

591V Multiscale Materials Modeling

Computational Lab-2

Outline: Today's class

Outline:

Part A: CHARMM forcefield.

Part B: Steered Molecular Dynamics (SMD)

Part C: Stretching simulation of protein (nanoHUB).

Part D: Hydrogen bond analysis

PART A: CHARMM forcefield

CHARMM Force Field

Chemistry at HARvard Macromolecular Mechanics

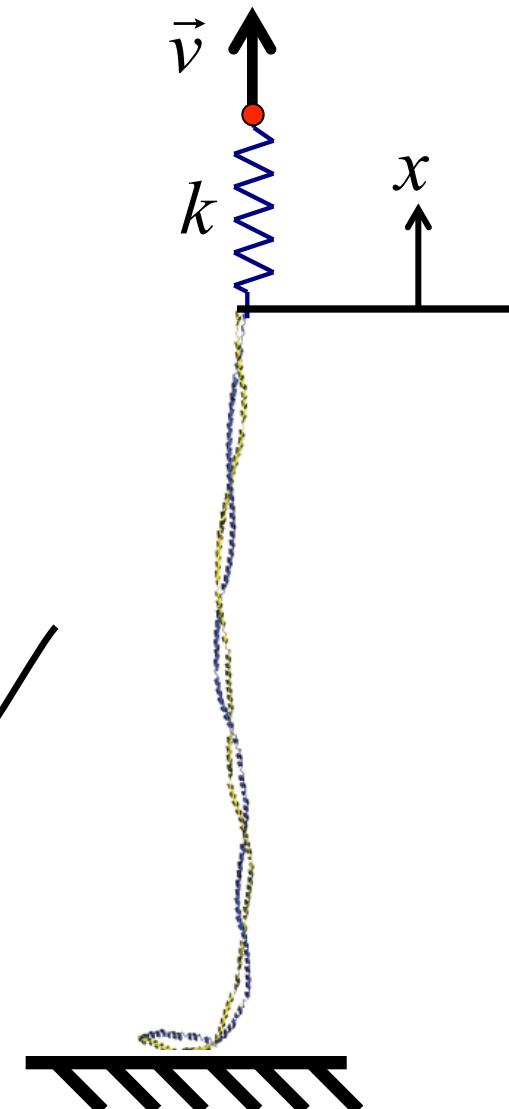
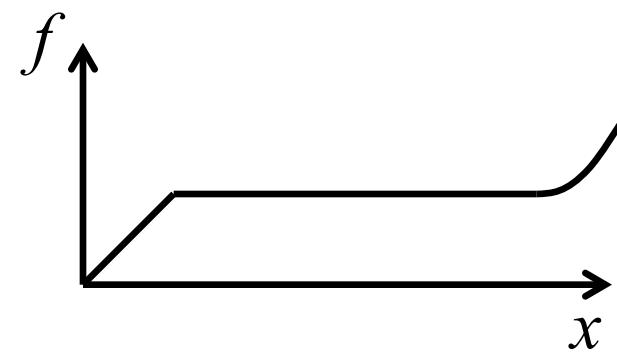
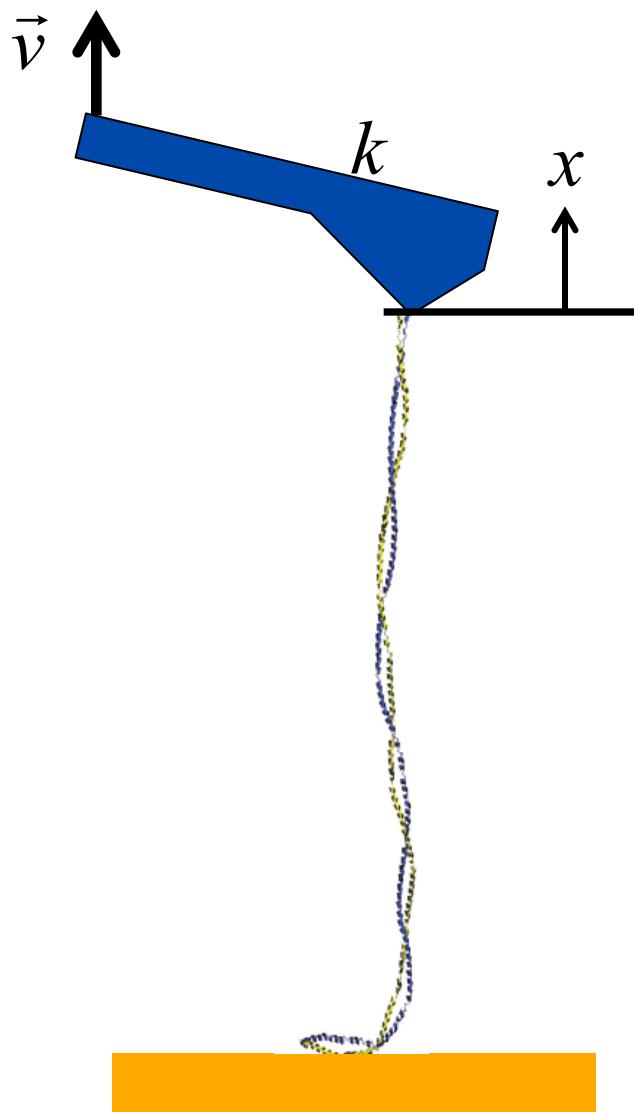
- A set of force fields for molecular dynamics.
- MD simulation and analysis package.
- Originally developed in 1983, and evolved over the years.
- Focused on molecules of biological interest including proteins, peptides, lipids, and so on.
- Comprehensive recent review is available at
Journal of Computational Chemistry 30, 1545 (2009).

