Smooth Particle Applied Mechanics: The Method, with Three Example Problems

Carol G. Hoover & William G. Hoover
Ruby Valley Research Institute
Ruby Valley, NV 89833, USA

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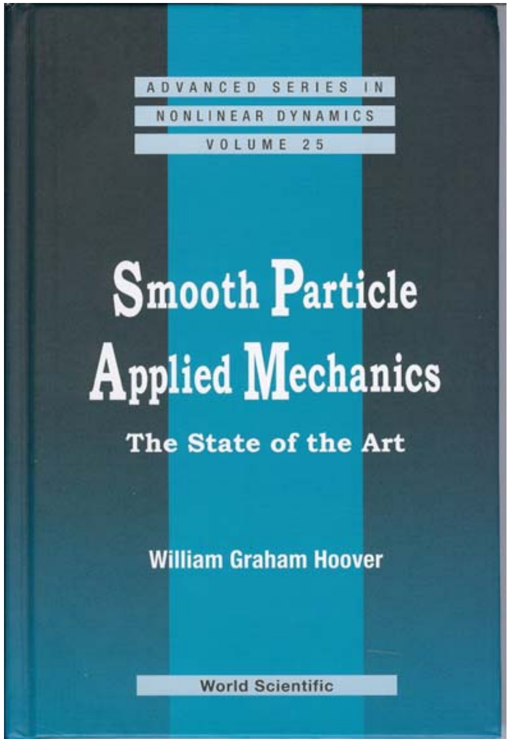


1.0 Motivation
2.0 SPAM method
3.0 Three applications:
- Free expansion of a gas
- Column of water, acted on by gravity
- Convecting, conducting, compressible fluid flow

1.1 Microscopic *versus* Macroscopic Material Descriptions

Atomistic Length & time scales

L ~ Å
t ~ ps - μs

Atomistic motion satisfies ordinary differential equations

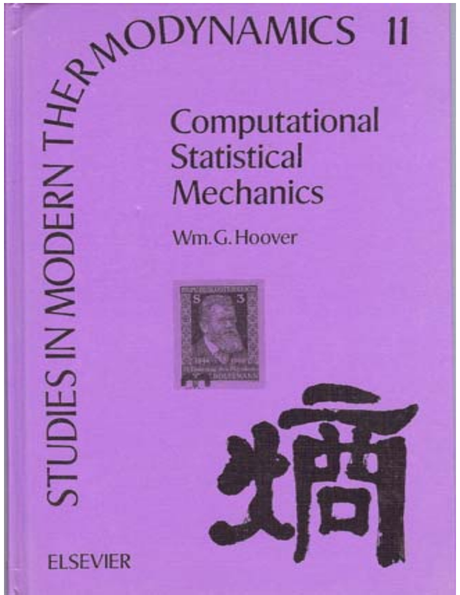
Specify: $m\dot{v} = -\nabla \cdot \Phi$

Laboratory Length & time scales

L ~ cm or meters
t ~ ms or seconds

Fluids and solids satisfy partial differential flow equations

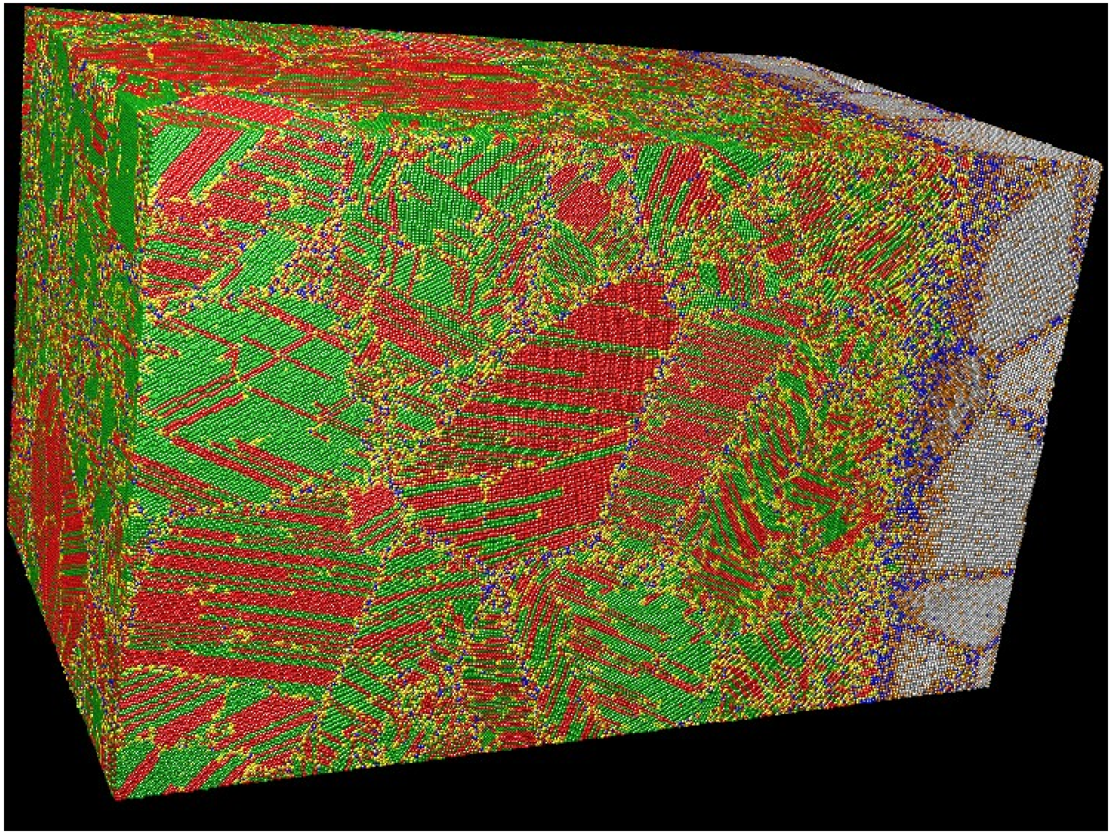
Specify: $\rho\dot{v} = -\nabla \cdot P$



