From atoms to the continuum: Use of Molecular Dynamics and SPH for engineering applications

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Applications of Current Interest

- Fragmentation of liquids
- Swelling of nuclear fuel rods
- Joule Thomson throttling of gases
- Deep Borehole Disposal of nuclear waste
- Closed die forging
- Clogging of sand bed filters
Molecular Dynamics

• Pioneered in 1950s by Bernie Alder.

• Newton’s equations of motion are solved using a finite difference integrator

• Generates time ordered sets of positions and momenta

Basic algorithm conserves energy and linear momentum.

Using the machinery of Boltzmann’s statistical mechanics, contact can be made with classical thermodynamics - an isolated system.
• The **Joule-Thomson effect** refers to the drop in temperature experienced by a gas flowing through a narrow restriction.

• Originated from Joule’s experiments to determine the mechanical equivalent of heat.

• The process is now known as **Throttling**.

• It has played a role in developing our understanding of intermolecular forces, is a key step in the industrial liquification of gases by the Linde process, and the basis of refrigeration.
A non-equilibrium steady state is rapidly established, with constancy of mass and energy fluxes.

\[
\begin{align*}
\rho u & \quad \text{mass flow} \\
\rho u^2 & \quad \text{momentum flow} \\
(\rho u) \left[ e + \left( \frac{P_{xx}}{\rho} \right) + \left( \frac{u^2}{2} \right) \right] & \quad \text{energy flow}
\end{align*}
\]

Tensor Temperature

- Results suggest Fourier’s law of heat conduction will require modification:

\[ Q_x = -\kappa \left( \nabla T_{xx} + \nabla T_{yy} \right) / 2 \]
• Flow of fluid between two parallel crystalline walls driven by an external field provides a useful method of studying non-equilibrium steady states.

• The simulation is fully periodic

• A constant force is applied to all atoms in the flow direction.

• System remains homogeneous in the longitudinal direction.

Results show that a **non-local** generalisation of Newton’s law of viscosity is required:

$$\Pi_{zx}(z) = -\int_0^z \eta(z; z - z')\gamma(z')dz'$$
Fragmentation of Liquids. I

- Fragmentation of liquids has many interesting applications: e.g. atomisation of liquid diesel through a nozzle prior to ignition.

- Cavitation is of considerable interest to engineers due to its ability to cause wear on components.

- A study of fragmentation of liquids (including cavitation) is also interesting for its own sake: the problem is complex involving, surface tension, shockwave formation, viscosity and heat conduction.
The Holian-Grady method

- Infinite checkerboard is linearly expanded in time

\[ \eta L_y \]
\[ \eta L_x \]

- Constant, homogeneous velocity profile is imposed at \( t = 0 \), thereafter the expansion is adiabatic
One (of many!) interesting questions is: **What is the mechanism for fragmentation?**

Adiabatic expansion of a 2D Lennard-Jones spline fluid follows a pathway which crosses through the liquid-vapour coexistence dome – is it spinodal decomposition?

Expansion at rate $\eta = 0.107$
Expansion pathway in $T$-$\rho$ plane

**Expansion at rate** $\eta = 0.107$

- **Expansion: $\rho=0.500, T=0.384$**
- **Expansion: $\rho=0.595, T=0.359$**
- **Expansion: $\rho=0.636, T=0.383$**
- **Expansion: $\rho=0.388, T=0.413$**
- **Expansion: $\rho=0.175, T=0.387$**
- **Expansion: $\rho=0.669, T=0.419$**
- **Expansion: $\rho=0.719, T=0.524$**

The expansion pathway is shown with points at various temperatures and densities. The phase transitions G + L and G + S are also indicated on the graph.
Equilibrium states sampled from expansion pathway

Expansion at rate $\eta = 0.107$

$\rho$ vs. $T$

- Expansion pathway
- EMD 1
- EMD 2
- EMD 3
- EMD 4
- EMD 5
- EMD 6
- EMD 7

G + S

G + L
Clogging of sand bed filters - background

- The Site Ion Exchange Plant (SIXEP) is designed to reduce discharge of Cs and Sr to the sea.

