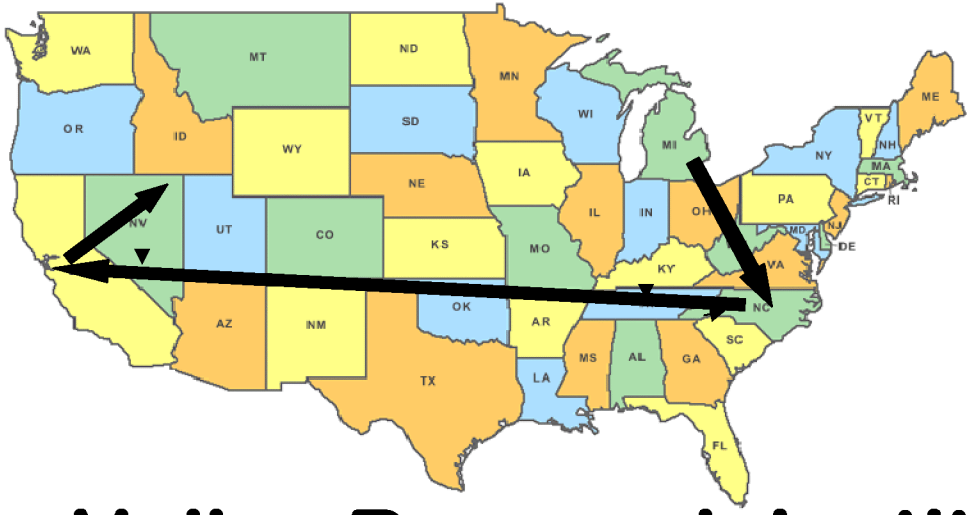
Computational Physics with Particles

Wm G Hoover & Carol G Hoover

[no longer at UCDavis & LLNL!]



Ruby Valley Research Institute

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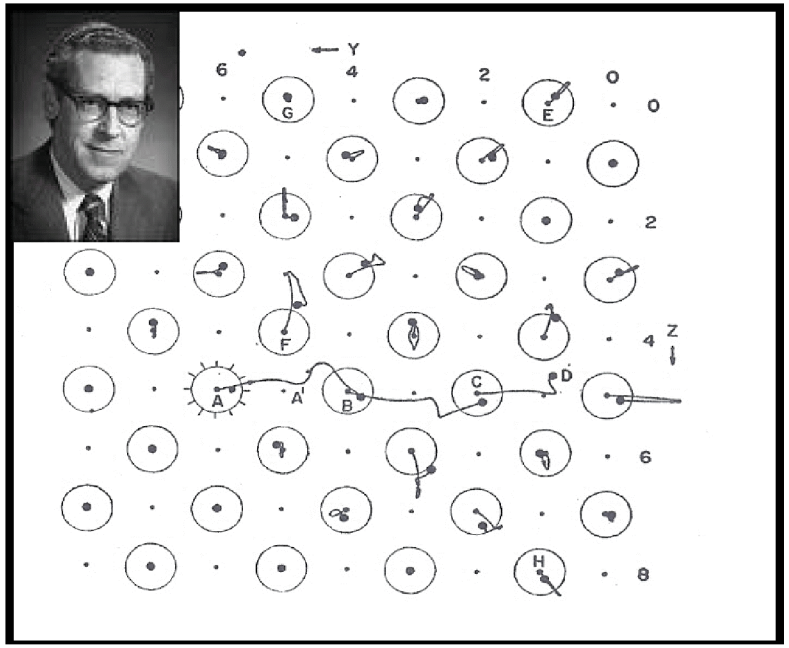
Historical/AutoBiographical Summary

@ University of Michigan 1958-1961 and saw “Molecules in Motion” by Berni Alder & Tom Wainwright Scientific American (1959) .



Historical/AutoBiographical Summary

@ Lawence Livermore Laboratory & "Teller Tech" [UCDavis] 1962-2004 [10,000 people/square mile]

Historical/AutoBiographical Summary

Bill Ashurst's PhD Thesis 1972-1975 :
"Nonequilibrium Molecular Dynamics"
Oyeon Kum's PhD Thesis 1992-1995 :
"Smooth Particle Applied Mechanics"

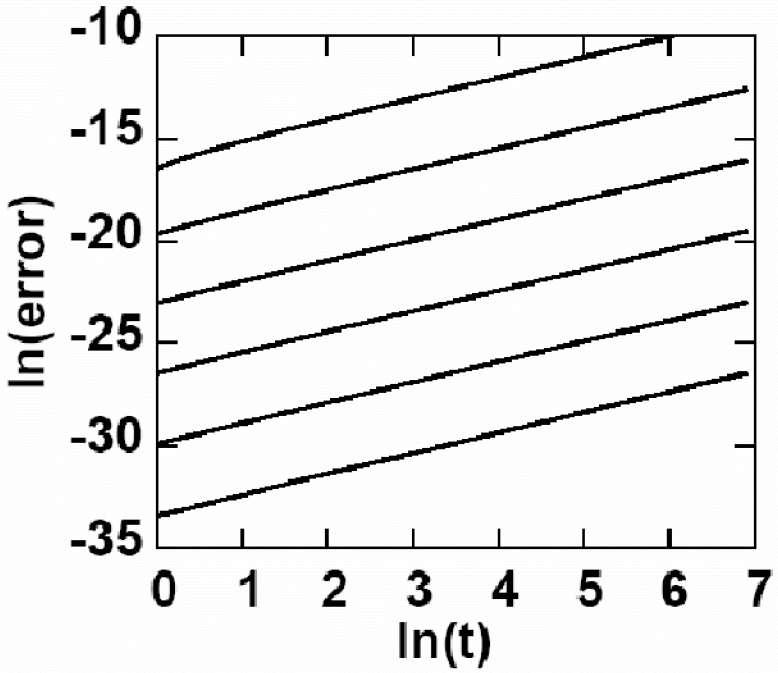
Historical/AutoBiographical Summary

Retirement @ Ruby Valley, Nevada 2004

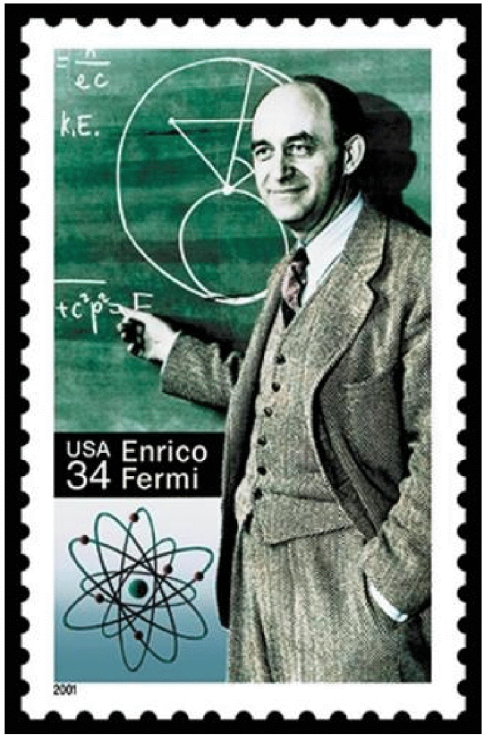
Computational Physics with Particles

- Particles obey Ordinary Differential Equations
- Molecular Dynamics + Control Theory [NEMD]
- Continuum Mechanics with Particles [SPAM]
- Future Needs for both these Particle Methods

Equilibrium Case, using Runge-Kutta



$\Delta t = 0.01$ to 0.32



Particles → Ordinary Differential Equations

Equilibrium & Nonequilibrium Simulations Need Numerical Solutions *via* Runge-Kutta .

