

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

Recitation #4

Creating molecules and crack propagation lab

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Massachusetts Institute of Technology

Review from last week

- Review about ensembles
- MC vs MD
- Ergodic hypothesis
- Questions?

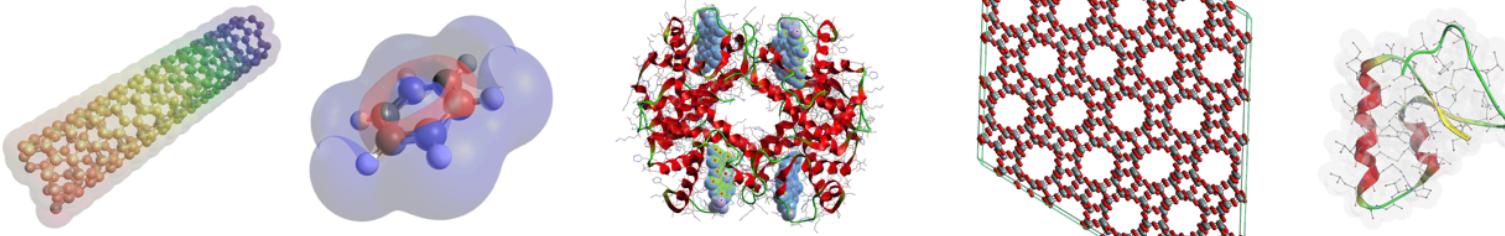
Creating initial coordinates

Creating molecules: Avogadro

<https://avogadro.cc>

[Download](#)[Manual](#)[Discuss](#)[Thanks](#)[Contribute](#)[Teach](#)

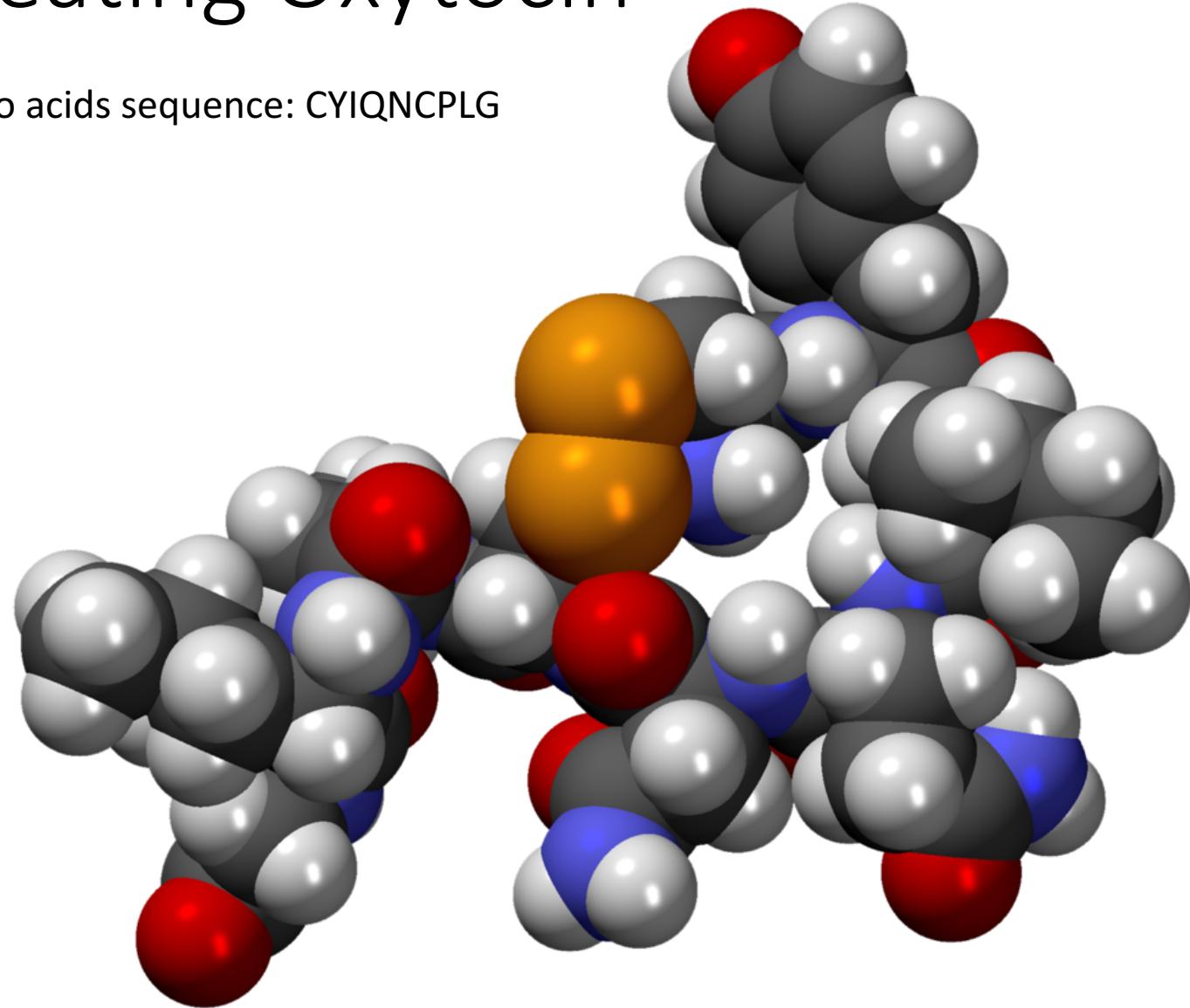
Avogadro is an advanced molecule editor and visualizer designed for cross-platform use in computational chemistry, molecular modeling, bioinformatics, materials science, and related areas. It offers flexible high quality rendering and a powerful plugin architecture.