Different force fields for different problems

PART B: Steered Molecular Dynamics (SMD)

SMD mimics AFM single molecule experiments

Atomic force microscope



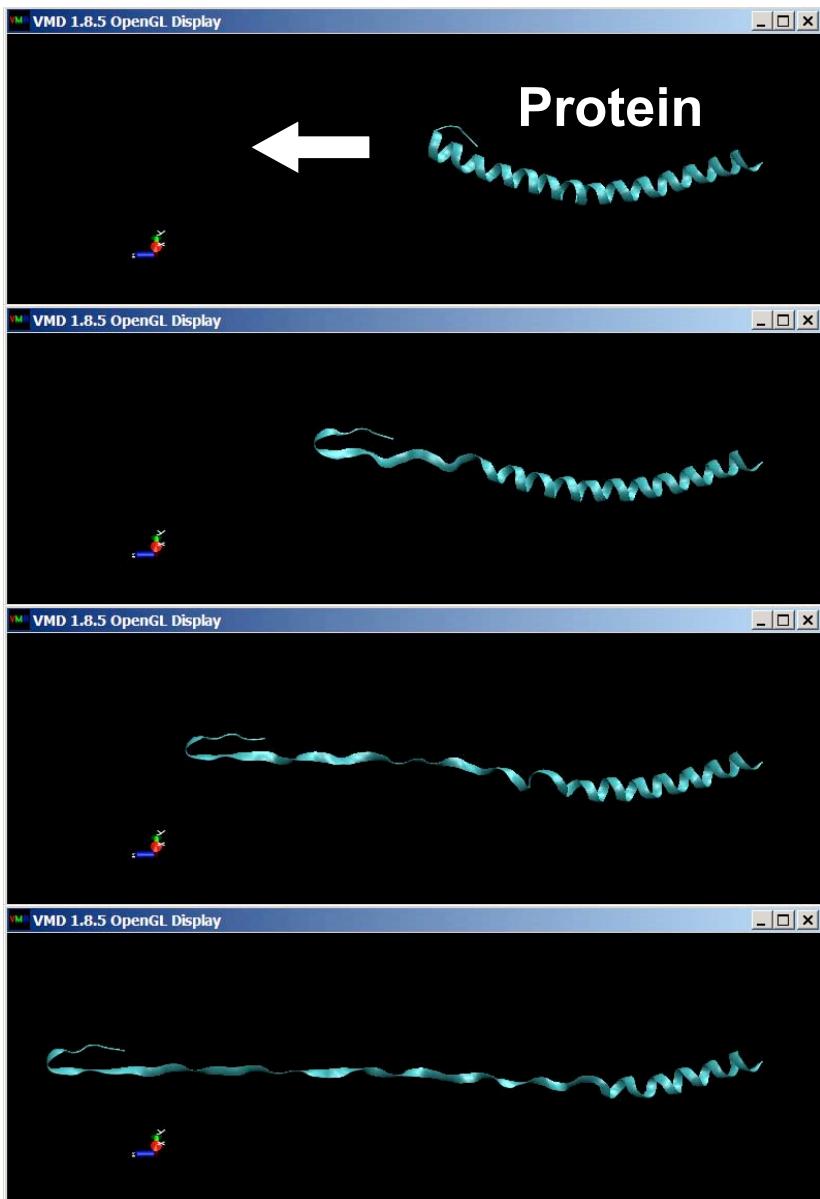
Steered Molecular Dynamics

- A method of applying external force to study various (biological) processes such as unfolding of macromolecules and elastic response of mechanical proteins.
- We apply a tensile load to the ends of a protein (stretching out a protein molecule).
- Knowledge of the mechanism of association and dissociation of macromolecules is important for many biological structures and processes.

PART C: Stretching simulation of protein

Outline

- NAMD
- CHARMM Force Field
- SMD