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

1.2 Particle Methods: Molecular Dynamics and SPAM

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



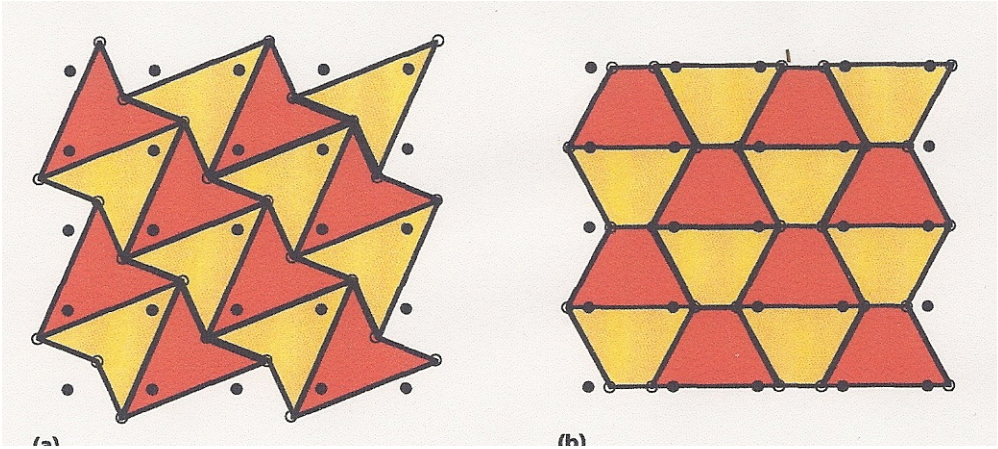
From Kai Kadau's Los Alamos Webpage 2007

1.3 SPAM *versus* Finite-Element Methods

SPAM is MUCH simpler than finite-element algorithms:
No mesh generation, no node and element lists,
no element integration

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

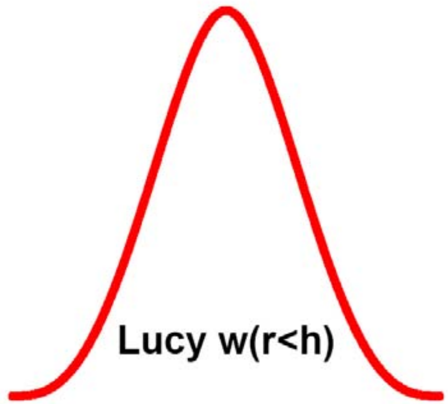
SPAM avoids mesh tangling and shear instabilities;
no unstable butterfly or hourglass modes



2.1 SPAM and Continuum Mechanics

Smooth Particle Applied Mechanics

Used for astrophysical problems (Lucy, Monaghan)
Used in the 80s & early 90's for fluids – SPH
Method is applied to many fields: heat conduction, electricity & magnetism, fluid-structure interaction, fragmentation



Particle weight function

Lagrangian (comoving) Equations of Continuum Mechanics

Continuity equation $d\rho/dt = -\rho \nabla \cdot u$

Equation of motion $\rho du/dt = -\nabla \cdot P$

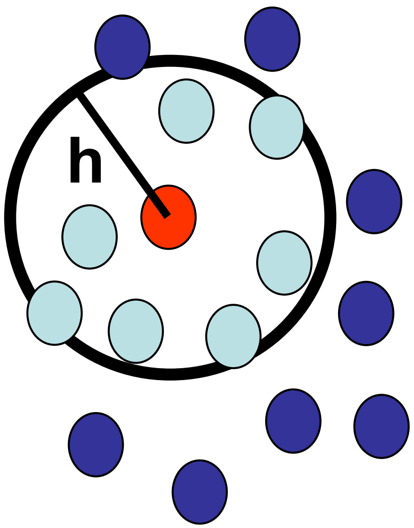
Energy equation $\rho de/dt = -\nabla u : P - \nabla \cdot Q$

