Utilization of LAMMPS in a Rapid-Response Production Environment to Solve Manufacturing Challenges

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Outline

• About NSC
• Simulation Technology
• Molecular Dynamics Concepts
• Molecular Dynamics
• Origination of need for molecular dynamics
  – Choosing how to implement
  – Rapid response to production issue
• Summary

If we have time, we will show additional applications where we used molecular dynamics in rapid response to production issues
National Security Campus
ELECTRICAL/ ELECTRONIC
- Microelectronics
- Arming, Fusing and Firing Systems
- Embedded Software
- Fiber Optics
- Fire sets / Initiators
- Optics and Initiators
- Radars
- Secure Electronics
- Sensors
- RF / Antenna Design
- Telemetry
- RF / Microwave
- Film Deposition
- Systems Integrator

MECHANICAL
- Containers
- Mechanisms
- Machining
- Solid Modeling
- Prototyping
- Special Materials and Processes
- Welding Technologies

ENGINEERED MATERIALS
- Ceramics
- Polymer Develop. and Production
- Materials Engineering
- Organic / Inorganic / Metallurgy
- Gas Transfer Systems

-60 Years of Continuous Service to Dept. of Energy
- Associates ~ 2500
- Area ~1.5 million sq. ft.
- Kansas City, Missouri
Simulation Technology

Value in Using Simulation Tools for Small Lot Production Environments

- Reduce or eliminate actual prototype builds.
- Reduce time to evaluate processes, designs, and/or fixturing.
- Allows for a more robust process, product or fixture.
- Uncover production problems before they occur.
- Allows for environmentally friendly ‘virtual’ evaluations.
- Aid if production failures do occur.

Simulations can make you agile and flexible to change for rapid response to needs and requirements.
Simulation Technology History

- Have used Finite Element Analysis (FEA) to troubleshoot mechanical issues since 1979
  - 1979 – 1985: NASTRAN
  - 1985 – 2015: Abaqus

- Simulation group, AESA, has grown from a few individuals to ~23 FTEs and conducts 150-200 projects per year

- First molecular dynamics simulation in 2014

- First *ab initio* simulation in 2015
Molecular Dynamics Fundamentals

\[
\frac{d^2 r_i}{dt^2} = \frac{F_i}{m_i} \quad F_i = -\nabla_{r_i} V(r_1, ..., r_N)
\]

Numerically solve them from \( t \) to \( t+\Delta t \), \( t+2\Delta t \) to obtain a trajectory (output data). Temperature and Pressure are calculated and controlled by thermostat and barostat.

\[
K = \frac{3}{2} N \kappa_B T
\]

\[
P V = N \kappa_B T + \frac{1}{D} \left( \sum_{i=1}^{N} r_i \cdot F_i \right)
\]

Physical material properties are emergent

Initial positions and velocities

Interatomic potentials

Symplectic Time Integration
Model & Simulation Applicability

Molecular and Quantum Modeling
- Density
- Young Modulus
- Shear Modulus
- Shear Yield Stress
- Heat Capacity
- Thermal Conductivity
- Thermal Expansion
- Mass Diffusion
- Transition Temps
- Cohesive Energy
- Surface Tension
- Molar Volume
- Solubility
- Gas Permeability

Continuum Modeling
- Product Performance
- Energy Absorption
- Mechanical response
- Thermal conductivity

Length Scales
- Å
- nm
- μm
- mm
- m
- km

Time Scales
- min
- s
- ms
- μs
- ns
- ps

Molecular Dynamics
\[ F = ma \]

Quantum Mechanics
\[ H \Psi = E \Psi \]

Continuum
\[ \sigma = C \varepsilon \]
Activation Energy: Why we took the plunge

• In 2013 an employee with 30+ years of experience of processing the base material for cellular silicones retired.

• Loss of “tribal knowledge” led process to the brink of being out-of-control. Questions arose:
  – What will happen if we replace the mixing blade?
  – What affect does filler particle size/distribution have?
  – Do the variations in room temperature cause the variance?
  – If a butterfly flaps its wings…?

• NSC was preparing 3 years of experiments to regain knowledge and confidence in process.

NSC needed an answer, fast!
Glassware: Getting the Right Tool for the Job

• Polymer production requested help from AESA to model the process’s chemistry.
  • AESA has depth in continuum solutions (EM/Thermal/Mech/Fluid), but none in discrete chemistry.

• The task was wide-open, all solution methods were on the table. Should we:
  – Write our own computational chemistry software to model this specific issue?
  – Outsource to academia?
  – Use open-source / free software exclusively?
  – Use commercial software?