- **Cross-Platform:** Molecular builder/editor for Windows, Linux, and Mac OS X.
- **Free, Open Source:** Easy to install and all source code and documentation is [available to modify or extend](#).
- **International:** Translations into Chinese, French, German, Italian, Russian, Spanish, and others, with [more languages to come](#).
- **Intuitive:** Built to work easily for students and advanced researchers both.
- **Fast:** Supports multi-threaded rendering and computation.
- **Extensible:** Plugin architecture for developers, including rendering, interactive tools, commands, and Python scripts.
- **Flexible:** Features include [Open Babel](#) import of chemical files, input generation for multiple computational chemistry packages, crystallography, and biomolecules.
- **How to cite Avogadro:** [The Avogadro Paper](#)

Creating Oxytocin

Amino acids sequence: CYIQNCPLG





Avogadro File Edit View

Build

Select Extensions

Crystallography

Window

Help

Cartesian Editor...

Change H to Methyl

Add Hydrogens

Add Hydrogens for pH...

Remove Hydrogens

Insert

DNA/RNA...

Fragment...

SMILES...

Peptide...

Invert Chirality

Super Cell Builder...

Nanotube Builder...

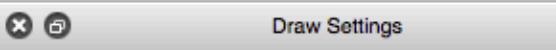


Messages



Tool Settings...

Display Settings...



View 1

Element: Carbon (6)

Bond Order: Single

 Adjust Hydrogens

Insert Peptide

Peptide Builder

Amino Acids:

Ala	Arg	Asn	Asp
Cys	Glu	Gln	Gly
His	Ile	Leu	Lys
Met	Phe	Pro	Ser
Thr	Trp	Tyr	Val

Sequence (N to C):

Structure:

Stereochemistry:

Straight Chain

Phi: 180.00°

Psi: 180.00°

N Terminus: NH₂

C Terminus: CO₂H

Chain Number: A

Insert Peptide

Messages

From one to three letters sequence

http://molbiol.ru/eng/scripts/01_17.html

Name (not necessary):

Amino acid sequence:
(case insensitive, all symbols, except standard symbols of
amino acids and stop-codons ("*", "****" and "end") are disregarded.)