Nonequilibrium Simulations require additional Boundary, Control, and Driving Forces .

For example, temperature control :

$$m\ddot{r} = F_{Atomistic} - \zeta p \; ; \; \dot{\zeta} \equiv [\,(K/K_{AVG}) - 1\,]/\tau^2 \; .$$

This generates Gibbs' canonical ensemble .

Nonequilibrium Ordinary Differential Equations

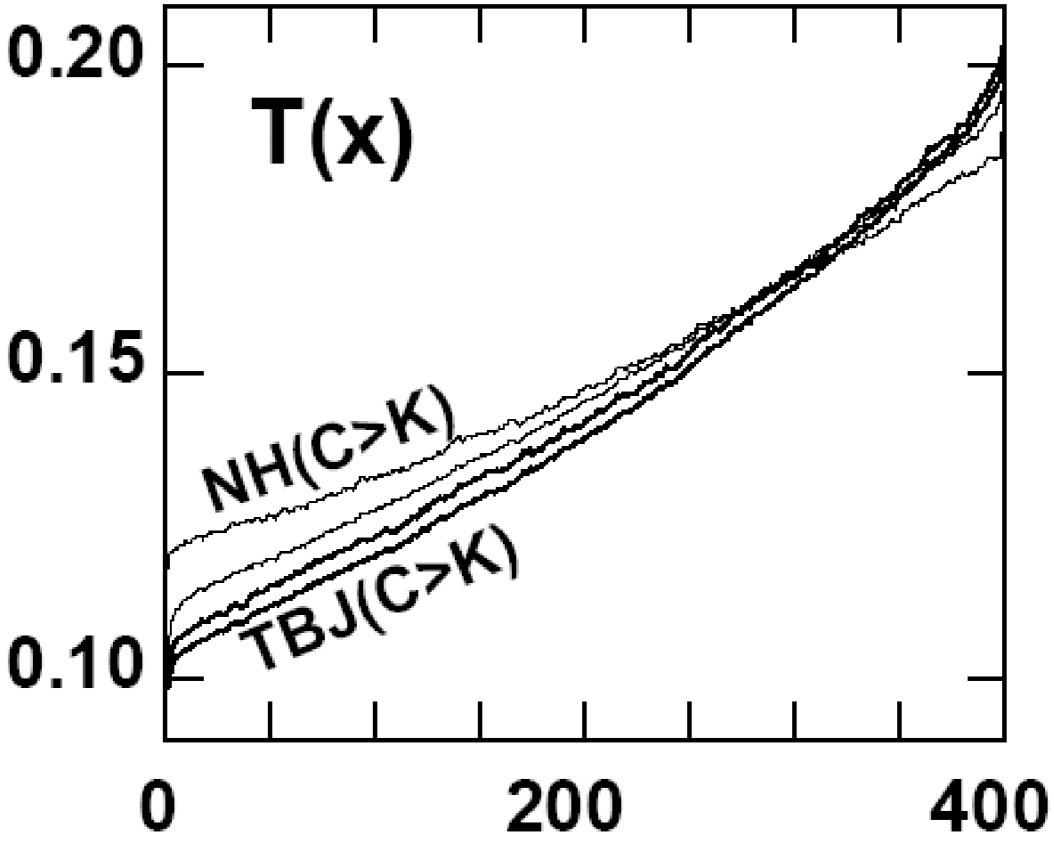
Heat Flow Solutions *via* Runge-Kutta
For Harmonic Chain with Quartic Tethers

$$\Phi_{\text{Harmonic}} = \frac{1}{2}\Sigma(|\,\mathbf{x}_{ij}\,| - \mathbf{d})^2$$

$$\Phi_{\text{Tether}} = \frac{1}{4}\Sigma(\delta\mathbf{x})^4$$

First (cold) and Last (hot) Particles *Thermostated* with Kinetic or Configurational Thermostat Forces .

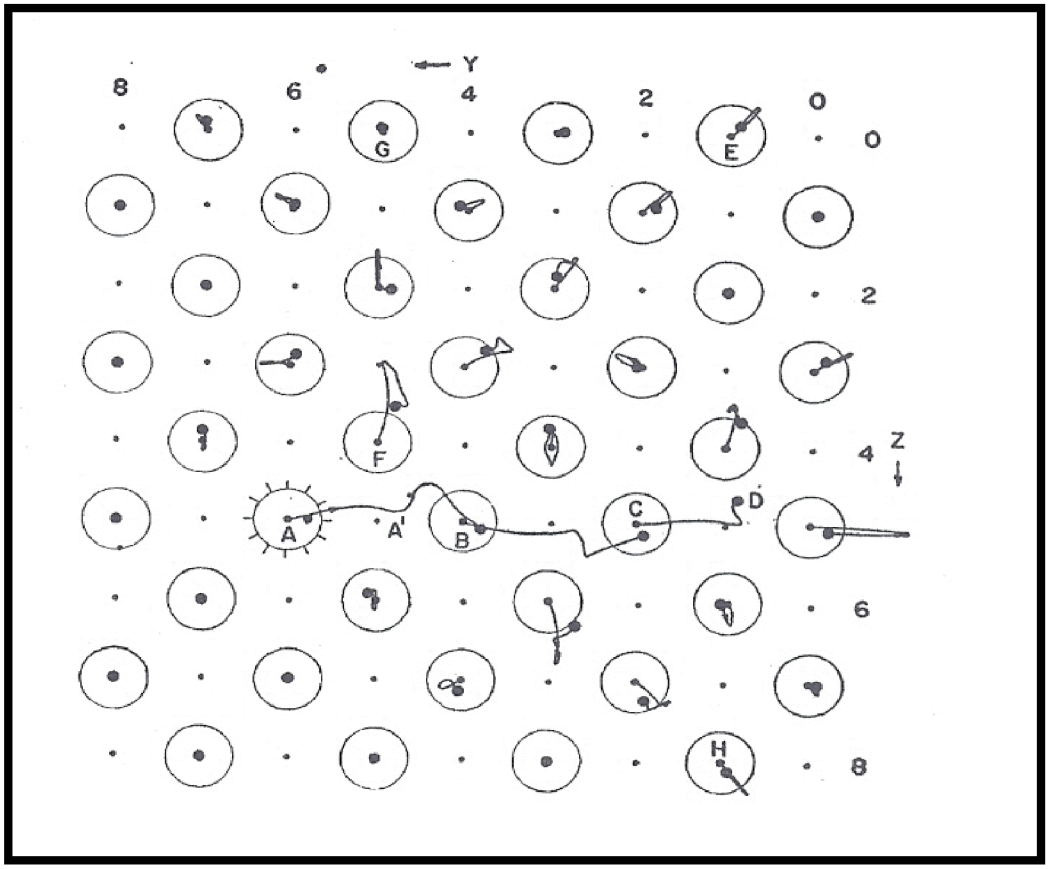
Nonequilibrium Case:
Aoki-Kusnezov ϕ^4 model



