/vmd/

THEORETICAL and COMPUTATIONAL BIOPHYSICS GROUP
NIH RESOURCE FOR MACROMOLECULAR MODELING AND BIOINFORMATICS
UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

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  - VMD Molecular Graphics Viewer
  - NAMD Molecular Dynamics Simulator
  - BioCoRE Collaboratory Environment
  - MD Service Suite
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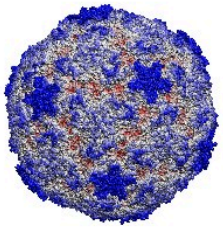
VMD
Visual Molecular Dynamics

VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting. VMD supports computers running MacOS X, Unix, or Windows, is distributed free of charge, and includes source code.
(more details...)

Spotlight

VMD is capable of working with very large structures up to the limits of available memory. The 64-bit versions of VMD allow huge simulation trajectories to be loaded into physical memory and accomodate large volumetric datasets. This 400,000 atom virus structure is just a simple example of what can be done with VMD on an appropriately equipped graphics workstation.
Other Spotlights



Overview

Molecular representations
Supported molecular file formats
GPU-accelerated computing
Interactive molecular dynamics
Programs that use VMD
VMD research publications
How to cite VMD, List of **4,872 papers citing VMD** (Oct 2010)

Download

Download (all versions)
VMD 1.9 (MacOS X, Unix, Windows)
VMD 1.8.7 (MacOS X, Unix, Windows)
VMD plugin library
VMD script library
License, Copyright and Disclaimer

News and Announcements

Immersive out-of-core visualization of large-size and long-timescale molecular dynamics trajectories, LNCS, 2011 NEW
VMD 1.9 released for MacOS X, Unix, and Windows (March 2011) NEW
Fast Analysis of Molecular Dynamics Trajectories with Graphics Processing Units — Radial Distribution Function Histogramming, J. Comp. Phys, 2011 NEW
2011 VMD Calendar
Setting up a simple stereo system
Illinois Researcher Named NVIDIA CUDA Fellow
Immersive Molecular Visualization and Interactive Modeling with Commodity Hardware, ISVC 2010
GPU-Accelerated Molecular Modeling Coming of Age, JMGM, 2010
VMD included in Tesla Bio Workbench portal
Investigating Interfaces of Macro-Molecular Complexes with Intervor
VMD QuicktimeVR/Flash rendering of PDB structures
Past announcements

Gallery

Software Downloads

Download VMD:

VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting.

