Purdue, Norfolk State, Northwestern, MIT, Molecular Foundry, UC Berkeley, Univ. of Illinois, UTEP

Publishing Simulation Tools on the nanoHUB

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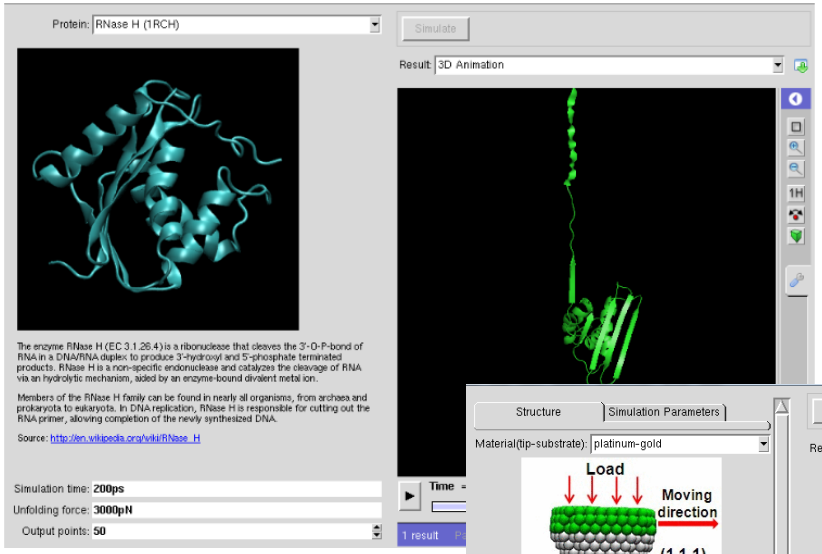
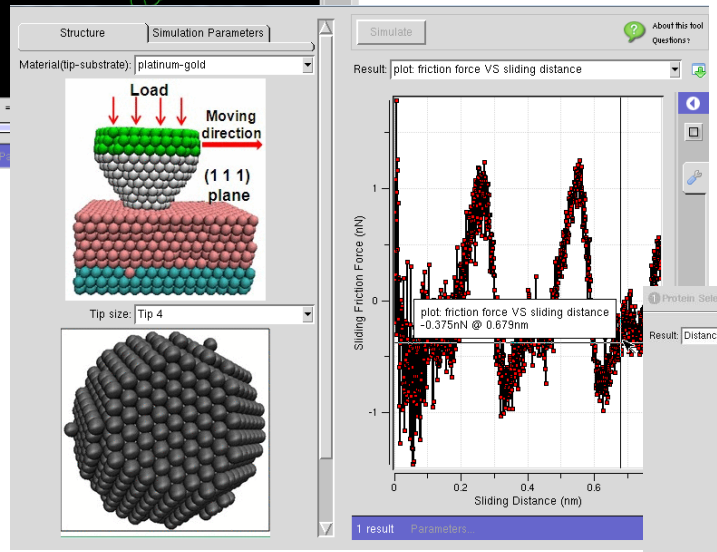
Simulation Tools



