SI2-SSE Collaborative Research: Molecular simulations for polymeric systems in the cloud

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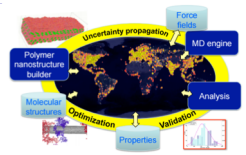
Awards: 1440727
1613155

Approach and Goals

GOAL: enable pervasive, high-quality molecular simulations of polymers and their nanostructures



Develop a framework for molecular simulations of polymers and their nanostructures, universally accessible and useful to the community for cloud computing via NSF's nanoHUB.

1. Powerful simulation tools for polymer nanostructures (molecular builders, a parallel MD engine for property characterization and post-processing);
2. A UQ framework to orchestrate the molecular simulations and propagate uncertainties in input parameters to predictions and compare the predictions to experimental values;
3. Databases of force fields and molecular structures as well as predicted and experimental properties.

Impact: tool usage

PolymerModeler

1200+ users
42,000+ simulation runs

nuSIMM

320+ users
47,000+ simulation runs

Struc2LAMMPS: 100+ users

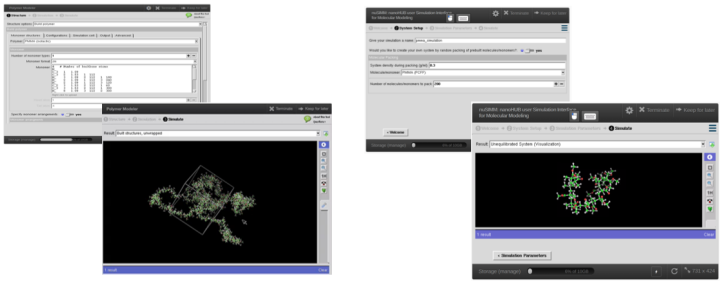
Use in research by outside groups

- Sahputra IH, Alexiadis A, Adams MJ. Molecular Simulation. 2018 Mar 24:1-7.
- Rzeznik L, Fleming Y, Wirtz T, Philipp P. Beilstein Journal of Nanotechnology. 2016 Aug 2;7(1):1113-28.
- Sebeck K, Shao C, Kieffer J. ACS Applied Materials & Interfaces. 2016 Jun 10.
- Rashidi V, Coyle EJ, Sebeck K, Kieffer J, Pipe KP. The Journal of Physical Chemistry B. 2017 Apr 24;121(17):4600-9.
- Sundarram SS, Li W. Polymer Engineering & Science. 2013 Sep 1;53(9):1901-9.
- Ingvason GA, Rollin V. In MRS Proceedings 2014 (Vol. 1700, pp. 61-66). Cambridge University Press.

Tool set for polymer simulations

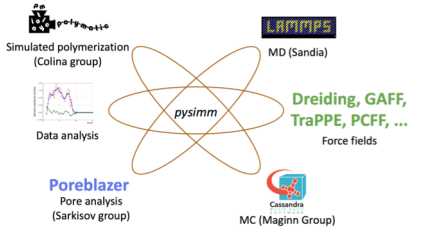
PolymerModel – https://nanohub.org/tools/polymod

nuSIMM – https://nanohub.org/tools/nusimm

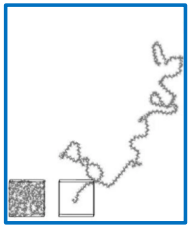


pySIMM – http://github.com/polysimtools/pysimm

Fortunato ME, Colina CM. pysimm: A python package for simulation of molecular systems. SoftwareX. 2017 Dec 31;6:7-12.



Self-avoiding random walk



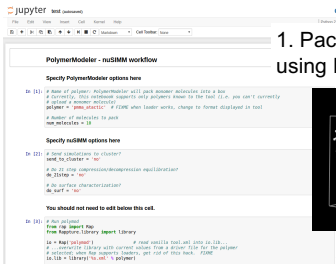
Setting up MD simulations

https://nanohub.org/tools/struc2lammpsdf

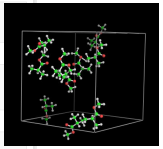
- Determine bond connectivity and topology
- Perform atom typing
- Create energy expression for LAMMPS
- Create required LAMMPS input files

Scientific workflows

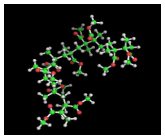
Jupyter notebooks running in nanoHUB



1. Pack monomers using PolymerModeler



2. Polymerize with nuSIMM

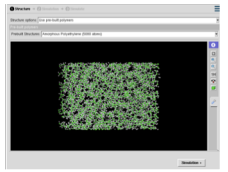


Jupyter notebooks:
- Combine text, graphics and live code
- nanoHUB notebooks seamlessly connect to simulation tools

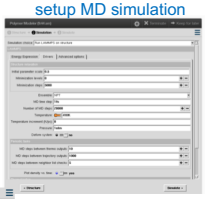
Impact: classroom use

Learning module: heat of fusion of PE

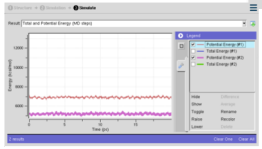
STEP 1: select initial structure



STEP 2: setup MD simulation



STEP 3: data analysis



Students use MD simulations of heat of fusion together with DSC experiments to learn about crystallization dynamics

Classroom use:
- U of Florida CHM6586: Computational Chemistry. Total of 23 students, with 2 being undergrads.
- Purdue University MSE 697: Atomistic view of materials: Modeling and Simulations. Total of 18 graduate students.
- Purdue University MSE 235 Materials Properties Laboratory. Instructor: Prof. Michael Titus.