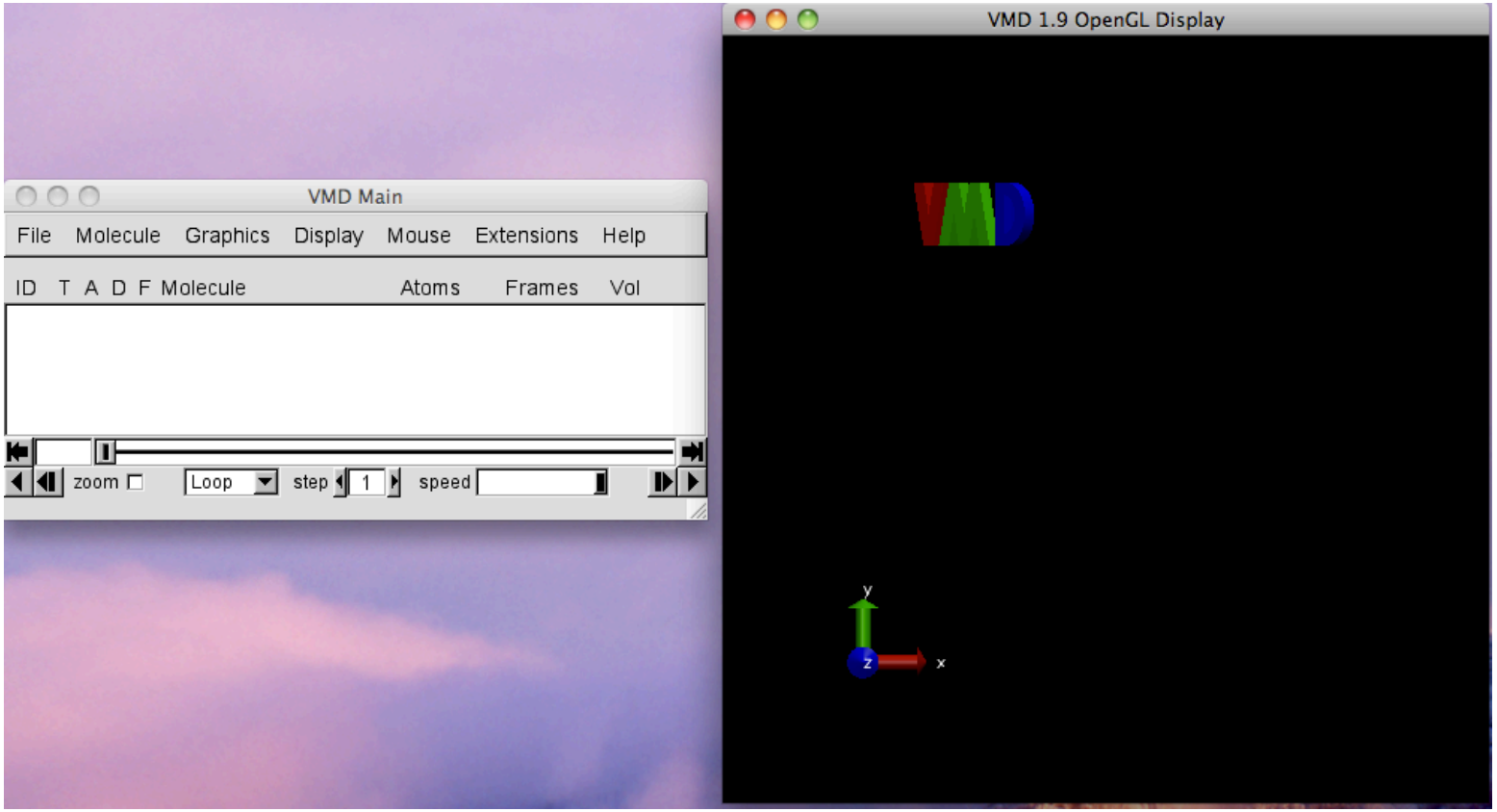
Selecting an archive below will lead to a user registration and login page. Your download will continue after you have registered or logged in.

Version 1.9.2 (2014-12-29) Platforms:

We recommend that all users upgrade to VMD 1.9.2

- **Source Code**
- **Blue Waters (64-bit Cray XK7)** (NCSA Blue Waters (64-bit Cray XK7) MPI, CUDA, OpenGL Pbuffers, TachyonL-OptiX)
- **LINUX_64 OpenGL, CUDA, TachyonL-OptiX** (Linux (RHEL 5.5 and later) 64-bit Intel/AMD x86_64 SSE, with CUDA and TachyonL-OptiX)
- **LINUX_64 OpenGL, CUDA** (Linux (RHEL 4.6 and later) 64-bit Intel/AMD x86_64 w/ SSE, with CUDA)
- **LINUX_64 Text-mode** (Linux (RHEL 4.6 and later) 64-bit Intel/AMD x86_64 w/ SSE, Text-mode)
- **LINUX OpenGL, CUDA** (Linux (RHEL 4.6 and later) Intel/AMD x86 w/ SSE, with CUDA)
- **MacOS X OpenGL, CUDA (32-bit Intel x86)** (Apple MacOS-X 10.5.x or later with CUDA)
- **MacOS X OpenGL (32-bit Intel x86)** (Apple MacOS-X (10.4.7 or later) with hardware OpenGL (native bundle))
- **SOLARISX86_64 OpenGL** (Sun Solaris 10 (64-bit x86) with OpenGL)
- **Windows OpenGL, CUDA** (Windows XP/Vista/7/8 (32-bit) with OpenGL and CUDA)
- **Windows OpenGL** (Microsoft Windows XP/Vista/7/8 (32-bit) using OpenGL)

New user registration


VMD Main
File
Molecule
Graphics
Display
Mouse
Extensions
Help
ID T A D F Molecule
Atoms
Frames
Vol
zoom
Loop
step
1
speed
VMD 1.9 OpenGL Display
y
z
x

To view your output file