Forced Protein Unfolding

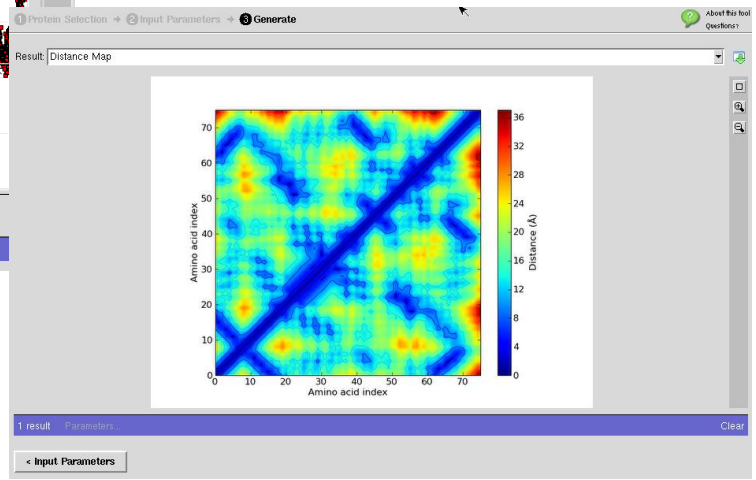
Published Summer 2009

Updated Summer 2010



Atomic Stick-Slip Toolkit

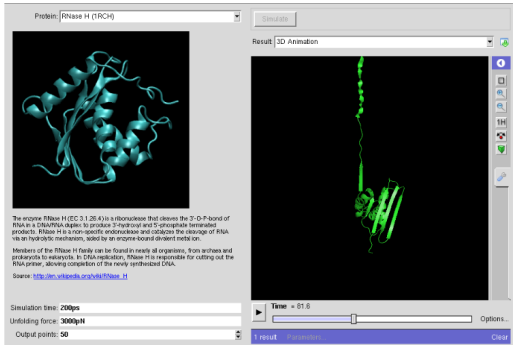
Published Spring 2010



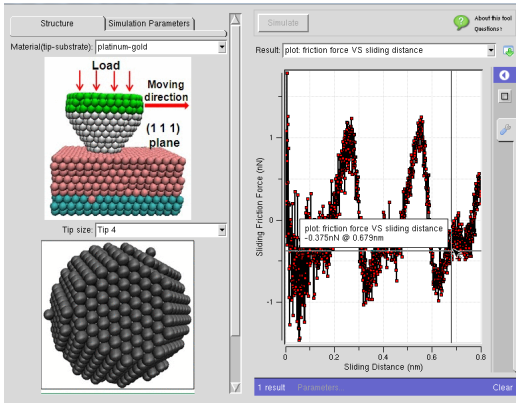
Protein Contact Maps

In Progress

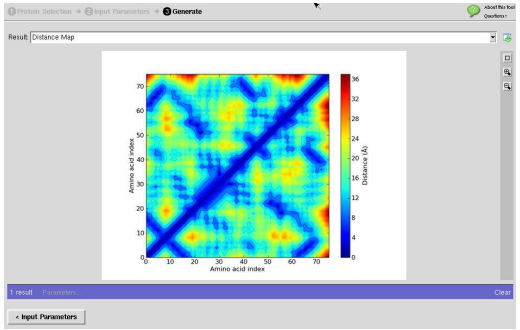
Simulation Tools



Primary Developer: Bejamin Rafferty
Undergraduate Senior
Electrical and Computer Engineering

