High Value from High Throughput: Harness the Power of LAMMPS with MedeA®

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Materials Design

LAMMPS Workshop
15 August 2019
MedeA® Software Environment
MedeA® Software Environment

- **Engines**
  - VASP, GIBBS, LAMMPS, GAUSSIAN, MOPAC

- **Databases**
  - ICSD, Pauling, Pearson’s, NIST, COD, InfoMaticA Query Engine, MPDS

- **Builders**
  - Crystals, nanoparticles, amorphous materials, interfaces, molecules, polymers, conformers, thermosets, docking

- **Force Fields (potentials)**
  - Forcefields bundle, Forcefield Optimizer

- **Property Modules**
  - MT, TSS, Phonon, Electronics, UNCLE, LAMMPS (Diffusion, Thermal Conductivity, Viscosity, CED, Surface Tension), P3C,

- **High Throughput**
  - HT-Launchpad, HT-Descriptors, HT-Correlation

- **Analysis**
  - Broad range of analysis tools

- **JobServer & TaskServer**
Potentials in MedeA

- **Metallic forcefields:**
  - EAM
    - All LAMMPS eam, eam/fs, and eam/alloy variants
  - MEAM

- **Inorganic forcefields:**
  - Buckingham
  - BKS
  - Clay-FF
  - CVFF_aug

- **Semiconductor forcefields:**
  - Tersoff
  - Stillinger-Weber
  - REBO

- **Organic (valence) forcefields:**
  - PCFF/PCFF+
  - Compass/Compass+
  - OPLS-AA/OPLS-AA+
  - AUA/AUA+
  - Trappe+

- **Variable charge forcefields**
  - Streitz-Mintmire
  - COMB3
  - ReaxFF

- **All other potentials in LAMMPS can be invoked via some additional lines of LAMMPS commands**

*Also available in MedeA®-GIBBS
Current Approach…
... Going to High-Throughput

Model & Simulation Definition

Data Mining

Statistical Analysis

Machine Learning

Job & Data Control

Model Building

Simulation

Analysis

Data Collection
Warmup:
$T_g$ of PPE
Glass Transition $T_g$ of a Polymer

Where is the $T_g$?

Polyphenylene ether (PPE)
Amorphous System V vs T

Automatically build 50 configurations

Variables
- nMols = 5
- nConfigs = 50
- T = 300 K
- P1 = 100 atm
- P2 = 1 atm
...

Amorphous Builder
- Geometry: bulk cell
- Density: 0.5
- Temperature: $T$
# configurations: nConfigs

Table
- Name: Densities

For Each Structure
- sequential loop
- file: amorphous.trj

Custom Stage
- Plot density distribution of final cooled models

Table: Print
- Table: Densities
- File: /Densities.csv
- Type: csv

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Glass Transition $T_g$ of a Polymer

Variability in individual V vs. T curves (gray lines)
Fit yields properties for the simulated system
Automatic procedure: single high throughput flowchart

Value of high throughput calculations:
- Clear signal from noisy simulation data

Gradient change (least squares fit) = 405.1K +/- 8.6K

Volume vs Temperature Analysis

- Variability in individual V vs. T curves (gray lines)
- Fit yields properties for the simulated system
- Automatic procedure: single high throughput flowchart
High-throughput Sampling:
Mechanical properties of a high performance thermoset resin
Building a Monomer

- Use the SMILES string
Modifying into a Repeat Unit

- Edit into a repeat unit with the **Molecular Builder**
  - Break bond, delete H atoms, then define a repeat unit
Turning into a Polymer

- Build with MedeA Polymer Builder
  - DP = 5 in this example
Building Initial Amorphous Material

- Use MedeA Amorphous Materials Builder
  - Combine poly(dicyclopentadiene) with cross-linkers

Initial density: 0.3 g/cc
Equilibrating the Amorphous Material

- With MedeA LAMMPS using **PCFF+** forcefield
  - Design simulation workflow with Flowchart

```
Equilibrium density at 300K: 0.963 g/cc
```
Creating Cross-links

- With MedeA Thermoset Builder
Predicting Mechanical Properties

- Final equilibration and calculate mechanical properties
  - Includes elastic constants, modulus, and thermodynamic functions

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<th>Modulus</th>
<th>Voigt</th>
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<th>Hill</th>
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<td>Young’s</td>
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</table>
| Longitudinal  | 3.73  | 3.35  | 3.54  | GPa