$kT_K = \langle p^2/m \rangle$ or

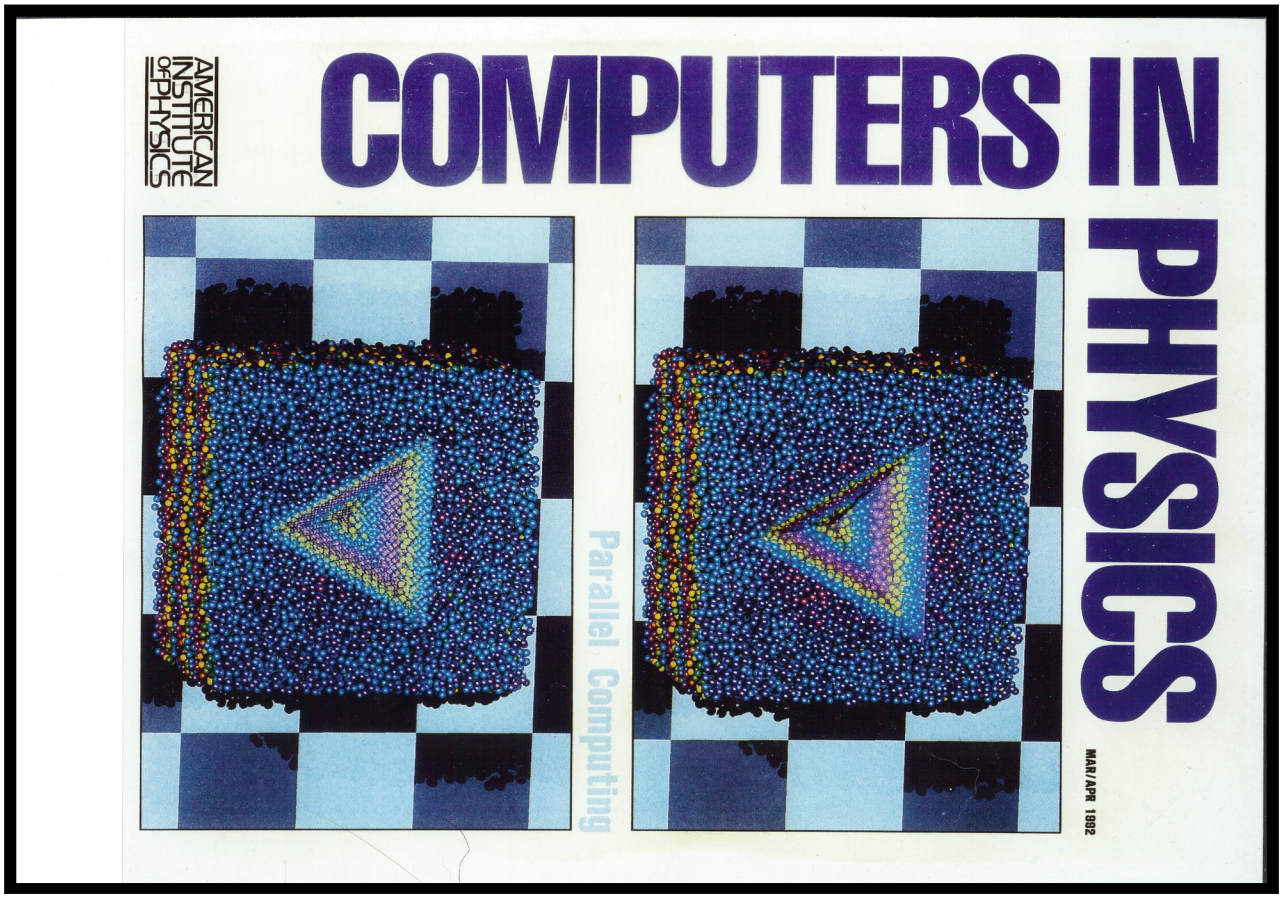
$kT_C = \langle F^2 \rangle / \langle \nabla^2 \mathcal{H} \rangle$

1959: Dynamics with 500 Particles



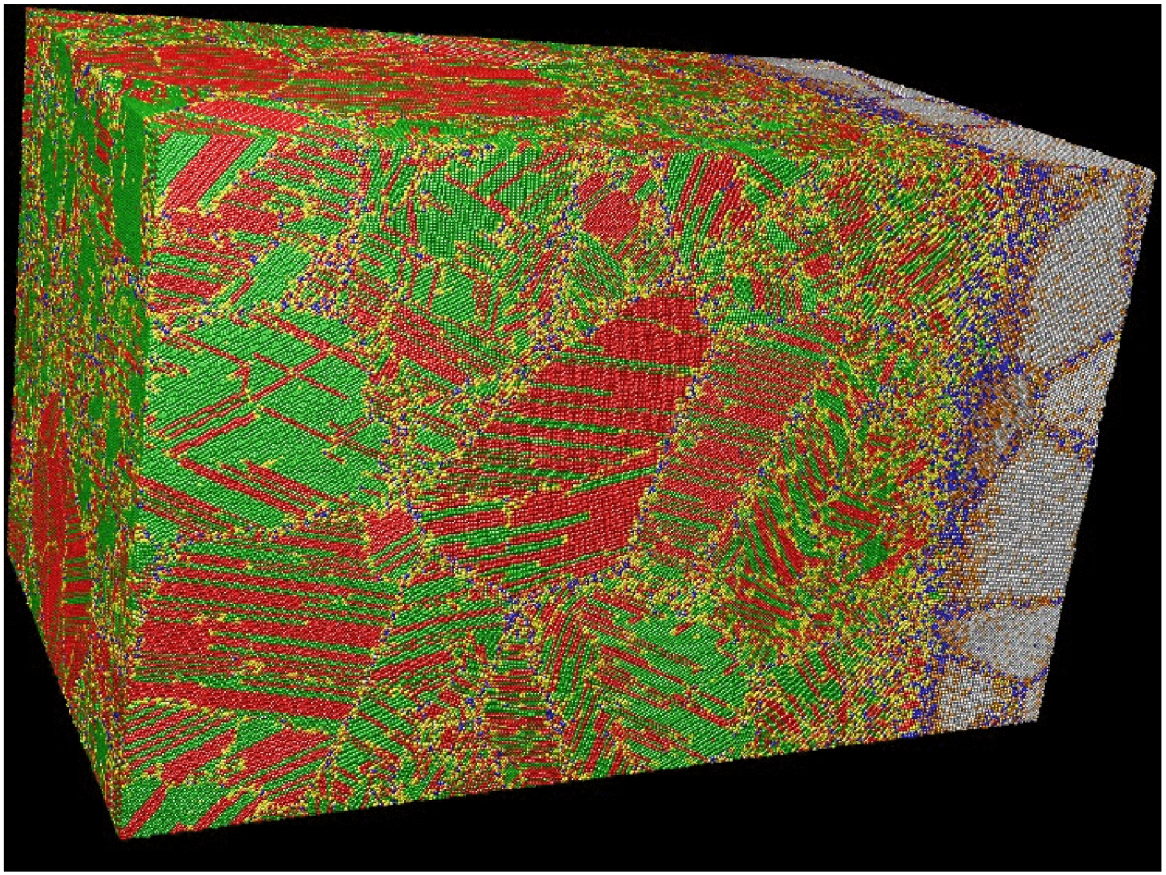
From Vineyard's 1960 Physical Review Article