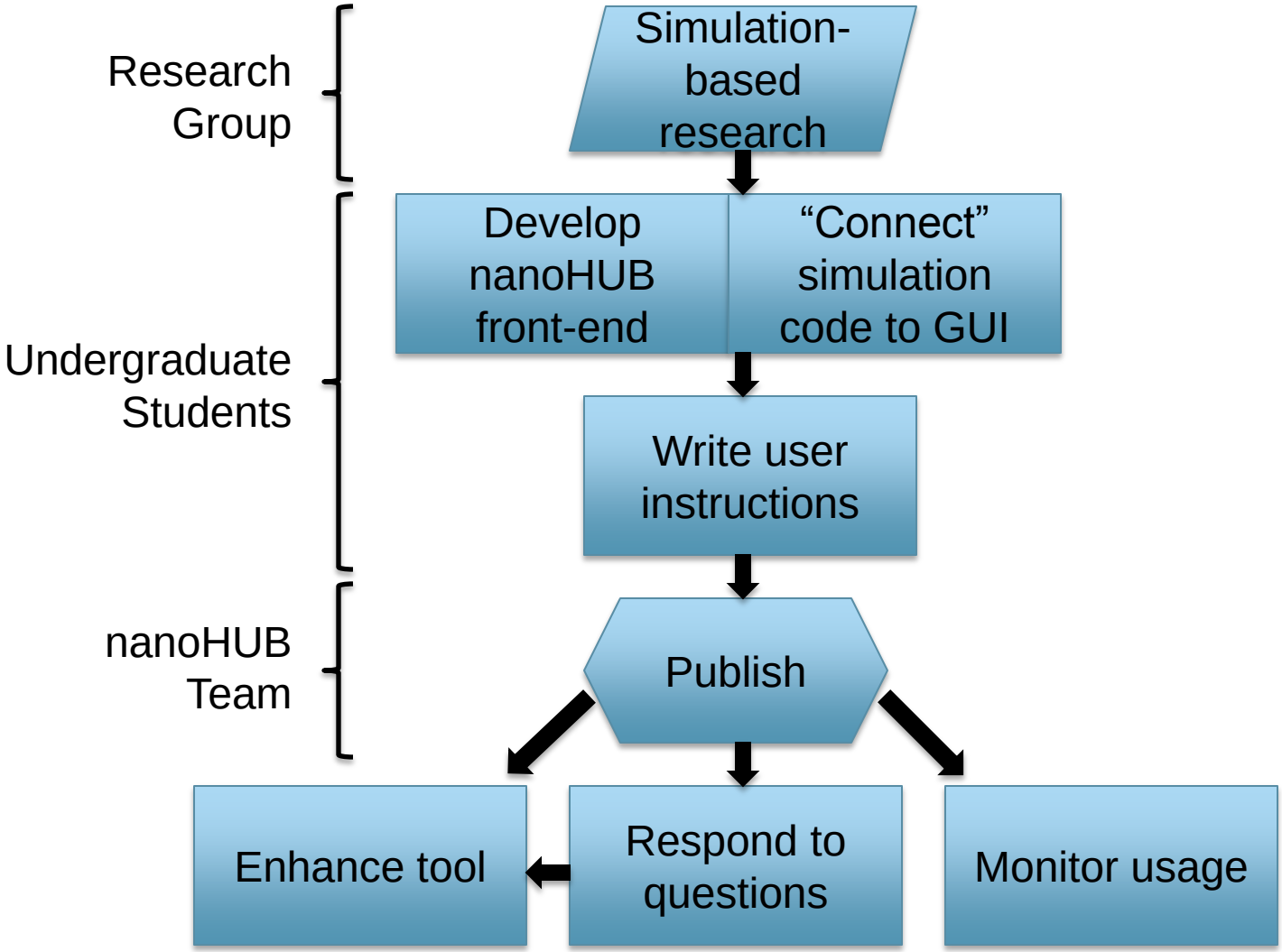


Primary Developer: Jianguo Wu
First Year Masters Student
Mechanical Engineering



Primary Developer: Zachary Flohr
Undergraduate Junior
Biomedical Engineering

Publishing Simulation Tools



Develop Tool Using Rappture

```
<?xml version="1.0"?>
<run>
  <tool>
    <title>Graphing Calculator</title>
    <about>Press Simulate to view results.</about>
    <command>python @tool/graph.py @driver</command>
  </tool>
  <input>
    <string id="formula">
      <about>
        <label>Formula</label>
        <hints>Example: 2*x + 1</hints>
      </about>
      <size>30x5</size>
    </string>
    <number id="min">
      <about> <label>From x</label> </about>
      <default>0</default>
    </number>
    <number id="max">
      <about> <label>To x</label> </about>
      <default>1</default>
    </number>
  </input>
  <output>
    <curve id="result">
      <about> <label>Formula: Y vs X</label> </about>
    </curve>
  </output>
</run>
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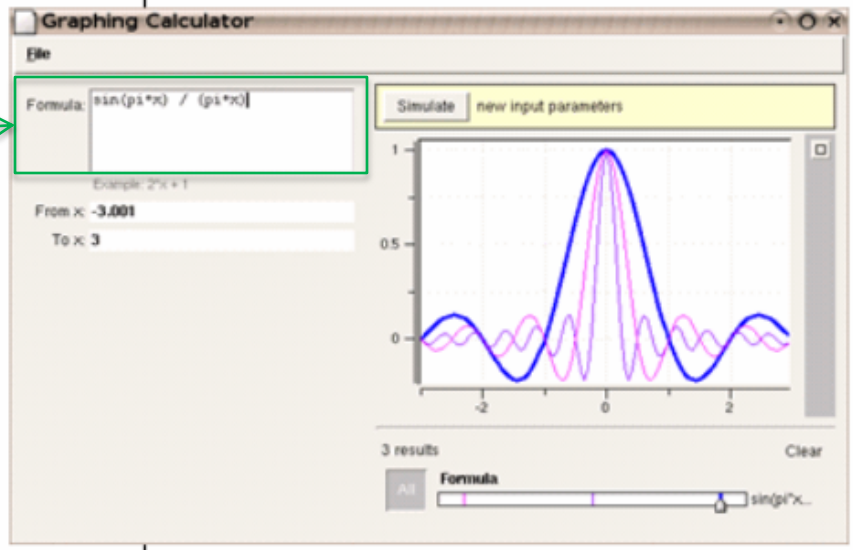
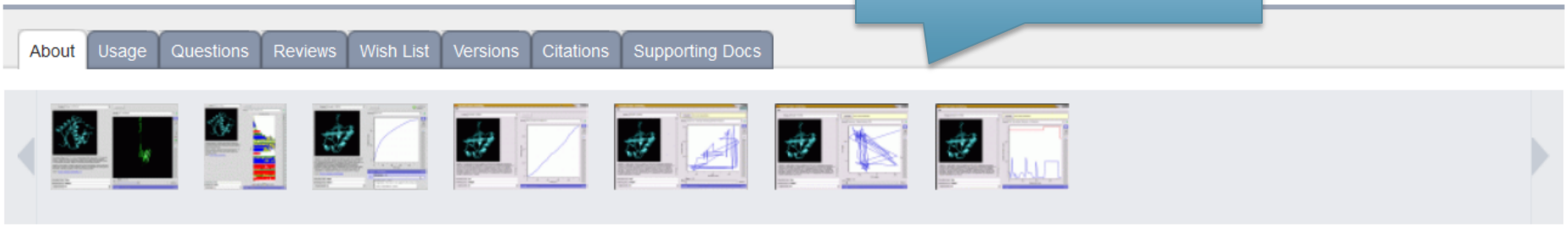


Rapid **app**lication infrastruc**ture**

Write User Instructions

Screen snapshots of the tool



Description

The Forced Protein Unfolding toolkit enables users to easily perform non-equilibrium molecular dynamics simulations of a protein subject to an external force and then analyze their simulation results both quantitatively and through animations of the protein dynamics.