Start

Variables

- tstep = 1 fs
- T = 300 K
- P = 1 atm

LAMMPS

Mechanical Properties

Strains: 0.005
Use MedeA High-Throughput Flowchart to turn 1 initial configuration to hundreds of samples and perform property calculations automatically.
## High-Throughput Sampling

Results written in a table

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<tr>
<th>Density (g/cm³)</th>
<th>Energy (kcal/mol)</th>
<th>Hill Bulk Modulus (GPa)</th>
<th>Hill Shear Modulus (GPa)</th>
<th>Hill Young's Modulus (GPa)</th>
<th>Stability</th>
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...
Sampling over 200 configurations

- 65.5% of the 200 samples were mechanically stable
- $Y$ in good agreement with experimental results of ~2.6 GPa

![Histogram of Hill Young's Modulus (GPa)]

Expt: 2.6 GPa

Hill Young’s Modulus (GPa)

- [0.49, 0.95]
- (0.95, 1.41]
- (1.41, 1.87]
- (1.87, 2.33]
- (2.33, 2.79]
- (2.79, 3.25]
- (3.25, 3.71]
- (3.71, 4.17]
Summary

- Sampled through 200 cross-linked thermoset resins for their mechanical stability and elastic moduli
  - Generated 200 resin samples from 1 set of molecules and cross-linker
    - From molecules to amorphous materials to thermoset
  - Distribution of Young’s modulus in excellent agreement with experiment
High-Throughput Screening
HT Implementation in MedeA

Specify InfoMaticA query

Structural databases: ICSD, Pearson, Pauling, COD

Primary Hit List

Select unique structures

Store unique structures

Define properties to be computed and set computational protocol

Perform calculations: Foreach Loop

Store computed results

Analyze results

Create crystal structures, substitute atoms, create surfaces, interfaces, nanoparticles, layers, defects

Build set of molecules

Create polymer models

Create crystal structures, substitute atoms, create surfaces, interfaces, nanoparticles, layers, defects

Build set of molecules

Create polymer models

VASP

LAMMPS

GIBBS

MOPAC

GAUSSIAN
O Removal Energy of Actinide Oxides

- Ce/O, Am/O, Cm/O, Np/O, Pu/O, Th/O, and U/O compounds
O Removal Energy of Actinide Oxides

- Retrieve all Ce/O compounds
  - With MedeA® InfoMaticA
O Removal Energy of Actinide Oxides

- Retrieve all Ce/O compounds
  - With MedeA® InfoMaticA
O Removal Energy of Actinide Oxides

- Retrieve all actinide oxide compounds
Save in a structure list:

- 56 Ce/actinide oxide compounds in various space groups
O Removal Energy of Actinide Oxides

- Assign the Cooper force field for actinide oxides

---

1 http://abulafia.mt.ic.ac.uk/potentials/actinides
Prepare a High-throughput flowchart

Energy of perfect compound

Energy of compound less 1 O
Run HT calculations in parallel or serial

- Value: Highly efficient screening of large number of compounds
O Removal Energy of Actinide Oxides

- View results from Job.out
  - 112 (56*2) calculations finished in 749 seconds on an 8-core Intel Linux box

- Can further convert O removal energy to O vacancy formation energy by considering energy of $O_2$
Summary

- Screened 56 Ce/O, Am/O, Cm/O, Np/O, Pu/O, Th/O, and U/O compounds for their oxygen removal energies
  - Directly imported structures from MedeA® databases to structure list
  - Set up LAMMPS calculations with Cooper potential
  - Results written to a table and a csv text file

- Same flowchart and strategy can be applied to other materials properties using other potentials
Conclusions

- The MedeA® environment hosts a variety of versatile tools required for creation of realistic models of materials:
  - Molecules, amorphous liquids and solids
  - Bulk polymer, crosslinked resins
  - Interfacial systems and composites

- Integration of highly regarded simulation codes, including LAMMPS, VASP, GIBBS, MOPAC, and Gaussian enables multiple types of property calculation on materials of interest.

- MedeA® High Throughput Launchpad enables the automated, massive screening, exploring, and sampling of materials properties:
  - Young’s modulus of thermoset resins
  - Oxygen removal energy of actinide oxides
Acknowledgements

- Aidan Thompson, Steve Plimpton, and Stan Moore
MedeA®

Your partner in the world of atoms