1989: Dynamics with 1,000,000 Particles



From our work in Japan, 1989-1990, simulating silicon .

2007: Dynamics with 30,000,000 Particles



From Kai Kadau's Los Alamos Webpage

Molecular Dynamics → Continuum Mechanics

Long **MD simulations represent nanoseconds .**
Large **MD simulations represent microns .**
Continuum Mechanics uses Finite Elements rather than Atoms .

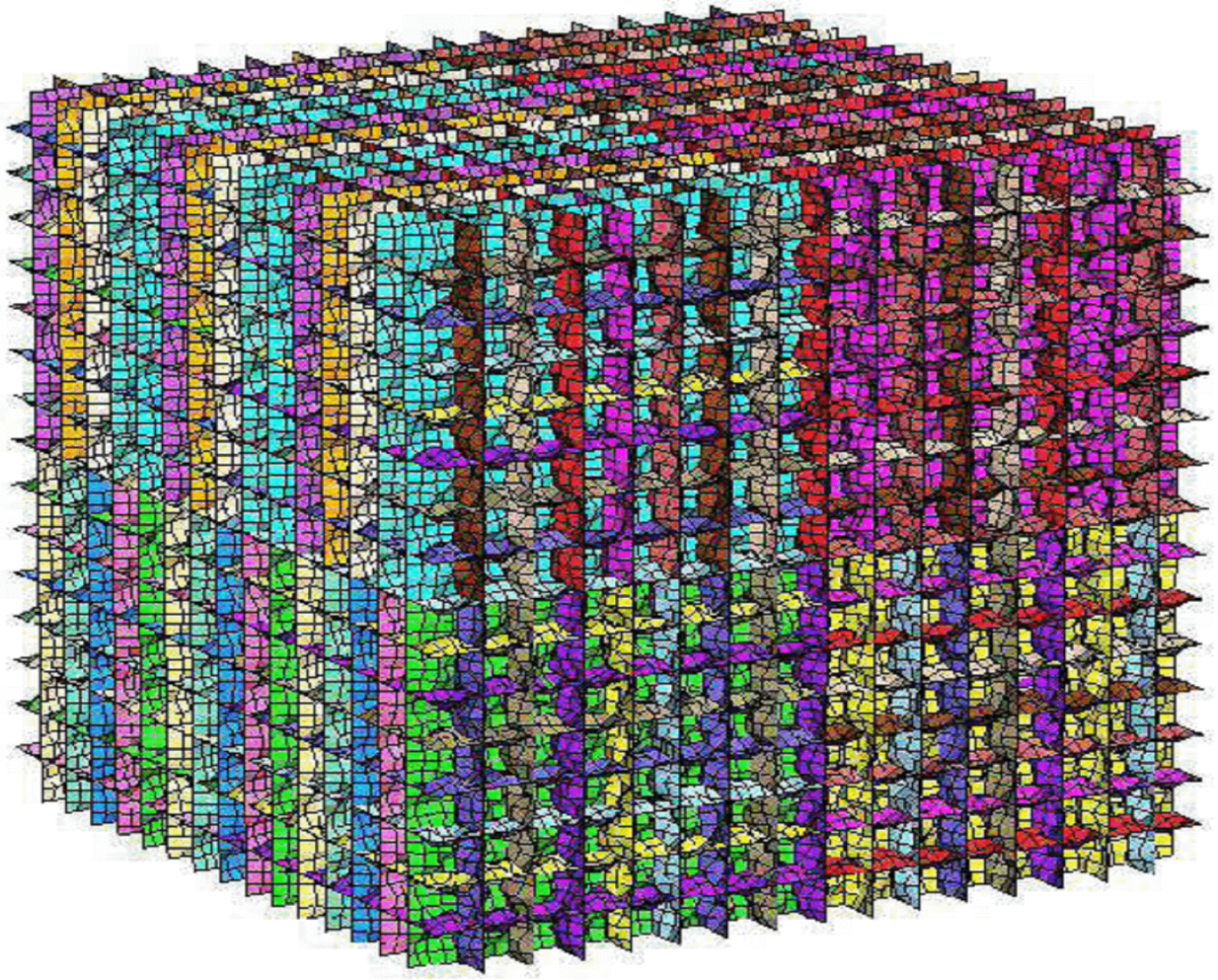
$$\dot{\rho} = -\rho \nabla \bullet \mathbf{v}$$

$$\rho \dot{\mathbf{v}} = -\nabla \bullet \mathbf{P} + \rho \mathbf{g}$$

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

The Finite Elements can be either
Eulerian (fixed) or Lagrangian (comoving) .

Auxetic Material Modeled with 208,896 Elastic-Plastic Shell Finite Elements .



Simpler Way: use Particles governed by SPAM !
SPAM uses w(r) to sum Particle Contributions

The "weight function" w(r<h) smoothes out the particles .
This provides also very smooth averaged field variables .

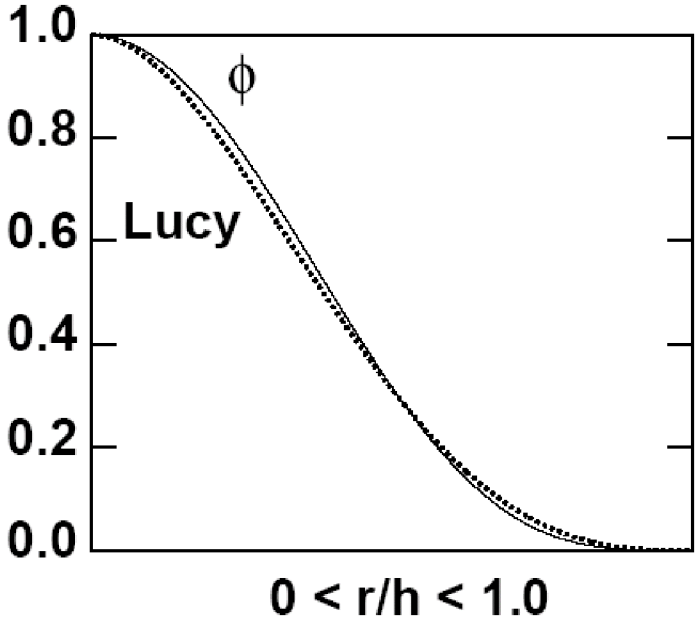
$$\rho_i = \sum_j m w_{ij}$$

$$\rho_i F_i = \sum_j m F_j w_{ij} \Rightarrow \nabla(\rho_i F_i) = \sum_j m F_j \nabla w_{ij}$$

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

Motion governed by *Ordinary* Differential Equations !