20 amino acids in one line;
 capital letters (for one letter code);
 print out the original sequence.



untitled.cml - Avogadro

Tool Settings... Display Settings...

Draw Settings

Element: Carbon (6)

Bond Order: Single

Adjust Hydrogens

Insert Peptide

Peptide Builder

Amino Acids:

Ala	Arg	Asn	Asp
Cys	Glu	Gln	Gly
His	Ile	Leu	Lys
Met	Phe	Pro	Ser
Thr	Trp	Tyr	Val

Sequence (N to C):

Cys-Tyr-Ile-Gln-Asn-Cys-Pro-Leu-Gly

Structure:

Straight Chain
Alpha Helix
Beta Sheet
3-10 Helix
Pi Helix
Other

Stereochemistry:

L D

N Terminus: NH₂

C Terminus: CO₂H

Chain Number: A

Insert Peptide

Messages



Tool Settings...

Display Settings...

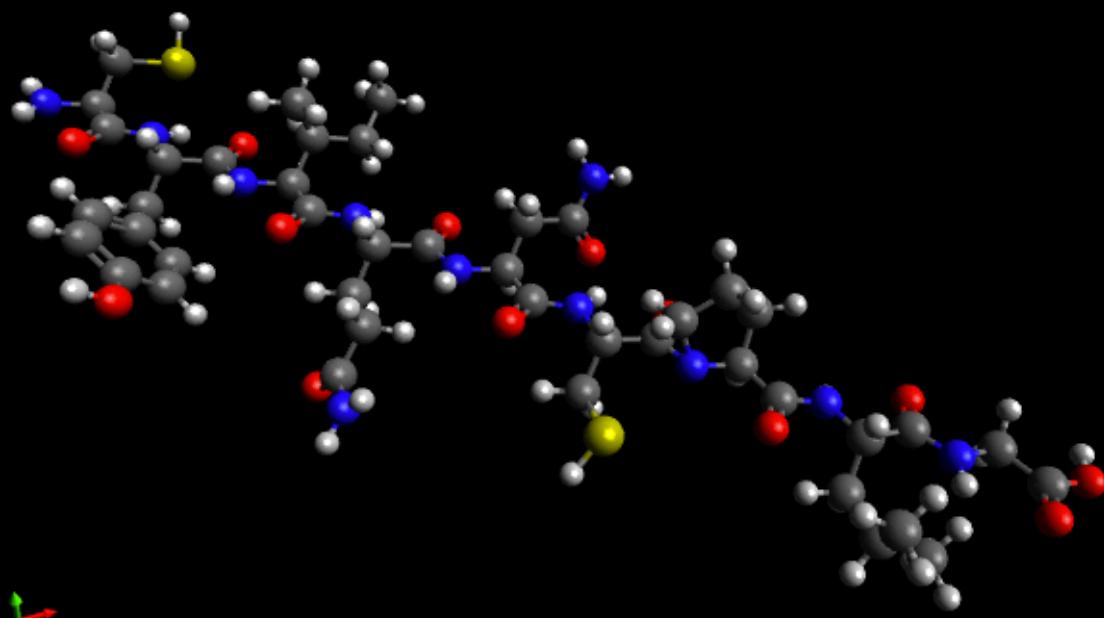
Selection Settings

Selection Mode: Atom/Bond

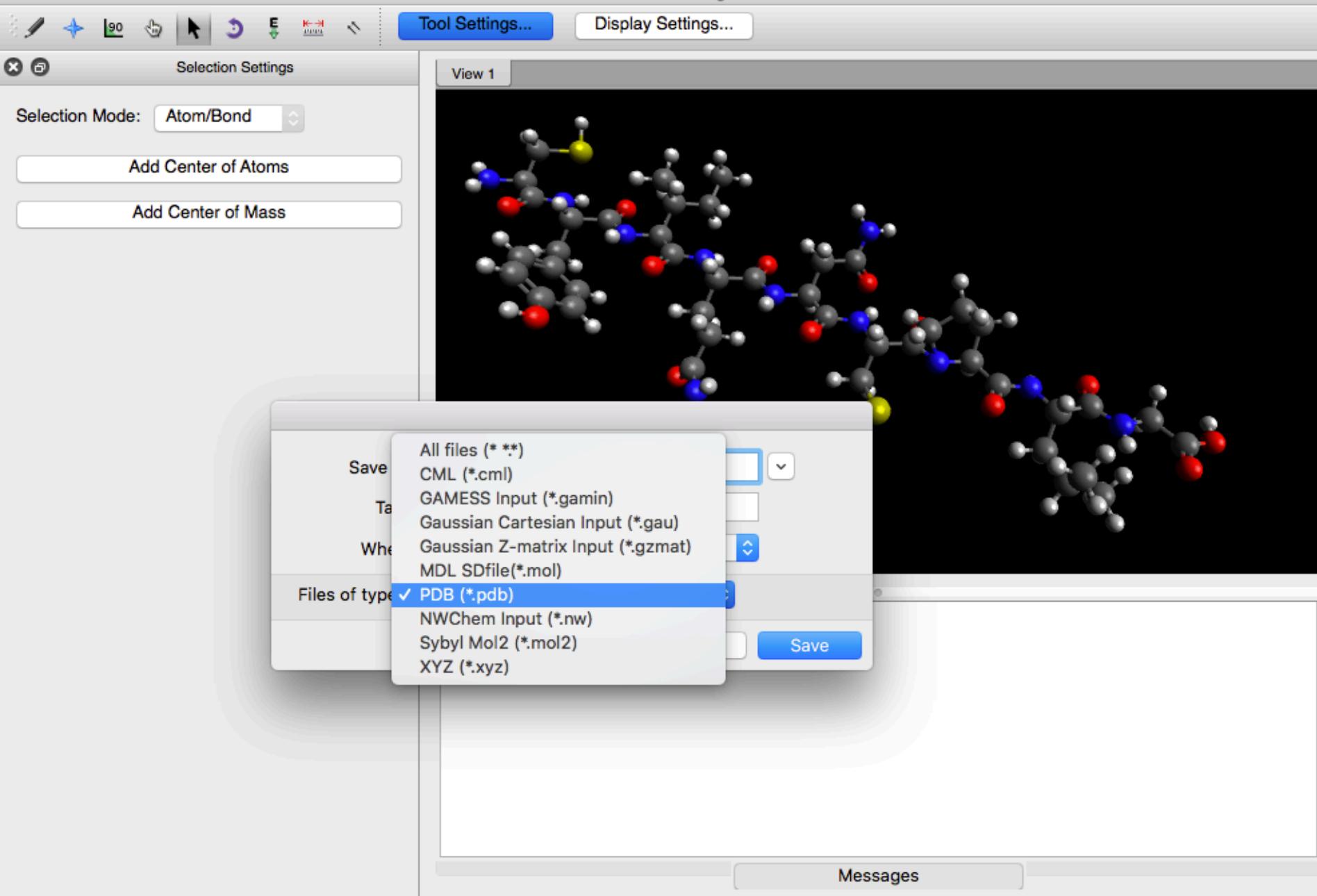
Add Center of Atoms

Add Center of Mass

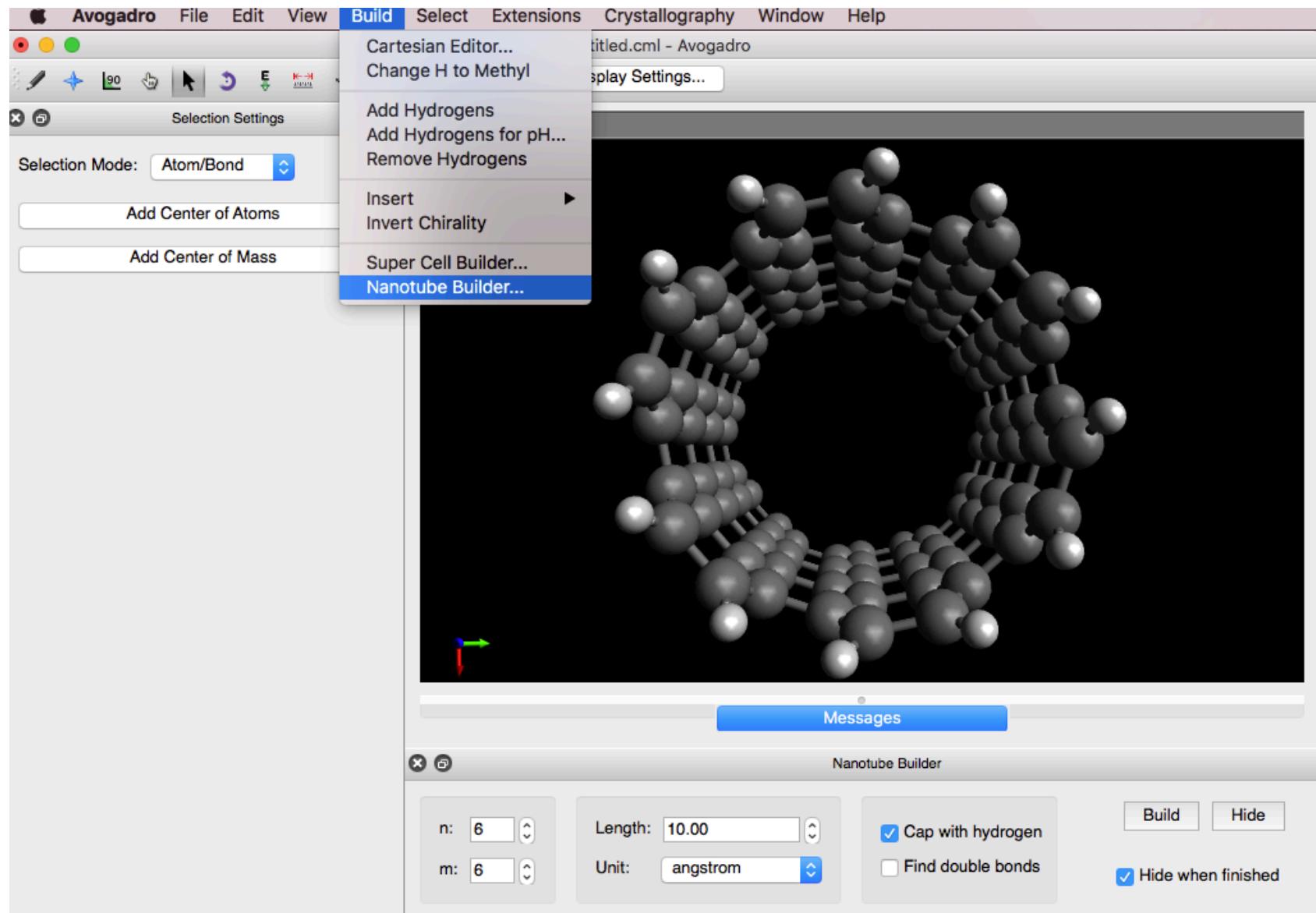
View 1



Messages



Creating nanotubes



Getting to work with crack propagation lab

