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

Recitation #6

Protein stretching

Recitation instructor: Francisco Martin-Martinez

email: fmartinm@mit.edu

Massachusetts Institute of Technology

Necessary files:

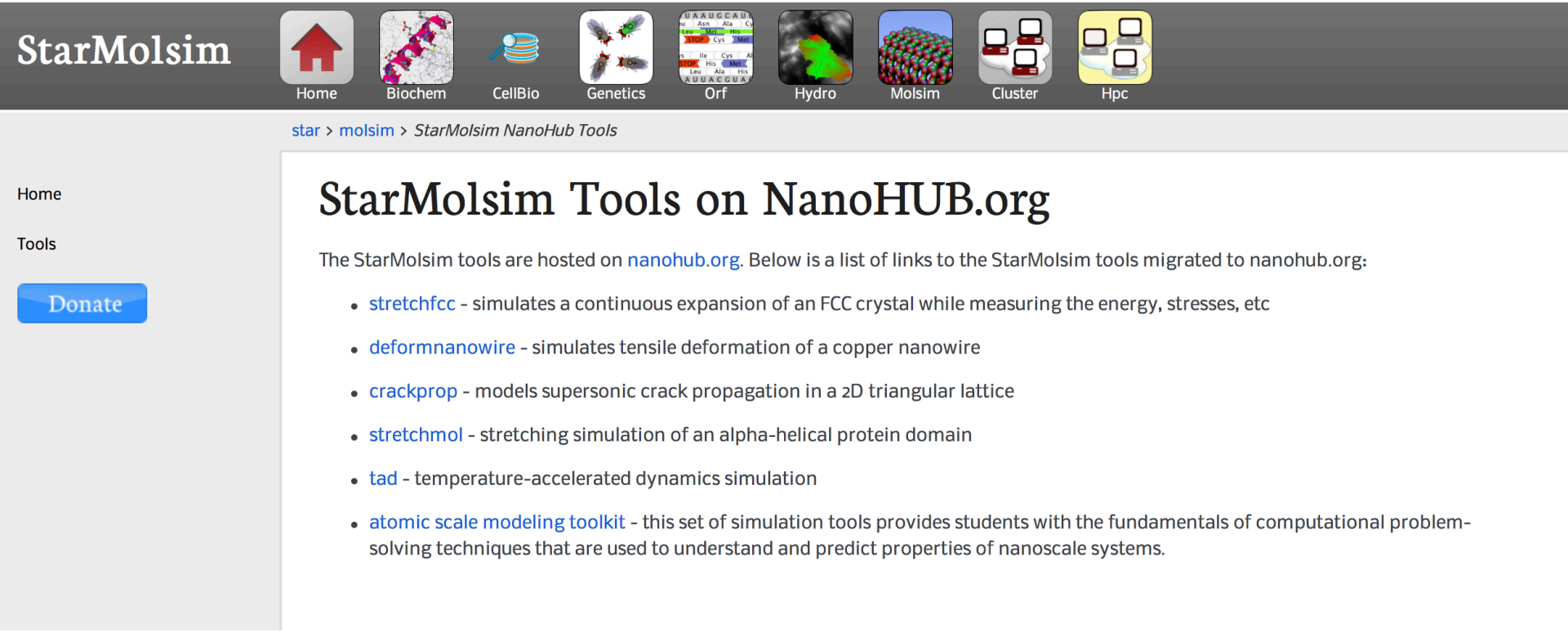
- Vimentin stretching

pset3_vimentin.zip

- Download those files first from stellar

Run stretchmol lab

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



Stretching simulation of an alpha-helical protein domain

Launch Tool

Version 1.0w - published on 19 Mar 2015

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View All Supporting Documents

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

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

Initial Geometry

Upload Files:

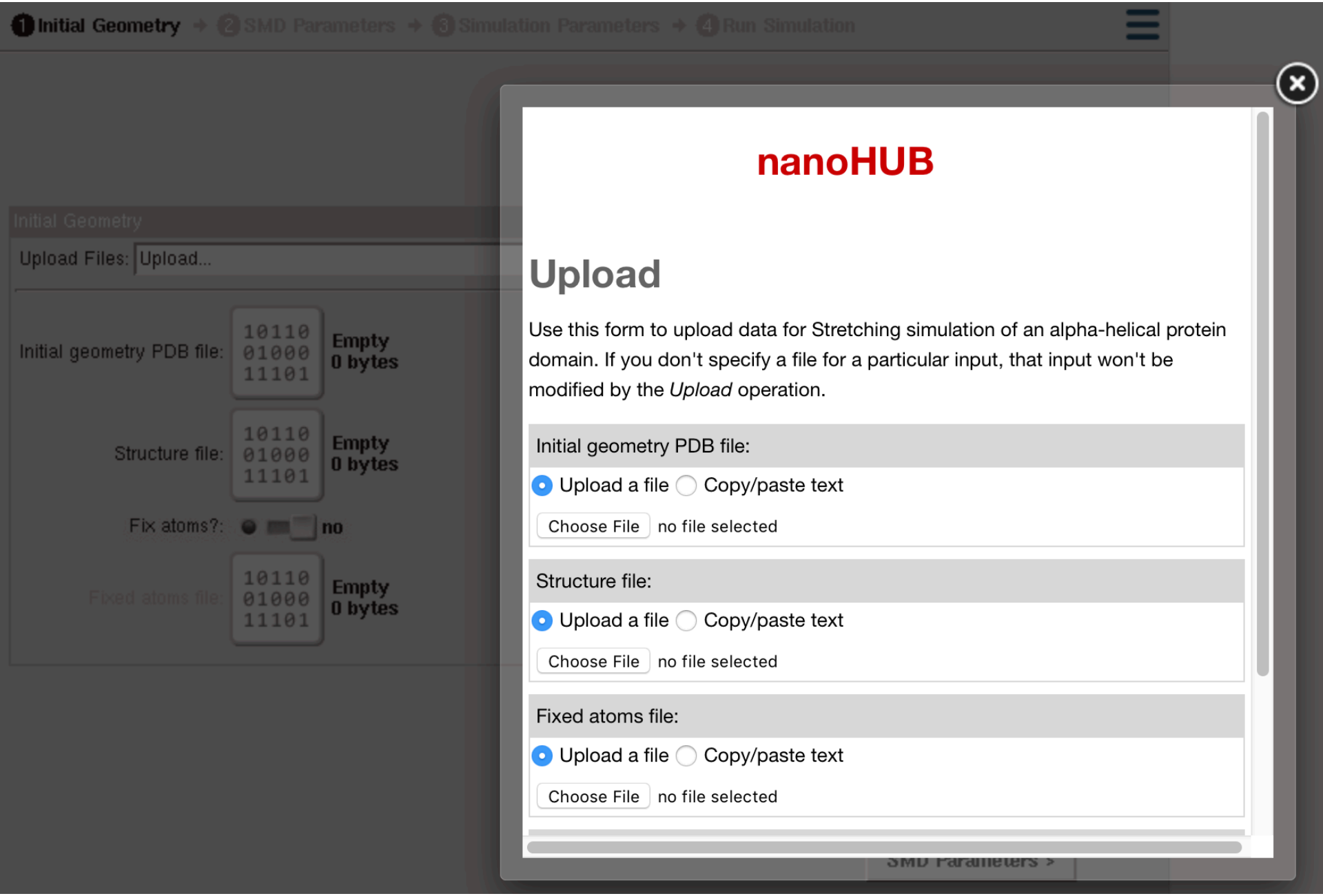
Initial geometry PDB file: 10110 01000 11101 **Empty** **0 bytes**