Lucy's weight function, $w = 1 - 6r^2 + 8r^3 - 3r^4$.



Short-range repulsive potential, $\phi = (1 - r^2)^4$.

SPAM can be isomorphic to Molecular Dynamics

Consider the case where P and ρ vary slowly in space .

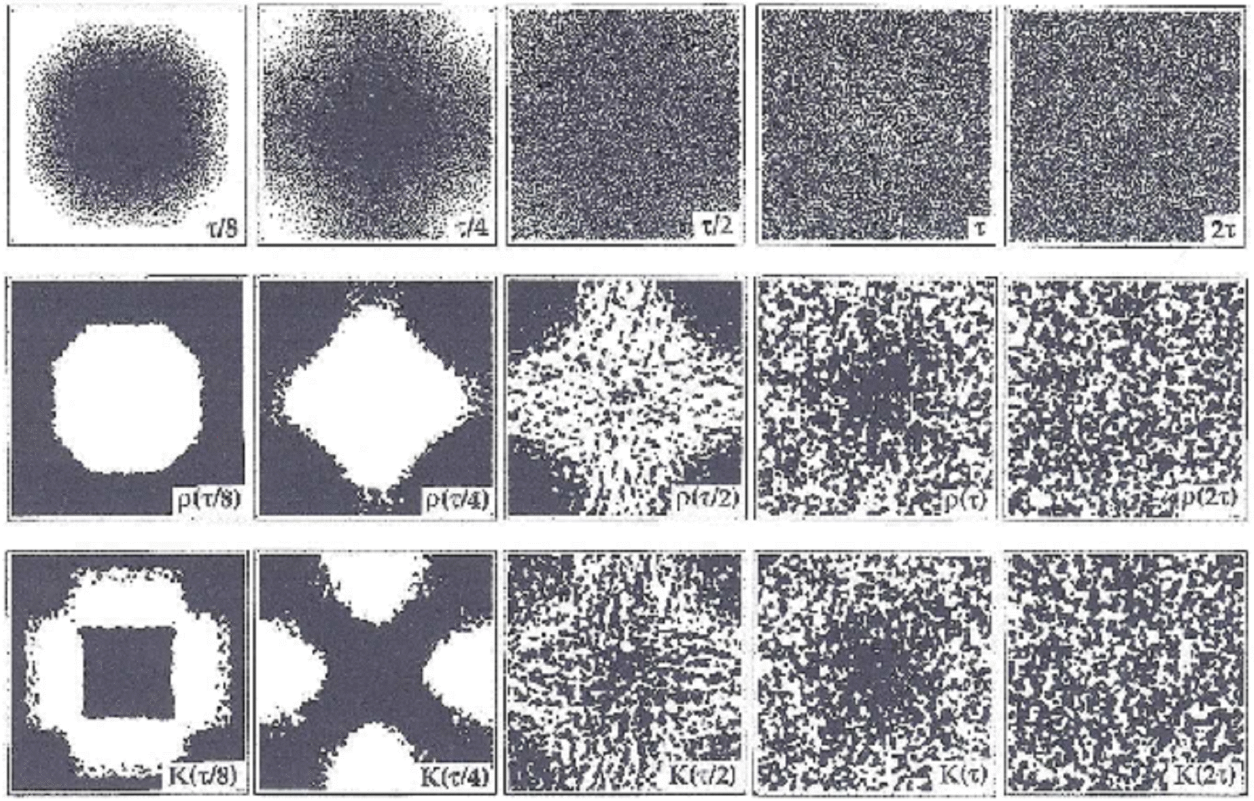
Consider the case of a gamma law fluid with $\gamma = 2$.

$$\dot{\mathbf{v}}_i = -\sum_j \mathbf{m}[(\mathbf{P}/\rho^2)_i + (\mathbf{P}/\rho^2)_j] \bullet \nabla_i \mathbf{w}_{ij} \approx$$

$$\dot{\mathbf{v}}_i \propto -\nabla_i \mathbf{w}_{ij} \; [\,\text{here SPAM is just like MD}\,]$$

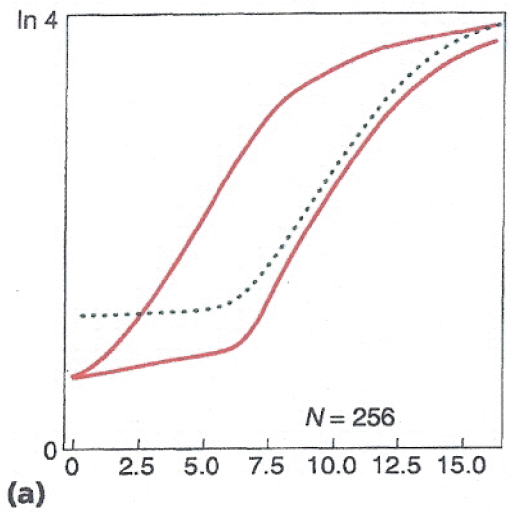
Consider a pedagogical example: Free Expansion .

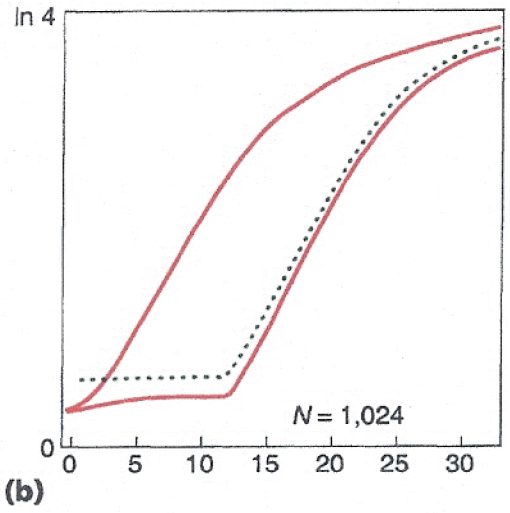
Fourfold Free Expansion Simulation : SPAM calculation of ρ and K contours .