The three proteins currently implemented in this version of the Forced Protein Unfolding toolkit are RNase H (1RCH), Barnase (1BNR), and Ubiquitin (1UBQ). These three proteins present contrasting structural forms: Barnase has five central antiparallel β strands with small peripheral α helices; RNase H is larger containing more extensive α helices; Ubiquitin has parallel and antiparallel β strands. In addition, the folding and unfolding pathways of these proteins have been extensively investigated numerically and experimentally

The following simulation parameters can be specified on the left-hand side of the Force Protein Unfolding toolkit window.

Protein: This is a drop down box containing the names and Protein Data Bank ids of proteins currently available for simulation. As a protein is selected from the drop down box, a diagram of the protein and brief description will appear below it.

Text description and instructions

Respond to Questions

Questions and Answers: Open Question

Question asked by a tool user

1

high T

Dear developers,

I would like to ask you 2 questions: 1 ...tting close to the melting temperature of the tip?

2) How did you compute, with LAMMPS, the adhesive energy? Are you using it in the hybrid method combining EAM with LJ?

kind regards, maurizio

tool:stickslip

RESPONSES (1)

Answer posted by tool developer

0 0

Dear Maurizio Zaccheddu,

Thank you for your good questions. I wil... to you.

Question 1: What it would happen if you...

