Kharagpur Lectures

Smooth Particles, Molecular Dynamics, and Finite Elements

Carol G. Hoover & William G. Hoover
Ruby Valley Nevada

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Outline

Introduction
Continuum Mechanics
Continuum Equations: comoving and Eulerian, derivation of the continuity equation in Eulerian and Lagrangian forms, equilibrium fluid constitutive equations, nonequilibrium constitutive equations

Numerical Methods
Finite-elements, molecular dynamics, smooth particles (SPAM)

Smooth Particle Method
History, characteristics of smooth particles, weight functions, spatial averaging, gradient interpolation, smooth particle conservation equations, smoothing algorithms for molecular dynamics, boundary conditions, initial conditions, lattice stabilization, smooth particle and molecular dynamics analogs, surface tension, tensile instability, artificial viscoscity and Monaghan's velocity correction

Smooth Particle Averages of Molecular Dynamics Data

SPAM Results
Free expansion, collapsing water column, Rayleigh-Bénard flow, ball-plate fragmentation

Parallel Computing

1. Introduction

Microscopic versus Macroscopic Material DescriptionS

Atomistic Length & time scales
L ~ Å
~ ps - ms
Atomistic motion satisfies ordinary differential equationst

Particle equations

Solve: $m\dot{v} = -\nabla \cdot \Phi$
Specify force laws for atoms

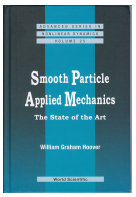
Laboratory Length & time scales
L ~ cm or meters
t ~ ms or seconds
Fluids and solids satisfy partial differential flow equations

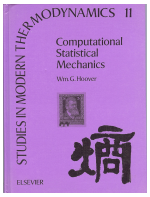
Continuum equations

Solve : $\rho\dot{v} = -\nabla \cdot P$
Specify : Constitutive relations for the materials

A particle method for solving the equations of continuum mechanics

For a pdf files, go to www.williamhoover.info





2. Continuum Mechanics

Continuum Equations Conserve Mass, Momentum, & Energy

Particles are material points and the evolution of particle points is expressed in the comoving Lagrangian coordinate frame .

Comoving Lagrangian Equations

$$\dot{\rho} = -\rho\nabla \cdot v \;\; ; \;\; \dot{v} = -\nabla \cdot P/\rho \equiv \nabla \cdot \sigma/\rho$$

$$\rho\dot{e} = \rho\left(\frac{\partial e}{\partial t} + v \cdot \nabla e\right) = [-\nabla \cdot Q] - (\nabla v) : P$$

Constitutive Equations

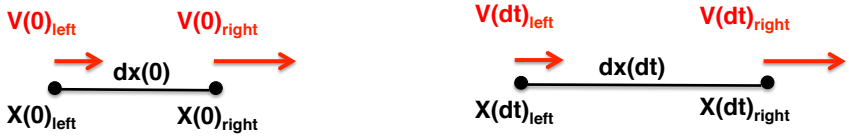
$$P = P(\rho, e, \nabla u)$$
$$Q = Q(\rho, e, \nabla T)$$

Laboratory-Frame Eulerian Equations

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho v) \;\; ; \;\; \frac{\partial (\rho v)}{\partial t} = -\nabla \cdot (P + \rho v v)$$

$$\rho\dot{e} = \rho\left(\frac{\partial e}{\partial t} + v \cdot \nabla e\right) = [-\nabla \cdot Q] - (\nabla v) : P$$

Continuity Equation - Conservation Law for Mass
Comoving Lagrangian Coordinates



The coordinate at the center of the interval is x_0 and it moves at the flow velocity.

$$v\left(x_0+\frac{dx}{2}\right)\approx v(x_0)+\frac{dx}{2}\left(\frac{\partial v}{\partial x}\right)_t$$
$$v\left(x_0-\frac{dx}{2}\right)\approx v(x_0)-\frac{dx}{2}\left(\frac{\partial v}{\partial x}\right)_t$$

$$x_{right}(dt)=x_{right}(0)+v\left(x_0+\frac{dx}{2}\right)dt$$
$$x_{left}(dt)=x_{left}(0)+v\left(x_0-\frac{dx}{2}\right)dt$$

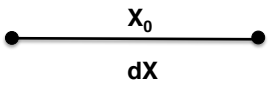
$$dx(dt)=dx(0)\left[1+\left(\frac{\partial v}{\partial x}\right)_t dt\right] \longrightarrow \frac{[dx(dt)-dx(0)]}{dtdx(0)}=\frac{dln(dx)}{dt}$$

$$-\frac{dln\rho}{dt}=\frac{\partial v}{\partial x}\ ;\qquad \frac{dln\rho}{dt}=-\nabla\cdot v$$

Student Problem

Using a similar analysis, develop the momentum conservation equation in Lagrangian coordinates.

Continuity Equation - Conservation Law for Mass
Laboratory Eulerian Coordinates



In the time interval *dt* the net change of mass within the interval dx is the difference in the mass flow into the interval at the end points.

$$\Delta m=\left[(\rho v_x)_{x-dx/2}-(\rho v_x)_{x+dx/2}\right]dt$$

Notice that for a fixed interval the time derivative of the mass is

$$\frac{\partial(\rho dx)}{\partial t}=dx\,\frac{\partial\rho}{\partial t}\ ;$$

$$\frac{\partial\rho}{\partial t}=\left((\rho v_x)_{x+dx/2}-(\rho v_x)_{x-dx/2}\right)/dx=-\frac{\partial\rho v_x}{\partial x}$$

$$\frac{\partial\rho}{\partial t}=-\frac{\partial\rho v_x}{\partial x}\ ;\quad \frac{\partial\rho}{\partial t}=-\nabla\cdot(\rho v)$$

Equilibrium Fluid Constitutive Equations

Mechanical equation of state (adiabatic and isothermal):

$$P = B_o\left(\frac{\rho^3}{\rho_o^3} - \frac{\rho^2}{\rho_o^2}\right)$$

Thermal equation of state and Mechanical equation of state:

$$E = NDkT/2;\ PV = NkT = \frac{2}{D}E$$

Heat capacity and compressibility:

$$dE/dT_{V\,or\,P} > 0;\ -(1/V)(\partial V/\partial P)_{T\,or\,S} > 0$$

Van der Waals' equation:

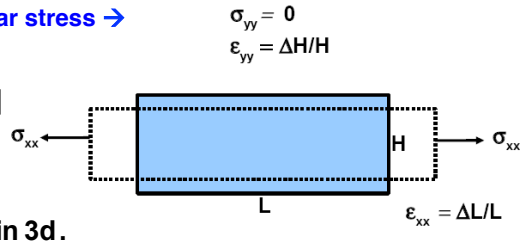
$$P = \frac{NkT}{V - Nb} - \frac{N^2a}{V^2};\ E = \frac{DNkT}{2} - \frac{N^2a}{V}$$

Nonequilibrium Constitutive Relations

- **Nonequilibrium dissipation: viscosity, conductivity, plasticity, …**
- **Fourier's law:** $Q = -\kappa\nabla T.$
- **Newton's formulation of shear stress → symmetrized stress tensor :**

$$\sigma = \sigma_{eq}I + \lambda I\nabla\cdot v + \eta[\nabla v + \nabla v^t]$$

$$\eta_v = \eta + \lambda \text{ in 2d};\ \eta_v = \tfrac{2}{3}\eta + \lambda \text{ in 3d}.$$



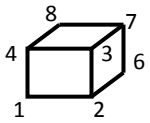
$$E = \sigma_{xx}/\varepsilon_{xx};\ \nu = -\varepsilon_{yy}/\varepsilon_{xx}$$

- **Use von Mises shear stress condition for plasticity :**

$$(s_{xx}^2 - s_{yy}^2) + 4s_{xy}^2 \le Y^2 \text{ in 2d}.$$

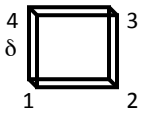
3. Numerical Solution Methods
Finite Elements DYNA3D

- **Use space-filling volumes to approximate the continuum:**
  8-Node brick has isoparametric velocity interpolation for strain rates:



$$v(x,y,z) = a_1 + a_2x + a_3y + a_4z + a_5xy + a_6yz + a_7zx + a_8xyz$$

- **4-Node shell elements are two-dimensional.**
  They have a thickness δ and various underlying through-the-thickness integration schemes.

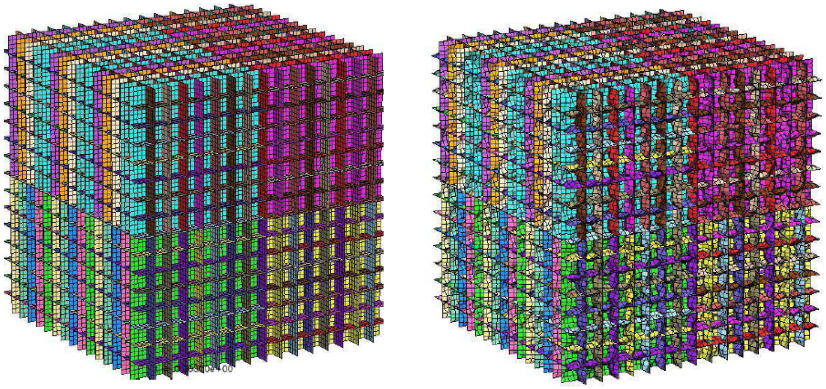


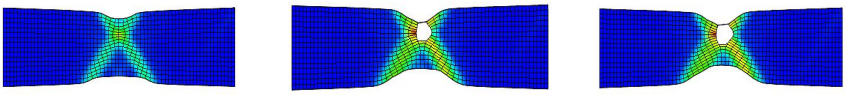
$$v(x,y) = a_1 + a_2x + a_3y + a_4xy$$

- **Calculate pressure, energy, stress by integrating over elements**
  For example, nodal strain/strain rates, element integration → stresses.