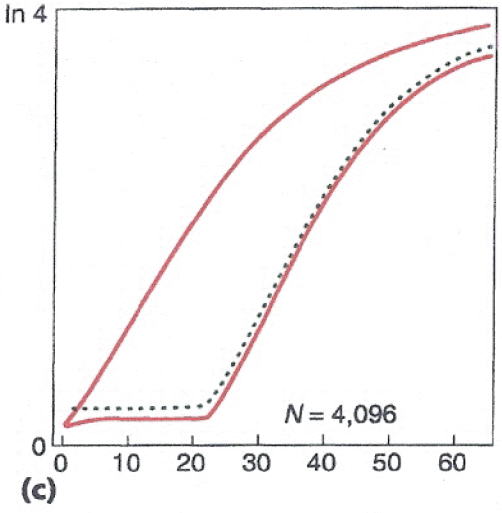


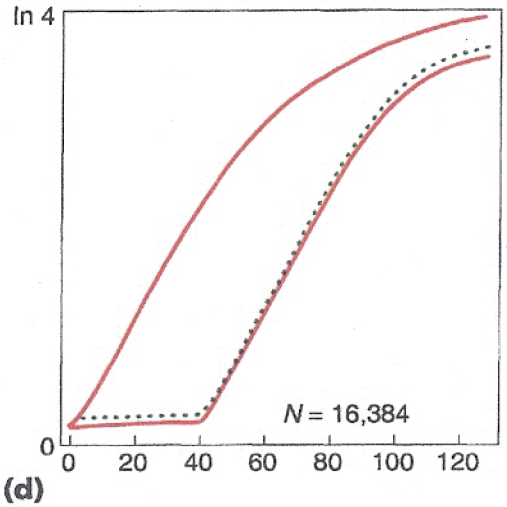
Equilibrates at the Sound Speed .

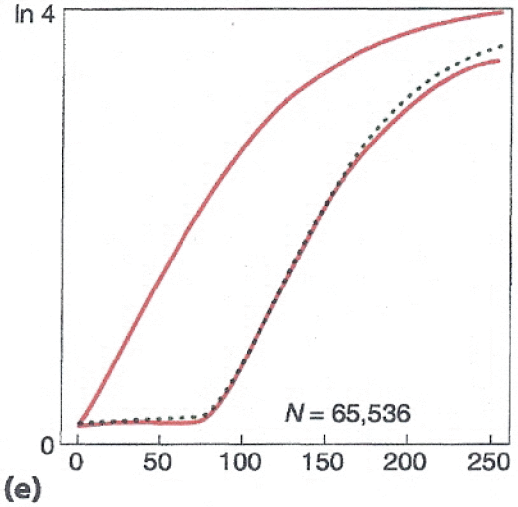
Fourfold Free Expansion Simulation : SPAM calculation of fluctuations in v .

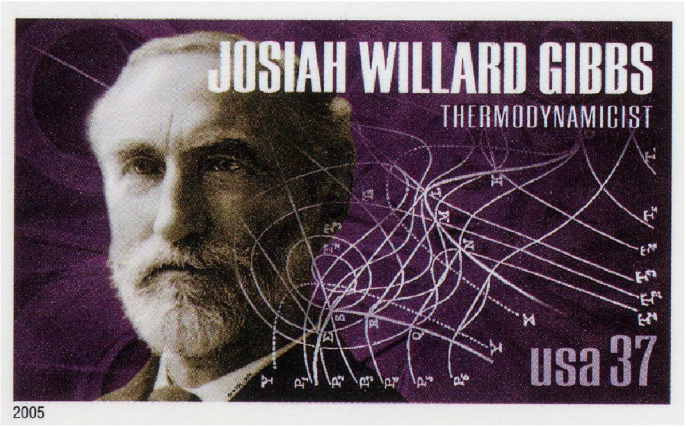




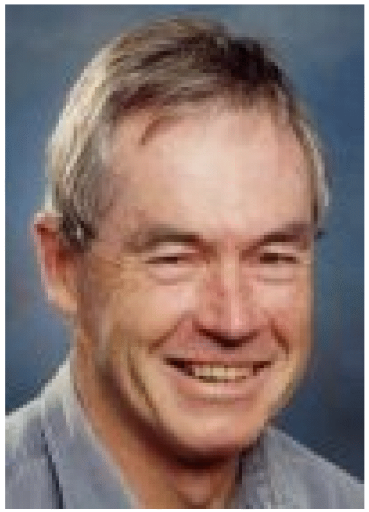


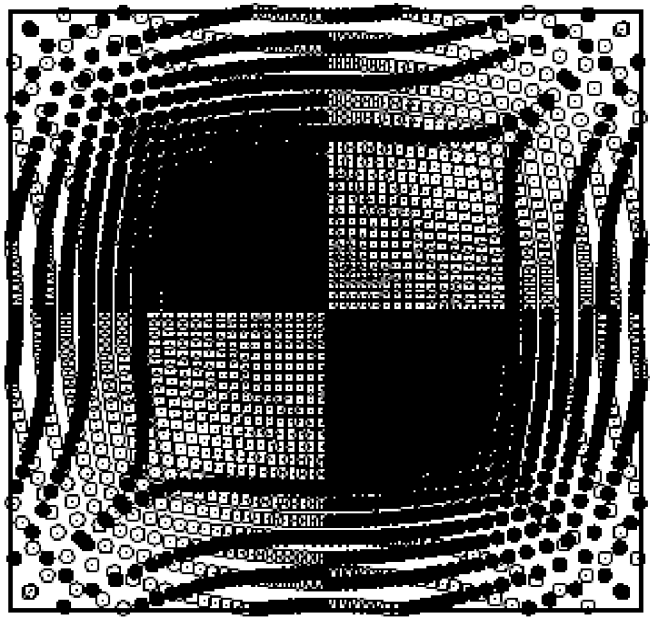


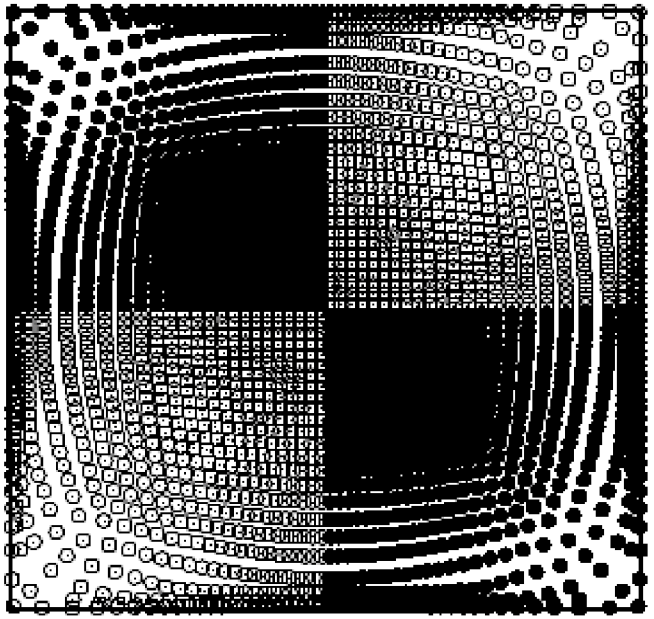




For Continuum Simulations use Monaghan's Trick to Limit Fluid-Fluid Interpenetration .