Answer: With the increase of temperatu... ion of each atom in the tip and the substrate will increase significantly which will result in more noise in the friction data. When the temperature close to or above the melting temperature, the tip will be not stable. As a result, the shape of the tip will change and some atoms of the tip will be transferred or stuck to the substrate. In this condition, the periodic stick-slip pattern of the friction force will disappear.

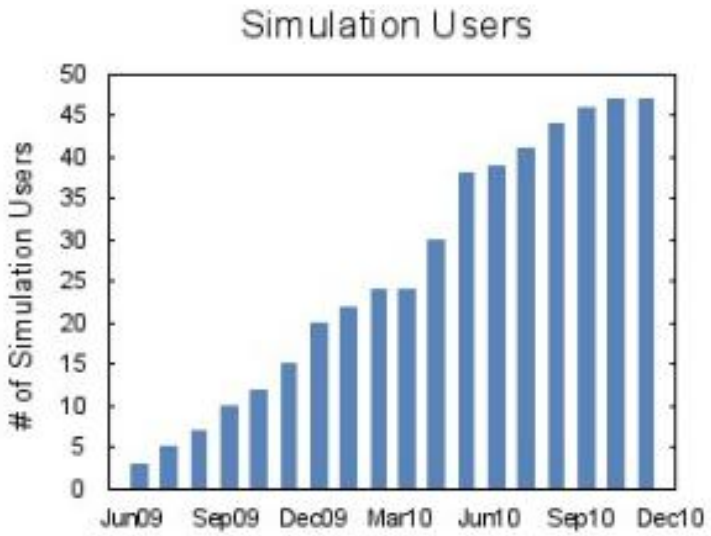
Question 2: How did you compute, with LAMMPS, the adhesive energy? Are you using it in the hybrid method combining EAM with LJ?

Answer: Do you mean the energy that is needed to separate the tip from the substrate? I just computed the force in separating process and then calculated the integration. Energy=Sum{Force*Velocity*dt} As for the force, I use "compute group/group" command. We use EAM potentials for all of the inter-atomic interactions. But when using the group/group command, EAM potentials for metals only include the pair potential portion of the EAM interaction, not the embedding term. However, we performed the same simulation with another simulation tool and found that the influence of the embedding term was very small and could be neglected.

I hope the answers could be of help to you.

Best regards

Monitor Usage



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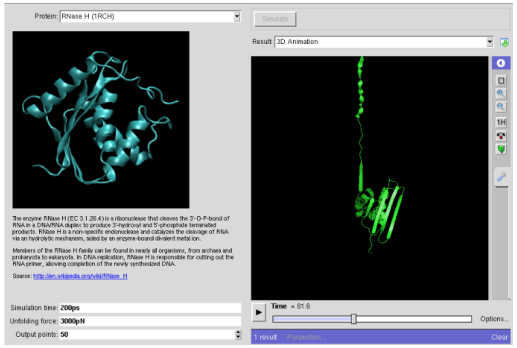
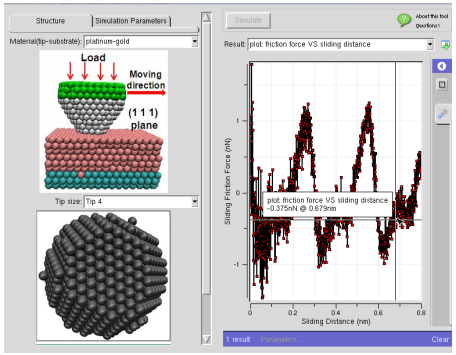
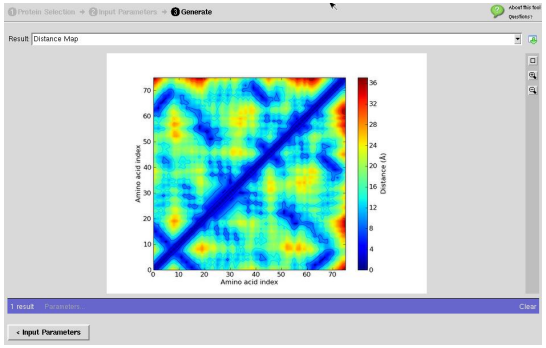
Thank You.
Questions?







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