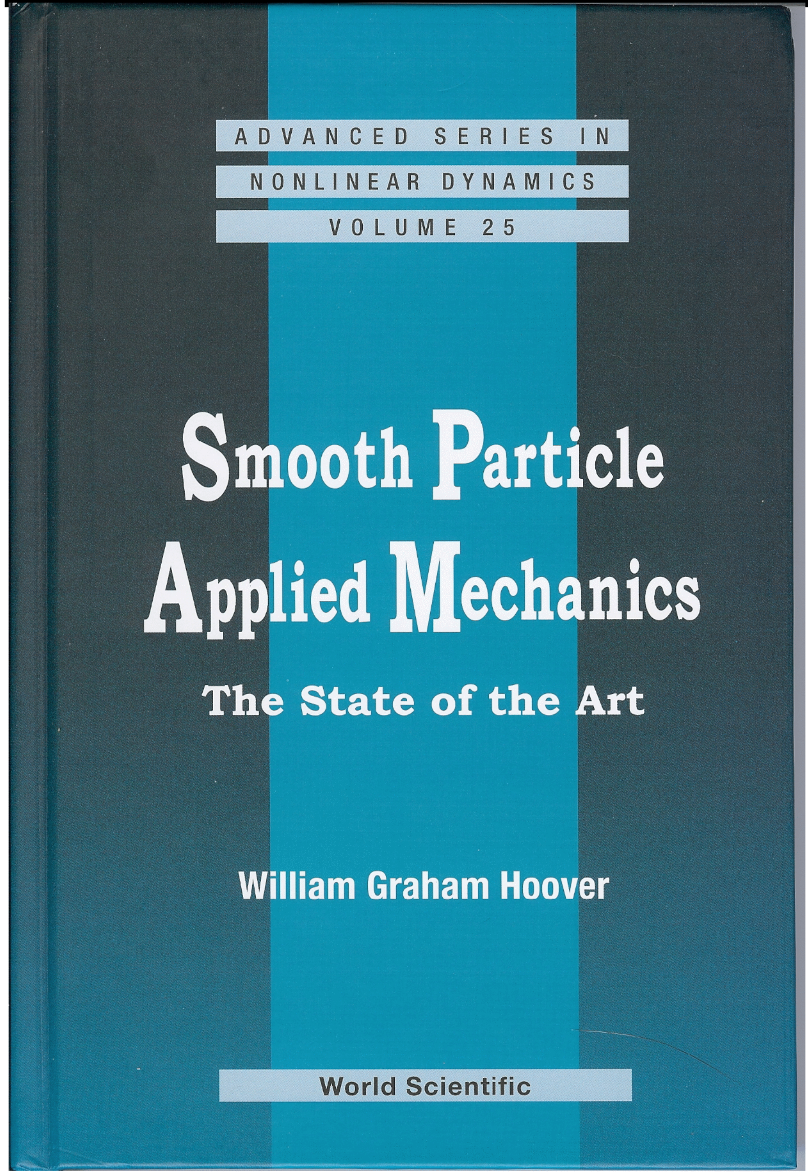
Smooth Particle Applied Mechanics



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Mexico City, Mexico
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SPAM: A Novel and Simple Method for Solving the Continuum Equations

- SPAM Theory
  1. Continuum Mechanics (PDEs)
  2. Numerical Solution Methods
     a) Finite Element Method
     b) Particle Method (Motivation)
  3. SPAM Interpolation & Gradients
  4. SPAM ODEs
  5. Runge-Kutta Time Integration
  6. Molecular Dynamics Analogs
  7. Mesh Generation & Boundary Conditions
  8. Maladies and Cures

- SPAM Results
  9. Free Expansion
  10. Parallel Techniques
  11. Collapsing Fluid Column
  12. Rayleigh-Bénard Flow
  13. Research problems
      a) Tension Test
      b) Ball Plate Problem

1. Continuum Theory : Microscopic *versus* Macroscopic Material Descriptions

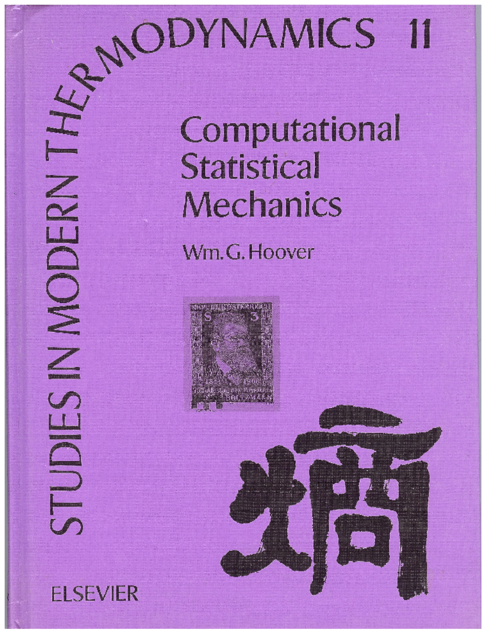
Microscopic Description

Atomistic length & time scales

L ~ Å
t ~ ps-ms (vibrational frequencies)

Follow atomic motion with ordinary differential equations

Specify force laws for atoms



Macroscopic Description

Laboratory length & time scales

L ~ cm or meters
t ~ ms or seconds

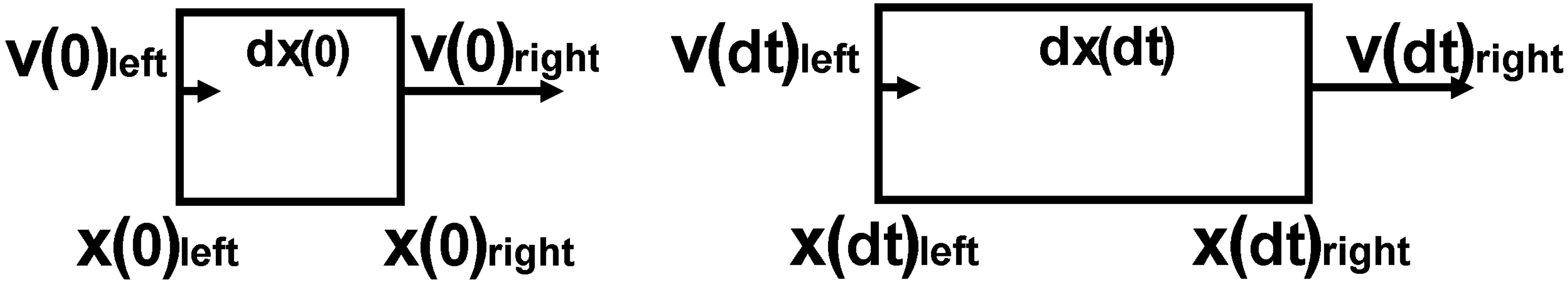
Material flow or solid deformation satisfy partial differential equations

Specify constitutive relations for the materials

← For a pdf file, go to www.williamhoover.info

1. Continuum Theory: Continuity Equation - Conservation Law for Mass

Lagrangian description follows the motion of material points:



$$x_{right} \to x_{right} + vdt + \frac{dx}{2}(\partial v/\partial x)_t dt$$

$$x_{left} \to x_{left} + vdt - \frac{dx}{2}(\partial v/\partial x)_t dt$$

$$dx(0) \to dx(0)[1 + (\partial v/\partial x)_t dt] = dx(dt)$$

$$\frac{dx(dt) - dx(0)}{dtdx(0)} \to \frac{d(\ln dx)}{dt} \equiv -\frac{d\ln\rho}{dt} = \frac{\partial v}{\partial x}$$

1. Continuum Theory: Lagrangian Equations, Pressure, Heat Flux

$$\dot{\rho} = -\rho \nabla \cdot v$$

$$\rho \dot{v} = -\nabla \cdot P$$

$$\rho \dot{e} = -\nabla v : P - \nabla \cdot Q$$

with

$$P = P(\rho, e, ?) \, ; \, Q = Q(\rho, e, ?) \, .$$

1. Continuum Theory
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:

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

Van der Waals' :

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

1. Continuum Theory
Nonequilibrium Constitutive Relations

- **Nonequilibrium dissipation: viscosity, conductivity, plasticity, ...**
- **Fourier's law:**

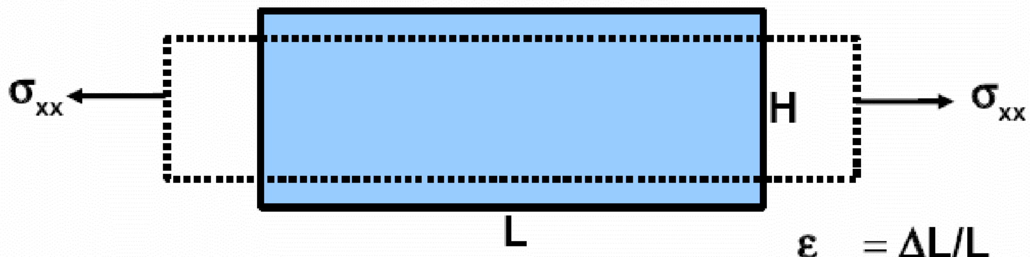
$$\mathbf{Q} = -\kappa \nabla \mathbf{T}.$$

- **Newton's formulation of shear stress → symmetrized stress tensor :**

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

$$\sigma_{yy} = 0$$

$$\varepsilon_{yy} = \Delta H/H$$



$$\varepsilon_{xx} = \Delta L/L$$

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

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

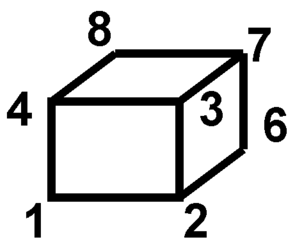
- **Use von Mises shear stress condition for plasticity :**

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

2. a) Numerical Solution Methods
Finite-Elements (DYNA3D and ParaDyn)

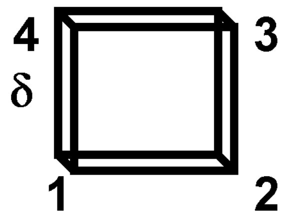
Use space-filling volumes to approximate the continuum:

- **8-Node brick has *isoparametric* velocity interpolation for strain rates:**



$$v(x,y,z) = a_1 + a_2 x + a_3 y + a_4 z + a_5 xy + a_6 yz + a_7 zx + a_8 xyz$$

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

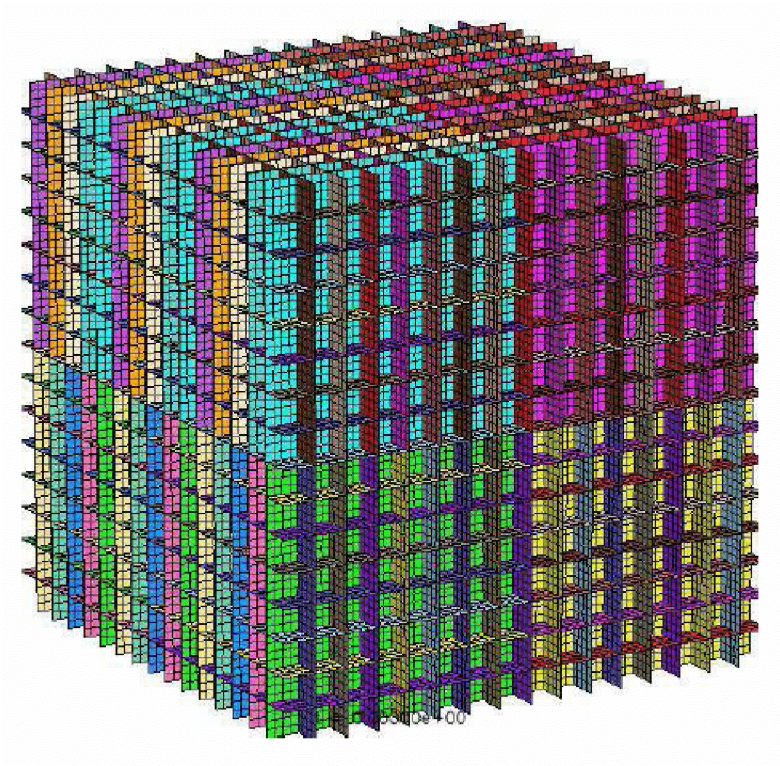


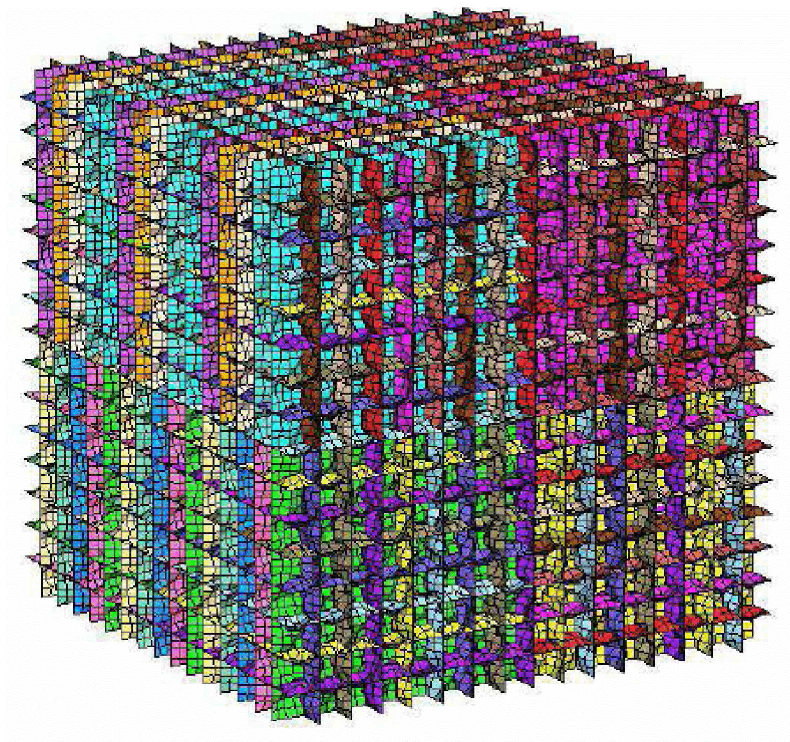
$$v(x,y) = a_1 + a_2 x + a_3 y + a_4 xy$$

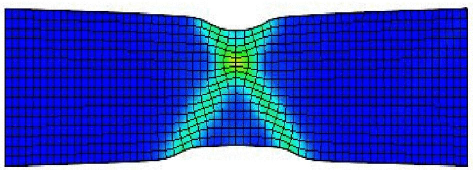
- **Calculate pressure, energy, stress by integrating over elements (for example, nodal strain/strain rates, element integration → stresses)**

Lin, DYNA3D, UCRL-MA-107254 & Hoover, *et alii*, ParaDyn, UCRL-MA-140943 from Methods Development Group, Lawrence Livermore National Laboratory .

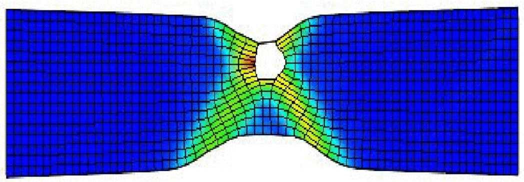
Two Example Finite-Element Calculations



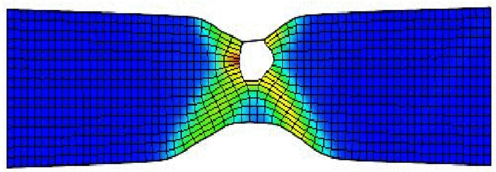




Time = 32



Time = 48



Time = 64

2. b) Numerical Solution Methods
Particle Methods – Motivation & Example

History

- Smooth particles used for astrophysics problems :
- Gingold, Lucy, and Monaghan - 1977
- Smooth particles applied to fluids and solids (~1990)

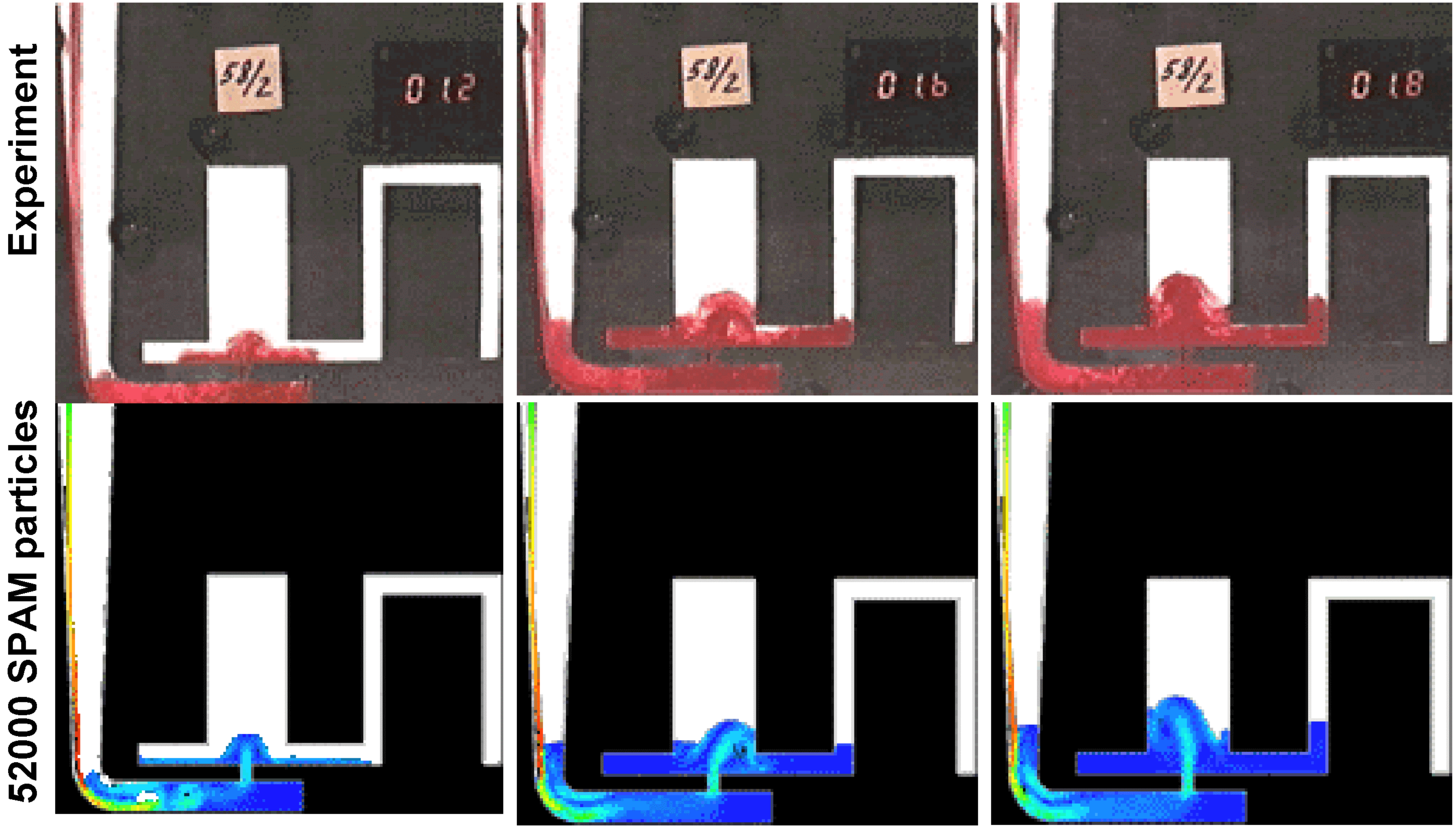
Motivation

- Fluids and solids satisfy the *same* motion equations
- No element integration
- No mesh tangling for flow problems
- Material failure is simple with Lagrangian particles
- Applications in *many* fields (heat conduction, electricity & magnetism, fluid structure interaction, fragmentation, …)

Simplify! Simplify! Simplify!
(Thoreau)