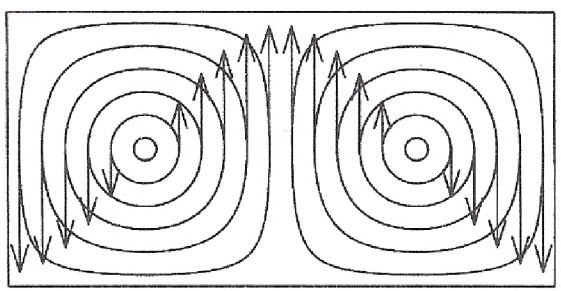


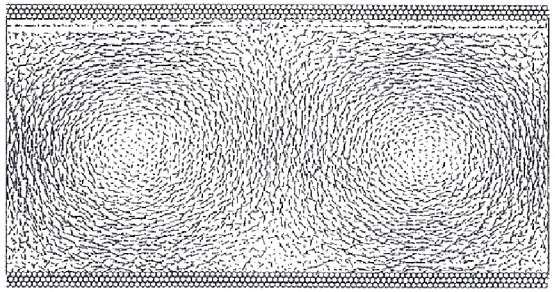


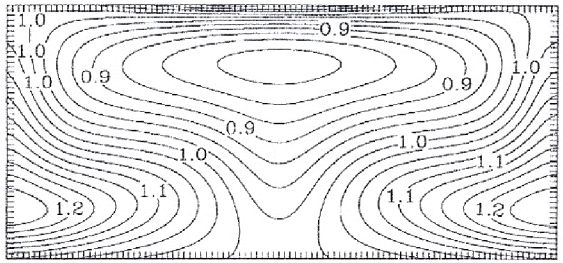
-25 < (x,y) < +25 -25 < (x,y) < +25

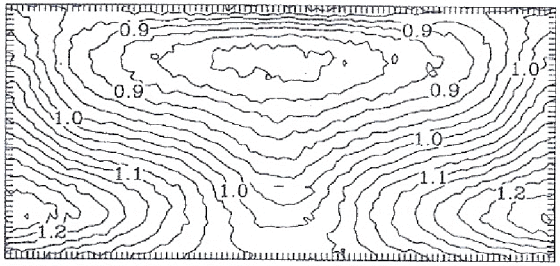
$$\{\dot{\mathbf{r}} = \mathbf{v}\} \Rightarrow \{\dot{\mathbf{r}}_i = \mathbf{v}_i + \Sigma_j \mathbf{m}(\mathbf{v}_j - \mathbf{v}_i)\mathbf{w}_{ij} / \rho_{ij}\}$$

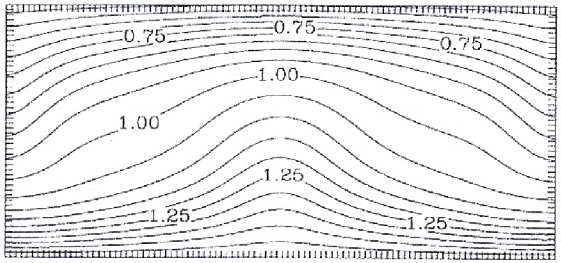
SPAM for Rayleigh-Benard Convective Instability

