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

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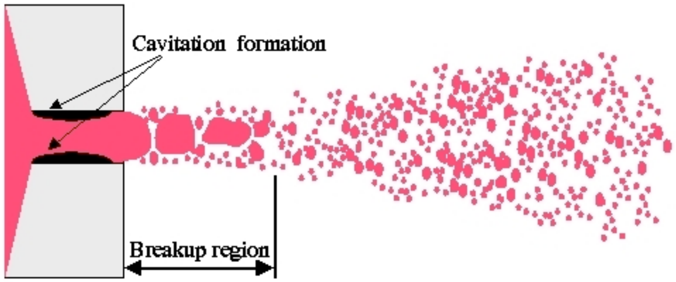
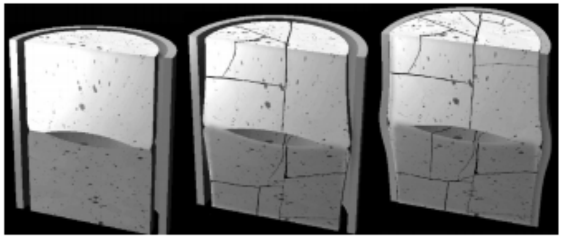
SPH and Industry Workshop, July 10th 2019

Applications of Current Interest

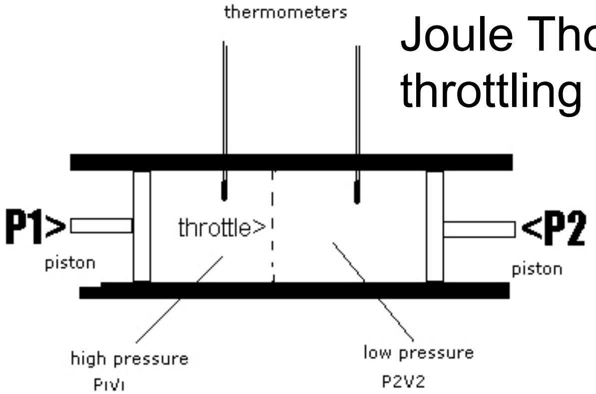
Fragmentation of liquids



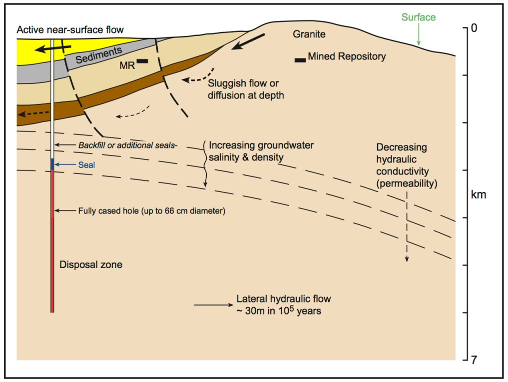
Swelling of nuclear fuel rods



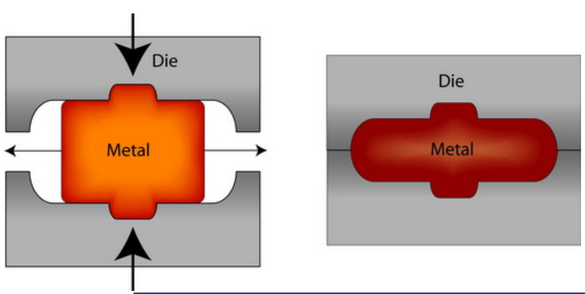
Joule Thomson throttling of gases



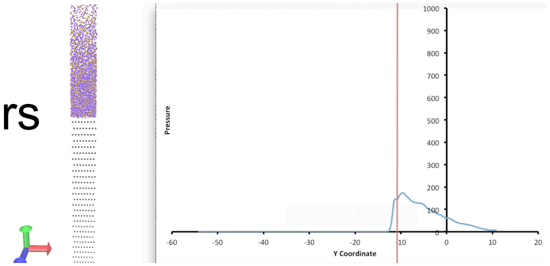
Deep Borehole Disposal of nuclear waste



Closed die forging



Clogging of sand bed filters



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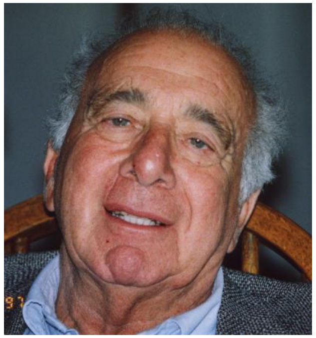
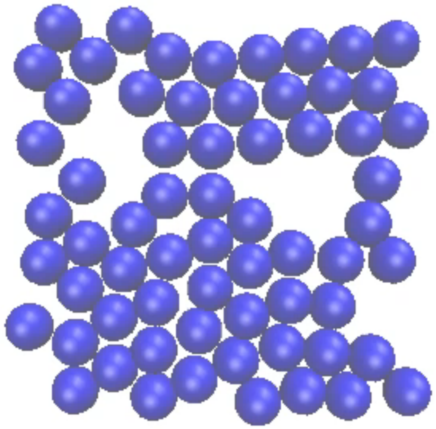
Molecular Dynamics



Bernie Alder, inventor of The Molecular Dynamics Method



- 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.

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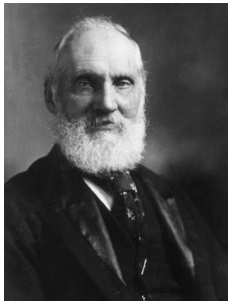
Joule Thomson Throttling process

- 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.

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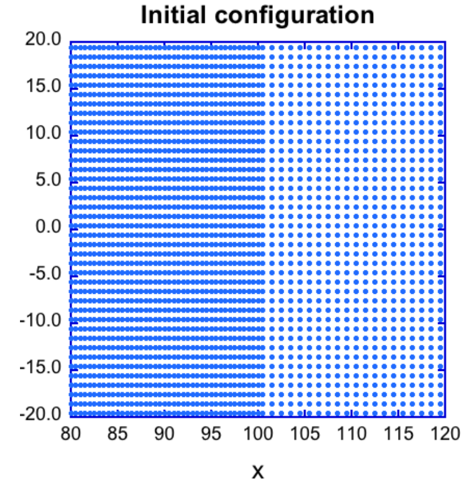
NEMD simulation of JT throttling. I

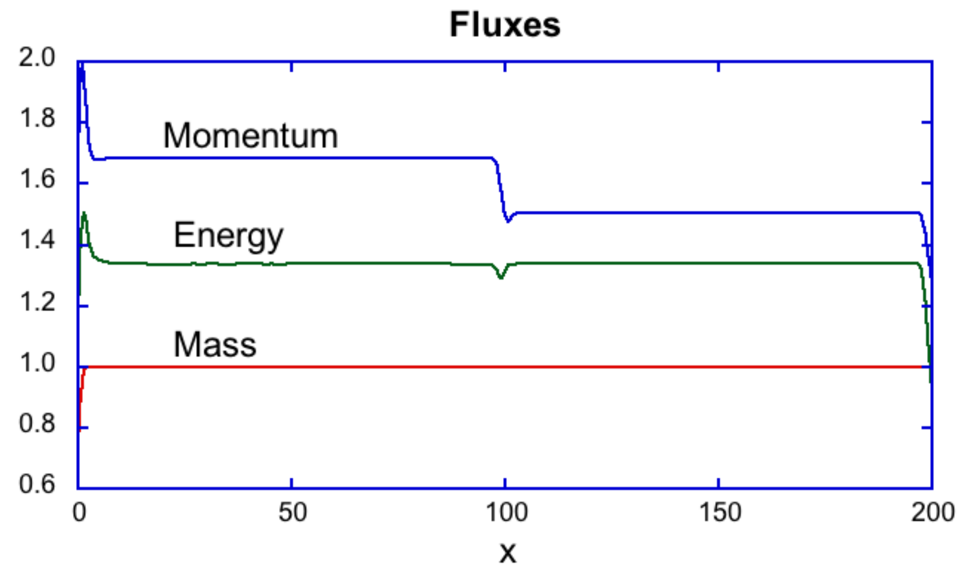
- A non-equilibrium steady state is rapidly established, with constancy of mass and energy fluxes.