- **Isoparametric elements are not rotationally invariant**
  Hourglass control is needed to prevent instability

Two Example Finite-Element Calculations

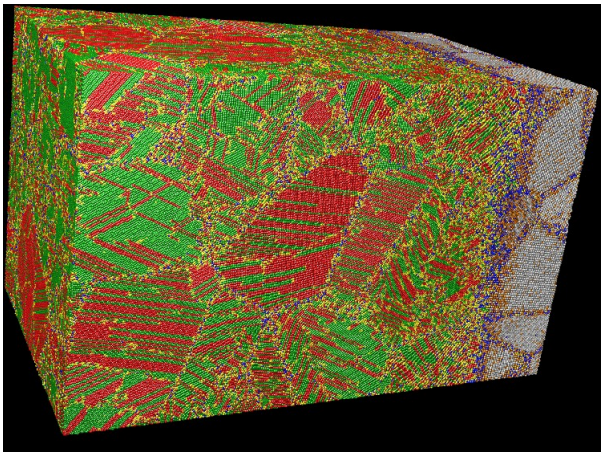




Time = 32 **Time = 48** **Time = 64**

Particle Methods: Molecular Dynamics and SPAM

30,000,000 atomistic particles + parallel computer → **5000-65,000 smooth particles + workstation**



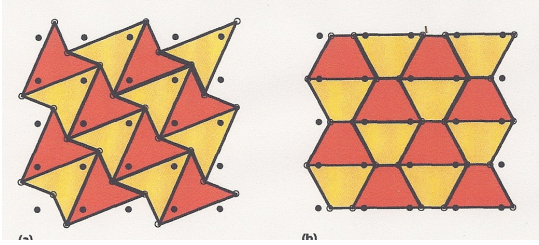
From Kai Kadau's Los Alamos Webpage 2007

SPAM versus Finite-Element Methods

SPAM is **MUCH simpler** than finite-element algorithms: no element lists, no element integration

SPAM solves **ordinary differential equations**; not partial differential equations; **rezoning is easy** with SPAM

SPAM avoids mesh tangling and shear instabilities; **no unstable butterfly or hourglass modes**

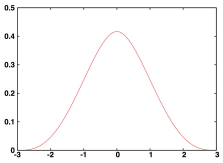


SPAM versus Molecular Dynamics

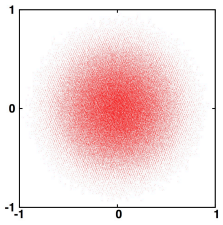
- SPAM and Molecular Dynamics are both *particle* methods.
- SPAM particles are mass points with a finite extent. Molecular dynamics particles are point masses.
- Molecular dynamics follows motion of point particles on an atomic length and time scale with ordinary differential equations. Input to the calculations is fundamental, the potential energy function.
- The SPAM method approximates the partial differential equations of continuum mechanics with particles that satisfy ordinary differential equations for conservation of mass, momentum and energy. Input to these equations are equations of state (constitutive equations).
- There are two interesting cases of trajectory isomorphism for SPAM and molecular dynamics. Trajectory isomorphism means identical trajectories.

4. Smooth Particle Method – History and Motivation

- **Smooth particles**
  Smooth particles have a finite extent h. The density at a point is the sum of smooth particles within a distance h of the point. Molecular dynamics uses point masses.
- **History**
  Smooth particles are used for astrophysics problems : (Gingold, Lucy, and Monaghan) - 1977
  Smooth particles were first used in the 1980's (Monaghan, Swegle) and early 1990's for fluids – SPH
  Smooth particles were applied to solids and fluids in 1990's (Wingate, Hoover, Cloutman)
  Today the method is applied in many fields: heat conduction, electricity and magnetism, fluids, fluid-structure interaction, and fragmentation.
- **Motivation → "Simplify, Simplify, Simplify" Thoreau**
  Partial differential equations are converted to ordinary differential equations
  Fluids and solids satisfy the same motion equations
  No element integration
  No mesh tangling for flow problems
  Material failure is simple with Lagrangian particles



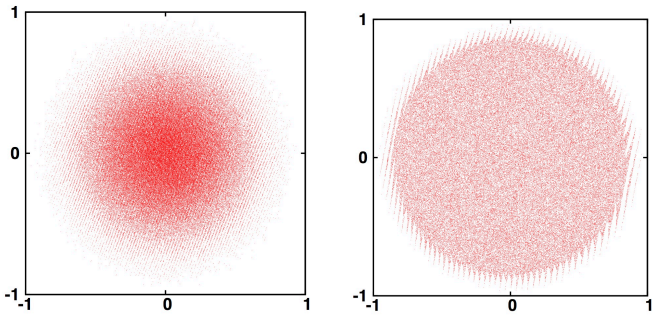
Particle in one dimension



Particle in two dimensions

A Random Number Problem!

These are plots of points generated randomly in [0,1] and then selected if the random number is less than the value of the Lucy weight function in two-dimensions.



Clearly, with the diagonal stripes that are quite visible at the edges, there is a problem with the random number generators. Possibly these are serial correlations?

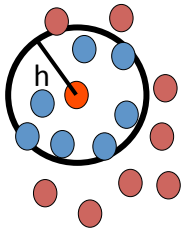
Student Problem

Do some research on random number generators and identify problems or find a better random number generator.

Characteristics of Smooth Particles

Very Smooth approximation: The functional form for a particle is chosen so that the density at a point is a smooth interpolant for continuum field variables. A smooth interpolant has at least continuous first and second derivatives. Polynomials of at least third degree or spline fits are good choices.

Finite extent: The range of a particle, h, overlaps with other particles. The density at a particle point is the sum of density contributions from all particles within the range h including the particle itself.



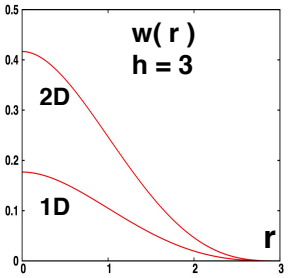
Define: $\rho(j) = \sum_i w(r_i - r_j)$

Interpolation satisfies physical laws: The smooth particle interpolation substituted into a continuum equation converts a partial differential equation into an ordinary differential equation. Such an interpolation is selected to satisfy conservation of mass, momentum or energy. One exception to this is the conservation of angular momentum.

Lucy's Weight Function

$$w(r<h) = C_D\left[1+3\frac{r}{h}\right]\left[1-\frac{r}{h}\right]^3$$

From a family → $w_n \propto \left[1+n\frac{r}{h}\right]\left[1-\frac{r}{h}\right]^n$; n = 3



Lucy' function is a quartic polynomial satisfying 5 conditions

Conditions on the function and derivatives

A smooth function with two continuous derivatives everywhere :

$$w'(0) = 0\,;\; w(h) = 0\,;\; w'(h) = 0\,;\; w''(h) = 0$$

Normalization

$$\int_0^h 2w_{1d}dr = 1\,;\; \int_0^h 2\pi r w_{2d}dr = 1\,;\; \int_0^h 4\pi r^2 w_{3d}dr = 1$$

$$C_{1D} = 5/4h \;\;;\;\; C_{2D} = 5/\pi h^2 \;\;;\;\; C_{3D} = 105/16\pi h^3$$

Student Problem

Write a program to calculate Lucy's weight function in one and two dimensions. Verify your program is correct by integrating the weight function from 0 to h.

Lucy's Weight function and derivative

```
c This is Lucy's function and its derivative in two dimensions
      function w(r)
      implicit double precision( a-h,o-z )
      common h

      pi = 3.141592653589793d00

      if(r.gt.h) stop
      z = r/h
      w = (5/(pi*h*h))*(1 - 6*z*z + 8*z*z*z - 3*z*z*z*z)
      return
      end

      function wp(r)
      implicit double precision( a-h,o-z )
      common h

      pi = 3.141592653589793d00
      z = r/h
      if(r.gt.h) stop
      wp = (5/(pi*h*h*h))*(-12*z+24*z*z-12*z*z*z)
      return
      end
```

Monaghan's Weight Function

Monaghan developed a weight function that is cubic rather than quartic by smoothly connecting two cubic splines and imposing 6 conditions conditions on the function and its derivatives and two additional conditions as shown below.

$$w_{Monaghan} = C_D\left(\frac{1}{2} - 3\frac{r^2}{h^2} + 3\frac{r^3}{h^3}\right) \quad for\ 0 < \frac{r}{h} < \frac{1}{2}$$

$$w_{Monaghan} = C_D\left(1 - \frac{r}{h}\right)^3 \quad for\ \frac{1}{2} < \frac{r}{h} < 1$$

Two cubic splines smoothly connected at r = 1/2 and satisfying 8 conditions

Normalization constants

$$C_{1D} = 8/3h \ ; \ C_{2D} = 80/7\pi h^2 \ ; \ C_{3D} = 16/\pi h^3$$

Smoothly connects the two spline matching at r = 1/2

$$w, w', w'' are\ continuous\ at\ r = 1/2$$

Maximum particle density in the center

$$w' = 0 \ at \ r = 0$$

Student Problem

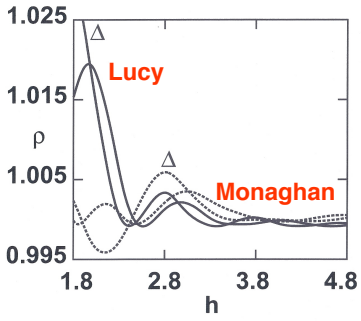
Write a program that calculates Monaghan's weight function in one and two dimensions. Check your results by integrating from 0 to h.