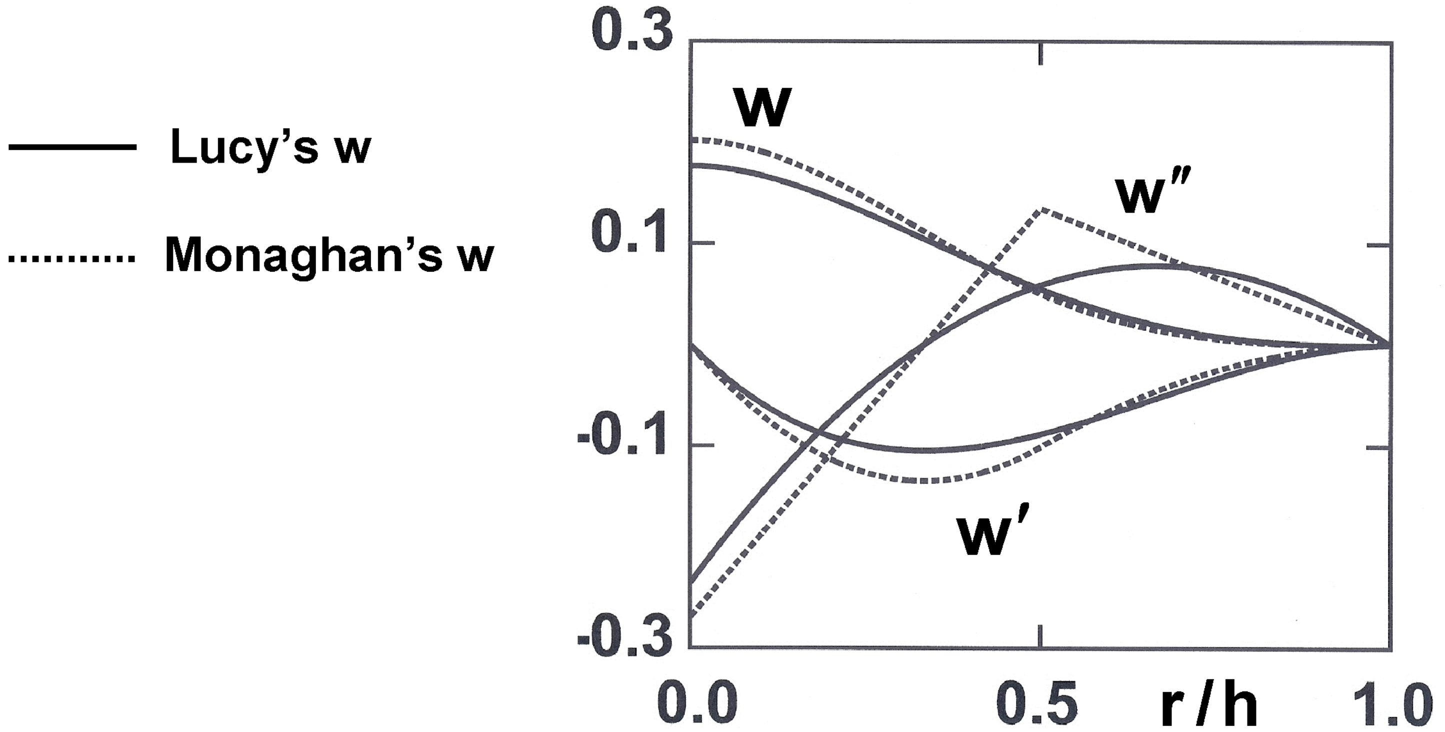
High Pressure Die Casting Experiment/Simulation

Ha, Cleary, Alguine & Nguyen@http://www.cmis.csiro.au/cfd/sph/



3. Spatial Interpolation and Gradients
Particles of Finite Extent Represent the Continuum .

Particles with an extent h represent a continuum.
The particle weight function, w, as well as its first two spatial derivatives are continuous.

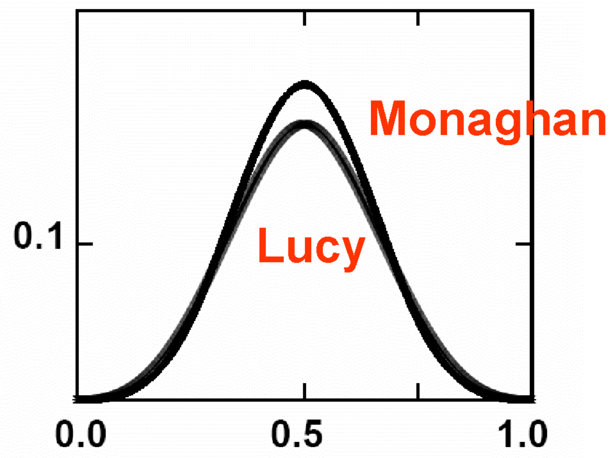


3. Spatial Interpolation and Gradients
Monaghan and Lucy weight functions in 2 dimensions

$$w_{Lucy}\ (r < h) = (5/9\pi h^2)[1 + 3(r/h)][\ 1 - (r/h)\ ]^3$$

w is normalized and w, w′, w″ vanish at r = h = 3.

$$\rightarrow w_n \propto [1 + n(r/h)][\ 1 - (r/h)\ ]^n$$



$$w_{Monaghan} = (40/7\pi h^2)[1 - 6(r/h)^2 + 6(r/h)^3] \quad \text{for } 0 < \frac{r}{h} < \frac{1}{2}$$

$$w_{Monaghan} = (80/7\pi h^2)[1 - (r/h)]^3 \quad \text{for } \frac{1}{2} < \frac{r}{h} < 1$$

3. Spatial Interpolation and Gradients
Density interpolation converges with ~ 20 neighbors

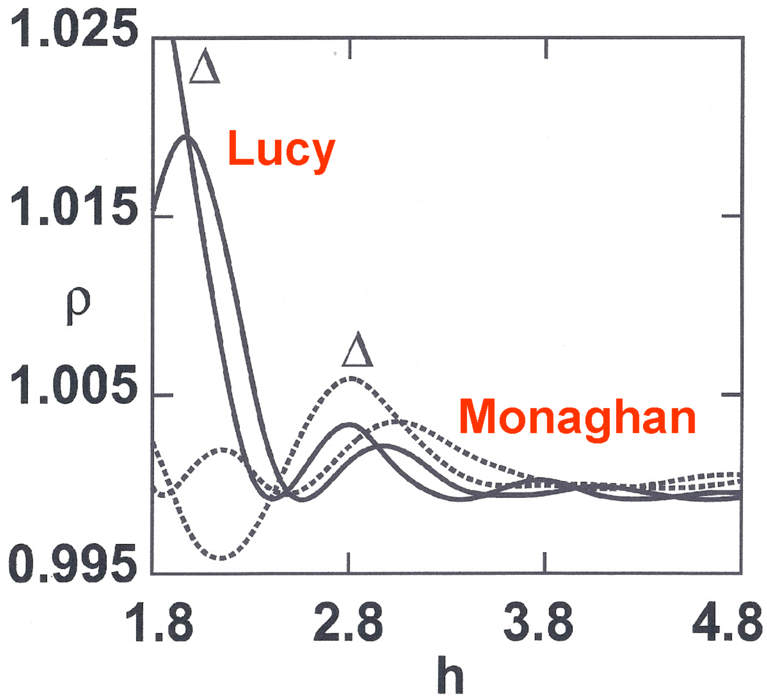
$$\rho_i = \sum_j w(|r_i - r_j|)\,;\ |r_i - r_j| \le h\,.$$

- 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% for both weight functions .



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

4. Spatial Interpolation and Gradients
Interpolation for Variables/Gradients Use Particle Sums

- Continuum variables & gradients :

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

- Use weighted sums of particle variables for interpolation :

$$\rho f(r) = \sum_j f_j w(|r - r_j|) \, ; \quad \rho_r = \sum_j w(r - r_j) \, ;$$

$$\nabla(\rho f)_r = \sum_j f_j \underline{\nabla_r w}(|r - r_j|) \, .$$

- Other powers or functions of density can be used, e. g. ,

$$f(r) = \sum_j (f/\rho)_j w(|r - r_j|) \, ;$$

$$f(r)/\rho = \sum_j (f/\rho^2)_j w(|r - r_j|) \, .$$

4. SPAM versions of the ODEs
Spatial interpolation → Ordinary Differential Equations

$$\dot{\rho}_i = \sum_j (v_i - v_j) \bullet \nabla w_{ij} \quad \text{or} \quad \rho_i = \sum_j w_{ij} \ ;$$

$$\dot{v}_i = -\sum_j [(P/\rho^2)_i + (P/\rho^2)_j] \cdot \nabla_i w_{ij} \ ;$$

$$\dot{e}_i = -\sum_j [(P/\rho^2)_i + (P/\rho^2)_j] : \frac{1}{2}(v_i - v_j)\nabla_i w_{ij}$$

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

Time integration with 4th Order Runge-Kutta .

5. Runge-Kutta Time Integration (Fourth Order)

$$\dot{r}_i = v\,;\;\; \dot{v}_i = -\sum_j [(P/\rho^2)_i + (P/\rho^2)_j] \cdot \nabla_i w_{ij}\,.$$

Compute r,v by averaging 4 values of derivatives t = {0, dt/2, dt} :

$$r(dt) = r(0) + \frac{dt}{6}(v_1 + 2v_2 + 2v_3 + v_4)\,;$$

$$v(dt) = v(0) + \frac{dt}{6}(a_1 + 2a_2 + 2a_3 + a_4)\,.$$

$$r_1 = r(0)\,;\;\; \dot{r}_1 = v_1 = v(0)\,;\quad \dot{v}_1 = a_1(r_1)\,;$$

$$r_2(\tfrac{dt}{2}) = r_1 + \frac{dt}{2}v_1\,;\quad v_2(\tfrac{dt}{2}) = v_1 + \frac{dt}{2}a_1\,;\;\; a_2 = \dot{v}_2\,;$$

$$r_3(\tfrac{dt}{2}) = r_1 + \frac{dt}{2}v_2\,;\quad v_3(\tfrac{dt}{2}) = v_1 + \frac{dt}{2}a_2\,;\;\; a_3 = \dot{v}_3\,;$$

$$r_4(dt) = r_1 + v_3 dt\,;\quad v_4(dt) = v_1 + a_3 dt\,.$$

6. Molecular Dynamics Analogs
Trajectory Isomophisms

- **Two interesting cases of trajectory isomorphisms occur with SPAM and molecular dynamics .**

Lucy fluid For $P = \rho^2 / 2$ trajectories are the same if

$$w_{ij} \text{ spam} \rightarrow \Phi_{ij} \text{ md} .$$

Embedded-atom fluid For $P = \rho^3 - \rho_0 \rho^2$ trajectories are the same if