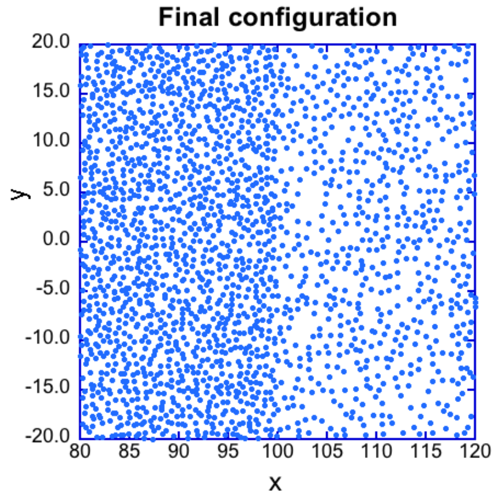
ρu mass flow

$P_{xx} + \rho u^2$ momentum flow

$(\rho u)\left[e + (P_{xx}/\rho) + (u^2/2)\right]$ energy flow

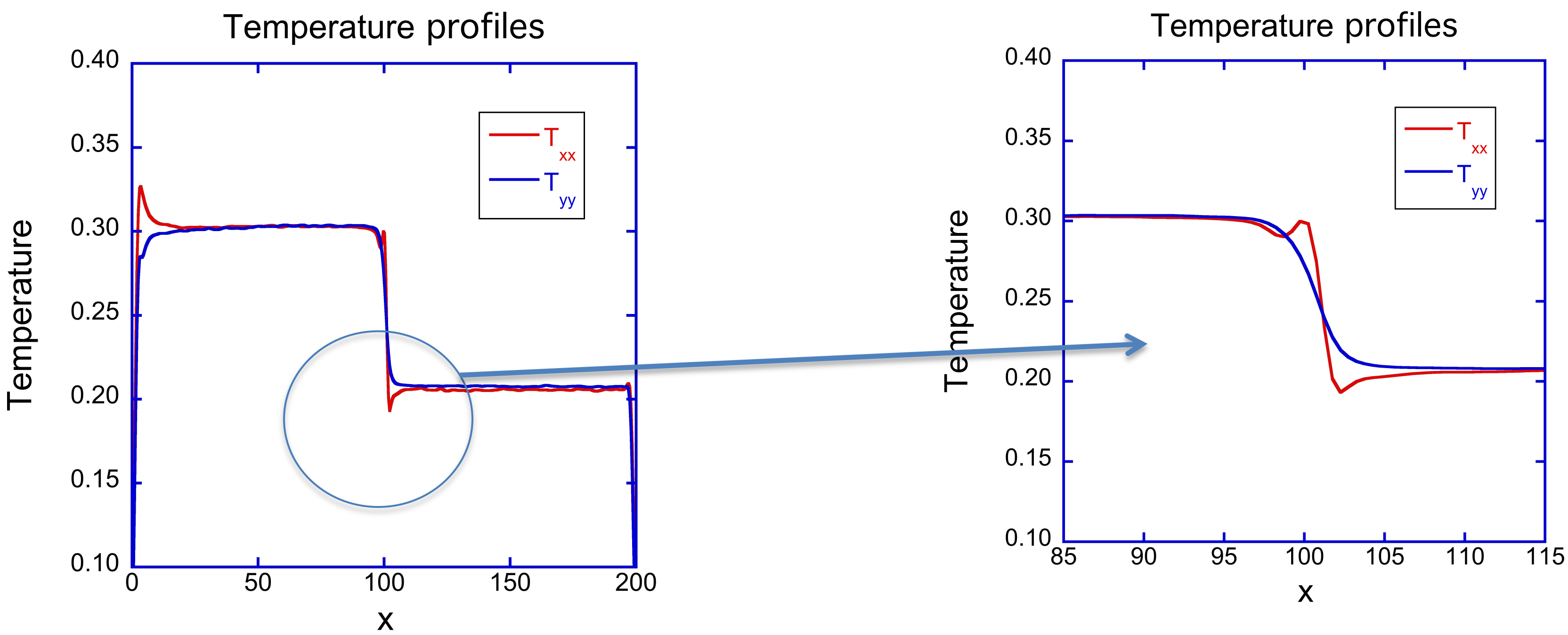






Hoover, Hoover and Travis, *PRL*,**112**, 144504 (2014).

Tensor Temperature



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

$$Q_x = -\kappa\left(\nabla T_{xx} + \nabla T_{yy}\right)/2$$

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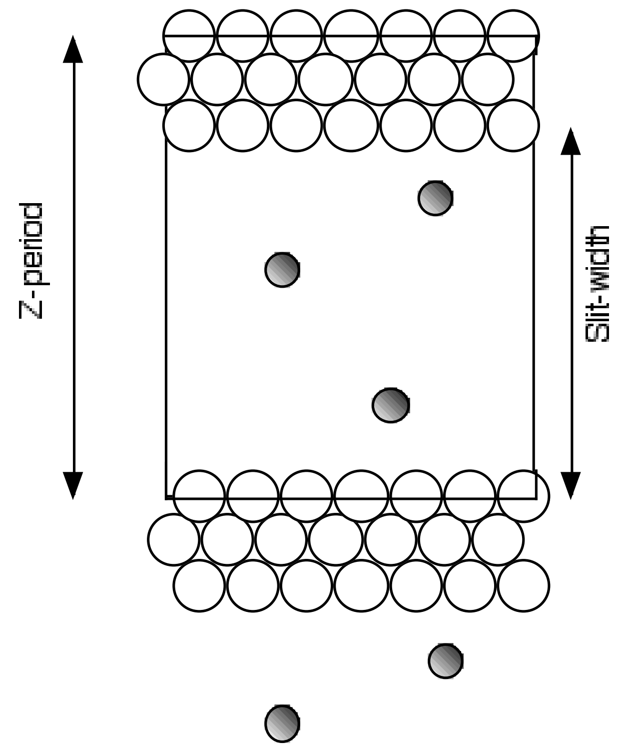
Planar Poiseuille/channel Flow I

- 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.



Travis and Gubbins, JCP, **112**, (2000).

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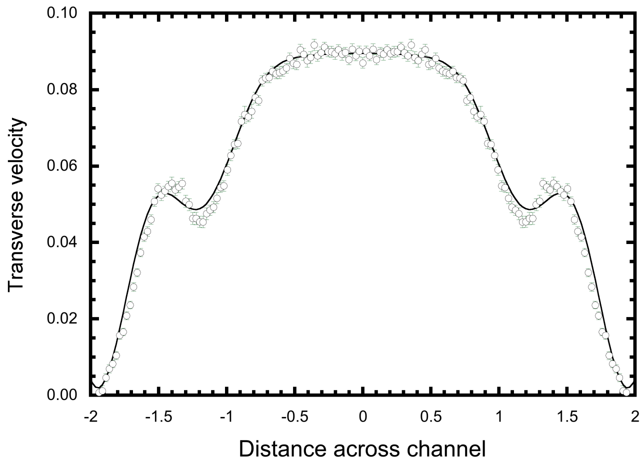
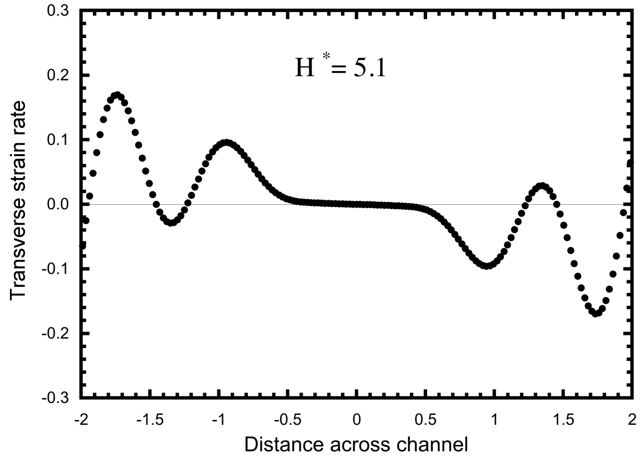
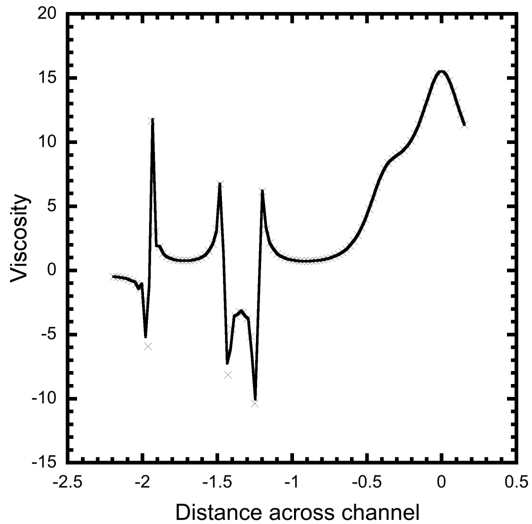
Planar Poiseuille/channel Flow II

- With channels as narrow as 10 molecular diameters, agreement between Navier-Stokes and simulation is good.