Spatial Interpolation

Density interpolation converges with ~ 20 neighbors

$$\rho_i = \sum_j w(|r_i - r_j|); \ |r_i - r_j| \le h.$$

Good estimate for particle smoothing length comes from the summed up densities at regular lattice sites .



2D square and triangular lattices with

$$h \ge 3$$

lead to errors less than 1% in the density for both weight functions

Continuum field variables & derivatives (at any point in space) are particle sums .

Student Problem

Calculate the density in a square lattice with the Monaghan weight function.

Density Calculation in Two Dimensions

```
c This is the summed-up density calculation
      subroutine getrho(x,y,rho)
      implicit double precision(a-h,o-z)
      parameter(N=400,iwide=20)
      dimension x(N),y(N),rho(N)
      common h

      do i = 1,N
      rho(i) = w(0.0d00)
      enddo

      do i = 1,99
      do j = i+1,100
      xij = x(i) - x(j)
      yij = y(i) - y(j)
      if(xij.gt.+iwide/2) xij = xij - iwide
      if(xij.lt.-iwide/2) xij = xij + iwide
      if(yij.gt.+iwide/2) yij = yij - iwide
      if(yij.lt.-iwide/2) yij = yij + iwide
      rij = dsqrt(xij*xij + yij*yij)
      if(rij.lt.h) then
        rho(i) = rho(i) + w(rij)
        rho(j) = rho(j) + w(rij)
      endif
      enddo
      enddo

      sumrho = 0.0d00
      do i = 1,N
      sumrho = sumrho + rho(i)
      enddo

      return
      end
```

$$\rho(j) = \sum_i w(r_i - r_j)$$

SPAM Interpolants Are Averages Formed by Particle Sums

Smooth particle interpolation uses particle averages

Averages are very easy to implement for an irregular set of points compared to the usual method of fitting functions to the points. Averages are not unique.

Smooth particle weight functions

Although the Lucy and Monaghan weight functions are most often used other choices may work equally well. The requirement that the weight function have continuous first and second derivatives must be met in order to apply the averages to the continuum equations. The order of the derivatives determine the choice of the smoothness of the weight function.

Smooth particle averages are based on defining the density in terms of the weight function

Define: $\rho(j) = \sum_i w(r_i - r_j)$

Applying the averages to partial differential equations converts them to ordinary differential equations which can be integrated with Runge-Kutta

Alternative Averages for Irregular sets of material points

The average value of a field variable at a point r is defined in terms of the sum of particle points within a distance h of the field points. The particle points are mass points whose motion is governed by ordinary differential equations. The ordinary differential equations for particle mass, momentum, and energy evolution are designed to approximate the partial differential equations of continuum mechanics. There are three averages (f_0 , f_1 , and f_2) useful in defining the continuum field variables.

$$\rho(r) f_0(r) = (f\rho)_r \equiv \sum_i f_i m_i w_{ri} \; ; \; w_{ri} \equiv w(r - r_i) \; ; \; \rho(r) = \sum_j m_j w_{rj} \; ;$$

$$f_1(r) \equiv \sum_i (f/\rho)_i m_i w_{ri} \; ; \; (f/\rho)_i \equiv f_i/\rho_i \; ; \; \rho_i = \sum_j m_j w_{ij} \; ; \; w_{ij} \equiv w(r_i - r_j)$$

$$f_2(r)/\rho(r) \equiv \sum_i \left(f/\rho^2\right)_i m_i w_{ri} \; ; \; \left(\rho^2\right)_i = \rho_i^2 \, .$$

where f_i = the value of a physical variable at a particle point (such as x, v, T, e, ..)
f_r = the average value of a field variable at a point r (sum over particles)
w_{ij} = the weight function at particle i including all particles j in the range h
w_{ri} = the weight function used in the sum over particles to create the average value at field point r.

Smooth Particle Approximation to the Continuity Equation

Consider the Lagrangian continuity equation $\dot{\rho} = -\rho \nabla \cdot v$

$$\dot{\rho}_i = \frac{d}{dt} \sum_j m_j w_{ij} = \sum_j m_j \left(\dot{r}_i \nabla_i w_{ij} + \dot{r}_j \nabla_j w_{ij} \right) = \sum_j m_j v_{ij} \nabla_i w_{ij}$$

$$with \; v_{ij} = \dot{r}_i - \dot{r}_j = v_i - v_j$$

Consider $\rho \nabla \cdot v = \nabla \cdot \rho v - v \cdot \nabla \rho \longrightarrow (\rho \nabla \cdot v)_i = (\nabla \cdot \rho v)_i - (v \cdot \nabla \rho)_i$

$$(\nabla \cdot \rho v)_i = \nabla_i \cdot \sum_j m_j v_j w_{ij} = \sum_j m_j v_j \nabla_i w_{ij} \; using \; the \; approximation \; \rho f_0$$

$$(v \cdot \nabla \rho)_i = v_i \cdot \sum_j m_j \nabla_i w_{ij}$$

$$(\rho \nabla \cdot v)_i = \sum_j m_j v_j \nabla_i w_{ij} - \sum_j m_j v_i \nabla_i w_{ij} = -\sum_j m_j v_{ij} \nabla_i w_{ij}$$

$$\dot{\rho}_i \equiv -(\rho \nabla \cdot v)_i \; exactly \, !$$

We don't need to solve for the evolution of the density!! Limitation: Surfaces need special treatment. Use density sums for bulk calculations.

Interpolation for Gradients Using Particle Sums

Continuum field variables & gradients include the following in two dimensions:

$$r, v, e, P_{xx}, P_{xy}, P_{yy}, Q_x, Q_y, \nabla v, \nabla T, \nabla \cdot Q, \nabla \cdot P$$

SPAM approximations for computing gradients

Evaluate derivatives using the three function approximations defined previously.

$$\nabla(f\rho)_r \equiv \sum_j m_j f_j \nabla_r w_{rj} \; ; \quad \nabla_r f \equiv \sum_j (f/\rho)_j m_j \nabla_r w_{rj} \; ; \quad \nabla(f/\rho)_r \equiv \sum_j (f/\rho^2)_j m_j \nabla_r w_{rj}$$

Nonequilibrium fluxes

Use the **first one** for evaluating ∇v *and* ∇T. It is ideal for describing the gradients leading to nonequilibrium fluxes of momentum and energy

Energy and momentum conservation

Use the **third one for evaluating** $\nabla \cdot P$ *and* $\nabla \cdot Q$ so as to conserve the overall system's momentum and energy.

Smooth Particle Motion Equation

Consider the Lagrangian momentum equation : $\rho \dot{v} = -\nabla \cdot P$

Use $\nabla \cdot \frac{P}{\rho} = -\frac{P}{\rho^2}\nabla\rho + \frac{1}{\rho}\nabla \cdot P$

$$\dot{v} = -\frac{1}{\rho}\nabla \cdot P = -\frac{P}{\rho^2}\nabla\rho - \nabla \cdot \frac{P}{\rho}$$

The smooth particle approximation is given by

$$\dot{v}_i = -\left(\frac{P}{\rho^2} \cdot \nabla\rho\right)_i - \left(\nabla \cdot \frac{P}{\rho}\right)_i$$

$$\left(\frac{P}{\rho^2} \cdot \nabla\rho\right)_i = \left(\frac{P}{\rho^2}\right)_i \cdot \sum_j m_j \nabla_i w_{ij}$$

$$\left(\nabla \cdot \frac{P}{\rho}\right)_i = \nabla_i \cdot \sum_j m_j \left(\frac{P}{\rho^2}\right)_j w_{ij} = \sum_j m_j \left(\frac{P}{\rho^2}\right)_j \cdot \nabla_i w_{ij}$$

Combining terms and multiplying by m_i gives the smooth particle motion equation

$$m_i \dot{v}_i = -\sum_j m_i m_j \left[(P/\rho^2)_i + (P/\rho^2)_j\right] \cdot \nabla_i w(r_i - r_j)$$

Use mean value for the mass product : $m_{ij} = \frac{1}{2}(m_i + m_j)$ *or* $\sqrt{m_i m_j}$

Smooth Particle Approximation to the Continuum Equations

We use 4th order Runge-Kutta to integrate these ordinary differential equations. They are smooth particle approximations to the continuum equations. The particle equations satisfy conservation of energy, mass, and momentum.

$$\dot{\rho}_i \equiv -(\rho \nabla \cdot v)_i \quad \textit{exactly !}$$

$$m_i \dot{v}_i = -\sum_j m_i m_j \left[\left(P/\rho^2\right)_i + \left(P/\rho^2\right)_j \right] \cdot \nabla_i w(r_i - r_j)$$

$$m_i \dot{e}_i = -\sum_j m_j \left[\left(P/\rho^2\right)_i + \left(P/\rho^2\right)_j \right] : \frac{1}{2} v_{ij} \nabla_i w_{ij}$$

$$-\sum_j m_i m_j \left[\left(Q/\rho^2\right)_i + \left(Q/\rho^2\right)_j \right] \cdot \nabla_i w_{ij}$$

There are three steps to deriving the energy equation

- The heat-flux divergence needs to be written in a symmetric pair-sum form, just as was the divergence of the pressure tensor.
- The antisymmetry of the derivatives ,

  $$\nabla_i w_{ij} + \nabla_j w_{ij} = 0$$

  guarantees that the summed up heat-flux contributions to the total energy change vanish.
- As a consistency check the rate of change of the internal energy must cancel the rate of change in the kinetic energy.