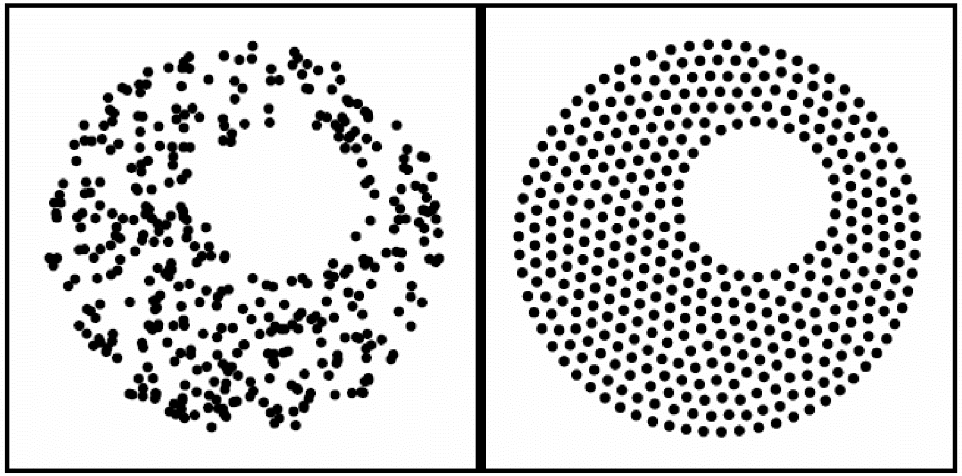
$$\Phi = \sum_j \frac{1}{2} \left(\frac{\rho_j}{\rho_0} - 1 \right)^2 .$$

- **Lucy fluid is used for the free expansion problem .**
- **Embedded atom can be used for structural relaxation and the collapsing water column .**

7. Mesh Generation & Boundary Conditions

Meshes for Irregular Shapes and Lattices

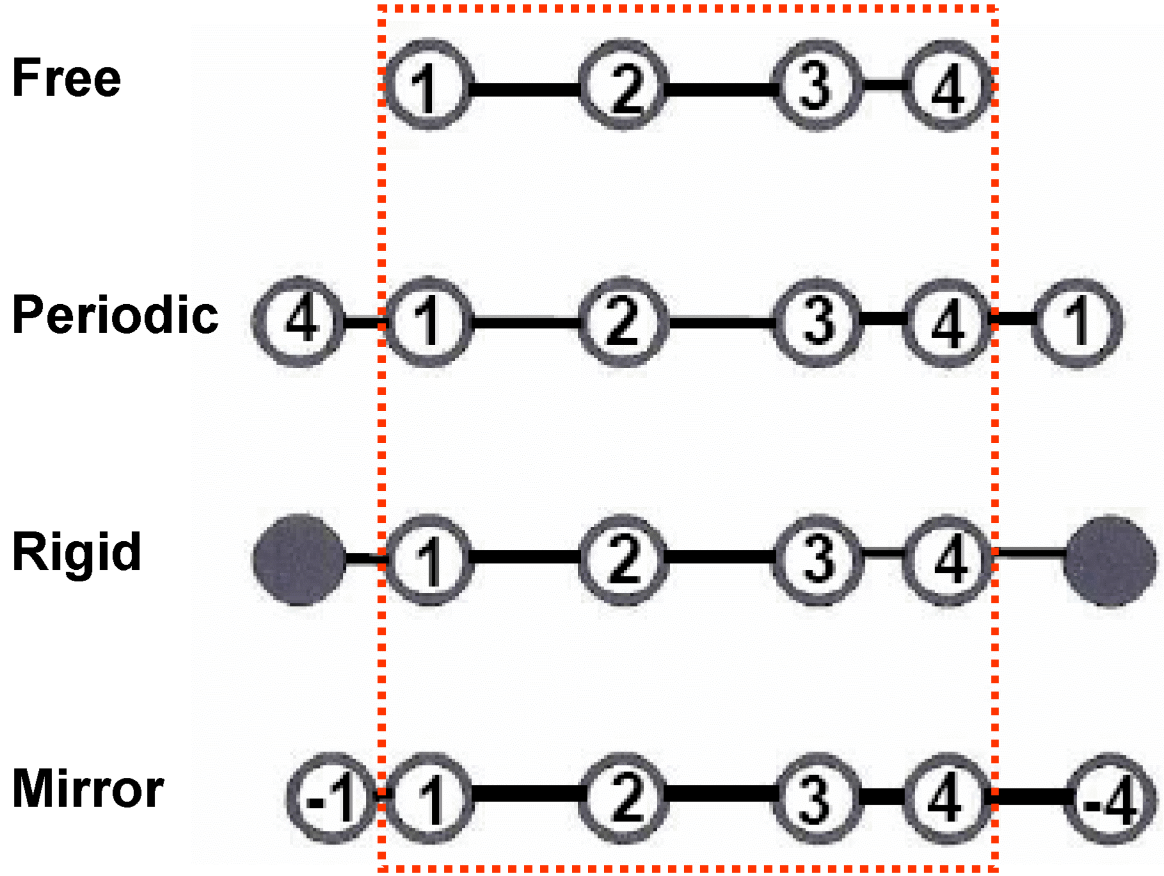
- Use viscous relaxation techniques from molecular dynamics .



- Test lattice structures for stability → Use density curvature potential .
- Select surface treatment using surface tension or $\sum_j (\nabla\rho)^2$ potential .

7. Mesh Generation & Boundary Conditions

Free, Periodic, Rigid & Mirror Boundaries



8. Maladies and Cures
Lattices with e(ρ) are typically unstable!

Two-dimensional MD lattices with the usual pair potentials are stable .

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

$$e_j \equiv \frac{1}{2}(\rho_j - \rho_0)^2 \longrightarrow P = \rho^2(\partial e / \partial \rho) = \rho^2(\rho - \rho_0)$$

$$\Phi_\rho \equiv \sum_j (\rho_j - \rho_0)^2 \; ; \rho = \sum_j w_{ij}$$

These lattices do not have any shear resistance and melt :

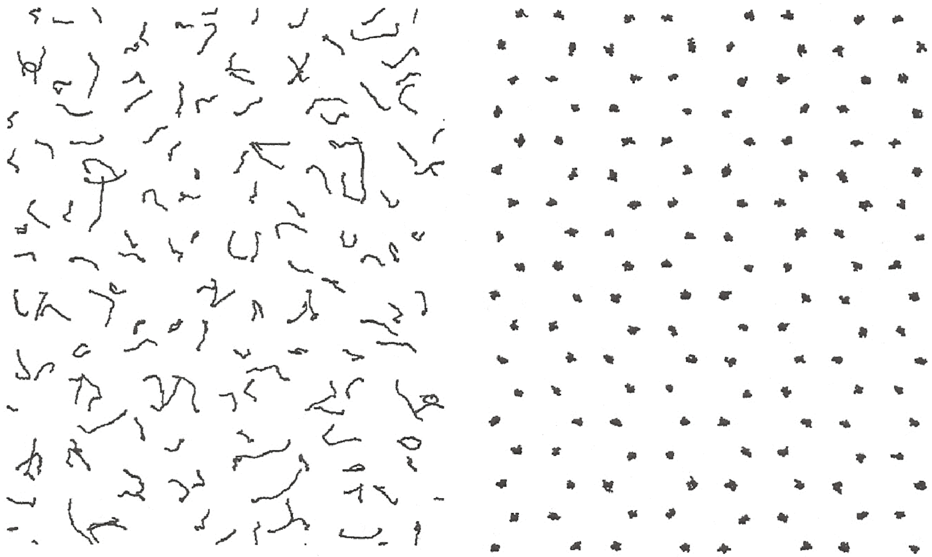
Particle sum estimates are misleading: $G \approx \nabla^2 e(\rho) \approx \frac{90}{7\pi h^4} \neq 0$;

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

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

Density-gradient potentials provide surface tension. An invariant curvature potential provides elastic shear strength, G > 0 .

8. Maladies and Cures
Invariant Curvature Potential Cures Lattice Instability

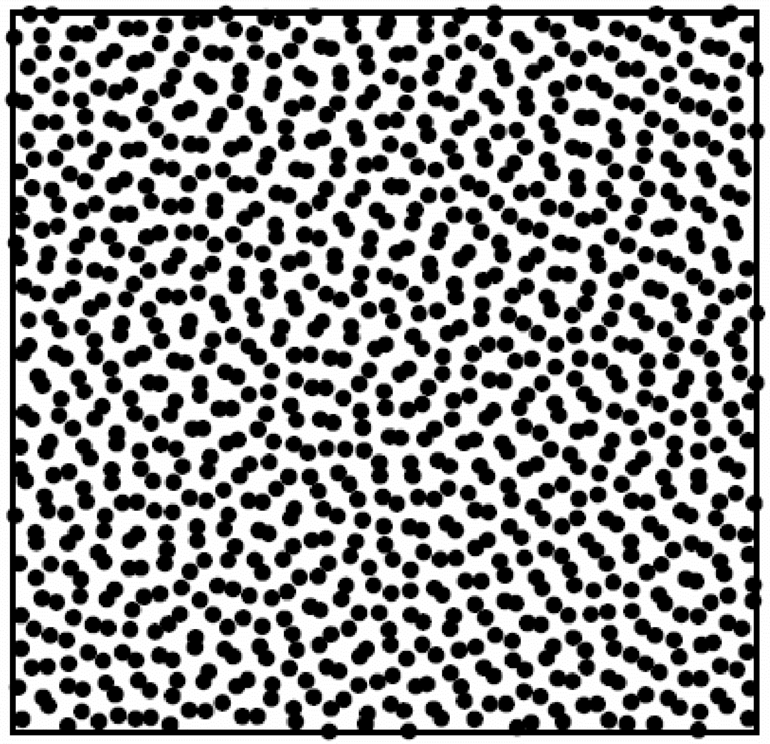


Particle trajectories in a two-dimensional hexagonal lattice. Initial particle displacements were chosen randomly with zero sum. Lattice is unstable (left) and is stabilized (right) by adding the invariant curvature potential .

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

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

8. Maladies and Cures
String Phases Are Cured with Core Potentials

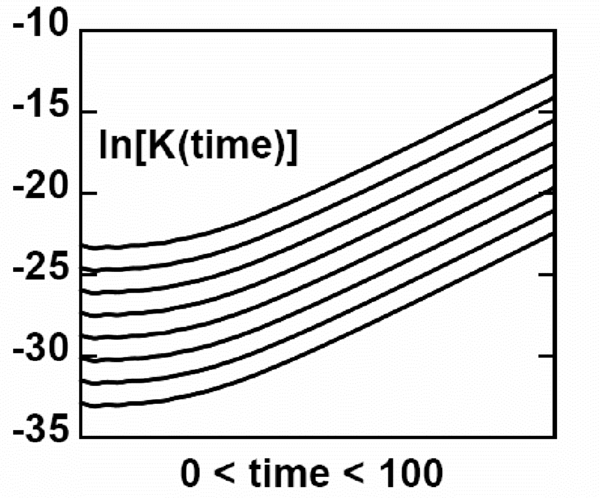


A relaxed periodic structure with an embedded atom equation of state, using Lucy's weight function with h = 3.5 . The cure for the string formation is to add a core potential so that particles cannot get too close .