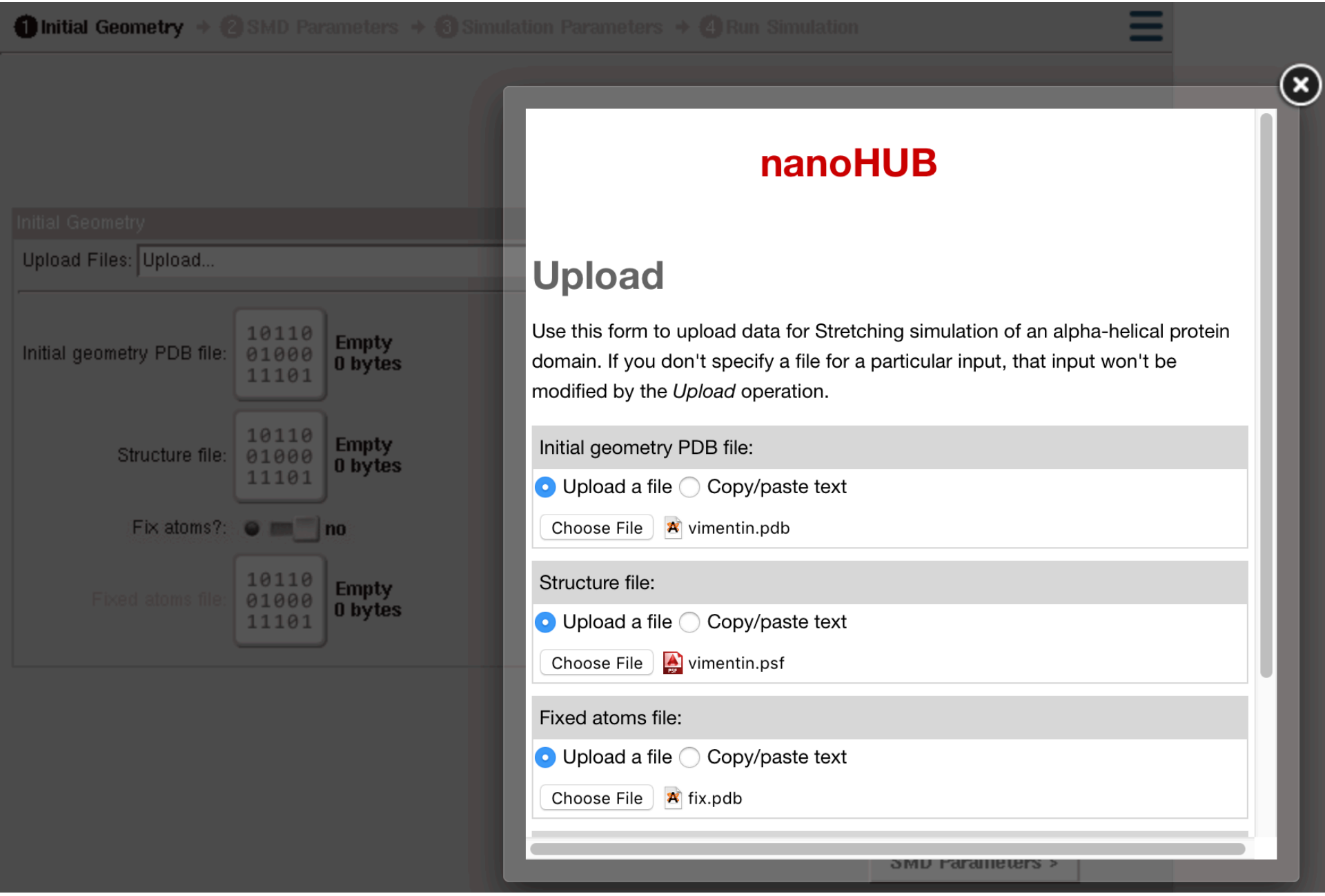
Structure file: 10110 01000 11101 **Empty** **0 bytes**