Smooth Particle Derivatives for Temperature and Velocity for Constitutive Relations

$$\text{Consider } \rho \nabla v = \nabla v \rho - v \nabla \rho$$

$$(\rho \nabla v)_r = \sum_j m_j v_j \nabla_r w(r - r_j) - v_r \sum_j m_j w(r - r_j) \quad \longleftarrow \quad \rho f_0$$

$$\textit{Using } r \to r_i \textit{ and combining terms gives}$$

$$(\rho \nabla v)_i = -\sum_j m_j v_{ij} w(r_i - r_j)$$

This expression for a pair of particles can be symmetrized using a mean density (arithmetic or geometric).

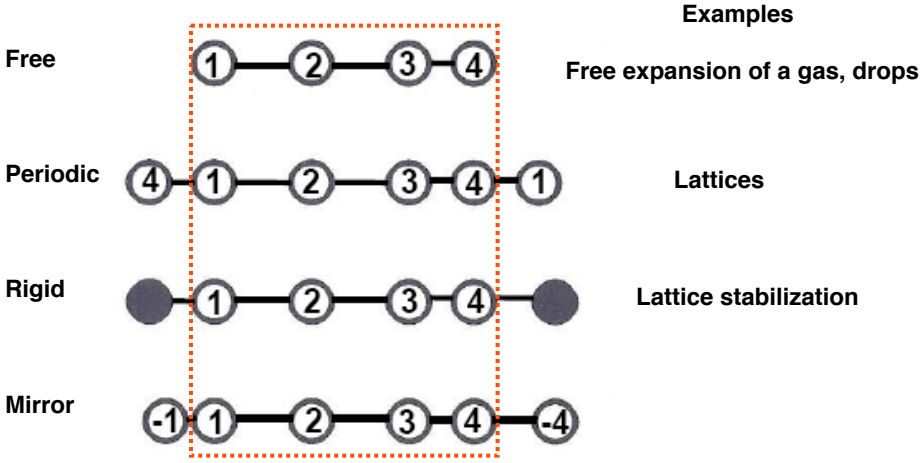
$$\rho_{ij} = \frac{1}{2}(\rho_i + \rho_j) \textit{ or } \rho_{ij} = \sqrt{\rho_i \rho_j}$$

For equal masses the velocity & temperature gradients have the form

$$\nabla T = \sum_j m_j [T_j - T_i] \nabla_i w_{ij} / \rho \; ; \quad \nabla v = \sum_j m_j [v_j - v_i] \nabla_i w_{ij} / \rho$$

Boundary Conditions

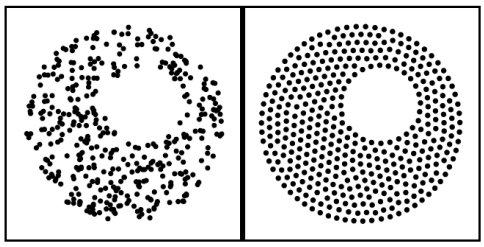
Free, Periodic, Rigid and Mirror Boundaries



Meshes for Lattices and Irregular Shapes

- **Generate lattice structures**
  Test lattice structures **for stability**

- **Use Monte-Carlo to fill an irregularly shaped region**
  Use viscous relaxation with molecular dynamics to equilibrate the particles.



- **Select surface treatment using** surface tension **or** $\sum_j (\nabla \rho)^2$ **potential .**

Equations of State Without Temperature Dependence
Tests for Lattice Stability

- **Families of equations of state without temperature dependence**

  In general energy is a function of both volume and temperature . Consider the special case without any temperature dependence. Then the pressure can be written as

$$P = -\frac{dE}{dV} = \rho^2 \frac{de}{d\rho}$$

  This is a complete specification for an equilibrium equation of state.

  We can construct families of equations of state expressing the pressure in terms of power laws of the density.

$$P = \frac{B_0}{n-m}\left[\left(\frac{\rho}{\rho_0}\right)^n - \left(\frac{\rho}{\rho_0}\right)^m\right]$$

- **Methods for stabilizing smooth-particle lattices**
  Add a core potential to prevent particles from overlapping at $r_{ij} = 0$
  Add a density dependent surface potential proportional to the square of the gradient of the potential
  Add a density dependent curvature potential to prevent shear instability for solid lattices

Molecular Dynamics Analogs : Trajectory Isomorphisms

- **Two cases of trajectory isomorphism with SPAM and molecular dynamics .**
  These isomorphisms simplify the SPAM programs by using molecular dynamics programs with potentials that are functions of the density where the density is defined with smooth particles.

Lucy fluid $P = \rho^2/2$

Trajectories are identical if $(w_{ij})_{SPAM} \rightarrow \phi_{ij}\ molecular\ dynamics$

Embedded-atom fluid $P = \left[\left(\frac{\rho}{\rho_0}\right)^3 - \left(\frac{\rho}{\rho_0}\right)^2\right]$

Trajectories are identical if $\emptyset = \sum_j \frac{1}{2}\left(\frac{\rho_j}{\rho_0} - 1\right)^2$

- **Lucy fluid is used for the free expansion problem .**

- **Embedded atom model can be used for structural relaxation and the collapsing water column .**

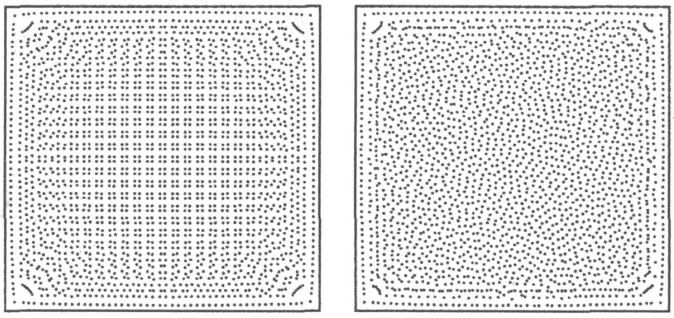
Student problem

Verify that the embedded-atom potential corresponds to the embedded-atom fluid. Hint: use the chain rule for differentiation.

Embedded Atom Approach to Structural Relaxation

$\Phi_{EA} = \frac{1}{2}\sum_i(\rho_i - 1)^2$; $w_{ij} = \left(1 + 3\frac{r}{h}\right)\left(1 - \frac{r}{h}\right)^3$; $h = 3$; $\phi_{core} = 10(\sigma^2 - r^2)^4$ *with* $\sigma = 0.2$

$Relaxation\ with\ F_i \propto -v_i$



Initial square lattice

Initial structure with random displacements

Boundary particles are doubled up and quadrupled at the corners. The goal is to generate a constant density. The original 48x48 particles were arranged in a square lattice (left) and at random (right) and then relaxed with a relaxation time of 2. A pairwise core potential was added to prevent particle overlap. The final embedded-atom potential energy of the relaxed structures was less than 10^{-6} per particle.

Lattices with e(ρ) are typically unstable!

- **SPAM/MD lattices with the following density-dependent internal/potential energy are typically NOT stable for any simple two dimensional lattice .**

Consider the embedded-atom fluid $P = \left[\left(\frac{\rho}{\rho_0}\right)^3 - \left(\frac{\rho}{\rho_0}\right)^2\right]$; $where\ B_0 = \rho_0\left(\frac{\partial P}{\partial \rho}\right)_{\rho_0}$

The trajectory in molecular dynamics with the smooth particle density is

$$\Phi = \sum_i \phi_i \ ; \quad \phi_i = \frac{mB_0}{2\rho_0}\left(\frac{\rho_i}{\rho_0} - 1\right)^2 \ ; \ \rho_i = \sum_j w_{ij}$$

Using the chain rule : $F_i = -\nabla_i\Phi = -\nabla_i\phi_i - \sum_j \nabla_i\phi_j = -\frac{m^2B_0}{(\rho_0)^2}\sum_j\left[\frac{\rho_i}{\rho_0} + \frac{\rho_j}{\rho_0} - 2\right]\nabla_i w_{ij}$

- **These two-dimensional lattices do not have any shear resistance and melt :**

$Particle\ sum\ estimates\ are\ misleading$: $G \approx \nabla^2 e(\rho) \approx \frac{90}{7\pi h^4} \neq 0$;

$Evaluation\ of\ elastic\ constants$: $G = C_{44} = 0$

Hoover and Hoover, Physical Review E **73**, 01672 (2006) .

- **Density-gradient potentials provide surface tension for solids and fluids.**

- **An invariant curvature potential provides elastic shear strength, G > 0**
  Prove this with molecular dynamics with the spam density sum.

Density Gradient Potential and Invariant Density Curvature Potential

The simple density gradient potential enhances shear resistance and minimizes the potential at the lattice sites. For systems with free surfaces it provides a surface tension for the embedded-atom Lucy fluid. The density gradient is maximized at the surface so that the square of the potential minimizes the extent of the surface.

$$\Phi_{\nabla\rho} \propto \sum_j \frac{1}{2}(\nabla\rho)_j^2$$

Even with the increased shear resistance the shear strength vanishes as shown previously with the calculation of the elastic constants.

