nanoHUB an open platform for simulation, data and publication

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Online simulations using nanoHUB

Developed & operated by the Network for Computational Nanotechnology
Supported by the US National Science Foundation

1.4 M visitors every year, 16,000+ simulation users per year
A growing community

- 500+ simulation tools
- 1,800+ contributors
- 16,000+ annual simulation users
- 1,000,000+ simulations per year

www.nanohub.org/usage
Powerful simulations, a few clicks away

https://nanohub.org/tools/nanomatmech

 Powered by LAMMPS
Tools are publications
Use in education

- Knowledge Transfer out of Research
- 29,000+ students
- 1,500+ courses
- 185 institutions
- 170+ companies in nanoHUB courses

Users:
- Soph. Materials Engineering
- Soph. Mechanical Engineering
- Freshmen
- Soph. Materials Engineering
- Experimentalist Researchers
- Computational Researchers
- Self-Study Users

Time (Days):
July 1, 2009 to June 30, 2010
Use for research

1,800+ citations
1,600+ use nanoHUB for research
283 papers with industrial authors
Reproducibility & dissemination of research
Your tool ... more powerful in nanoHUB

- Automatic UQ available for all Rappture tools
UQ in nanoHUB

Uncertainties in predicted quantities

Sensitivity analysis

Surrogate models
Reaching for Jupyter

Jupyter notebooks

• Web-documents with powerful visualization & code
• Graphics run on your browser for fast response & modern look
• 1,000,000+ developer community

Workflows using Jupyter

Results of the simulation
Chiral index $n = 5$
Chiral index $m = 5$
Bond length [Å]: 1.42
CNT length [nm]: 5.00
Thermal conductivity [W/mK]: 110.44

Note as we have excluded the first five groups at the ends from the fit to avoid errors due to the high temperature gradients close to the thermostats (effect of the thermal resistance).

Conclusions

In this tutorial, we have seen a generic procedure to estimate the thermal conductivity of carbon nanotubes. This tool is intended for pedagogical purposes only; indeed, in order to save in computational time, we have restricted the simulation time for the non-equilibrium part to 200 ps, which is clearly not enough to reach a steady temperature profile (you will get very different results with different runs). If you want to compute the conductivity for this case, please use the tool version with a suitable simulation time for the non-equilibrium simulation (e.g. at least, 1 ns).
Workflows using Jupyter

1. PolymerModeler (Rappture)
   - Amorphous builder
2. nglview
   - Visualizer
3. LAMMPS
   - Molecular dynamics

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**Calculate Tg using nanoHUB PolymerModeler and LAMMPS**

By Ben Haley, Purdue University

Import libraries and setup LAMMPS

```python
In [ ]:
import sys
import subprocess as sp
sys.path.append('/apps/share64/debian7/
from hubw import RapptureTask
import nglview
from ipywidgets import Label, VBox
import hublib.use
use lammps-10May15
sys.path.append('/home/nanohub/strachan/
from tcalc import getVDT, getVDTdata, getTg_BL, getHyperb
import matplotlib.pyplot as plt
import matplotlib notebook

Setup PolymerModeler variables

Setup monomer, number of monomers per chain and number of chains.
PolymerModeler uses Configurational Bias Continuous Monte Carlo to build relaxed polymer structures

In [ ]:
# First task: run PolymerModeler to pack chains into a box
task1 = RapptureTask('polymod')
```

---

Ben Haley
Jupyter and nanoHUB

nanoHUB hosts your notebook
- A custom environment for scientific computing
- Access 450+ Rappture tools and a range of community codes
- nanoHUB hardware and remote execution
- Permanent environments - your tool will always run the same - reproducibility

Publish
- Your tool, data and analysis
- DOIs and versioning

Tool mode
- Dashboard features
- nanoHUB custom extensions
A growing cyber-ecosystem for science
Commercial sites are well ahead
An interoperable cyber-ecosystem
An interoperable cyber-ecosystem
**KIM Models**

Click on an element in the periodic table for which you need an interatomic model.

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**KIM Models** (interatomic potentials and force fields) are software packages for describing atomic interactions that can be used with a variety of simulation codes, including LAMMPS, DL_POLY, IMD, ASE and GULP, that are compatible with the KIM API standard.
Explore KIM potentials & run MD
Data management system -> nanoHUB

- Launch simulations from data exploration or other simulation tools
- On-demand simulation seamlessly integrated into users workflows
nanoHUB simulations as web-service
An interoperable cyber-ecosystem
Thanks