- However, at widths of ~ 5 diameters and less, serious deviations occur.







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

$$\Pi_{zx}(z) = -\int_{0}^{z} \eta(z; z - z')\gamma(z')dz'$$

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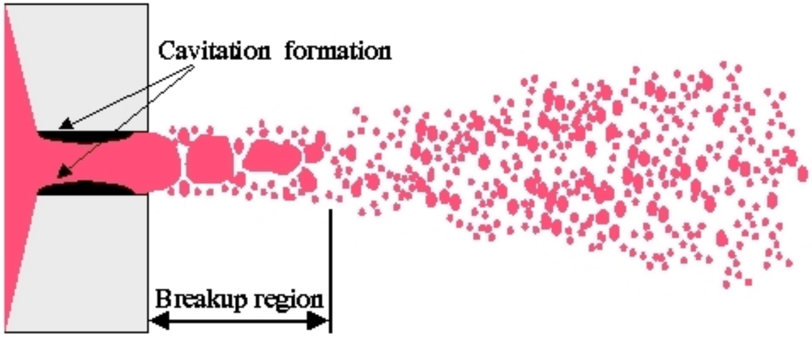
Fragmentation of Liquids. I



• 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.

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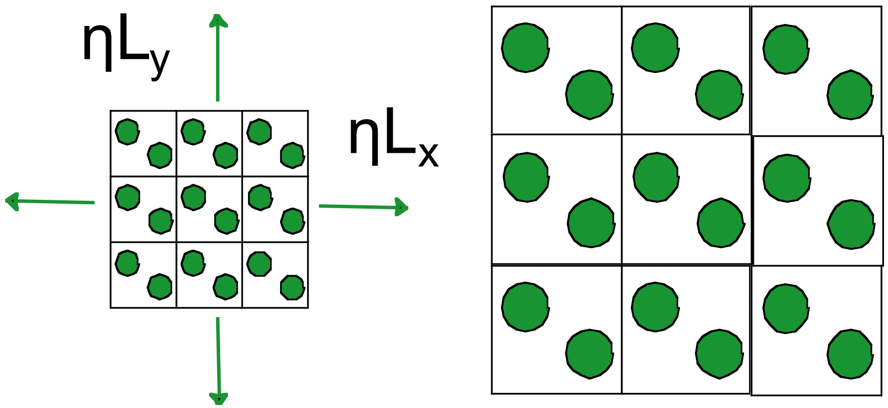
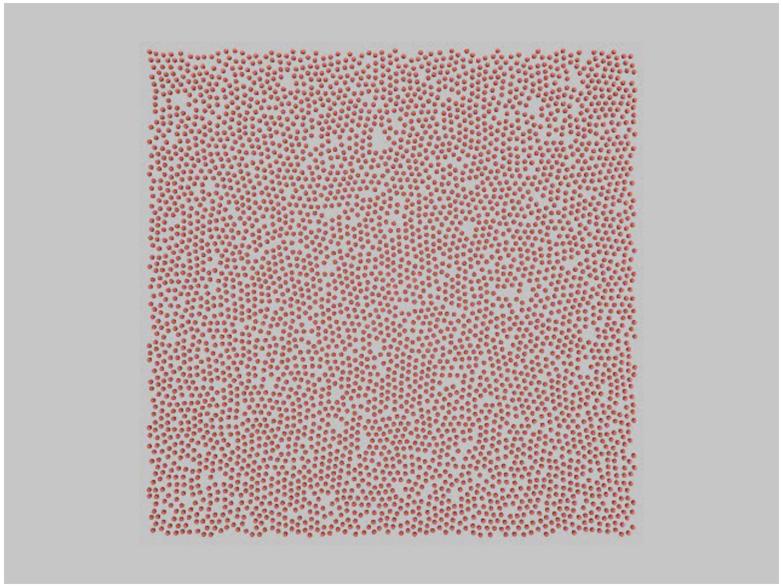
The Holian-Grady method

- Infinite checkerboard is linearly expanded in time





- Constant, homogeneous velocity profile is imposed at t = 0, thereafter the expansion is adiabatic

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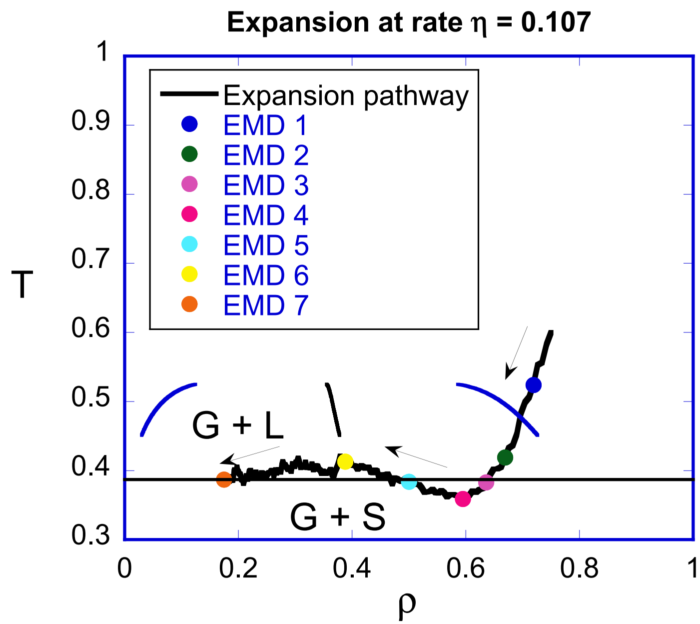
Fragmentation of Liquids. III

- 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?



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Expansion pathway in T-ρ plane

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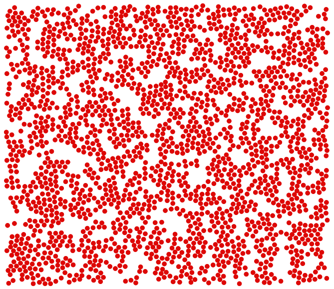
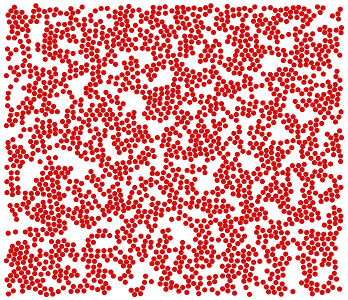
Expansion: $\rho=0.500, T=0.384$



Expansion: $\rho=0.595, T=0.359$



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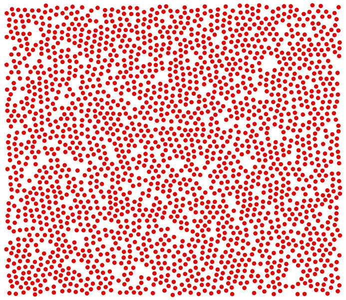
Expansion: $\rho=0.636, T=0.383$