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

StarMolsim



star > molsim > StarMolsim NanoHub Tools

Home

Tools

Donate

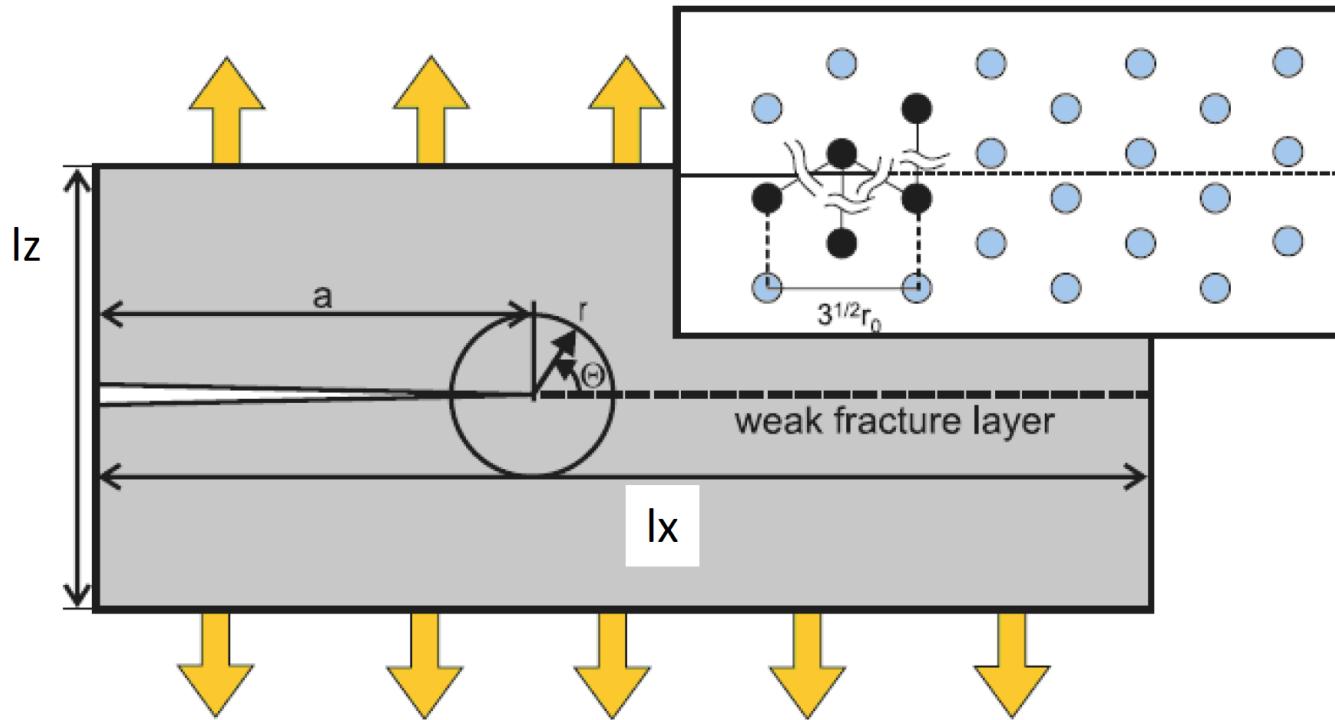
StarMolsim Tools on NanoHUB.org

The StarMolsim tools are hosted on nanohub.org. Below is a list of links to the StarMolsim tools migrated to nanohub.org:

- [stretchfcc](#) - simulates a continuous expansion of an FCC crystal while measuring the energy, stresses, etc
- [deformnanowire](#) - simulates tensile deformation of a copper nanowire
- [crackprop](#) - models supersonic crack propagation in a 2D triangular lattice
- [stretchmol](#) - stretching simulation of an alpha-helical protein domain
- [tad](#) - temperature-accelerated dynamics simulation
- [atomic scale modeling toolkit](#) - this set of simulation tools provides students with the fundamentals of computational problem-solving techniques that are used to understand and predict properties of nanoscale systems.