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

2.2 Smooth Particles and Weight Functions

Particle density from neighbors within a smoothing length

$$\rho_J = \sum_K m_{JK} w(|r_J - r_K|) \ , \quad |r_J - r_K| \le h$$



Properties of the weight function:

Normalization: $\int 2\pi r w(r) dr = 1$

Continuous first and second derivatives

$w'(0) = 0 \ ; \quad w, w', w'' = 0$ at $r = h$

Lucy's weight function

$$w_{2D}(r < h) = (5/\pi h^2)(1+3x)(1-x)^3 \ , \ x = r/h \ ;$$

$h = 3$

2.3 Particle Averages for Functions

Density-based interpolations for averages

$$\rho_R = \sum_J m_K w_{RJ}$$

Averages:	**Exact for:**
$f_R = \sum_J f_J \, m_J \, w_{RJ} / \rho_R$	$f_R = \text{constant}$
$f_R = \sum_J (f/\rho)_J \, m_J \, w_{RJ}$	$f_R \propto \rho$
$(f/\rho)_R = \sum_J (f/\rho^2)_J \, m_J \, w_{RJ}$	$f_R \propto \rho^2$

For h ~ 3 lattice spacings, error ~ 0.2%

Averages can be formed for any power of ρ or functions of ρ.

2.4 Particle Averages for the Gradients

Heat flux and Pressure Gradients

$$\nabla(p/\rho) = \frac{1}{\rho}\nabla\cdot P - \frac{P}{\rho^2}\nabla\rho$$

$$\left(\frac{\nabla\cdot P}{\rho}\right)_R = \sum_J \left[\left(\frac{P}{\rho^2}\right)_J + \left(\frac{P}{\rho^2}\right)_R \right] m_J \nabla_R w_{RJ}$$

Velocity and Temperature Gradients

$$\nabla(\rho u) = u\cdot\nabla\rho + \rho\nabla\cdot u$$

$$\left(\rho\nabla\cdot u\right)_R = \sum_J m_J(u_J - u_R)\nabla_R w_{RJ}$$

When R ⟶ particle K, then use m_{KJ} :

$$m_{KJ} = ½\,(m_K + m_J) \quad \text{or} \quad m_{KJ} = \sqrt{m_K m_J}$$

2.5 Smooth-Particle Equations

Continuity Equation is automatically satisfied.

Equation of Motion:

$$m_J(du_J/dt) = -\sum m_J m_K[(P/\rho^2)_J + (P/\rho^2)_K] \cdot \nabla w_{JK}$$

Energy Equation:

$$m_J(de_J/dt) = \text{heat in} - \text{work done}$$

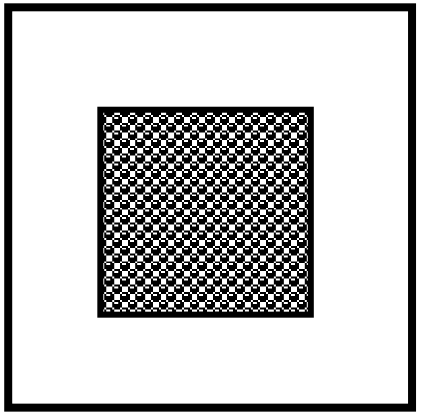
Work and heat are computed from pressure and gradients of the velocity, temperature, and heat flux.

Time integration with 4th order Runge-Kutta

Wm. G. Hoover, *et ux*, *SPAM-Based Recipes for Continuum Simulations,* Computing in Science & Engineering, p. 78 (2001).

3.1 Free Expansion of a Gas

$P = (\rho^2)/2$ for a 2D gas is the adiabatic equation of state;



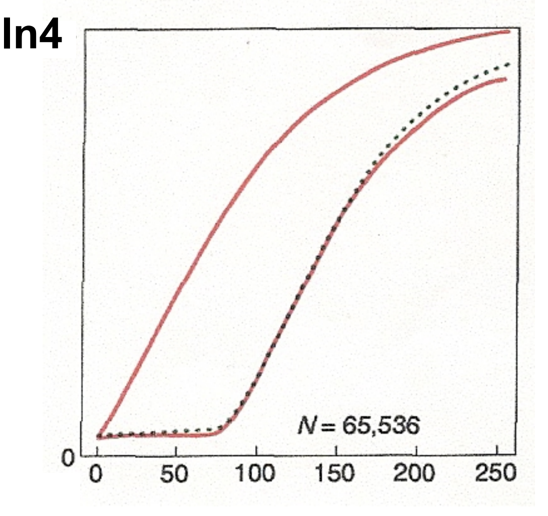
Trajectory isomorphism

Lucy's w_{IJ} SPAM $\longrightarrow$ Φ_{IJ} MD

$V_0 = 1/4V_F$

Calculate field values on a mesh:

$< \rho >, < u >, < e >$



Entropy increases!