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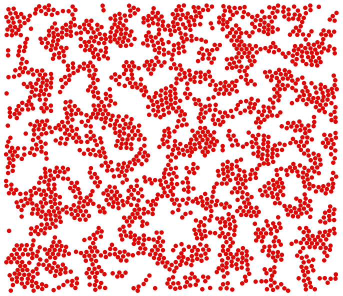
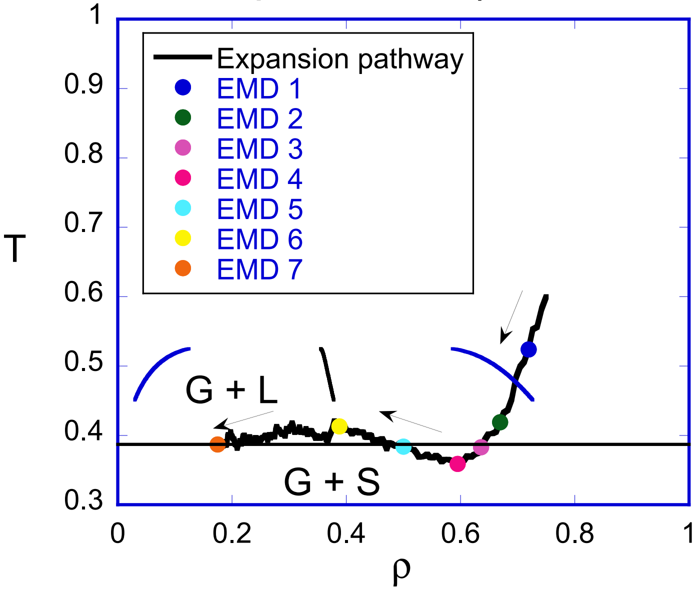
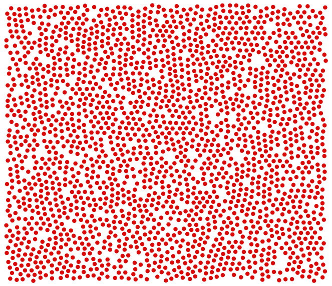
Expansion: $\rho=0.388, T=0.413$



Expansion at rate η = 0.107



Expansion: $\rho=0.669, T=0.419$



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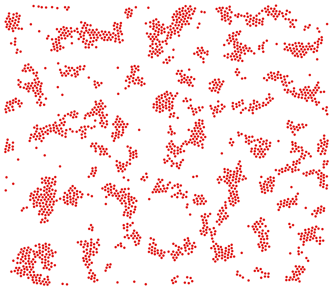
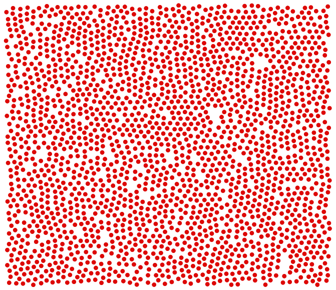
Expansion: $\rho=0.175, T=0.387$



Expansion: $\rho=0.719, T=0.524$



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Equilibrium states sampled from expansion pathway

EMD: ρ=0.500, T=0.384

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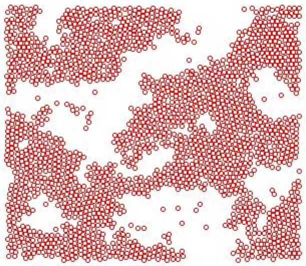
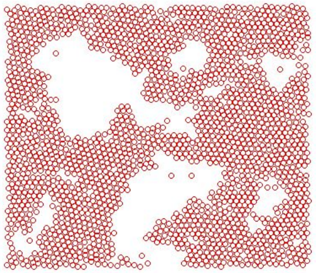


EMD: ρ=0.595, T=0.359



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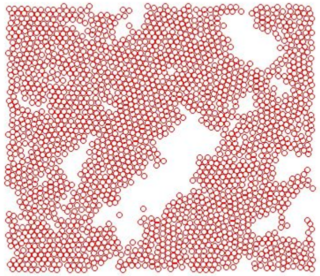
EMD: ρ=0.636, T=0.383



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EMD: ρ=0.388, T=0.413

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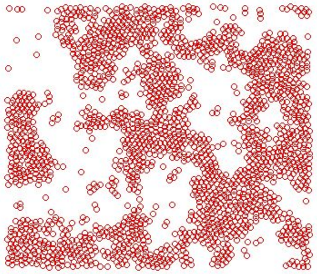
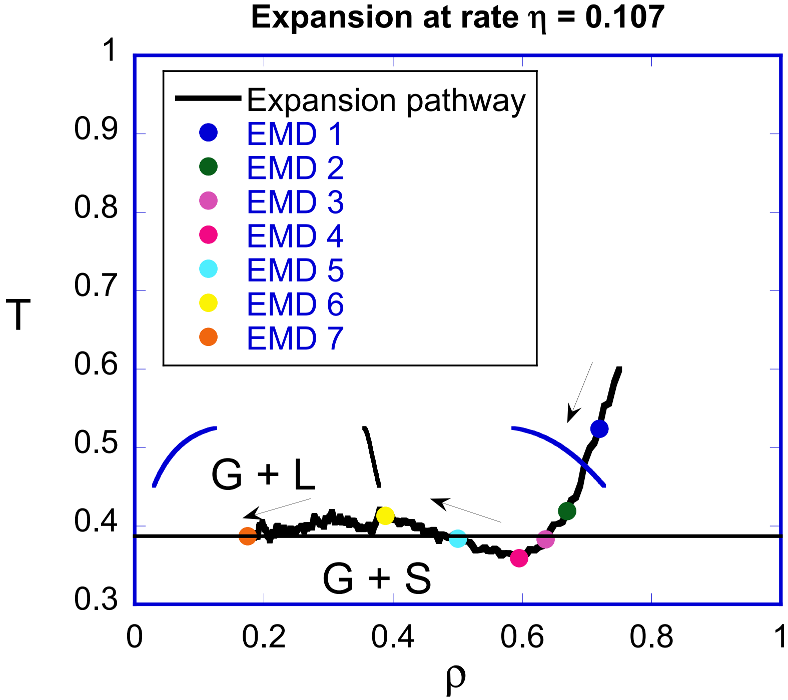
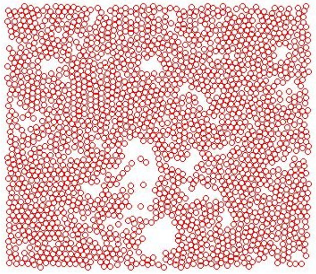




EMD: ρ=0.669, T=0.419



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EMD: ρ=0.175, T=0.387

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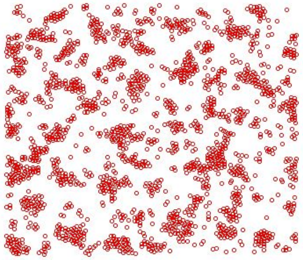
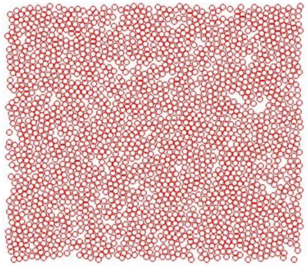


EMD: ρ=0.719, T=0.524



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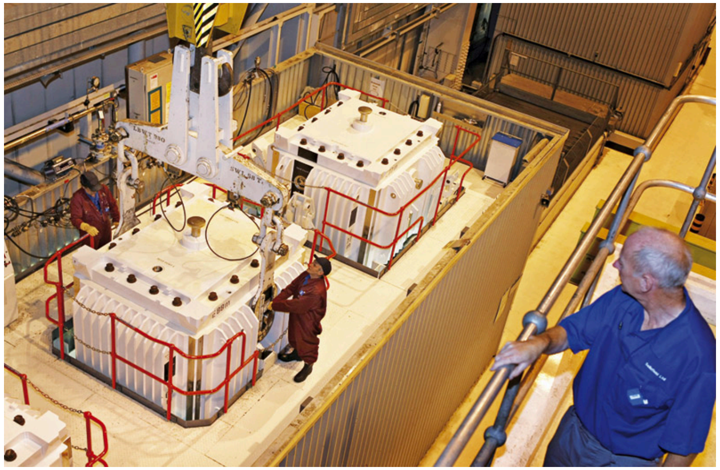
Clogging of sand bed filters - background

- 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, γ, depend on?