8. Maladies and Cures
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) .

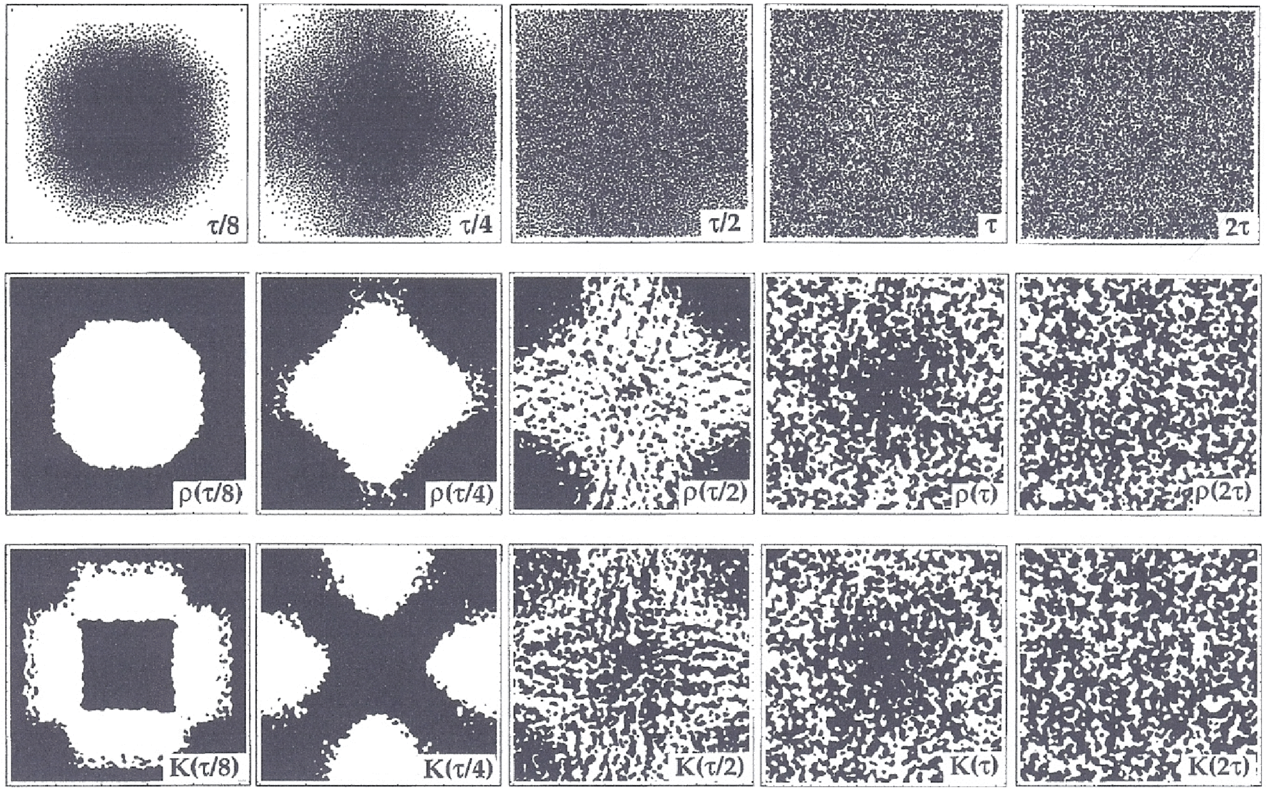
9. SPAM Results: Free Expansion of 16,384 particles:

τ is the time relative to the sound traversal time . Light regions are above the average and dark regions are below the average .

Particle motion

Density

Kinetic energy

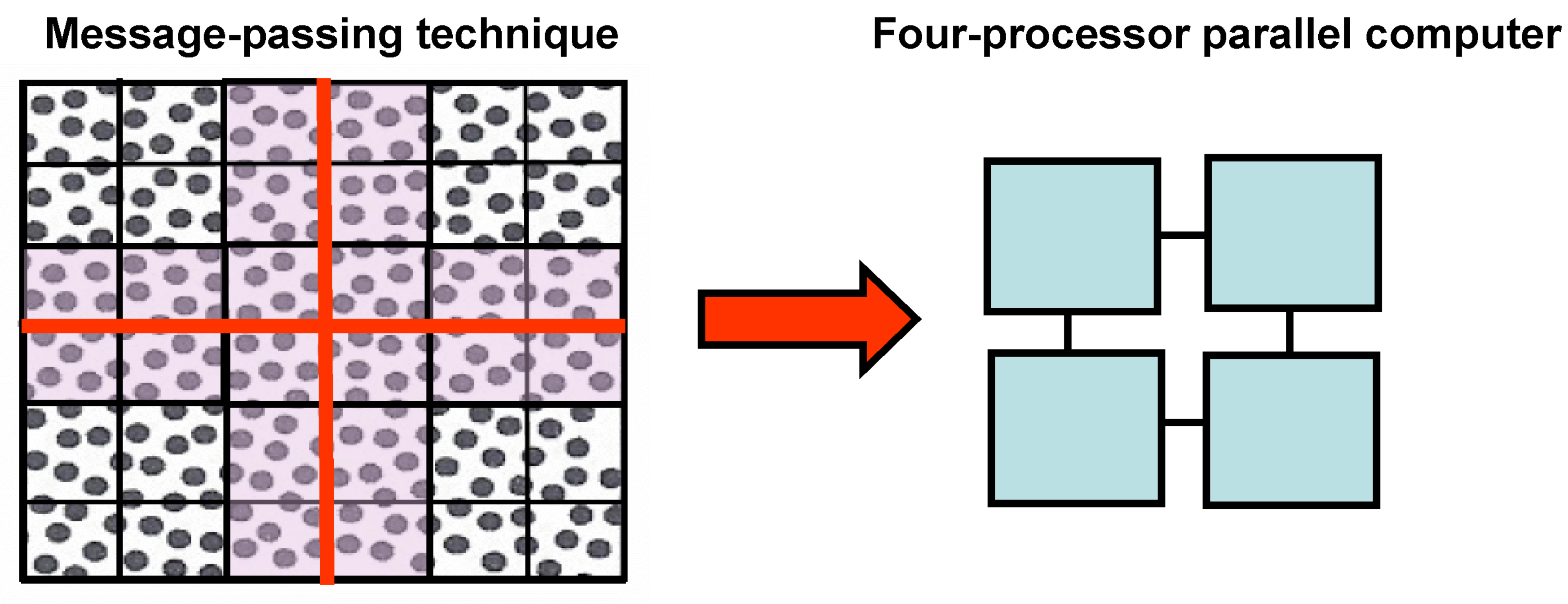


$V_0 = 1/4V_f$, Lucy fluid with h = 6 .

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

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

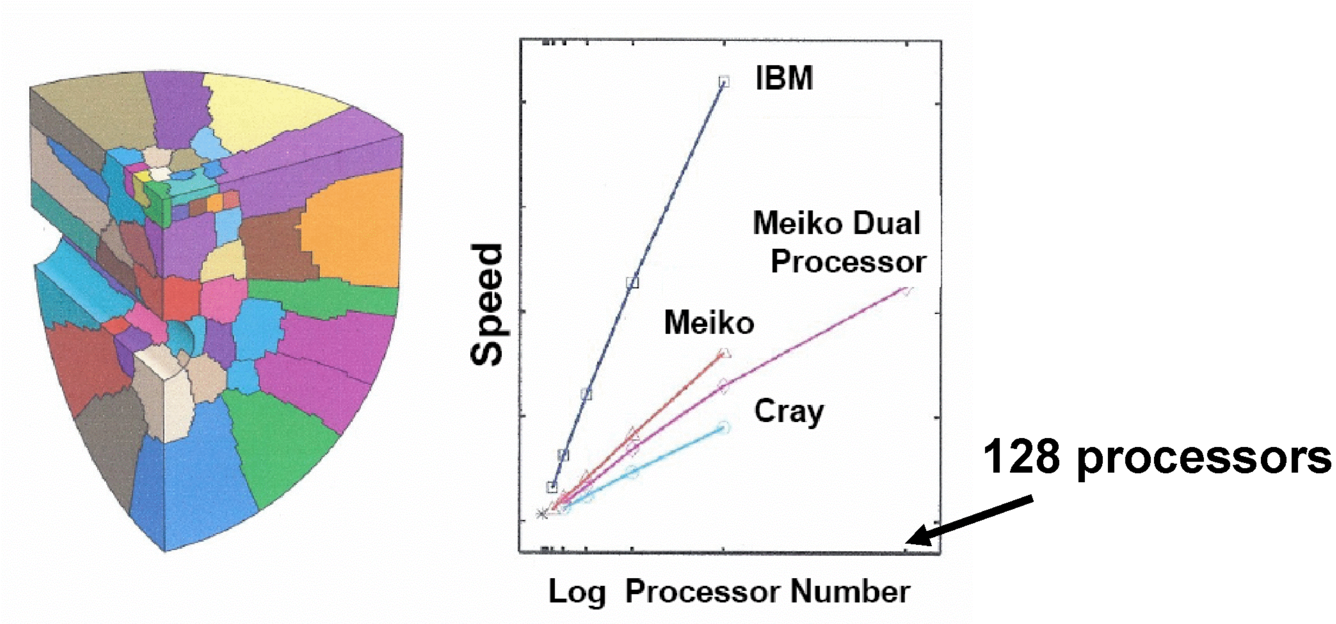
- Two forms of parallel are "shared memory" and "message-passing .
- Must use message-passing for large problems .
- Message-passing is more efficient, works for larger problems, but is much more difficult to program .