$2kT/m = < v^2 > - < v >^2$

$S/Nk = \ln(VT)$

$\Delta S/k = \ln 4$

The following reference discusses all 3 examples:

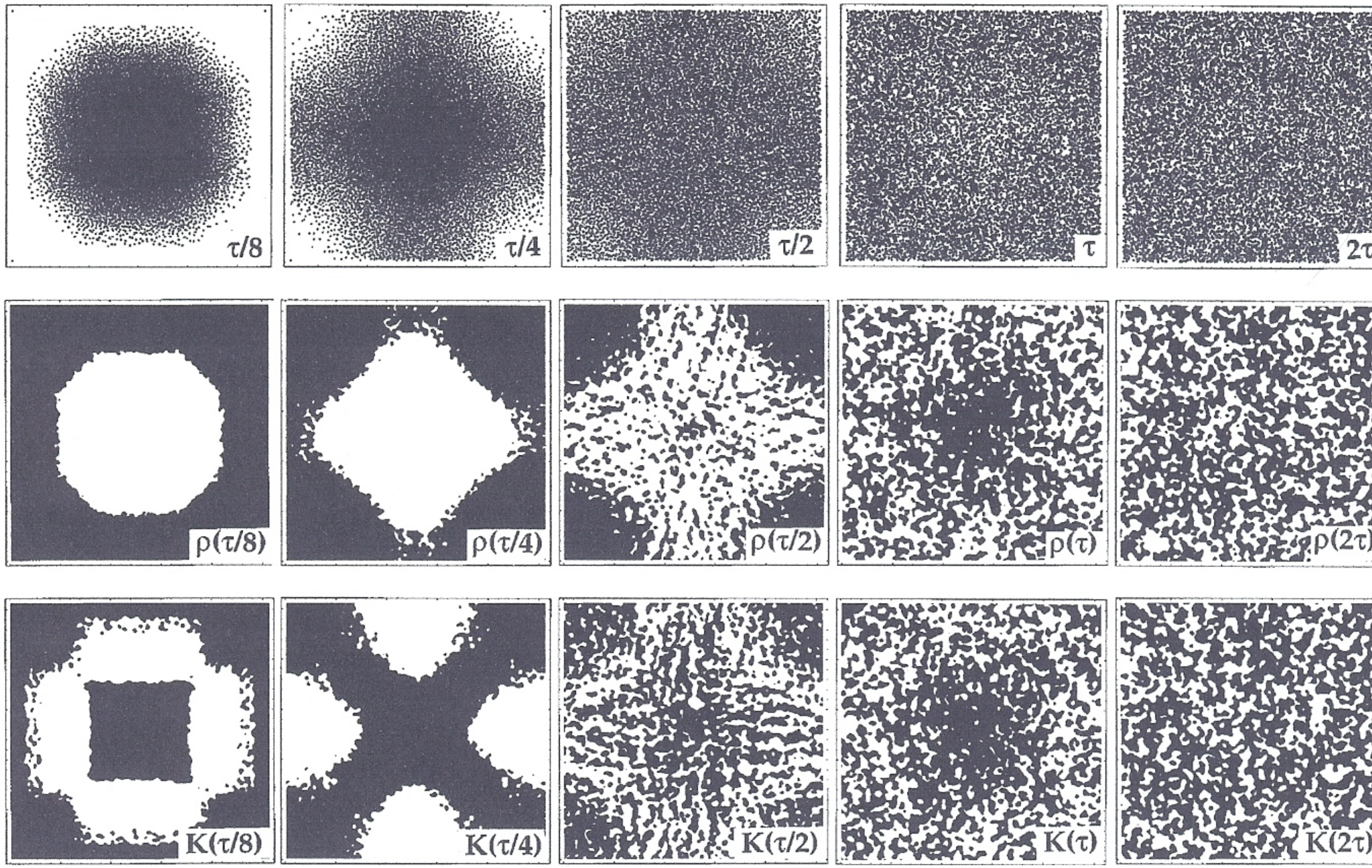
Wm. G. Hoover, *et ux, Computational Physics with Particles,* American Journal of Physics 76 (2008).

3.2 Free Expansion of a Gas - Results

Particle motion

Density

Kinetic energy



Hoover, Posch, Castillo, *et ux*, Journal of Statistical Physics 100, Numbers 1 and 2, (2000) .

4.1 Water Column Acted on by Gravity

Initialize

Equilibrate the water column with damping.
Periodic boundaries on the sides.
Reflecting boundary on the bottom.

Use a core potential to avoid particle clumps.