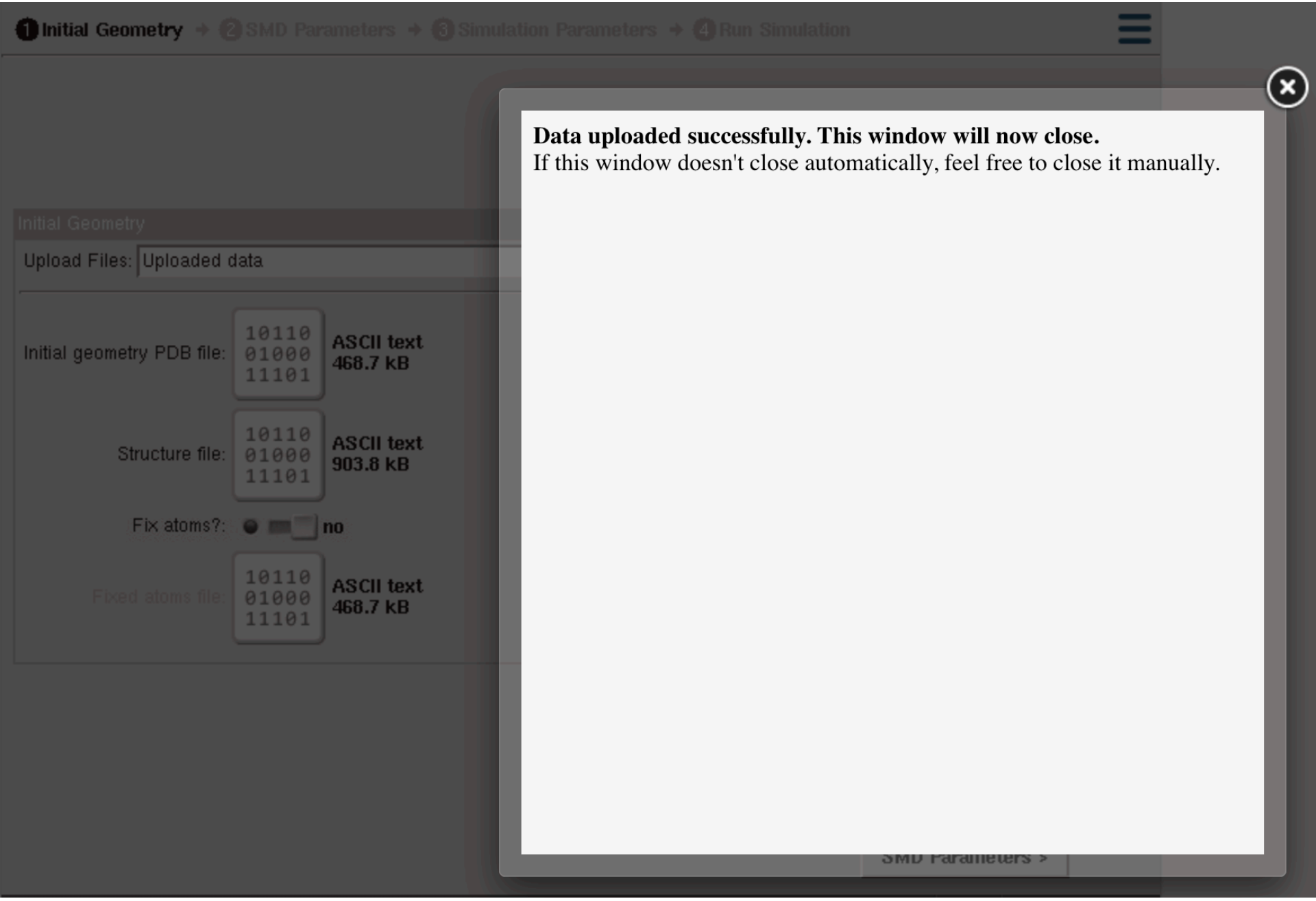
Fix atoms?: **no**

Fixed atoms file: 10110 01000 11101 **Empty** **0 bytes**

SMD Parameters >


1 Initial Geometry
2 SMD Parameters
3 Simulation Parameters
4 Run Simulation
Initial Geometry
Upload Files:
Upload...
Initial geometry PDB file:
Empty
0 bytes
Structure file:
Empty
0 bytes
Fix atoms?:
no
Fixed atoms file:
Empty
0 bytes
nanoHUB
Upload
Use this form to upload data for Stretching simulation of an alpha-helical protein domain. If you don't specify a file for a particular input, that input won't be modified by the Upload operation.
Initial geometry PDB file:
Upload a file
Copy/paste text
Choose File
no file selected
Structure file:
Upload a file
Copy/paste text
Choose File
no file selected
Fixed atoms file:
Upload a file
Copy/paste text
Choose File
no file selected


1 Initial Geometry
2 SMD Parameters
3 Simulation Parameters
4 Run Simulation
Initial Geometry
Upload Files: Upload...
Initial geometry PDB file:
Empty
0 bytes
Structure file:
Empty
0 bytes
Fix atoms?:
no
Fixed atoms file:
Empty
0 bytes
nanoHUB
Upload
Use this form to upload data for Stretching simulation of an alpha-helical protein domain. If you don't specify a file for a particular input, that input won't be modified by the Upload operation.
Initial geometry PDB file:
Upload a file
Copy/paste text
Choose File
vimentin.pdb
Structure file:
Upload a file
Copy/paste text
Choose File
vimentin.psf
Fixed atoms file:
Upload a file
Copy/paste text
Choose File
fix.pdb
SMD Parameters >