An invariant curvature potential vanishes for symmetric lattices such as the square, triangular, and hexagonal lattices but ceases to vanish under simple shear, thus stabilizing the lattices.

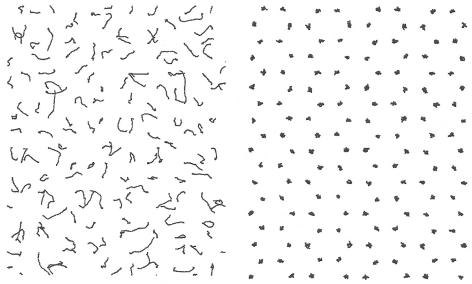
$$\Phi_{\nabla\rho\nabla\rho} = \frac{1}{2}(\rho_{xx} - \rho_{yy})^2 + 2\rho_{xy}^2$$

$$\rho_{xx} = \frac{\partial^2\rho}{\partial^2 x} \; ; \; \rho_{yy} = \frac{\partial^2\rho}{\partial^2 y} \; ; \; \rho_{xy} = \frac{\partial^2\rho}{\partial x \partial y} \; .$$

$$\longleftrightarrow \quad w(r < h) = C_D\left[1 + 4\frac{r}{h}\right]\left[1 - \frac{r}{h}\right]^4$$

The Lucy weight function must be replaced by a weight function with continuous first, second, and third derivatives. The very smooth weight function above comes from the Lucy family of weight functions with n = 4.

Invariant Curvature Potential Cures Lattice Instability

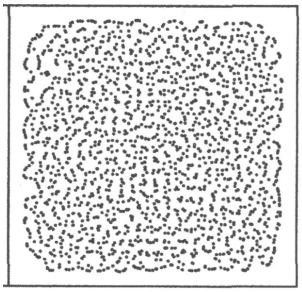


Particle trajectories in a two-dimensional hexagonal lattice. Initial particle displacements were chosen randomly with zero sum. Lattice is unstable (left) and is stabilized (right) by adding the invariant curvature potential .

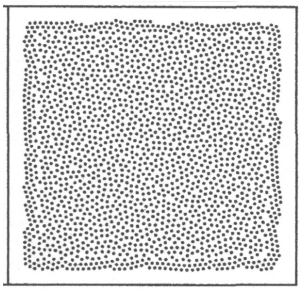
$$\phi = (\rho_{xx} - \rho_{yy})^2 + 4(\rho_{xy})^2 \; ;$$

$$\rho_{xx} = \frac{\partial^2\rho}{\partial^2 x} \; ; \; \rho_{yy} = \frac{\partial^2\rho}{\partial^2 y} \; ; \; \rho_{xy} = \frac{\partial^2\rho}{\partial x \partial y} \; .$$

String Phases Are Cured with Core Potentials



Relaxed structure
Embedded-atom only



Relaxed structure
Embedded-atom plus core potential

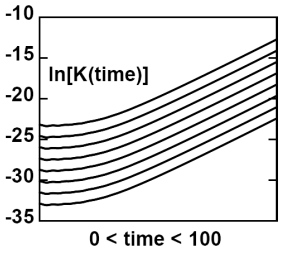
A relaxed periodic structure with an embedded-atom equation of state, using Lucy's weight function with h = 3 produces a string phase . The cure for the string formation is to add a core potential so that particles cannot get too close . Using a repulsive core pair potential prevents the string phase :

$$\phi_{core}(\sigma < r) \propto \left(\sigma^2 - r^2\right)^4$$

Tensile Instability

Kinetic energy growth in an isotropic solid under uniform tension .

The kinetic energy of a single particle moving slowly (~ 10^{-8} or smaller) will increase exponentially at a time longer than the inverse Einstein frequency .



Three useful cures :

1. Add von Neumann-Richtmyer artificial viscosity ;
2. Introduce a repulsive core potential ;
3. Modify the relationship between r and v (Monaghan) :

$$\dot{r} = v \rightarrow \dot{r} = v_i + \sum_j (v_j - v_i)\frac{w_{ij}}{\rho_{ij}} ;$$

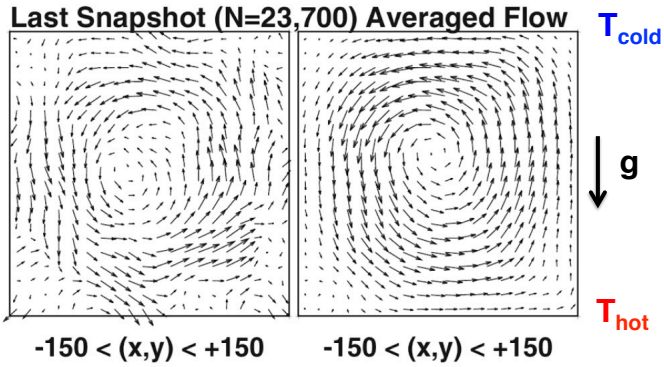
$$\rho_{ij} = \sqrt{\rho_i \rho_j} \text{ or } \rho_{ij} = \tfrac{1}{2}(\rho_i + \rho_j) .$$

Swegle, Hicks, Attaway, Journal of Computational Physics **116**, 123-134 (1995) .

5. SPAM Examples

Smooth Particle Averages of Molecular Dynamics Data

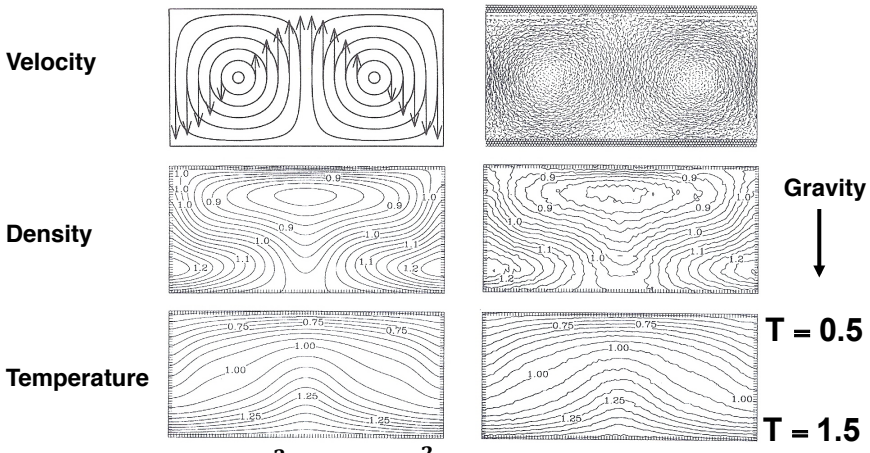
Smooth particle averages generate continuous, twice differentiable field values on any kind of grid or at any point r_i in space. SPAM averages are a very valuable tool for smoothing molecular dynamics data as shown below.



Rayleigh-Bénard flow velocity from molecular dynamics, using Lucy's weight function with h = 50, where the system width is 300. The longtime average shows a well-formed single roll similar to calculations using finite differences. The snapshot, from the last timestep, is spoied by thermal fluctuations. The Rayleigh number for this 23,700 particle simulation is 45,000.

Rayleigh-Bénard Flow (Gravity & T gradient)

Finite-Difference (left) & Smooth Particles (right)



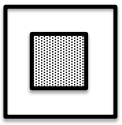
$$\mathcal{R} = \frac{gh^3}{(\upsilon D_T)} = \left(\frac{40}{0.4}\right)^2 = 10,000 \; ; \; \frac{\Delta T}{\langle T \rangle} = 1 \; ; \; \upsilon = D_T$$

5000 smooth particles & field quantities computed on a grid

Kum, Hoover, & Posch, PRE **52**, 4899-4908 (1995) .

Example SPAM Calculations

Four-Fold Volume Expansion of a γ–Law Gas



$V_i = 1\,;\; V_f = 4$

$\rho_i = 4\,;\; \rho_f = 1$

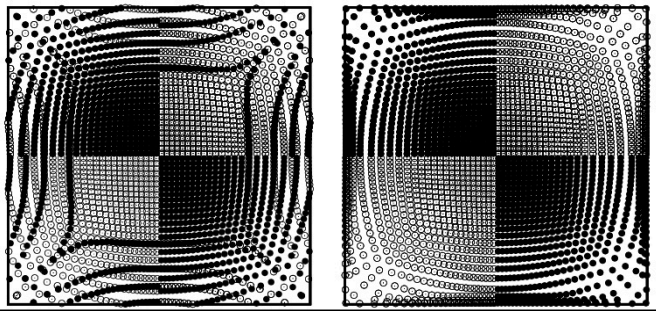
- Consider an isentropic equation of state, the Lucy Fluid :

  $P = \rho e \propto \rho^2/2 \;\rightarrow \dot{v}_i \propto \nabla_i w_{ij}$

- Equilibrate the initial condition
- Use Monaghan's velocity averaging to avoid interpenetration

$$\dot{r}_i = v_i \rightarrow \dot{r}_i = v_i + \sum_j (m_j v_j - m_i v_i)(w/\rho)_{ij}$$

This choice conserves momentum.



Steps in the SPAM Program for the Free Expansion Problem

- Choose the initial conditions

  $\{r_i\,, v_i\,, e_i\}$ at a density $\rho_i = 4$.