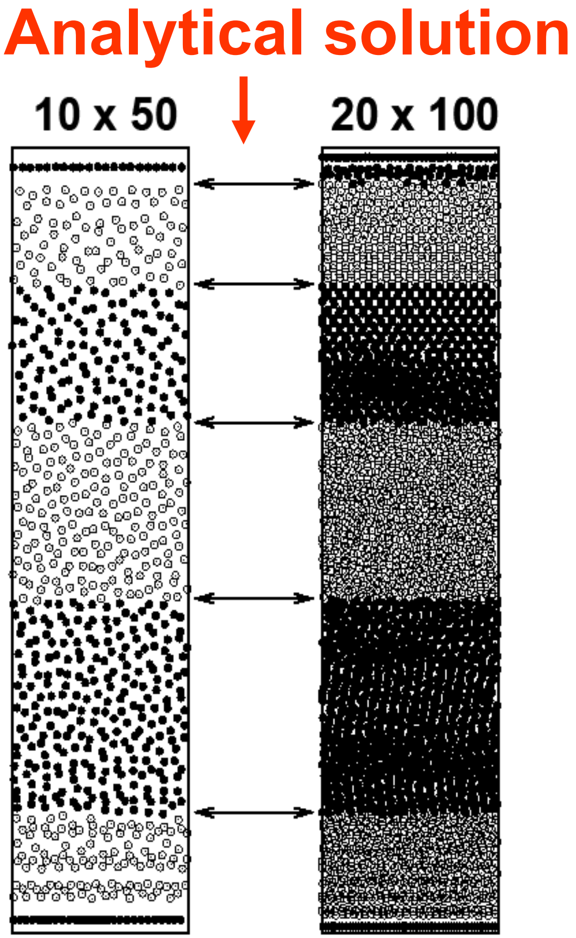
Dense fluid equation of state:

$$P = \rho^3 - \rho^2 .$$

Falling water column:

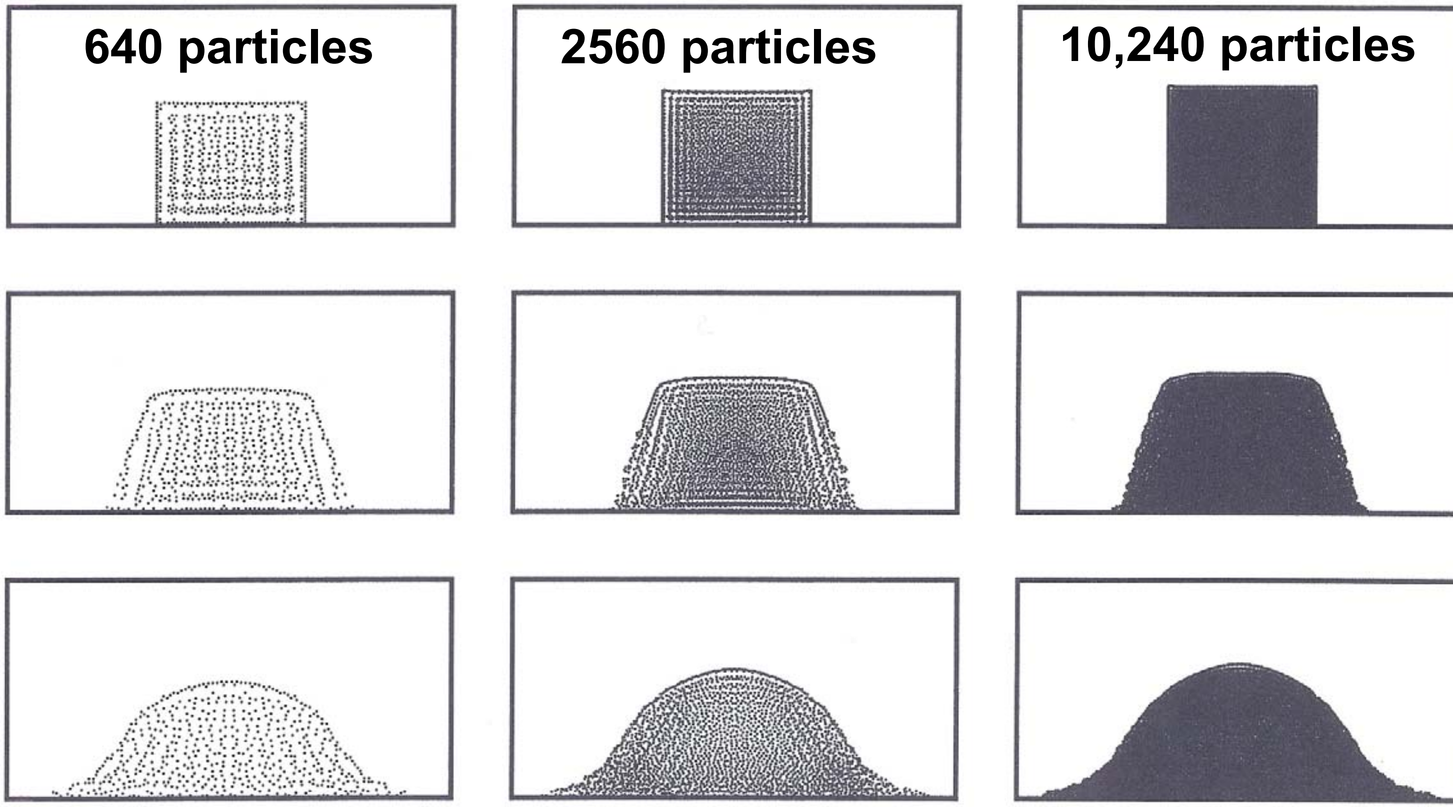
Remove the periodic side boundaries.
Add a surface tension with a potential.