10. Parallel Techniques
Efficiency, Scalability & Message-Passing

- **Communication time reduces parallel efficiency**

$$s = \tau_1 / \tau_N = N\eta \leq N = N\eta_{ideal}$$



- **Message-passing involves detailed lists tracking cells/particles in processors .**

10. Parallel Techniques
Create Subdomains from Optimized Cuts of Graphs

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

  cells $\Rightarrow$ vertices

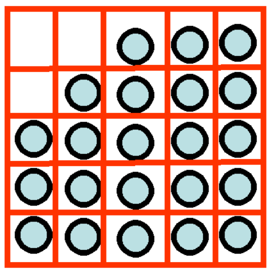
  cell connectivity $\Rightarrow$ lines

- **Optimized cuts of graphs are *partitions* (subdomains) .**

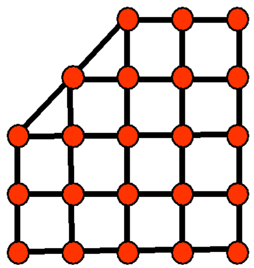
Method by Karypis and Kumar + free software :

http://www.cs.umn.edu/~metis/

Particles
in dx ~ h



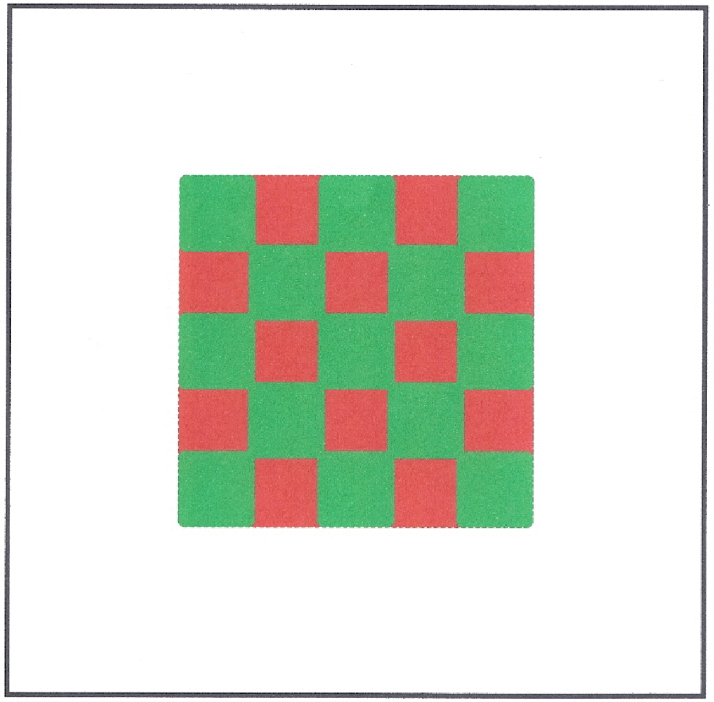
Graph with
connected cells



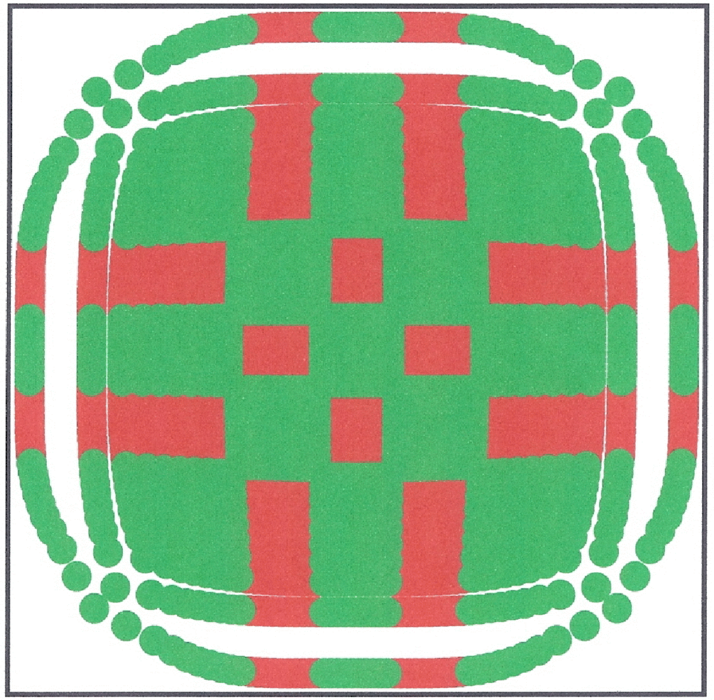
Vertex weights $\propto$ processor work time
Line weights $\propto$ communication time

10. Parallel Techniques
Example: Dynamically Partitioned Free Expansion

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

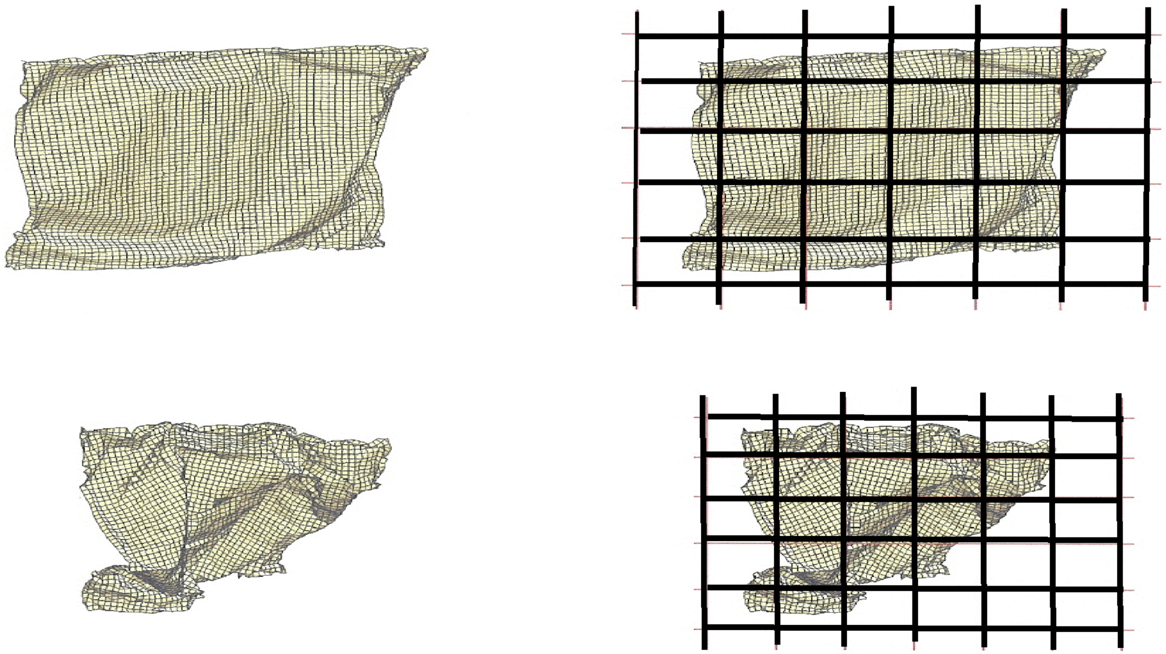


$-25 < (x,y) < +25$



$-25 < (x,y) < +25$

10. Parallel Techniques
Example: Dynamically Partitioning Crushed Sheet



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

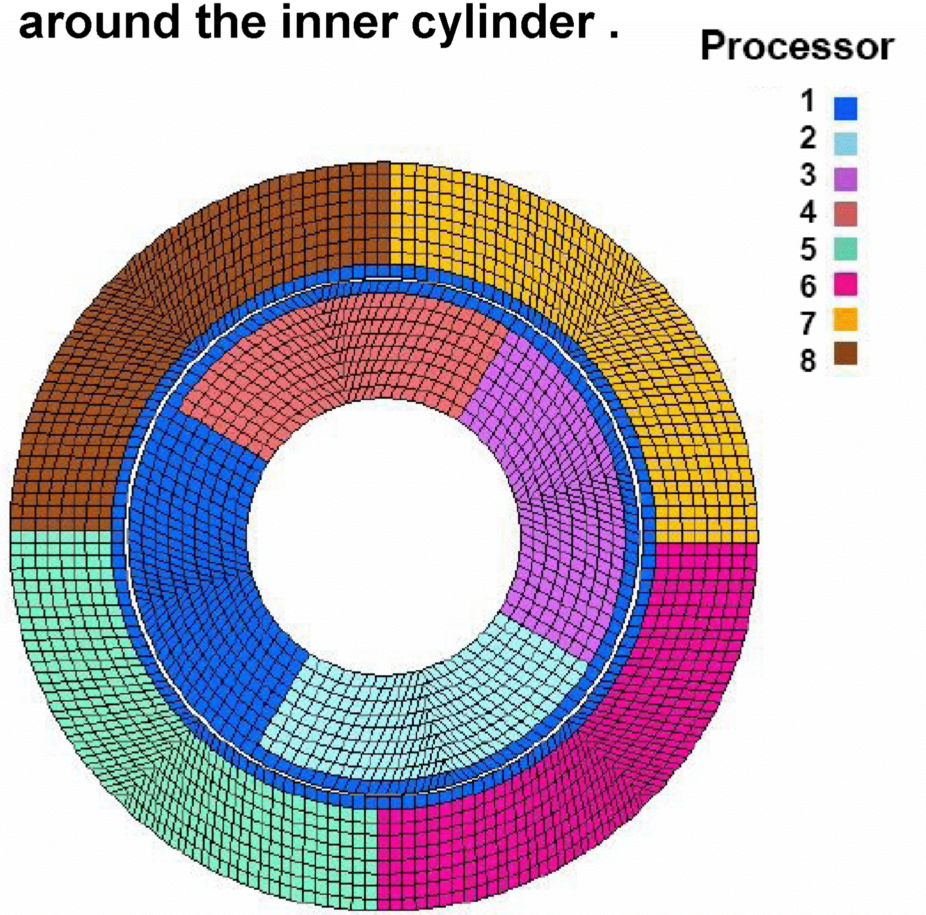
10. Parallel Techniques
Example: Partitioned “Nut-Bolt” Mesh and Interface

• Treat the surfaces as a separate partition ;

• For many surfaces, distribute them among several processors .