<https://nanohub.org/tools/deformnanowire>

Breaking a 2D lattice network



r_0 : equilibrium interatomic distance

a : initial crack length

Density: $1.155m_a/r_0$

l_x , l_y : system size

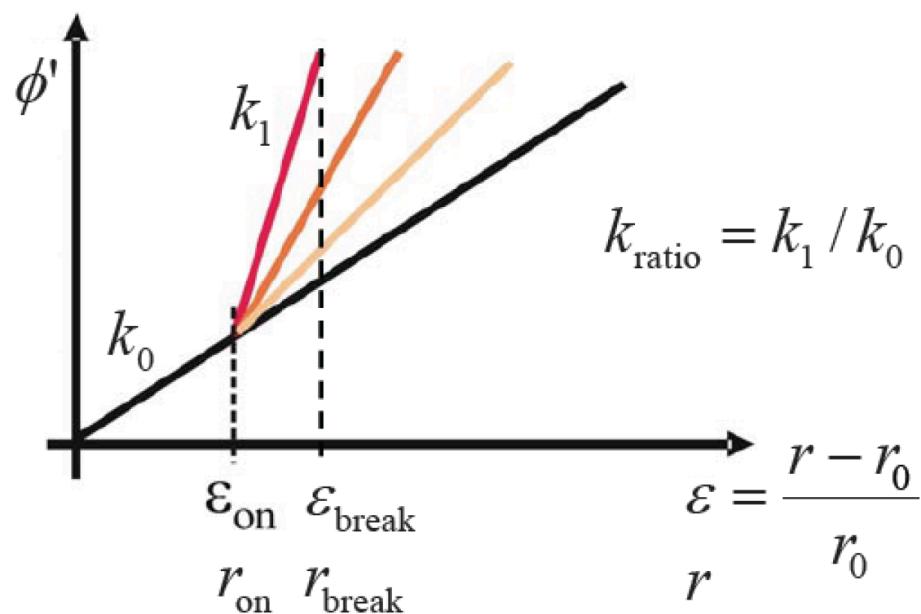
Interatomic potential: biharmonic potential

Spring constant k_0 associated with small perturbations from equilibrium distance r_0

Spring constant k_1 associated with large bond stretching for atomic separation $r > r_{on}$

$$\phi(r) \begin{cases} a_0 + \frac{1}{2} k_0 (r - r_0)^2 & \text{if } r < r_{on} \\ a_1 + \frac{1}{2} k_1 (r - r_1)^2 & \text{if } r > r_{on} \end{cases}$$

r_{on} – critical atomic separation for onset of the hyperelastic effect



$$K_{ratio} > 1$$

$$K_{ratio} < 1$$

Material characteristic

$$\varepsilon = \frac{r - r_0}{r_0}$$



RESOURCES EXPLORE NANOHUB-U PARTNERS COMMUNITY ABOUT SUPPORT

Logged in Help Search

Home > Tools > Crack Propagation Lab > About

Collect

Crack Propagation Lab

By Markus Buehler¹, Justin Riley¹, Joo-Hyoung Lee, Jeffrey C Grossman²

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

Models supersonic crack propagation in a 2D triangular lattice

[Launch Tool](#)

Version 1.1 - published on 03 Sep 2014

doi:10.4231/D31G0HW04 [cite this](#)

[View All Supporting Documents](#)

Tool Audience Unrated

276 users, [detailed usage](#)

0 Citation(s)

0 questions ([Ask a question](#))

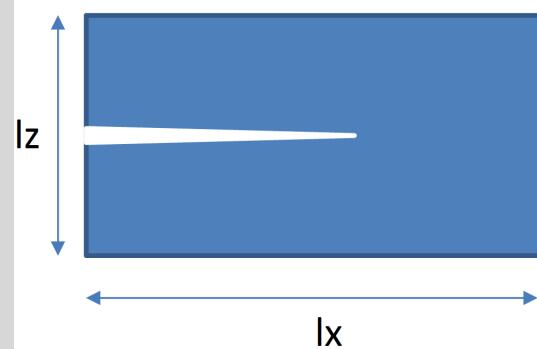
0 review(s) ([Review this](#))

0 wish(es) ([New Wish](#))

→ Share: ...