$$\Phi \propto \sum (\nabla \rho)^2$$



Equilibration

4.2 Collapsing Water Column with Gravity - Results

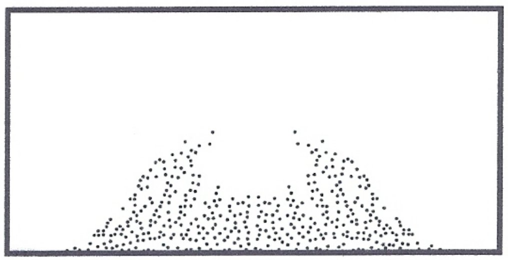


$$t_{10240} = 2t_{2560} = 4t_{640}$$

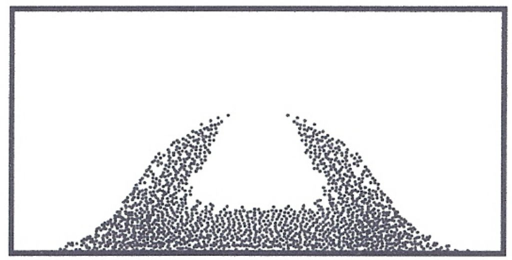
Uses Φ_{EA}, $\Phi_{surface} \propto \sum_j (\nabla\rho)_j^2$, Φ_{core} .

4.3 Collapsing Water Column with Gravity

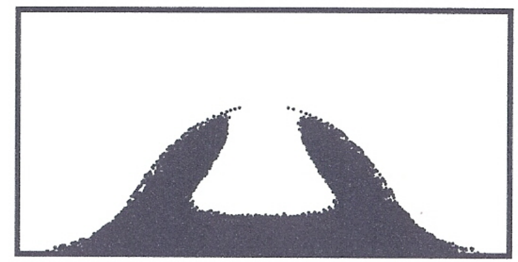
Tensile Regions – SPAM and Finite Elements



640 particles

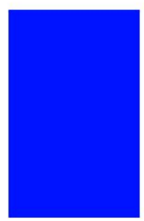


2560 particles

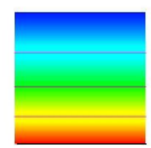


10,240 particles

WxH = 80x64 elements
dy = 2dx = 1



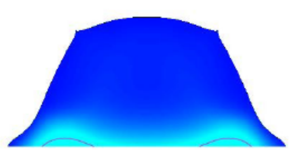
g = 0



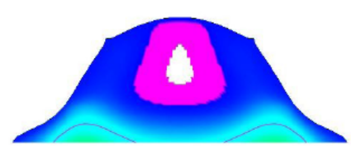
t = 0

Relaxation

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



t = 30



t = 40

Collapse

5.1 The Rayleigh-Bénard Problem

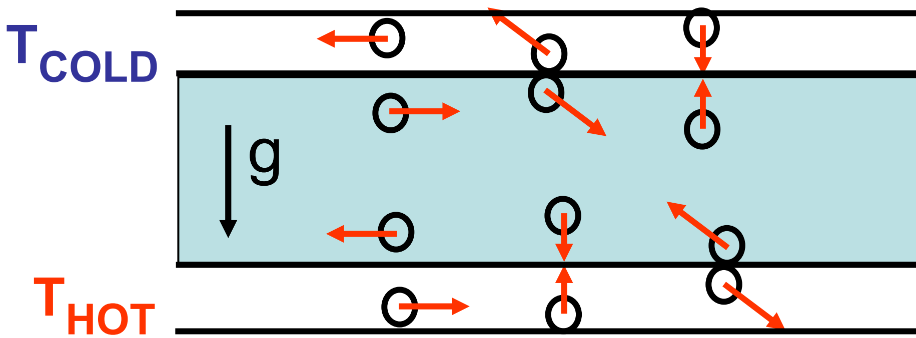
A conducting, convecting fluid in 2D is heated from below in the presence of gravity.

$$P = \rho T = \rho e \quad Q = -\kappa\,(\partial T/\partial y)$$

Periodic boundaries on the sides.

Image & fluid particle provide u, T at the top/bottom boundary.

$$< u_{IMAGE} + u_{FLUID} > = u_{BOUNDARY}$$
$$< T_{IMAGE} + T_{FLUID} > = T_{BOUNDARY}$$



Convection rolls are formed using 5000 smooth particles when the Rayleigh number exceeds a few thousand .