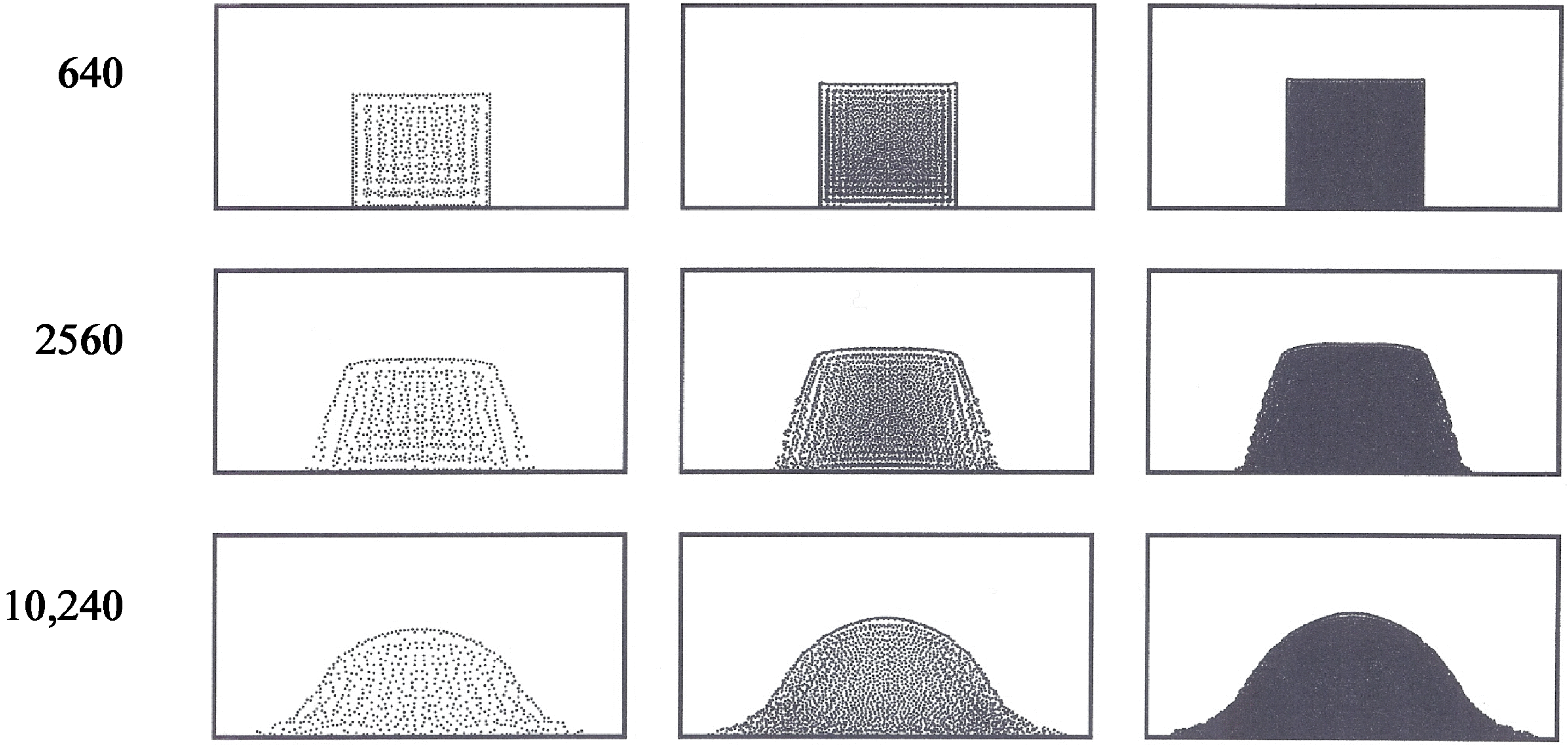
• Surface partition is computed only once for this problem .

The outer cylinder rotates around the inner cylinder .



11. Collapsing water column with gravity

N = 640, 2560, 10,240 particles

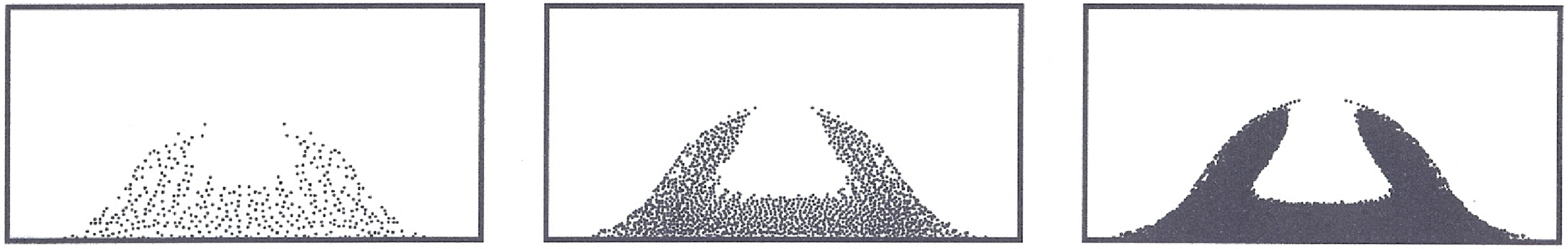


$$t_{10240} = 2t_{2560} = 4t_{640}$$

Uses Φ_{EA}, $\Phi_{surface} \propto \sum_j (\nabla\rho)_j^2$. , Φ_{core} .

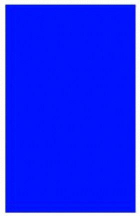
11.Collapsing water column with gravity

Tensile regions – SPAM and Finite Elements

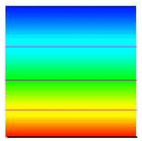


640 particles | 2560 particles | 10,240 particles

WxH = 80x64 elements
dy = 2dx = 1



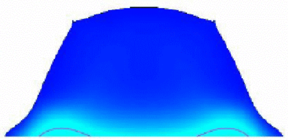
$g = 0$



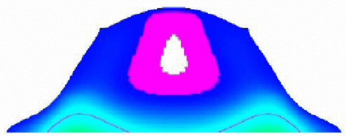
$t = 0$

Relaxation

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



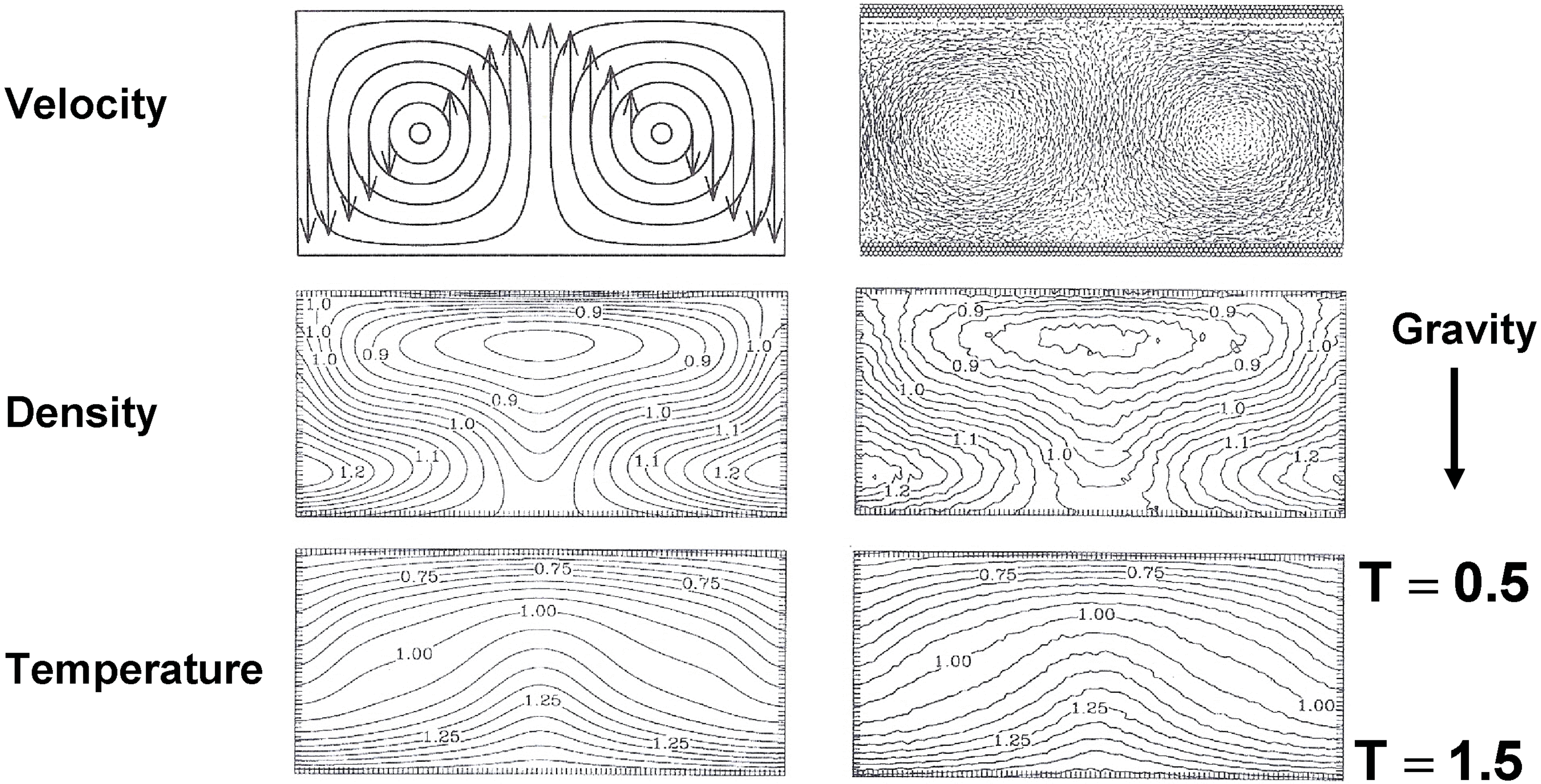
$t = 30$



$t = 40$

Collapse

12. Rayleigh-Bénard Flow (Gravity & T gradient)
Finite-Difference (left) & Smooth Particles (right)

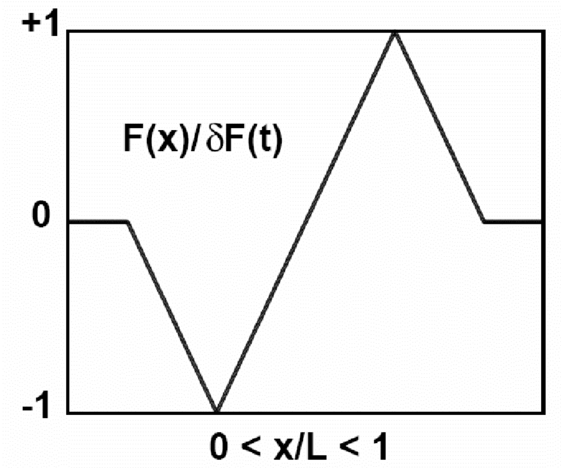


Rolls form for $R_c = \dfrac{gL^4 (d\ln T/dy)}{\upsilon D_T}$ & 5000 smooth particles

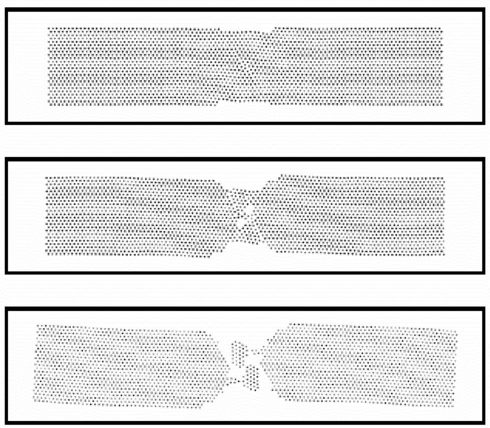
Kum, Hoover, & Posch, PRE 52, 4899-4908 (1995) .