- **Stretching simulation of an alpha-helical protein domain from nanoHUB**



NAMD

Not (just) Another Molecular Dynamics program

<http://www.ks.uiuc.edu/Research/namd/>

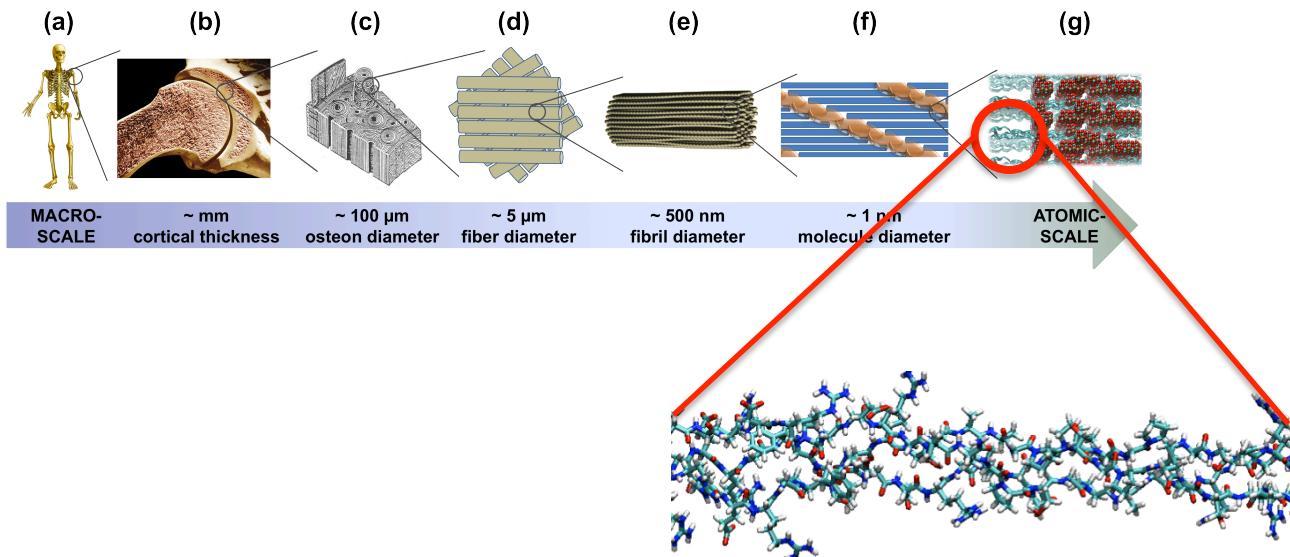
- Developed by the joint collaboration of the Theoretical and Computational Biophysics Group and the Parallel Programming Laboratory at the UIUC.
- A code designed for high-performance simulation of large biomolecular systems.
- NAMD is compatible other MD packages such as AMBER, CHARMM, GROMACS and X-PLOR.
- We use the CHARMM force field (J. Phys. Chem. B **102**, 3586 (1998)), which is a reasonable model for atomistic interaction within proteins and between different proteins.