To guide us, we used lessons learned through AESA’s extensive history with finite element analysis
# Building a Finite Element Code

## Geometry
- ACIS
- Parasolid
- Open CASCADE
- CGM
- SOLIDS++

## Discretization
- Topology
- Shape
- Unstructured
- Adaptive
- Higher Order

## Solve
- Linear Solvers
  - Trilinos
  - PETSc
  - Hypre
  - Paralution

## Analyze
- Excel
- Matlab
- Python
- Blot
- Paraview
- VisIt

Of course you can also write any of these yourself!
Code Development and Rapid Response

• This model does not suit well to a rapid-response production environment

• Would require either a few omniscient analysts, or an entire infrastructure built around developing codes (like that found at Sandia National Labs)

• Equal, if not more, time spent debugging issues with code than debugging production issues

• AESA instead uses a commercial FEA software with the following general characteristics:
High quality and easy to use interfaces to:

- We rely on vendor’s quality assurance
  We trust them!

- Rapidly construct accurate geometry

- Rapidly build an accurate physics model

- Rapidly analyze comprehensive results

Total time to build, run and analyze simulation: **4 hours**
Applying to Computational Chemistry

Software Functionality Criteria

<table>
<thead>
<tr>
<th>Low</th>
<th>Desired</th>
<th>Needed</th>
<th>Critical</th>
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</table>
| • Ease of installation  
• Simulate multiple materials?  
• User privilege level required  
• White docs (industry case studies) | • Correlation tool  
• Easy to simulate  
• Easy to post-process  
• Low Cost (<$50k)  
• LAMMPS engine  
• GPU capabilities  
• Quality of Tech Support  
• OS flexibility / interoperability  
• Ability to customize | • Graphics  
• Easy to build amorphous cells  
• Scripting interface  
• Ability to run jobs simultaneously  
• **Good** tutorials & documentation | • Atomistic capabilities  
• Mesoscale capabilities  
• Crosslinking capabilities  
• Works with our HPC platforms / queuing |
Software Selection

• After an initial review of nearly 30 software tools, 3 were selected for evaluation
  – Scienomics: MAPS
  – Materials Design: MedeA
  – Accelrys: Materials Studio

Now Dassault Systemes BIOVIA

• Now armed with a tool, we tackled the problem at hand!
Allowable branching limits were determined using MD. This matched predictions derived from experiment.
Investigating Silicone Polymer Production

Computed Tomography

Contours of Strain-Energy Density ($J/m^3$)

FEA to Compute Mechanical Response
Reinforced Silicone Polymer

Simulations were used to set parameters for experimental methods investigating particle/polymer interactions and aging.

Viscoelastic Stress/Strain

\[
\sigma = \sigma_0 \sin(t\omega + \delta) \quad \varepsilon = \varepsilon_0 \sin(t\omega)
\]

Loss Modulus

\[
E'' = \frac{\sigma_0}{\varepsilon_0} \sin(\delta)
\]

Storage Modulus

\[
E' = \frac{\sigma_0}{\varepsilon_0} \cos(\delta)
\]

\[
\tan(\delta) = \frac{E''}{E'}
\]

Experiment shows tan delta increased with time, as predicted by simulations.
Crosslinking in Silicone Polymer

Bond Distribution Analysis:
- Crosslink formation as function of process conditions
- Probability of secondary reactions (via Gibbs Energy)

Effect of End Group
Vinyl = Crosslinks <200°C
Silanol = No reaction below 200°C

Silanol vs Vinyl functional group
Molecular Dynamics can provide information regarding dynamic change of structure, yielding phase transformation.

Important for Direct-Ink-Write applications

Courtesy of Sid Yip. Used with permission
Professor Emeritus M.I.T
Results

• Cost savings of $210k per year (Materials and Labor)

• Provided confidence that production could downscale this process
  – Provided support for acquisition of $380k of capital equipment

• By providing parameters for experiments, simulations reduced the search space, thus reducing the number of experiments by 70%
Summary

• Molecular dynamics has proven to be a useful tool for NSC and its usage is being expanded
  – If we have time we will look at a few expansions

• NSC’s usage of LAMMPS is dependent on
  – External tools that accelerate and/or enable construction of simulations
  – Trusting that features in these tools and in LAMMPS have been thoroughly validated / verified

• With the right tools and people, molecular dynamics can provide value to rapid-response production environments
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Polymer solubility can be calculated for any given chemical formulation.

**Solubility** $(J/cm^3)^{1/2}$
- Molecular Dynamics = 18.5
- Experimental Value = 19.9

Total time to build, run and analyze simulation: 4 hours

Polymethylacrylate (PMA)
Thin Film Diffusion

Solder Material – Thermal Aging

**Goal:** Improve understanding of metal diffusion observations in thin film aging experiments

**Approach:** Model diffusion via molecular dynamics

\[
\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}
\]

\[
D = p \frac{\Delta x^2}{\Delta t}
\]

\[
\langle \Delta r^2(t) \rangle = \frac{1}{N} \sum_i (\bar{r}_i(t) - \bar{r}_i(0))^2
\]
Minimizing the total energy gaps minimizes residual stress. Control via annealing process.