- SIXEP uses a combination of sand bed filters and ion exchange columns.

- A regeneration cycle is implemented when clogging occurs.

\[
\frac{\Delta H}{\Delta H_0} = (1 + \gamma\sigma)^2
\]

- What variables does the clogging parameter, \( \gamma \), depend on?
MD Model of filtration

• Bottom elastic boundary removed when equilibrium is reached

• Particles allowed to fall between scatterers

• Pressure calculated at top and bottom

• Expand this model to match the experiment

Initial conditions  t = 0  t = 1000  t = 5000
Determination of the terminal velocity of a sinking waste package is important for:

1) Developing a safety case for DBD.

2) Establishing if canisters can be emplaced through a cement slug (sink under their own weight).
Sinking speed?

• 3-pronged approach to this problem:
  o Solve Navier-Stokes equations.
  o Conduct sinking experiments using scale model.
  o Model using atomistic simulation and SPH

\[
U^2 \frac{\rho_f R^2 \kappa^6}{L \mu (1 - \kappa^2)^2} + U \left( \frac{-2(1 + \kappa^2)}{(1 + \kappa^2) \ln(\kappa) + (1 - \kappa^2)} \right)
- \frac{R^2 \kappa^2 g}{\mu} \left( \rho_s - \rho_f \right) = 0
\]
NEMD Simulations of flow past solid objects

- Hard object: circle or rectangle modelled with elastic boundaries.

- Fluid atoms modelled with short ranged repulsive potential:

\[ \phi(r) = (1 - r^2)^4 \]

- Conveyor belt boundaries in flow direction drive particles at a fixed flow speed.
• At low Re, the advective term in the NS equations can be discarded.

• For an incompressible fluid we then have:

\[ \nabla p = \eta \nabla^2 \mathbf{v} - g \rho_0 \hat{e}_z \]

\[ \nabla \cdot \mathbf{v} = 0 \]

• The pressure must satisfy Laplace’s equation, \( \nabla^2 p = 0 \) from which follows the velocity field:

\[ v_r = U_\infty \left( 1 - \frac{a^2}{r^2} \right) \cos \theta \]

\[ v_\theta = -U_\infty \left( 1 - \frac{a^2}{r^2} \right) \sin \theta \]
Molecular Dynamics of flow past a confined disk

\[ R = 45, \, v = 0.5 \]
Molecular Dynamics of Flow past a confined rectangle

\( V = 0.5, \ L = 160, \ 2w = 80 \)

\( N = 90,000 \)
• Understanding why materials fail is evidently important.

• Length scales involved dictate the use of continuum modelling.

• Finite element/volume methods have limitations – mesh entanglement, need to re-mesh at failure.

• Continuum mechanics is clearly incomplete and failure modes have an atomistic origin: cracking <- bond breaking.
Example of fracture: Ball-plate penetration. II

• Use atomistic simulation to build better continuum models; use meshless continuum solvers e.g. SPH

• Ball-penetration problem in 2 dimensions provides a useful example in which to do this.
• Movie showing results from simulations using 8-4 potential, four different initial ball velocities \{1,2,4,8\}
Fragmentation of solids by SPAM. I

Stress tensor

\[ \dot{v}_i = \sum_j m_i m_j \left[ \left( \frac{\sigma}{\rho^2} \right)_i + \left( \frac{\sigma}{\rho^2} \right)_j \right] \cdot \nabla_i w(r_{ij}) \]

\[ \sigma = \sigma_{eq} \mathbf{1} + \lambda \mathbf{1} (\nabla \cdot \mathbf{u}) + \eta (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \]

- Where \( \lambda \) and \( \eta \) are the Lamé constants. In terms of the shear and bulk moduli, these are given by

\[
\begin{align*}
\lambda &= B - G \\
\eta &= G
\end{align*}
\]
In SPAM, strains are not readily available and so the deviatoric stress must be obtained indirectly from integration of stress rates.