NAMD

In order to perform NAMD simulations, we need 4 external files:

- **Coordinate file** : Positions of each atom (xyz coordinates) in a system (protein)
- **Structure file** : Structure of the protein and the kind of bonds and interactions between the individual atoms (e.g. single bond, double bond, etc.)
- **Fixed atom file** : To specify which atoms move and which don't.
- **SMD file** : To specify which atoms are pulled and which aren't.
(<http://www.ks.uiuc.edu/Research/namd/2.10/ug/node48.html>)

Hierarchical Structure of Bone



Type I collagen (Gautieri et al., Nano letters, 2011)

We are going to simulate a segment of the collagen molecule

Resources: Tools

[Start a new Tool](#)[Browse by Tags](#) [Browse Visually](#)Type:

Tag

[\[All \]](#)[NCN Supported \(44\)](#)[1D \(1\)](#)[1D conduction \(1\)](#)[2D \(3\)](#)[2D materials \(1\)](#)[2D solidification undercooled anisotropy \(2\)](#)[2D Spinodal Decomposition \(1\)](#)[3-D reconstruction \(1\)](#)[3D atom probe \(1\)](#)[3D object \(1\)](#)[3D Spinodal Decomposition \(1\)](#)[4-level system \(1\)](#)[AAE590D \(2\)](#)[What is this? About NCN Supported](#)

Resources

[Sort by Title](#)

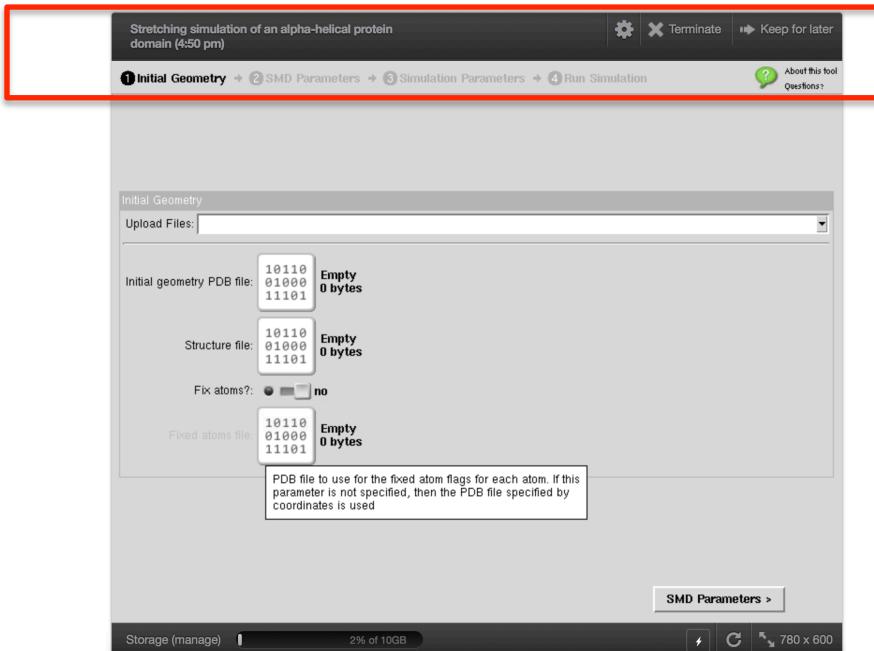
- > Simple Photonic Crystals
- > Simulate Knudsen Thermal Forces...
- > Simulation and Admittance Analysis...
- > Simulator for a T-stub transistor in...
- > Small Molecules in Intense Lasers...
- > SMC
- > Solar PV
- > Spice3f4
- > Spin Coupled Quantum Dots
- > Stick2D
- > StrainBands
- > Stretching simulation of an...
- > Stretching Simulation of FCC Crystal
- > Sugaraid

Stretching simulation of an alpha-helical protein domain

Uses steered molecular dynamics (SMD) to apply a tensile load to the ends of a molecule (such as an alpha-helical protein domain) [Learn more >](#)

[Launch Tool](#)[159 users, detailed usage](#)[0 Citation\(s\)](#)[1 question \(Ask a question\)](#)[0 review\(s\) \(Review this\)](#)[0 wish\(es\) \(New Wish\)](#)[Share: ...](#)

NanoHUB Tools



- Simulations take long time to complete.
- We will show how to do these simulations rather than actually run them.

Stretching a molecule

Stretching simulation of an alpha-helical protein domain (4:50 pm)

Initial Geometry SMD Parameters Simulation Parameters Run Simulation About this tool Questions?

You need to allow popup window to upload files

Initial Geometry

Upload Files: []

Initial geometry PDB file:
10110
01000
11101
Empty
0 bytes

Structure file:
10110
01000
11101
Empty
0 bytes

Fix atoms?: yes

Fixed atoms file:
10110
01000
11101
Empty
0 bytes

SMD Parameters >

Storage (manage) 2% of 10GB

780 x 600

File uploading

Initial geometry PDB file:

Upload a file Copy/paste text

No file selected.