1 Crystal Geometry → 2 Crack Properties → 3 Simulation Parameters → 4 Run Experiment 



Crystal Geometry

Unit cells in x-direction: **200**



Unit cells in z-direction: **100**



[Crack Properties >](#)

Storage (manage)



10% of 10GB



620 x 535

Crack Propagation Lab

X Terminate ▶ Keep for later

Crack Propagation Lab Jmol X

Geometry → ② Crack Properties → ③ Simulation Parameters → ④ Run Experiment About this tool
Questions?

Crack Properties

Crack length ratio (aa/dimension_X): **0.3**

Strain Rate: **0.0005**

Breaking distance (radius): **1.15**

ON radius for biharmonic potential: **1.2**

Spring constant: **28.57**

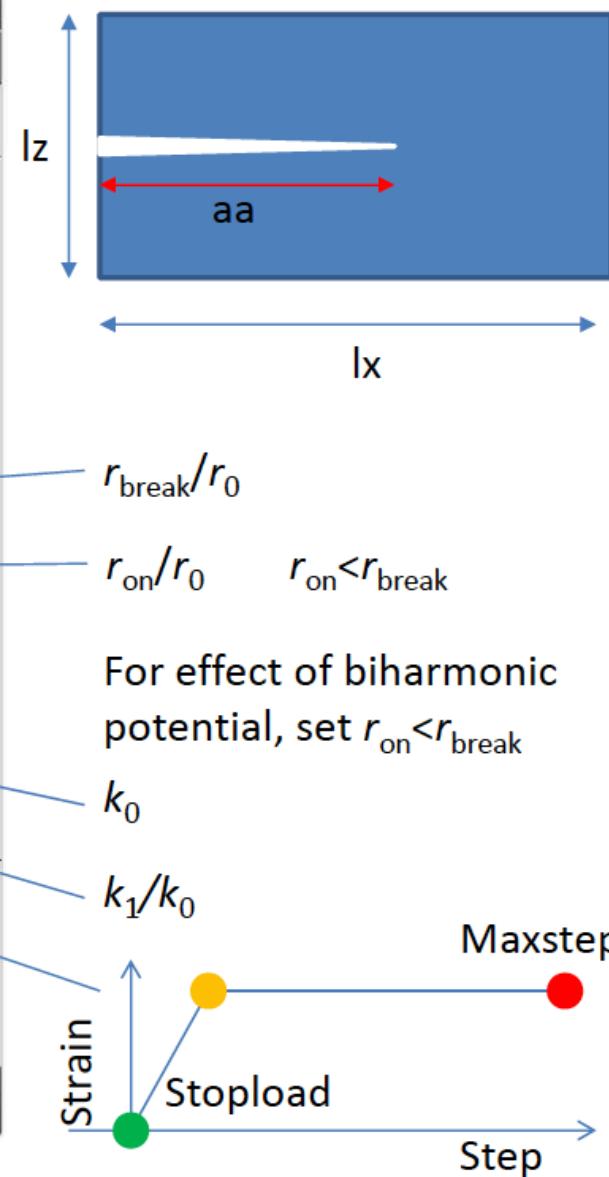
Spring constant ratio: **1.00**

stopload: **10000**

[Crystal Geometry](#) [Simulation Parameters >](#)

Storage (manage) 20% of 1GB

The diagram shows a blue rectangular domain representing a crystal. A horizontal white line segment within the rectangle is labeled 'aa', representing the crack length. The vertical dimension of the rectangle is labeled 'lx' at the bottom right, and the horizontal dimension is labeled 'lz' at the top left.





Simulation Parameters

Maximum number of steps: **30000** Timestep: **0.00450**How often is energy and stress information written: **5** How often is check-point information written: **500**

< Crack Properties

Run Experiment >



To do in class:

- Try different aa length for the crack.
- How does changing the ON radius affect the material behavior?