**SI2-SSE Collaborative Research:** Molecular simulations for polymer composites in the cloud

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**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.

**Cloud computing via NSF nanoHUB**

- **Online simulations using simply a web-browser:**
  - Go to: https://nanohub.org/tools
  - No need to download or install any software
  - Use NSF's computing resources at Purdue for large-scale parallel jobs

**Step 1: Build polymer structure**

**PolymerModeler tool**

**Step 1:** Build polymer structure
- Select monomer
- Specify energetics (torsions & vdW)

**Step 2:** Perform MD simulations
- Pre-built structures
- Structures from builder
- LAMMPS parallel simulator from Sandia

**Impact:** 584 users from 10 countries have performed 13,000+ interactive simulations

**Polymatic simulations @ nanoHUB in MSE curricula**

**Empowering educators & students**

- Learning modules to facilitate simulation-powered curricula

**References**