- Compute ρ_i at each particle.
- Compute the gradients (∇T_i) and (∇v_i) for each particle.

  These are typically required for computing the particle values of P_i and Q_i .

- Compute P_i and Q_i at each particle, using the equation of state.

  For the ideal-gas example both the viscous pressure and the heat fluxes { Q_i } vanish.

- Compute the righthandside of the equations

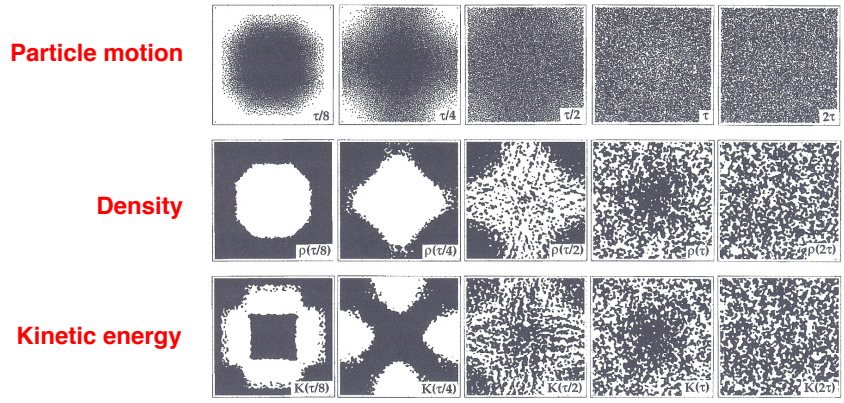
  SPAM equations of motion and energy include the pressure tensor and heat flux vector. Include Monaghan's velocity velocity average if needed.

- Integrate the equations with fourth-order Runge-Kutta

Molecular dynamics requires only three of these steps, with the third and fourth skipped entirely. Step 2, the smooth-particle density sum, is equivalent to the potential energy sum in molecular dynamics.

Four-fold Expansion of 16,384 SPAM particles:

Snapshots of particles, density, and kinetic energy. Light regions for density and energy are above the average and dark regions are below the average .



$V_0 = 1/4V_f$, Lucy fluid with h = 6 .

Hoover, Posch, Physical Review E **59**, 1770-1776 (1999) .
Hoover, Posch, Castillo, Hoover, Journal of Statistical Physics, **100**, Nos. 1/2, (2000) .

Embedded-Atom Gravitational Relaxation and Collapse

Consider a rectangular column of fluid L x (8/5)L at a stress-free density of unity. Using the embedded atom-equation of state we can calculate the gravitational field strength to equilibrate the fluid to a square with a density of two at the bottom of the column and the stress-free density of one at the top.

$$P = \left[\left(\frac{\rho}{\rho_0}\right)^3 - \left(\frac{\rho}{\rho_0}\right)^2\right] \; ; \; \rho_0 = 1 \; ; \quad \frac{dP}{d\rho}\frac{d\rho}{dy} = (3\rho^2 - 2\rho)\frac{d\rho}{dy} = -\rho g$$

$$\int_2^1 (3\rho - 2)\, d\rho = -\int_0^L g dy \; ; \quad g = \frac{5}{2L}$$

Relaxation step : Reflecting boundary walls on sides and bottom .

Three system sizes : $N = 20x32 \; g = \frac{1}{8}$; $N = 40x64 \; g = \frac{1}{16}$; $N = 80x128 \; g = \frac{1}{128}$

Use the embedded atom acceleration, a pair core potential and a damping force :

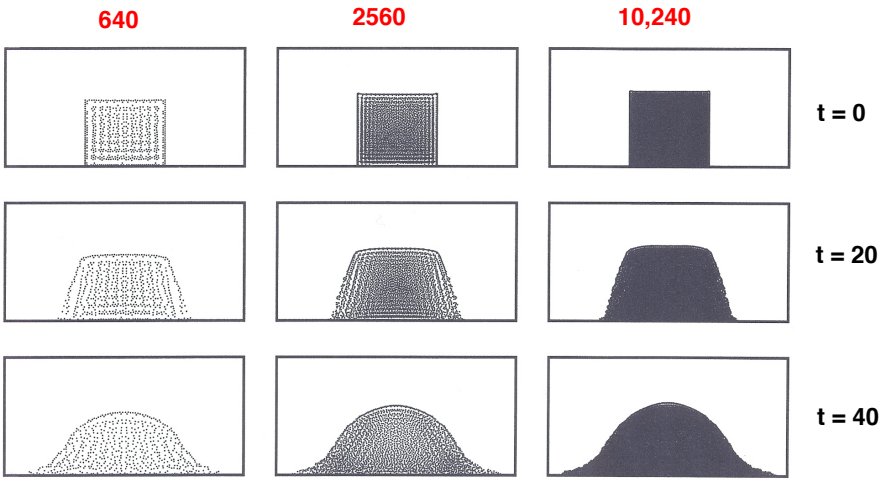
$$(\dot{v}_i)_{EA} = -\sum_i [\rho_i + \rho_j - 2]\frac{r_{ij}}{|r_{ij}|}w'_{ij} \; ; \quad \phi_{core} = \epsilon\left(1 - \frac{r^2}{\sigma^2}\right)^4 \; ; \; \epsilon = 1 \; ; \; \sigma = .6$$

$$(\dot{v}_i)_{damp} = -\frac{v}{\tau} \; ; \; \tau = \frac{L}{8} \; ;$$

Relaxation for about 10 sound traversal times and side constraints were removed.

Collapsing water column with gravity

N = 640, 2560, 10,240 particles



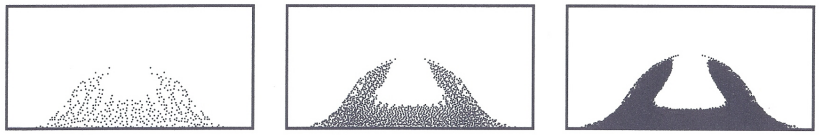
$t_{10240} = 2t_{2560} = 4t_{640}$

$Uses\ \phi_{EAM}\ ;\ \phi_{surface} \propto \sum_j (\nabla\rho)_j^2\ ;\ \phi_{core}\ .$

Collapsing water column with gravity

Tensile regions – SPAM and Finite Elements

No failure model needed for SPAM



640 particles 2560 particles 10,240 particles

WxH = 80x64 elements
dy = 2dx = 1

g = 0

t = 0

Relaxation

Cavitation model :
$P > P_c \rightarrow P = P_c$

t = 30

t = 40

Collapse

Penetration Mechanics : Failure Mechanisms
Molecular Dynamics and Continuum Mechanics

- **Molecular dynamics**

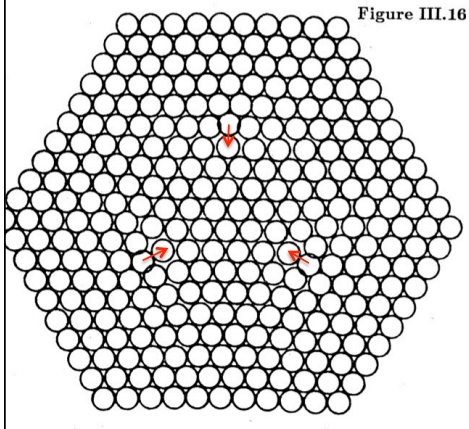
Plastic behavior begins with dislocation formation. Plastic flow is the result of coalescing of dislocations and motion along crystallographic directions. In the triangular lattice the dislocation core is identified by noticing adjacent sites, one with only 5 neighbors and the other neighbor with 7 neighbors. The Burger's vector locates the dislocation center with a vector from the site with 5 neighbors to the site with 7 neighbors.

- **Continuum models must specify failure criteria**

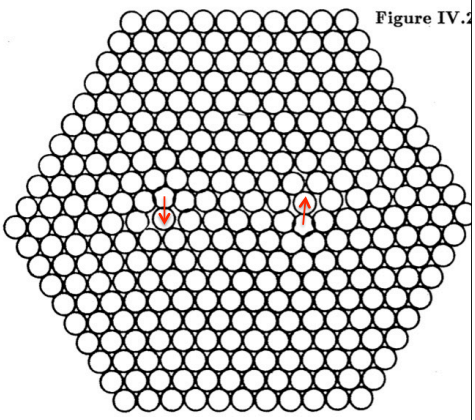
We model two failure modes. For tensile failure when the mean stress reaches the tensile failure limit the element strength is reduced to zero. In DYNA3D we use a plastic strain for a failure model which includes hardening. We model plastic failure in SPAM by specifying a plastic strain for failure and an algorithm for keeping the stresses on the yield surface until the failure strain is reached.

Dislocations in Crystals are identified with Burger's Vectors

3 dislocations



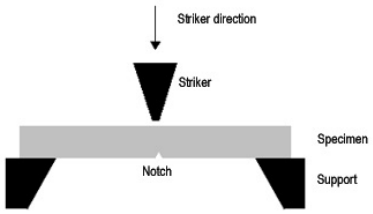
2 dislocations

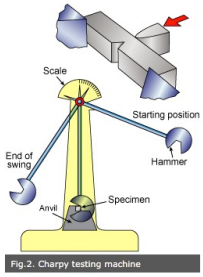


Anthony J. C. Ladd and William G. Hoover, "Energy and entropy of interacting dislocations", Phys. Rev. B, Vol. 26, Number 10, (15 November 1982).