$$R_c = gL^4(d\ln T/dy) / (\nu D_T)$$

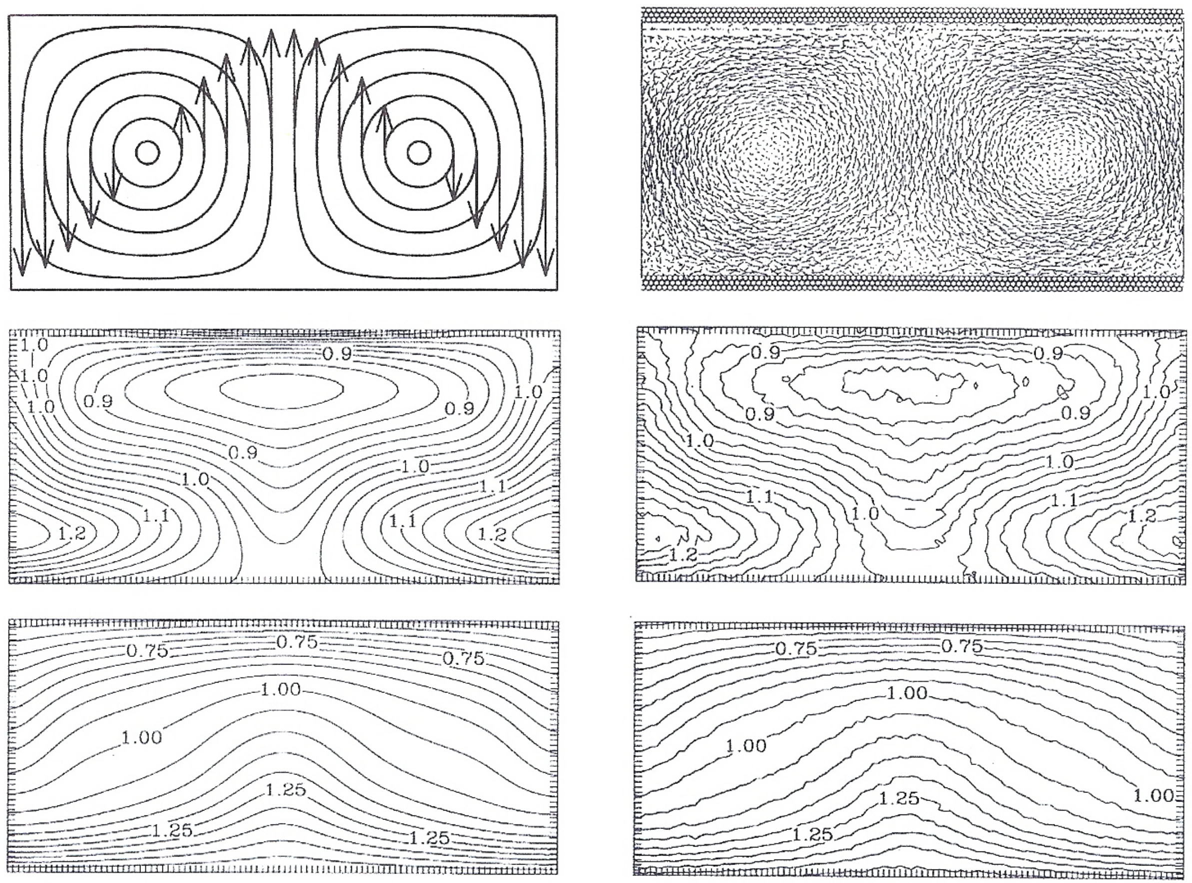
5.2 Rayleigh-Bénard Flow (Gravity & T gradient)

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

Velocity

Density

Temperature



Gravity

T = 0.5

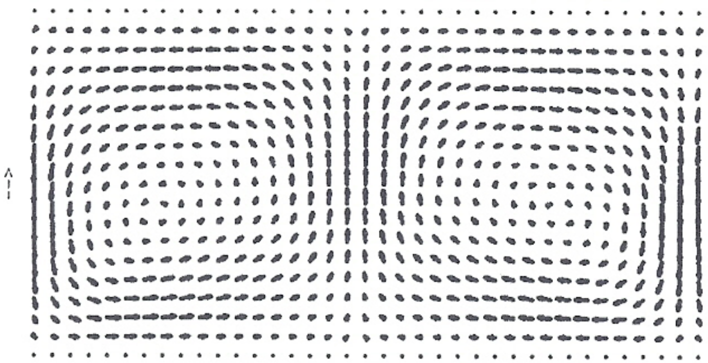
T = 1.5

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

Kum, Hoover, & Posch, Physical Review E 52, 4899-4908 (1995) .

5.3 Existence & Uniqueness in Continuum Mechanics

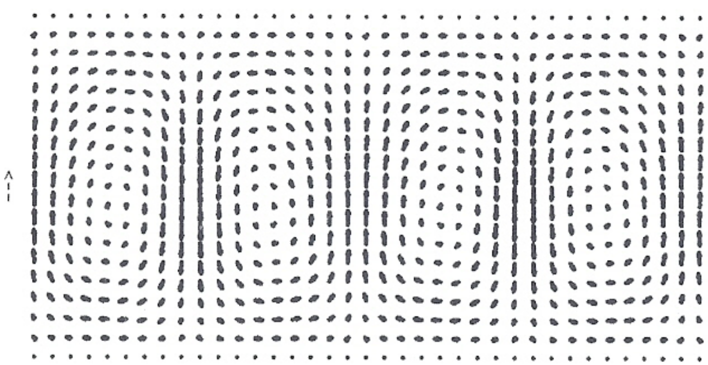
Multiple solutions for a specified boundary condition:
Initial velocity perturbation: sin(y) & sin(nx), or random