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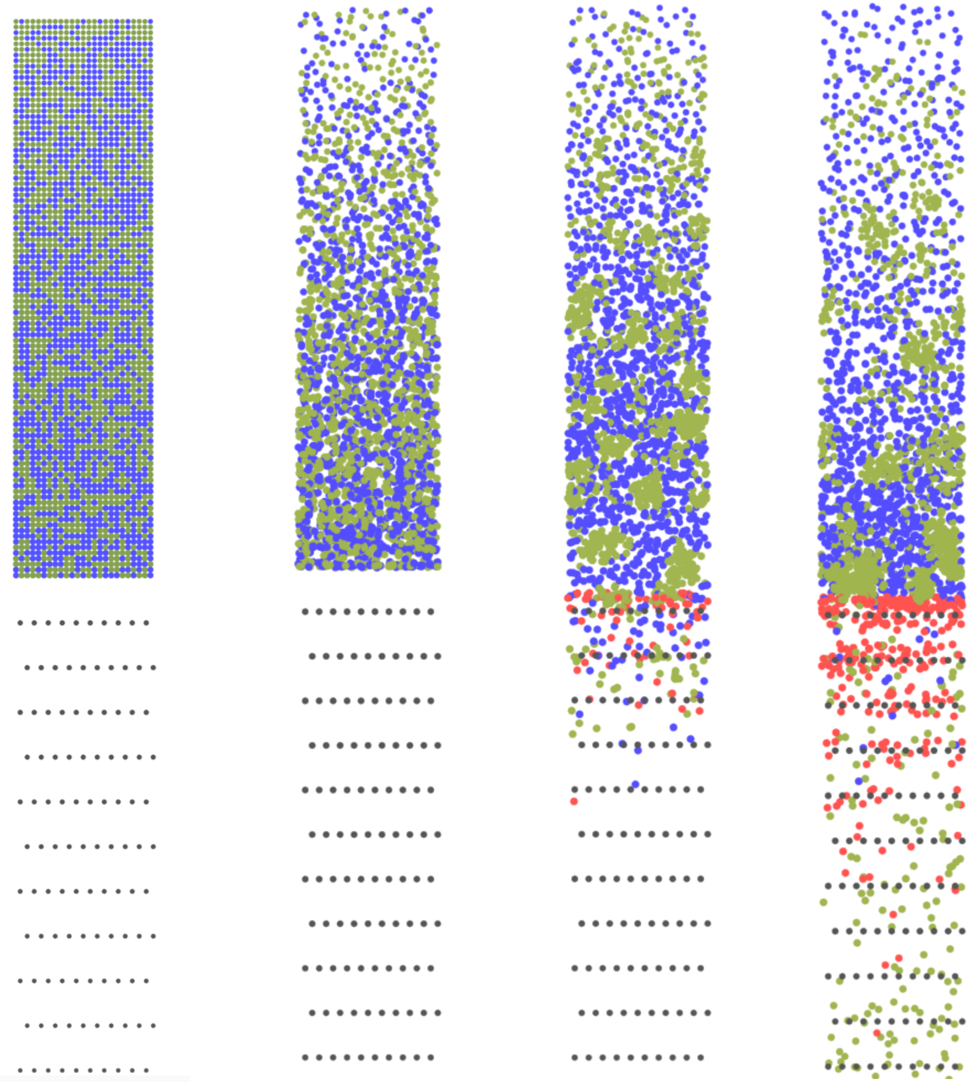
MD Model of filtration

- 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

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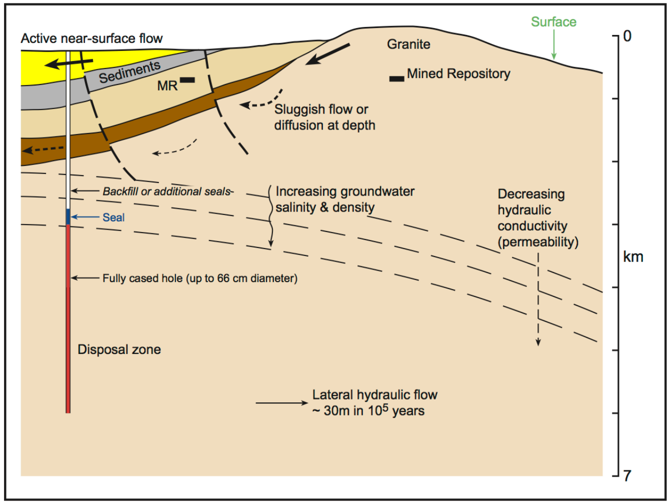
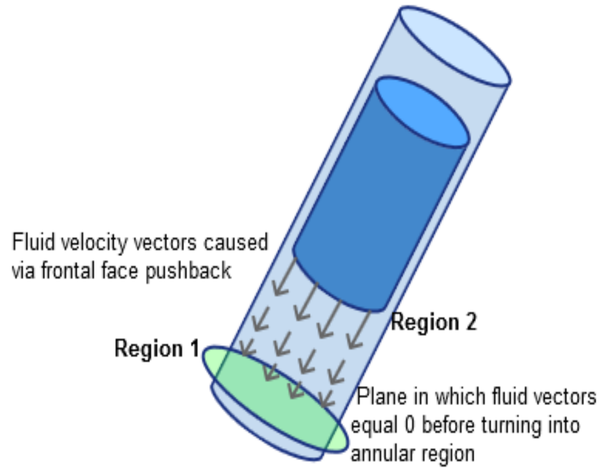
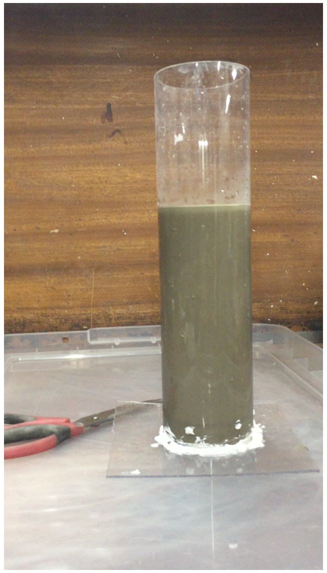
Deep Borehole Disposal (DBD) of HLW / Spent Fuel







- 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).

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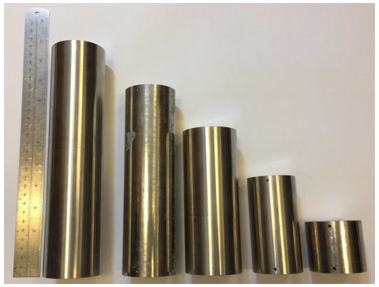
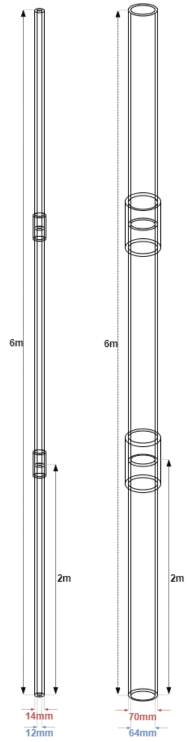
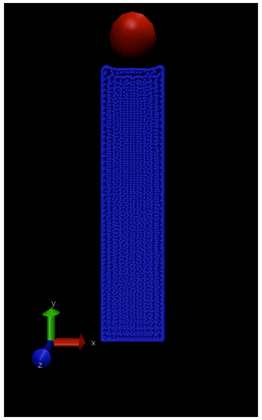
Sinking speed?

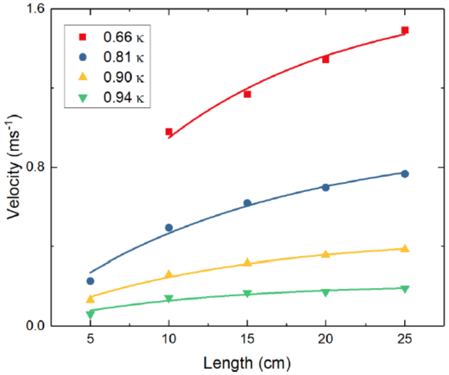
- 3-pronged approach to this problem:
  - Solve Navier-Stokes equations.
  - Conduct sinking experiments using scale model.
  - Model using atomistic simulation and SPH







$$U^2 \frac{\rho_f R^2 \kappa^6}{L\mu(1-\kappa^2)^2} + U\left(\frac{-2(1+\kappa^2)}{(1+\kappa^2)ln(\kappa)+(1-\kappa^2)}\right) - \frac{R^2\kappa^2 g}{\mu}(\rho_s-\rho_f) = 0$$