Penetration Mechanics

- **A prototypical experiment in penetration mechanics is the Charpy test*.**

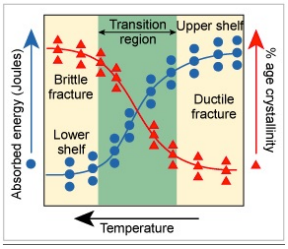




Reproducibility: At least 3 tests are needed.

- **Failure models are developed from energy considerations**

For sufficiently high velocities the plate material will fail in one of two ways : tensile failure or plastic flow. New surfaces are created resulting from melting, vaporization, plastic flow or brittle failure.



- http://www.azom.com/article.aspx?ArticleID=2763
- http://www.twi-global.com/technical-knowledge/job-knowledge/mechanical-testing-notched-bar-or-impact-testing-071/

Penetration Model
Finite Elements, Molecular Dynamics and SPAM

- **In our models we model the penetrator with a rigid ball**

This avoids possible numerical problems in the finite element program with a sharp point.

- **The finite-element model**

We use both a tensile failure and a plastic strain failure with hardening. The ball and plate have the same density. The plate bulk modulus is 2. The Young's modulus is Y = E/100 = .0025. Elements in the plate fail when the tensile stress reaches 0.1 or when the plastic strain reaches 1.0 or 2.0.

- **Molecular Dynamics**

We use a power-law potential and a triangular lattice.

- **For SPAM-like molecular dynamics**

We use the embedded-atom potential, a surface gradient potential, and a curvature potential for strength.

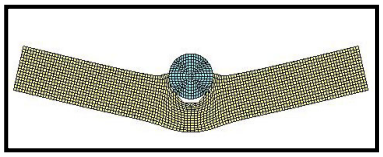
- **The SPAM model**

We use the cold equation of state matching the molecular dynamics potential.

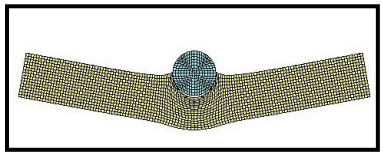
Ball-Plate Fragmentation
Ball-plate Penetration with Finite Elements

Tensile failure : $t_f = 0.1$; Plastic strain failure : $\varepsilon_p = \{ 1.0, 2.0)$

V_0=1/4 ; e_f = (1.0, 2.0)

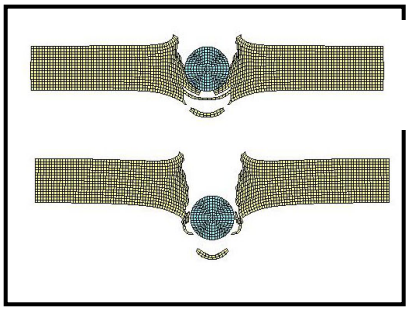


$e_p < e_f = 1.0$, $v_0 = 1/4$



$e_p < e_f = 2.0$, $v_0 = 1/4$

V_0=1/2 ; e_f = 1.0



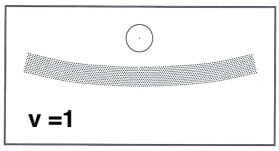
$e_p < e_f = 1.0$, $v_0 = 1/2$

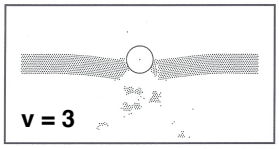
For the lower velocity (left) the ball bounces back, but leaves a permanent deformation . For the higher velocity the ball breaks through the plate .

Ball-Plate Penetration with Molecular Dynamics

$$\frac{Mv^2}{2\pi R^2} < -\frac{\Phi_{plate}}{A}$$

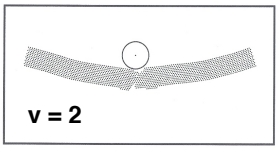
Ball bounces

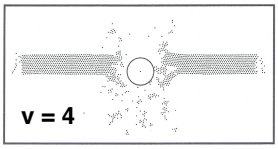




$$\frac{Mv^2}{2\pi R^2} \cong -\frac{\Phi_{plate}}{A}$$

Plate cracks





-70 < x < +70 ; v = 1, 2, 4, 8

Plate particles interact with a 4-8 potential in a triangular lattice with m = 1.

$$\phi_{pp}(r < \sqrt{2}) = (2 - r^2)^8 - 2(2 - r^2)^4$$

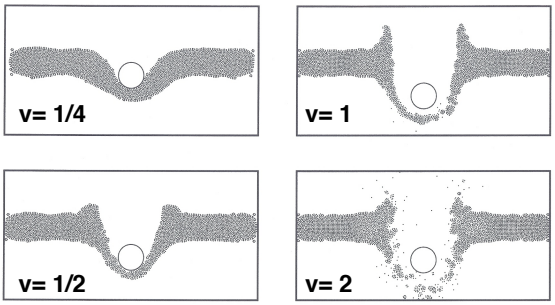
Ball-plate potential is an extended of the core potential.

$$\phi_{core}(r < \sigma) \equiv \phi_{bp}(r - R < \sigma) = 100\left[1 - \left(\frac{\delta r}{\sigma}\right)^2\right]^4 \; ; \; \delta r = r - R < \sigma$$

$$M = \pi R^2 \rho = \sqrt{4/3}\pi R^2$$

Ball-Plate Penetration SPAM-like Molecular Dynamics

Invariant Curvature potential provides strength.



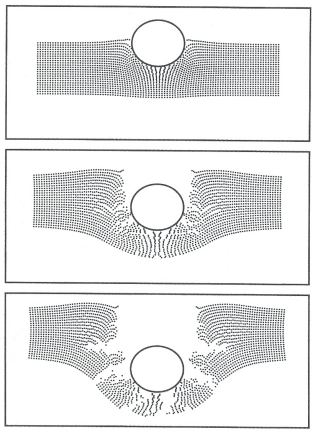
-100 < x < +100 ; v = 1/4, 1/2, 1, 2

$$\Phi = \Phi_{EA} + \Phi_{core} + \Phi_{surf} + \Phi_{curv}\,; \quad \rho_0 = \sum w_{smooth} \quad for\ h = 2.30\,;$$

$$\Phi_{EA} = \sum_j \frac{1}{2}\left(\rho_j - \rho_0\right)^2\,; \quad \Phi_{core} = \sum_{i<j} 100\left[1 - \left(\frac{r^2}{\sigma^2}\right)\right]^4$$

$$\Phi_{surf} = \frac{1}{20}\sum_j \frac{1}{2}(\nabla\rho)^2\,; \quad \Phi_{\text{curv}} = \sum\left[\frac{1}{2}\left(\rho_{xx} - \rho_{yy}\right)^2 + 2\rho_{xy}^2\right]$$

Ball-Plate Penetration with SPAM



-60 < x < +60 ; t = 4, 12, 20

Cold lattice mechanical equation of state

$$e_0 = 3\left(2 - \frac{v}{v_0}\right)^8 - 6\left(2 - \frac{v}{v_0}\right)^6\,;$$

$$P_0 v_0 = 24\left[\left(2 - \frac{v}{v_0}\right)^7 - \left(2 - \frac{v}{v_0}\right)^3\right]$$

We find $B = 2\sqrt{24}$

Plastic Flow Model

In prototypical yield strength measurements yielding first occurs when σ_{xx} is 2Y. A simple plastic flow model is to reduce the shear stress to Y after any timestep in which Y is exceeded. A correction factor to bring the shear stresses to the yield surface is :

$$f = Y/\sigma_{xx}\ with\ shear\ stress\ component\ updates$$

$$\sigma_{xy} \rightarrow f\sigma_{xy}$$

$$\sigma_{xx} \rightarrow \frac{1}{2}\left(\sigma_{xx} + \sigma_{yy}\right) + \frac{f}{2}\left(\sigma_{xx} - \sigma_{yy}\right)$$

$$\sigma_{yy} \rightarrow \frac{1}{2}\left(\sigma_{xx} + \sigma_{yy}\right) - \frac{f}{2}\left(\sigma_{xx} - \sigma_{yy}\right)$$

Tensile failure

Set the entire stress tensor to 0 on failure. Return the density to the stress-free value of $(4/3)^{1/2}$.

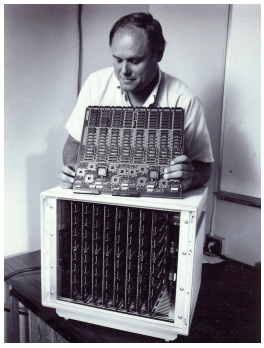
Conclusion – SPAM Is a Transparent, Pedagogical Particle Method for Simulating Continuum Dynamics

- **SPAM is useful for modeling continuum mechanics**
  - Algorithm is transparent to program & easier to debug ;
  - Algorithm avoids mesh tangling that stops mesh-based calculations ;
  - Rezoning is easy .
- **Various deficiencies have been cured**
  - Density-gradient potential for lattice surfaces ;
  - String phases cured with core potentials ;
  - Invariant density-curvature potential for strength .
- **Challenging research problems remain for developing failure models for penetration mechanics**
  - Fast desktop computers as well as array processors and massively parallel computers provide opportunities to investigate numerical models for failure.

Life in Japan at Keio University Yokohama
Molecular Dynamics : 1989 – 1990 and beyond

Parallel Algorithms

Tony De Groot
at LLNL



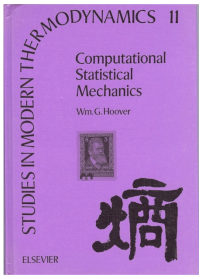
$30,000 SPRINT versus $30,000,000 Cray Computers

1,036,800 particles!!