\[
\begin{align*}
\dot{\sigma}_{xx} &= (\lambda + 2\eta)\dot{\varepsilon}_{xx} + \lambda\dot{\varepsilon}_{yy} \\
\dot{\sigma}_{yy} &= (\lambda + 2\eta)\dot{\varepsilon}_{yy} + \lambda\dot{\varepsilon}_{xx} \\
\dot{\sigma}_{xy} &= \eta\dot{\varepsilon}_{xy}
\end{align*}
\]

Which in turn depend on strain rates, requiring only relative velocities and symmetrised particle densities.
Cold lattice energy from pair potential

\[ \phi_{m,n}(r < \sqrt{2}) = \frac{m}{n-m}(2-r^2)^n - \frac{n}{n-m}(2-r^2)^m \]

\[ \rho = \frac{3}{6\sqrt{3}r^2} \quad \rightarrow \quad v = \frac{\sqrt{3}r^2}{2} \]

Minimum energy, \( \phi = -1 \), (stress free) when \( r = 1 \), \( v_0 = \frac{\sqrt{3}}{2} \)

\[ \therefore r^2 = \frac{v}{v_0} \]
Cold lattice energy equation

\[ e_0 = \frac{3m}{n-m} \left( 2 - \frac{v}{v_0} \right)^n - \frac{3n}{n-m} \left( 2 - \frac{v}{v_0} \right)^m \]

Cold lattice mechanical equation of state

\[ P_0 v_0 = -v_0 \frac{d e_0}{d v} = \frac{3nm}{n-m} \left\{ \left( 2 - \frac{v}{v_0} \right)^{n-1} - \left( 2 - \frac{v}{v_0} \right)^{m-1} \right\} \]

\[ \Rightarrow \sigma_{eq} = -P_0 \]
Bulk modulus from the equation of state:

\[ B_0 = -\nu_0 \left( \frac{dP}{dv} \right)_{v=v_0} \]

Shear modulus determined geometrically:

- Apply a small shear strain to an initially stress-free lattice

\[ G = \lim_{\varepsilon \to 0} \frac{1}{V} \frac{\partial^2 \Phi}{\partial \varepsilon^2} \]

- Compute the change in energy. Repeat for larger strains.
Need to account for plastic yield and tensile failure in continuum model

Plastic yield – von Mises’ energy based yield criterion

\[
\sigma_{\text{shear}} = \left[ \sigma_{xy}^2 + \frac{1}{4} \left( \sigma_{xx} - \sigma_{yy} \right)^2 \right]^{1/2} > Y \rightarrow \text{rescale shear stress}
\]

Tensile failure model:

\[
\frac{1}{2} (\sigma_{xx} + \sigma_{yy}) > \sigma_{\text{tensile}} \Rightarrow \sigma \rightarrow 0, \rho \rightarrow \rho_0
\]
Tensile and yield strengths from NEMD tension test.

- Use time varying periodic boundary conditions in longitudinal direction to pull material apart:

\[
L_x(t) = L_x(0) \left\{ 1 + \dot{\varepsilon} \Delta t \right\}
\]

**Stress**

\[
\sigma_{xx}(t) = -\frac{1}{V} \left[ \sum_i p_{xi}^2 / m_i + \sum_i \sum_{j>i} x_{ij} f_{ij}^x \right]
\]

**Engineering Strain**

\[
\varepsilon_{xx}(t) \equiv \varepsilon = \frac{L_x(t) - L_x(0)}{L_x(0)}
\]
SPAM Ball-Plate penetration – results for \( \{m,n\} = 4,8 \)

**SPAM**

- \( v = 1 \)
- \( v = 2 \)
- \( v = 4 \)
- \( v = 8 \)

**MD**

- \( v = 1 \)
- \( v = 2 \)
- \( v = 4 \)
- \( v = 8 \)
Summary

• Atomistic simulation provides insight and can be used to develop new constitutive equations

• Provides parameters for SPH – important validation step

• Improved models for surface tension, Fourier heat flow and viscous flow are emerging from this work.

• Using home-built codes to enable exploration of weight functions and boundary conditions.