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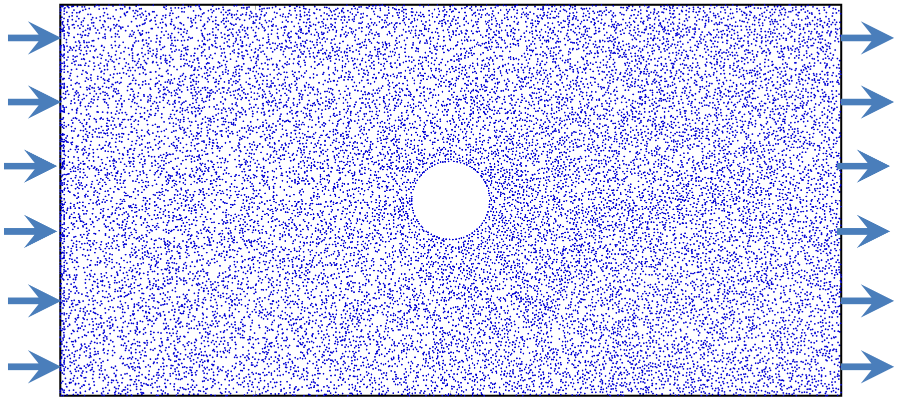
NEMD Simulations of flow past solid objects

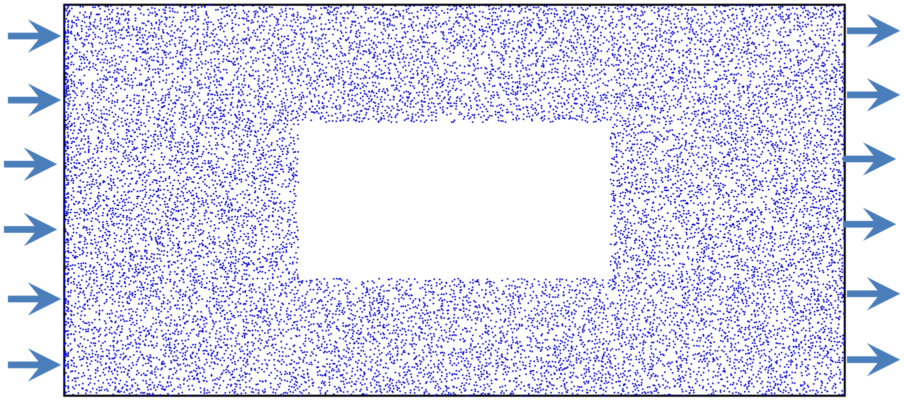
- Hard object: circle or rectangle modelled with elastic boundaries.

- 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.





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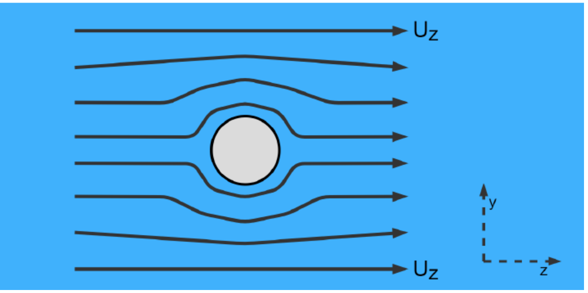
Creeping Flow past a disk: Theory



- At low Re, the advective term in the NS equations can be discarded.
- For an incompressible fluid we then have:

$$\nabla p = \eta \nabla^2 \boldsymbol{v} - g\rho_0 \hat{\boldsymbol{e}}_z$$

$$\nabla \cdot \boldsymbol{v} = 0$$

- The pressure must satisfy Laplace's equation, $\nabla^2 p = 0$ from which follows the velocity field:

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

$$v_\theta = -U_\infty \left(1 - \frac{a^2}{r^2}\right) sin\theta$$

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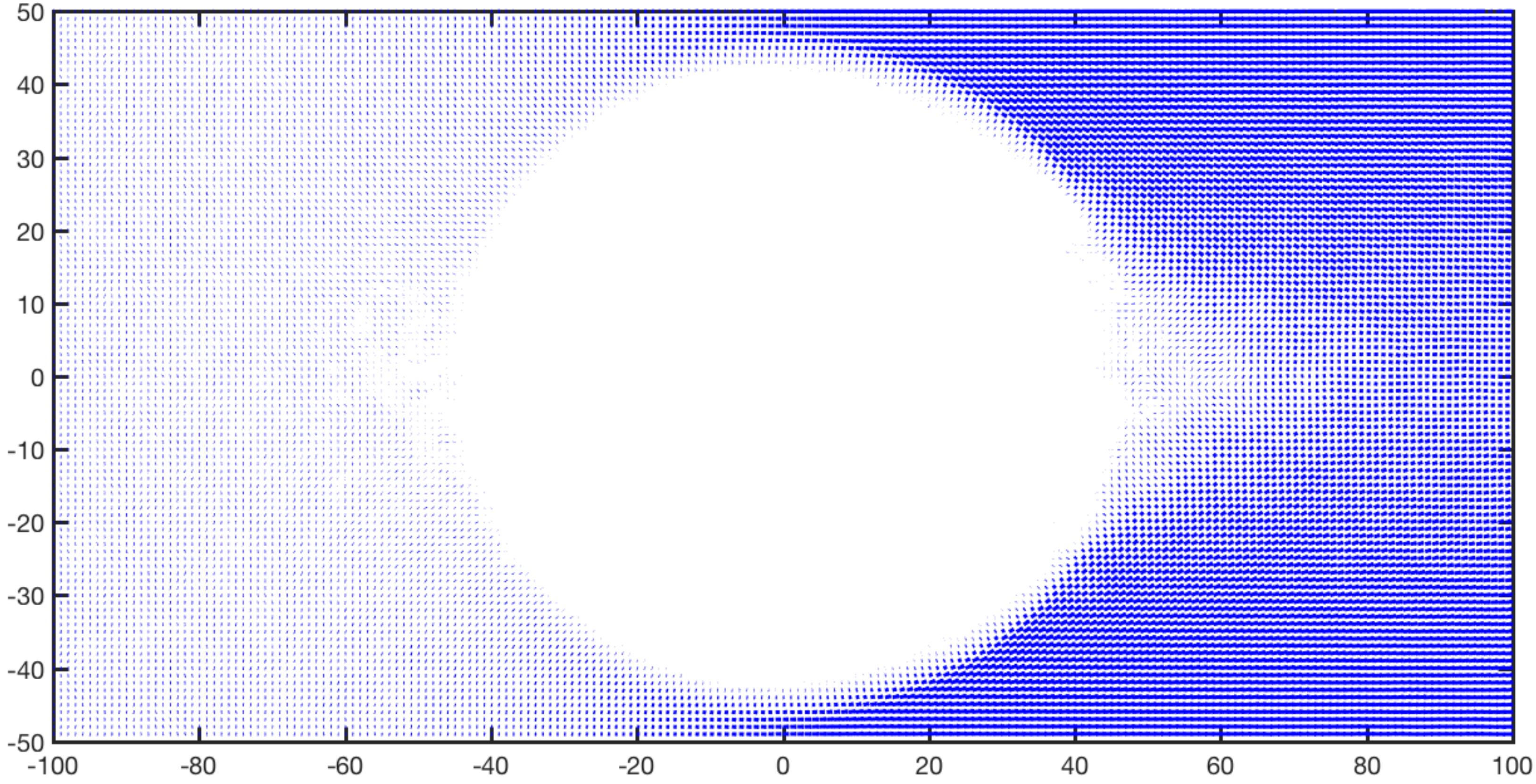
Molecular Dynamics of flow past a confined disk

R = 45, v = 0.5



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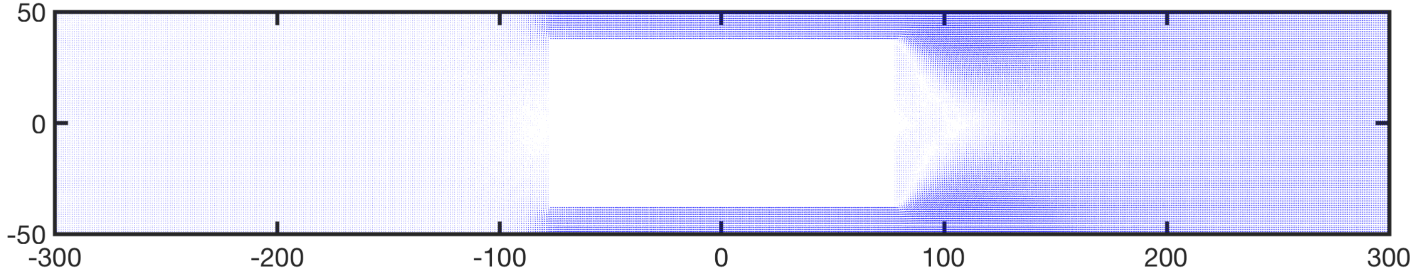
Molecular Dynamics of Flow past a confined rectangle