1 Initial Geometry → 2 SMD Parameters → 3 Simulation Parameters → 4 Run Simulation
Initial Geometry
Upload Files: Uploaded data
Initial geometry PDB file:
10110
01000
11101
ASCII text
468.7 kB
Structure file:
10110
01000
11101
ASCII text
903.8 kB
Fix atoms?:
no
Fixed atoms file:
10110
01000
11101
ASCII text
468.7 kB
Data uploaded successfully. This window will now close.
If this window doesn't close automatically, feel free to close it manually.
SMD Parameters >

Initial Geometry

Upload Files: Uploaded data

Initial geometry PDB file: 10110 01000 11101 **ASCII text 468.7 kB**

Structure file: 10110 01000 11101 **ASCII text 903.8 kB**

Fix atoms?: **yes**

Fixed atoms file: 10110 01000 11101 **ASCII text 468.7 kB**

SMD Parameters >

SMD Parameters

Upload Files: Uploaded data

Upload...

Use Steered M

Velocity: 0.00005

Direction X: 0

Direction Y: 0

Direction Z: 1

Force constant (k): 10.000

SMD PDB File: 10110 01000 11101 **ASCII text 468.7 kB**

< Initial Geometry

Simulation Parameters >

Simulation Parameters

Upload Files: Uploaded data

Temperature:	300
Number of Steps:	5000
Number of Averaging Bins:	100
DCD Frequency:	150

Force Field Parameters: 10110 01000 11101 **ASCII text 237.9 kB**

< SMD Parameters

Run Simulation >

Result: Output Log

- Output Log
- Energy Plot
- Force Displacement Plot
- Energy Data
- SMD Data
- NAMD Input File
- VMD Movie Files (ZIP)
- ---
- Download

```
Using
execut
retval
stdout
Charm
Charm
Charm
Conver
CharmL
Charm
Charm
Info: NAMD 2.9 for Linux-x86_64-MPI
Info:
Info: Please visit http://www.ks.uiuc.edu/Research/namd/
Info: for updates, documentation, and support information.
Info:
Info: Please cite Phillips et al., J. Comp. Chem. 26:1781-1802 (2005)
Info: in all publications reporting results obtained with NAMD.
Info:
```

Find: Select All

2 results Clear One Clear All

All ▸ **Simulation** = #2

SMD PDB File = REMARK original generated coordinate pdb file ATOM 1 N LEU P 70 12.152 25.138 10.399 0.00 ...
Upload Files = Uploaded data
Force Field Parameters = *>>>>> CHARMM22 All-Hydrogen Parameter File for Proteins <<<<<<<< *>>>>>>>>>>>>>>>>>>>> ...

< Simulation Parameters

Result: VMD Movie Files (ZIP)

```
<binary> 2.1 MB

000000: 50 4b 03 04 14 00 00 00  | PK......
0x0008: 08 00 4f 73 6b 4c be c3  | ..OskL..
0x0010: e7 b8 06 54 20 00 70 b9  | ...T .p.
0x0018: 24 00 07 00 00 00 6f 75  | $.....ou
0x0020: 74 2e 64 63 64 8c b8 07  | t.dcd...
0x0028: 54 8f 6f 18 37 ae 44 11  | T.o.7.D.
0x0030: 1a 46 cb 4e 42 0b 49 8a  | .F.NB.I.
0x0038: f8 5e 9f a4 90 a4 21 12  | .^....!.
0x0040: 4d 09 51 56 45 a1 bd f7  | M.QVE...
0x0048: de 69 6b ab 34 28 6d 4d  | .ik.4(mM
0x0050: ed a1 a1 29 25 33 a3 d0  | ...)%3..
0x0058: cf 78 bf ef 7f 9c f3 be  | .x......
0x0060: e7 bc e7 fc ff f7 39 d7  | ......9.
0x0068: 79 ce f3 3c f7 fd b9 af  | y..<....
0x0070: fb 7e ee eb 73 5d 9f 47  | .~..s].G
0x0078: 6b de bc 79 8a c7 35 0e  | k..y..5.
0x0080: 6e 60 5e 43 ff 1f 3b b9  | n`^C..;.
```

Find:

Select All

2 results Clear One Clear All

All

Simulation = #2

SMD PDB File = REMARK original generated coordinate pdb file ATOM 1 N LEU P 70 12.152 25.138 10.399 0.00 ...

Upload Files = Uploaded data

Force Field Parameters = *>>>>> CHARMM22 All-Hydrogen Parameter File for Proteins <<<<<<< *>>>>>>>>>>>>>>>>>>> ...

< Simulation Parameters