13. a) Tension Test with Particles
Pair Φ MD, core Φ, density-gradient Φ & strength

- External forces applied to the interior of a tension specimen ;
- Initially tapered bar .

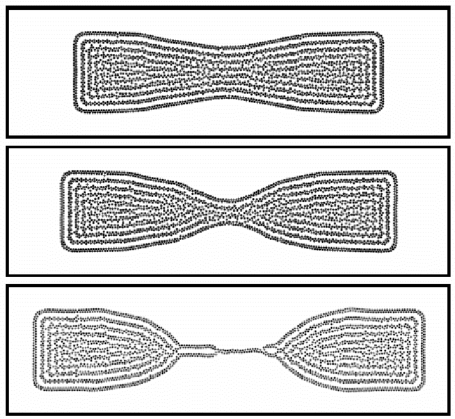


- Three tension-test particle simulations :



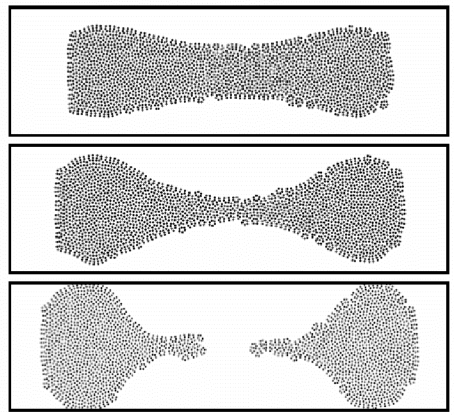
-60 < x < +60 ; t = 620, 624, 628

Pair-potential MD



-70 < x < +70 ; t = 375, 625, 875

SPAM + core potential



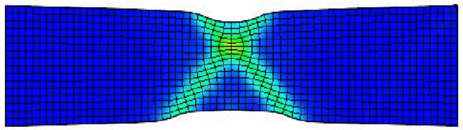
-70 < x < +70 ; t = 10000, 15000, 20000

SPAM-like MD: core + $\sum_j (\nabla\rho)^2$ + strength

13 a) Tension Test with DYNA3D

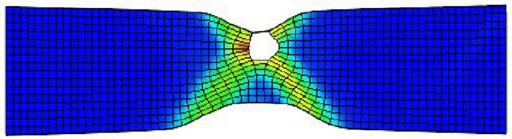
Finite-Element Simulation of Tension Test

A tapered bar is created with elements reduced in height by 10% from the end of the bar to the middle of the bar. A time dependent load is applied to the ends of the bar.



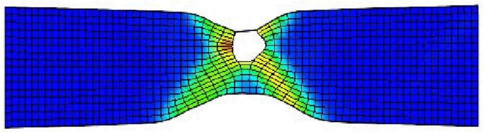
Time = 32

ε_p **= .05**



Time = 48

ε_p **= .075**

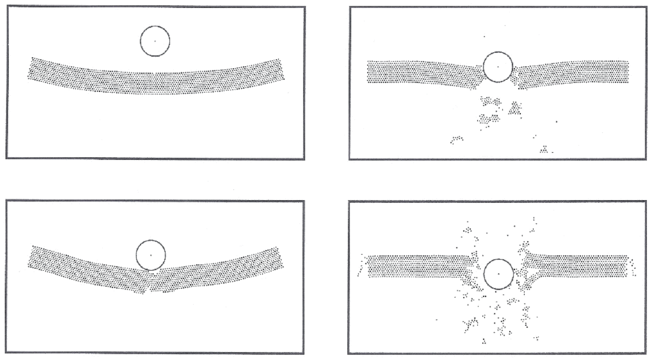


Time = 64

ε_p **= .100**

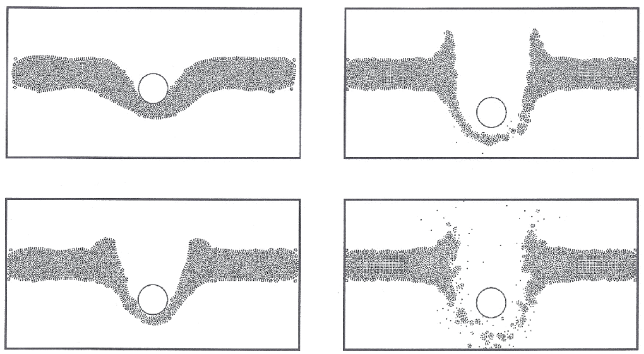
Plastic flow begins at $\varepsilon = \delta L/L = .01$

13 b) Ball-Plate Fragmentation
Ball-Plate Penetration with Particles



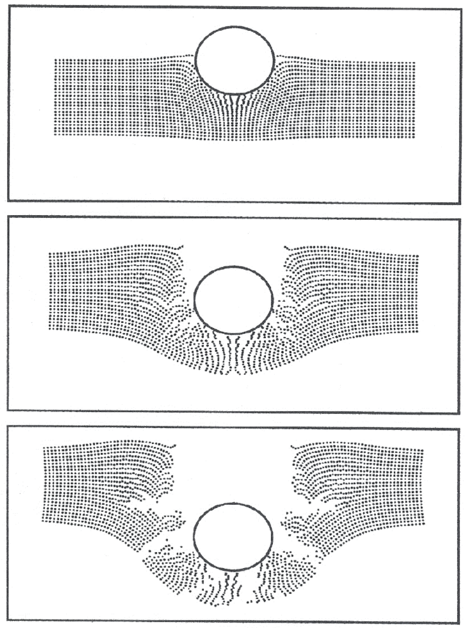
-70 < x < +70 ; v = 1, 2, 4, 8

Pair potential MD



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

MD + embedded-atom & strength

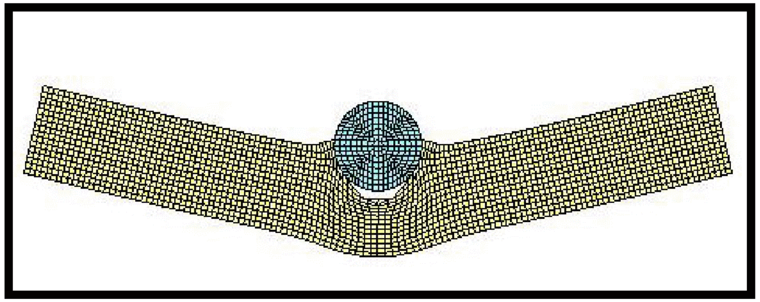


-60 < x < +60 ; t = 4, 12, 20

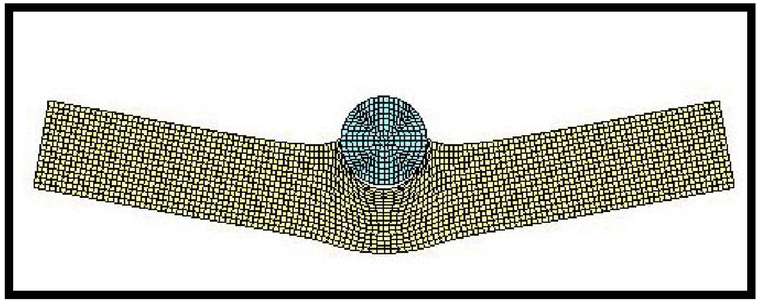
SPAM

13 b) Ball-Plate Fragmentation
Ball-plate Penetration with Finite Elements

$V_0 = 1/4$; $\varepsilon_f = (1.0, 2.0)$

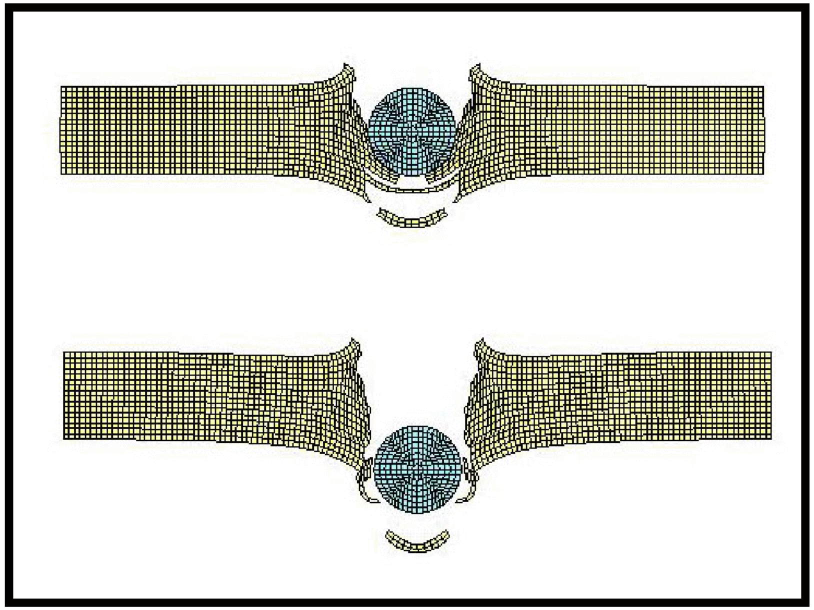


$\varepsilon_p < \varepsilon_f = 1.0$, $v_0 = 1/4$



$\varepsilon_p < \varepsilon_f = 2.0$, $v_0 = 1/4$

$V_0 = 1/2$; $\varepsilon_f = 1.0$



$\varepsilon_p < \varepsilon_f = 1.0$, $v_0 = 1/2$

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

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 ;
  Density-curvature potential for strength .