V = 0.5, L = 160, 2w = 80

N = 90,000



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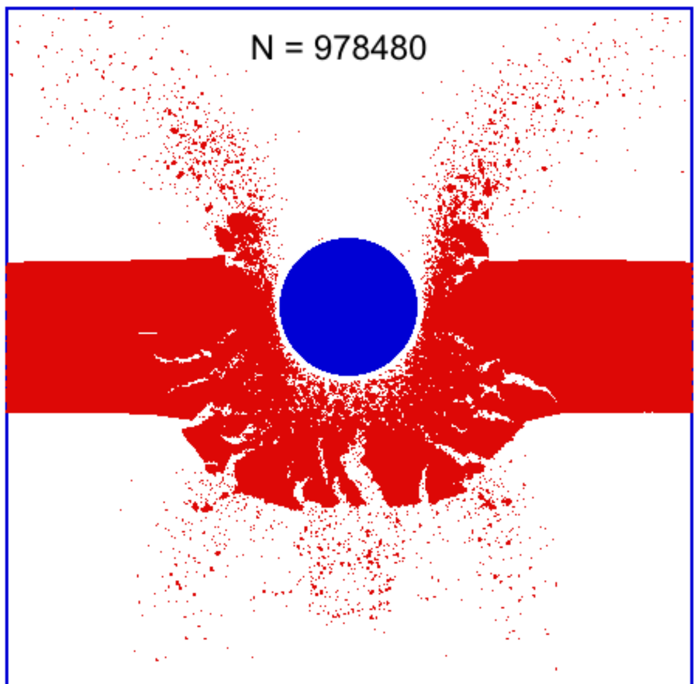
Example of fracture: Ball-plate penetration. I

- 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.



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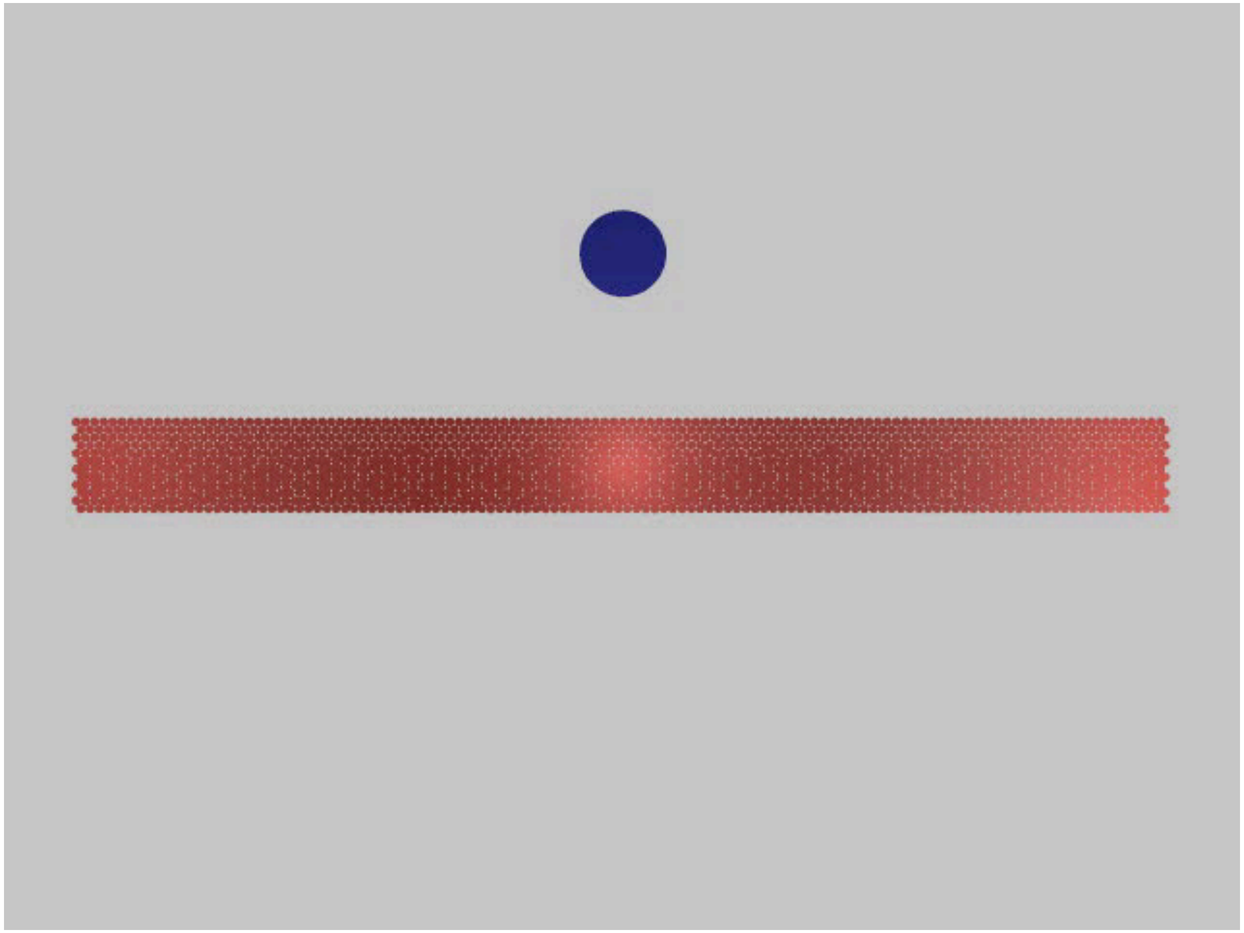
Molecular Dynamics – results I

- **Movie showing results from simulations using 8-4 potential, four different initial ball velocities {1,2,4,8}**



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Stress tensor

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

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

- Where **λ** and **η** are the Lamé constants. In terms of the shear and bulk moduli, these are given by

$$\lambda = B - G$$
$$\eta = G$$

Fragmentation of solids by MD and SPAM. II

- In SPAM, strains are not readily available and so the deviatoric stress must be obtained indirectly from integration of stress ***rates***.

$$\left.\begin{aligned}\dot{\sigma}_{xx} &= (\lambda + 2\eta)\dot{\varepsilon}_{xx} + \lambda\dot{\varepsilon}_{yy} \\ \dot{\sigma}_{yy} &= (\lambda + 2\eta)\dot{\varepsilon}_{yy} + \lambda\dot{\varepsilon}_{xx} \\ \dot{\sigma}_{xy} &= \eta\dot{\varepsilon}_{xy}\end{aligned}\right\} \leftarrow \quad (\nabla \boldsymbol{v})_i = \dot{\boldsymbol{\varepsilon}} = -\sum_j \left(\frac{\boldsymbol{v}_{ij}}{\rho_{ij}}\right)\nabla_i w_{ij}$$

- Which in turn depend on strain rates, requiring only relative velocities and symmetrised particle densities.