2 rolls

We also produced 6 roll solutions

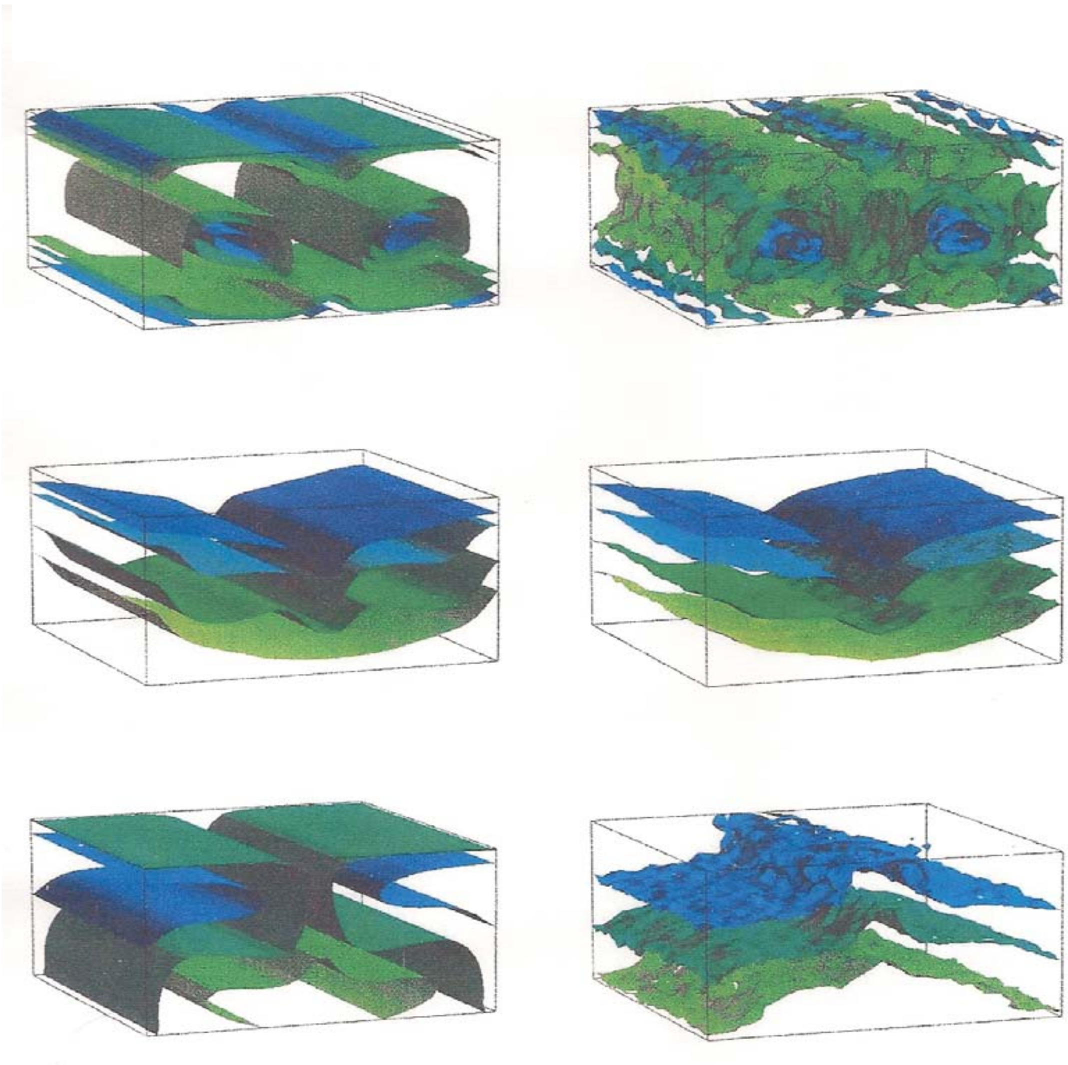
Max or min, S or dS/dt, solutions



4 rolls

V. M. Castillo, Wm. G. Hoover, and C. G. Hoover, Coexisting Attractors in Compressible Rayleigh-Bénard Flow, Physical Review E, **55**, No. 5, (May 1997).
V. M. Castillo, and Wm. G. Hoover, Entropy Production and Lyapunov Instability at the Onset of Turbulent Convection, Physical Rev E, **58**, No, 6, (December 1997).

5.4 Three-Dimensional Rayleigh-Bénard Flow



Finite Difference **SPAM**

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 .

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

SPAM is a useful for modeling continuum mechanics

- Algorithm is transparent to program and easier to debug ;
- Algorithm avoids mesh tangling ;
- Rezoning is easy .

Various deficiencies have been cured

Use density-gradient potential for lattice surfaces ;

String phases are cured with core potentials ;

Use density-curvature potential for strength .

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