Structure file:

Upload a file Copy/paste text

No file selected.

Fixed atoms file:

Upload a file Copy/paste text

No file selected.

The form contains three sections for file upload: 'Initial geometry PDB file', 'Structure file', and 'Fixed atoms file'. Each section has two options: 'Upload a file' (selected) and 'Copy/paste text'. Below each option is a 'Browse...' button and a message 'No file selected.'. At the bottom is a large 'Upload' button. Three black arrows point from the 'Upload a file' radio buttons to the right: the first arrow points to a red-bordered box containing 'file.coor', the second to another red-bordered box containing 'file.psf', and the third to a third red-bordered box containing 'fix.pdb'.

Click upload button

SMD Parameters

The screenshot shows the 'SMD Parameters' step of a molecular dynamics workflow. At the top, a navigation bar indicates the steps: 1 Initial Geometry, 2 SMD Parameters (which is active), 3 Simulation Parameters, and 4 Run Simulation. A 'About this tool' link is also present.

The main panel is titled 'SMD Parameters'. It includes the following fields:

- Upload Files:** An 'Upload...' button, circled in red.
- Use Steered Molecular Dynamics (SMD)?:** A checkbox labeled 'Yes' (checked), circled in red.
- Velocity:** A value of **0.0002**.
- Direction X:** Value **0**.
- Direction Y:** Value **0**.
- Direction Z:** Value **1**.
- Force constant (k):** Value **10.000**.
- SMD PDB File:** A file preview showing binary data: **10110
01000
11101**. To its right, it says **ASCII text** and **512.0 kB**.

Three callout boxes provide additional context:

- A blue-bordered box with a blue arrow pointing to the Velocity field contains the text: **Pulling velocity in Å/fs** (about 0.0001 is reasonable).
- A blue-bordered box with a blue arrow pointing to the Direction X, Y, and Z fields contains the text: **Direction of pulling force**.
- A blue-bordered box with a blue arrow pointing to the Force constant (k) field contains the text: **Virtual spring constant between moved atom and protein (kcal/(mol·Å²))**.

On the left side of the main panel, there are four small windows labeled 'VMD 1.9.5 OpenGL Display' showing molecular structures.

File uploading

Upload

Use this form to upload data for Stretching domain. If you don't specify a file for a parameter by the *Upload* operation.

SMD PDB File:

Upload a file Copy/paste text

smd.pdb

A diagram illustrating the file selection process. A red rectangular box surrounds the file name "smd.pdb". A thick black arrow originates from the right side of this red box and points downwards towards the "Upload" button located below the file input field.

Simulation Parameters

The screenshot shows a software interface for setting simulation parameters. At the top, a navigation bar indicates the current step: ③ Simulation Parameters. The main area is titled "Simulation Parameters".

Upload Files: An "Upload..." button is highlighted with a red circle.

Temperature: Set to 300.

Number of Steps: Set to 150000.

Number of Averaging Bins: Set to 300. A blue arrow points from this value to a callout box containing the text: "Averaging of the data to get rid of noise".

DCD Frequency: Set to 150. Another blue arrow points from this value to a callout box containing the text: "How often atomic configuration is stored".

Force Field Parameters: Shows binary data (10110, 01000, 11101), file type (ASCII English text), and size (123.6 kB).

File uploading

Upload

Use this form to upload data for Stretching simulation. This is a particular input, that input won't be modified by the simulation.

Force Field Parameters:

Upload a file Copy/paste text

CHARMM_Standard.prm
CHARMM_Collagen.prm

Note: Different force fields for different problems

The screenshot shows a software interface for simulation parameters. At the top, a navigation bar indicates the current step: ③ Simulation Parameters. Below this is a toolbar with a question mark icon and links for "About this tool" and "Questions?". The main area is titled "Simulation Parameters" and contains the following fields:

- Upload Files:
- Temperature: **300**
- Number of Steps: **1000**
- Number of Averaging Bins: **100**
- DCD Frequency: **150**
- Force Field Parameters:
10110
01000
11101

A tooltip for the Force Field Parameters section states: "Empty 0 bytes". At the bottom right of the main area is a red-bordered button labeled "Run Simulation >".

Simulations are very long, 6-8 (maybe 10) hours!

PART D: Hydrogen bond analysis

Example of studies on mutations in bone