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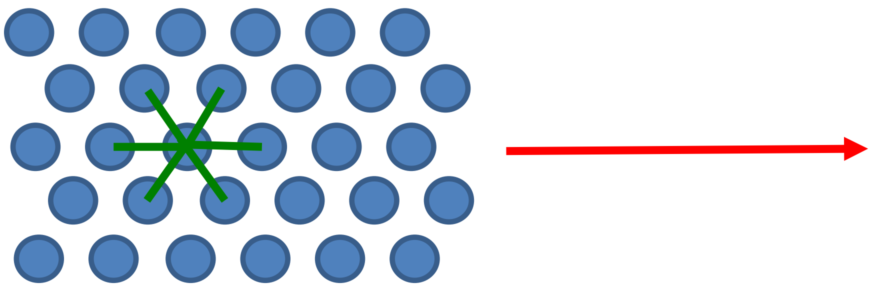
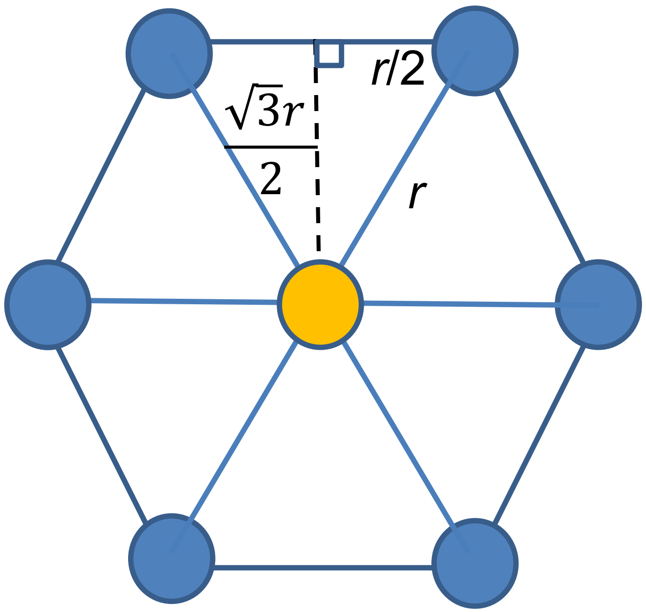
Cold lattice energy from pair potential

$$\phi_{m,n}\left(r<\sqrt{2}\right)=\frac{m}{n-m}\left(2-r^2\right)^n-\frac{n}{n-m}\left(2-r^2\right)^m$$





$$\rho=\frac{3}{6\frac{\sqrt{3}r^2}{4}}\longrightarrow v=\frac{\sqrt{3}r^2}{2}$$

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

$$\therefore r^2=\frac{v}{v_0}$$

Parameterisation I. Equation of state

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

$$P_0 v_0 = -v_0 \frac{de_0}{dv} = \frac{3nm}{n-m}\left\{\left(2 - \frac{v}{v_0}\right)^{n-1} - \left(2 - \frac{v}{v_0}\right)^{m-1}\right\}$$

$$=> \sigma_{eq} = -P_0$$

Parameterisation III. Shear modulus

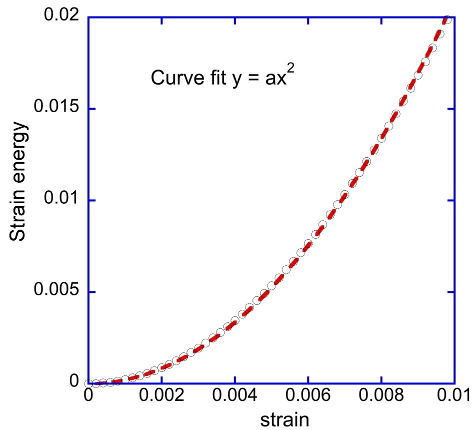
Bulk modulus from the equation of state:

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

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.

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Need to account for plastic yield and tensile failure in continuum model

Plastic yield – von Mises' energy based yield criterion

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

Tensile failure model:

$$\frac{1}{2}(\sigma_{xx} + \sigma_{yy}) > \sigma_{tensile} \Rightarrow \boldsymbol{\sigma} \rightarrow 0, \rho \rightarrow \rho_0$$

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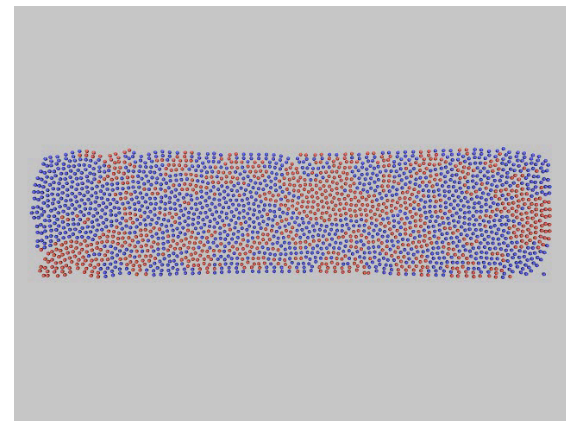
Tensile and yield strengths from NEMD tension test.

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



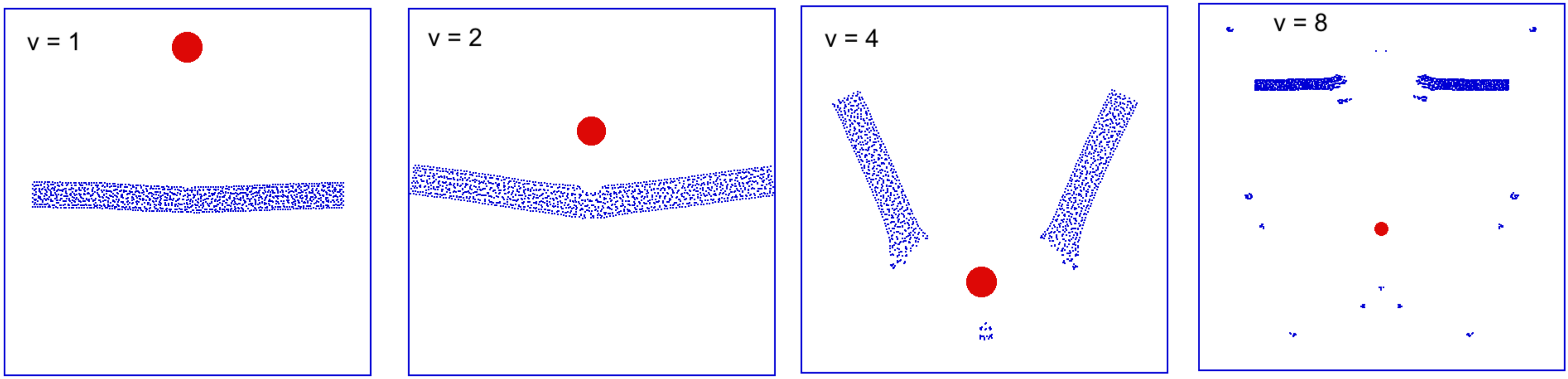
$$L_x(t) = L_x(0)\left\{1 + \dot{\varepsilon}\,\Delta t\right\}$$

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

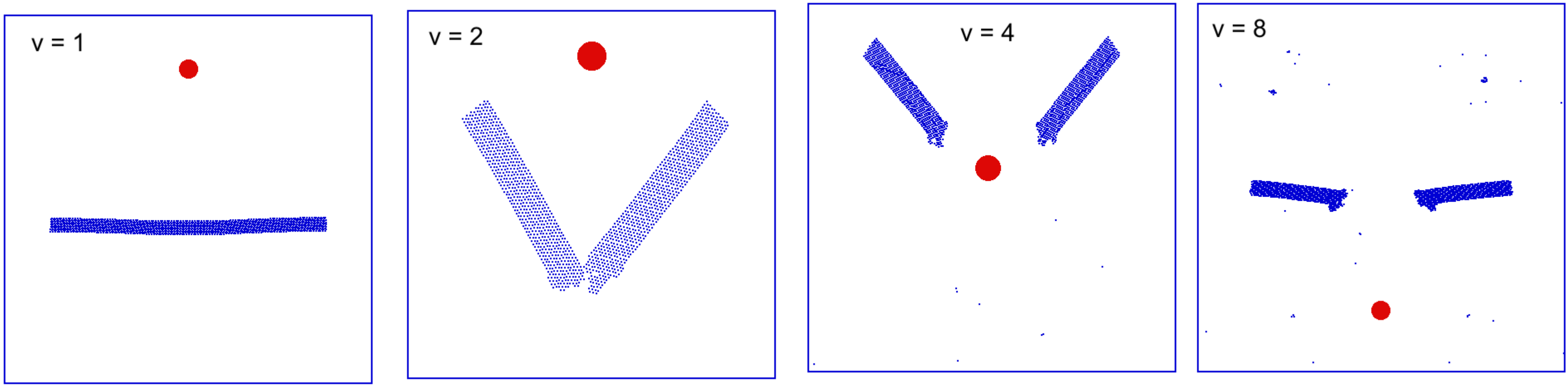
Engineering Strain $$\varepsilon_{xx}(t) \equiv \varepsilon = \frac{L_x(t) - L_x(0)}{L_x(0)}$$

SPAM Ball-Plate penetration – results for {m,n} = 4,8

SPAM



MD



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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.

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