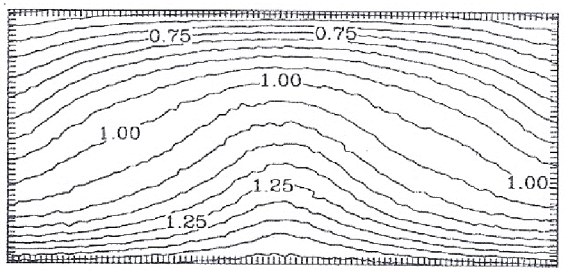










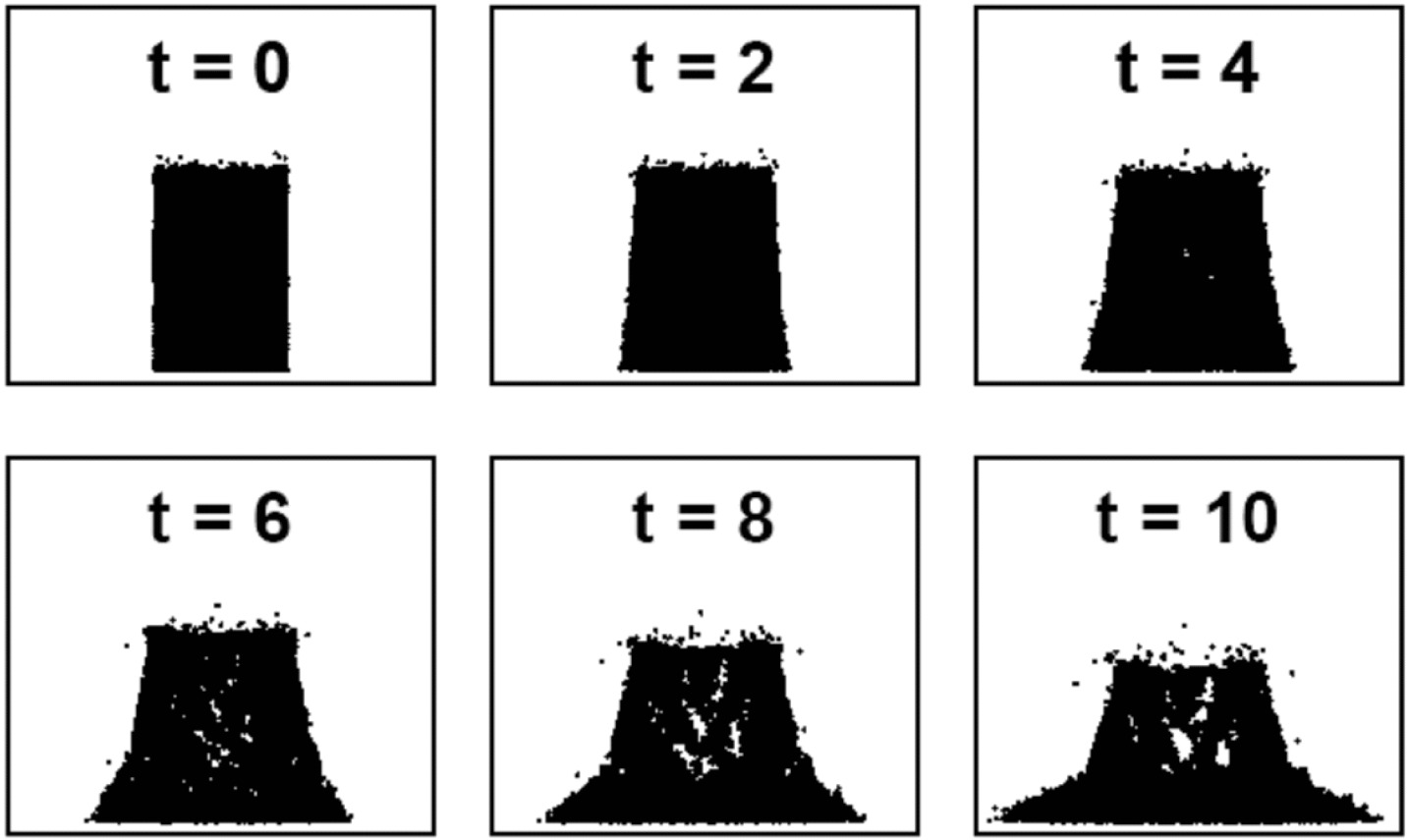


←N = 5000

0.5 < T < 1.5

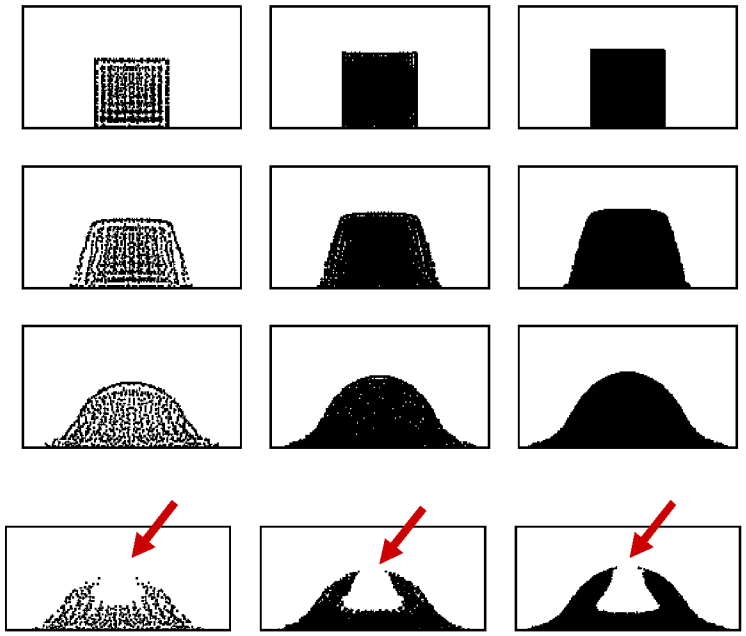
Continuum Mechanics *versus* SPAM, from Oyeon Kum's Thesis .

Column Collapse *via* Molecular Dynamics



$$\phi = (2 - r^2)^8 - 2(2 - r^2)^4 \text{ for } r^2 < 2 .$$

Column Collapse *via* SPAM with $P = \rho^3 - \rho^2$



N = 640 ;
N = 2560 ;
N = 10240 .

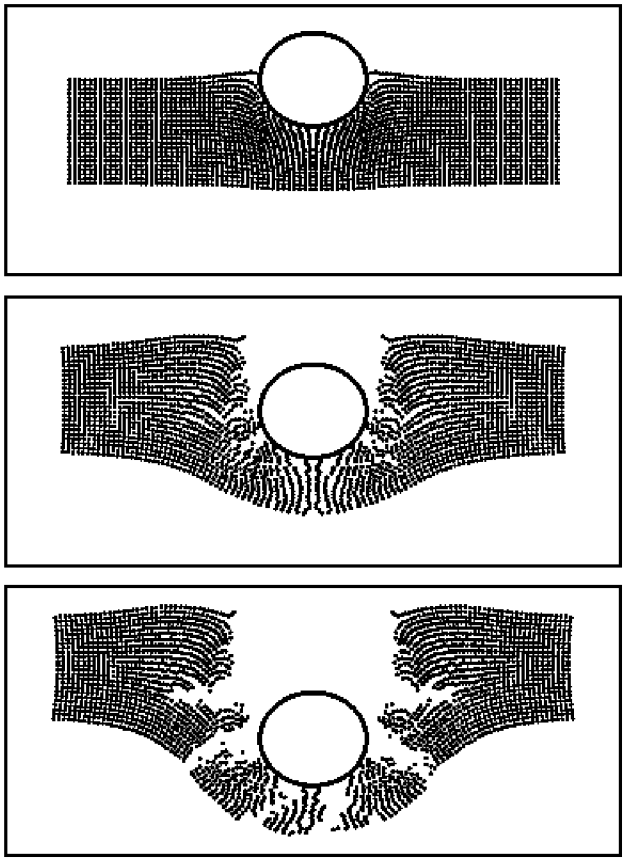
Tensile Regions

Surface potential and Core potential are both included:

$\Phi \propto (\nabla\rho)^2$ for minimizing surface .

$\Phi \propto \Sigma(\sigma^2 - r^2)^4$ for avoiding string formation .

Penetration using SPAM With Tensile Failure Model



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

$$\rho = \sqrt{4/3}\,; v = 4\,;$$

$$Y = \eta/100\,; \sigma = \eta/2\,;$$

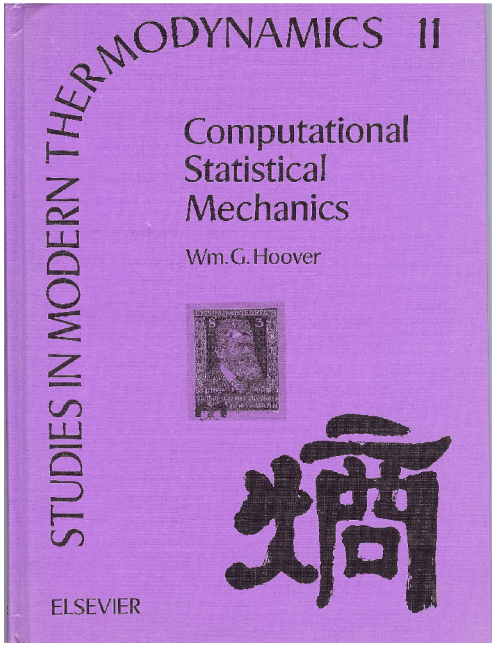
$$\eta = \lambda = \sqrt{24}.$$

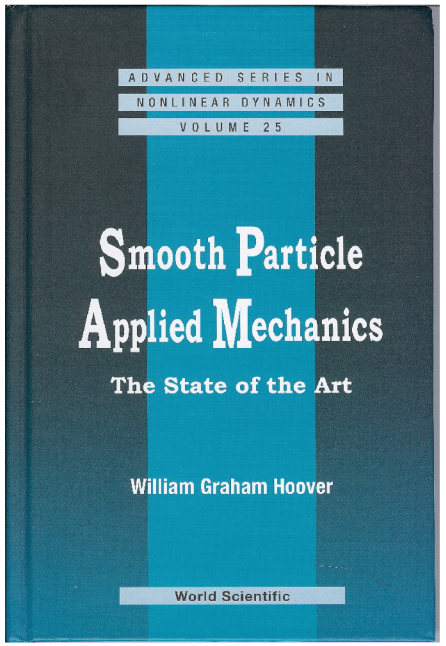
“What to do?” [Lenin]

Encourage Students to Implement Particle Methods .

Molecular Dynamics is Classical, while Real Life is not .

SPAM has a need for documented failure models .





http://williamhoover.info