Toshio Kawai
at Keio University

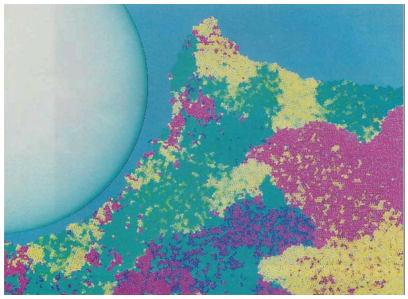
Taisuke Boku
Keio University

Evenings/Weekends

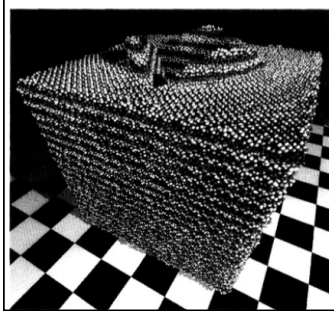


Sigeo Ihara
Hitachi

Two & Three-Dimensional Parallel Simulations of Indentation

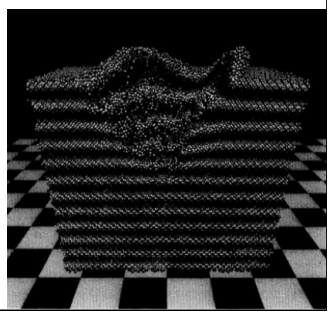


Nonequilibrium indentation for 720 x 1440 particles in two dimensions. Lennard-Jones with an embedded-atom potential models a granular solid representing metals such as copper or nickel . Molecular dynamics on Tony De Groot's SPRINT computer with message-passing processors.



Work of indentation → Surface + elastic energy Plastic yield strength.

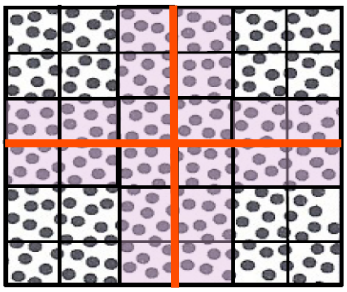
Tetrahedral indentation : 72 x 72 x72 silicon atoms with Stillinger-Weber ϕ

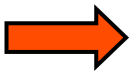


Parallel Techniques for Fluids and Solids
Eulerian Grid of Particle-Cells → Processors

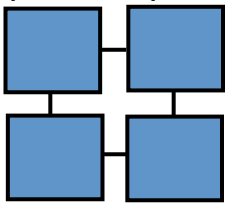
Two forms of parallel are shared memory and message-passing .
Must use message-passing for large problems .
Message-passing is more efficient, works for large problems, but is more difficult to program .

Message-passing technique





Four-processor parallel computer



Efficiency, Scalability & Message-Passing

- In practice, communication time reduces parallel efficiency

$$\tau_{wc} = \tau_{calc} + \tau_{comm}$$

τ_{wc} *is the total elapsed time taken for the calculation (wall clock time)*

τ_{calc} *is the elasped time the processors spend computing*

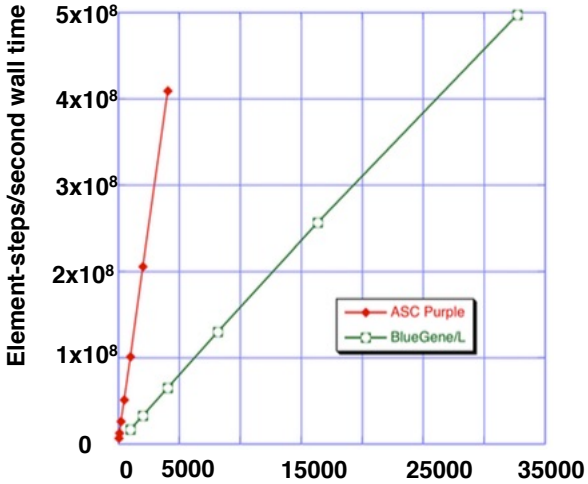
τ_{comm} *is the eplapsed time the processors spend communicating shared data.*

- **Scalability**

Ideally, if the number of processors is doubled, the rate for delivering results will be doubled. The term scalability or theoretical scalability refers to this linear scaling of the delivery rate with the number of processors. In practice scalability breaks down when the communication time becomes significant compared to the amount of time processors spend computing results.

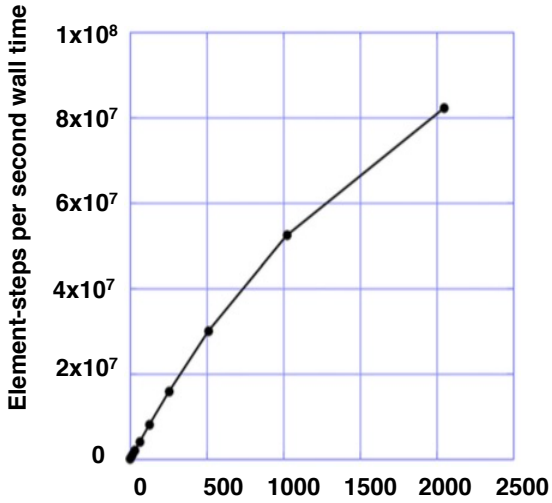
$$S = \frac{\tau_1}{\tau_N} = N\eta \leq N = N\eta_{ideal}$$

Parallel Scalability for two computers at the Lawrence Livermore National Laboratory



Parallel speedup for a 90-million element problem having no slide surfaces (material interfaces) defined. A small percentage of the nodes are communicating between processors. Note that performance is still increasing at more than 32000 processors.

Parallel Scalability with a single large material interface



Speedup for a one-million element problem having one large slide surface. Although performance continues to increase, the rate of speedup is beginning to decrease at approximately 1024 processors. For the 1024-processor case, there are only about 1000 elements per processor. Such small computational work per processor lowers the parallel efficiency.

Create Subdomains from Optimized Cuts of Graphs

- Goal: Domain split into subdomains . Subdomains → processor .
- Method: Convert domain → weighted graph :

  cells ⇒ vertices

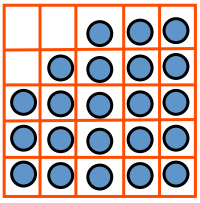
  cell connectivity ⇒ lines

- Optimized cuts of graphs are partitions (subdomains) .

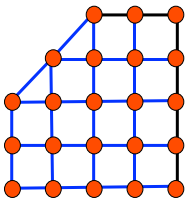
  Method by Karypis and Kumar + free software :

  http://glaros.dtc.umn.edu/gkhome/

Particles in cells
dx ~ h



Graph with connected cells

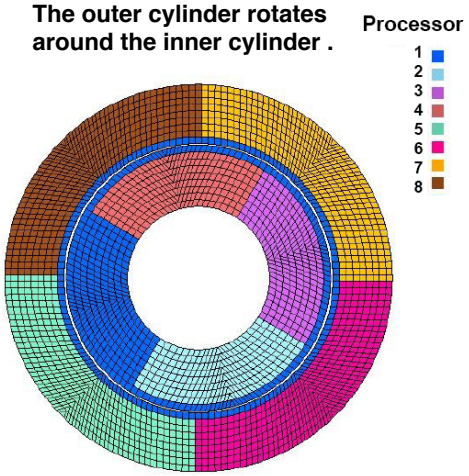


Vertex weights
processor work time
Line weights
communication time

Example: Partitioned "Nut-Bolt" Mesh and Interface

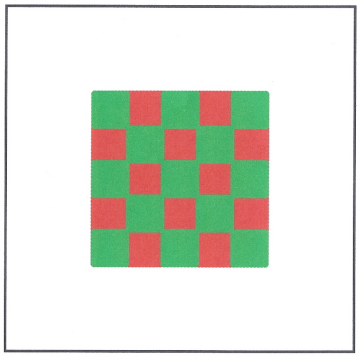
- Treat the surfaces as a separate partition ;
- For many surfaces, distribute them among several processors .
- Surface partition is computed only once for this problem .

The outer cylinder rotates around the inner cylinder .

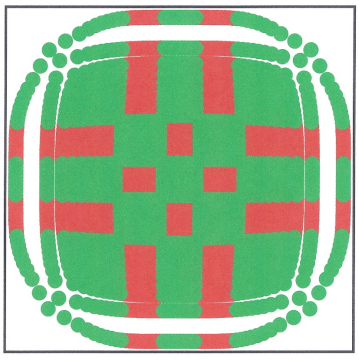


Example: Dynamically Partitioned Free Expansion

Repartition at any time during the calculation when there is a load imbalance .

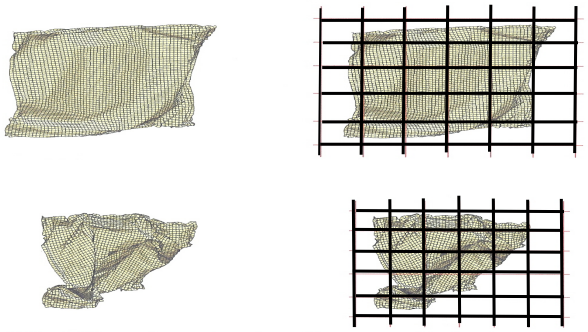


-25 < (x,y) < +25



-25 < (x,y) < +25

Example: Dynamically Partitioning Crushed Sheet



This complex surface folding leads to arbitrary "self contact".
This is a hard problem on single processor computers !!