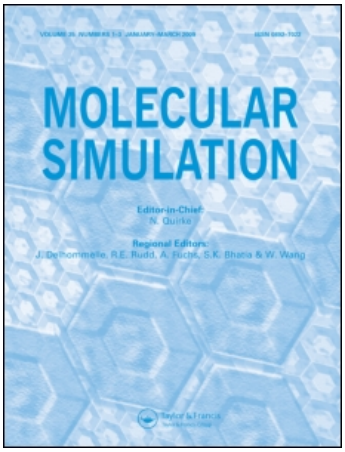

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Surface tension and strength in SPAM (smooth particle applied mechanics)

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Surface tension and strength in SPAM (smooth particle applied mechanics)

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Molecular dynamics is limited to small-size short-time situations in which the interparticle forces are known. Continuum mechanics applies at the time and distance scales relevant to men. Smooth particle applied mechanics (SPAM) is a simple, transparent, and flexible approach to solving continuum mechanics problems with particles. Here we point out cures for some of the maladies afflicting a straightforward implementation of SPAM. We present some example simulations to emphasize the intrinsic simplicity, utility, and appeal of the method.

Keywords: SPAM; Continuum methods; Surface tension; Strength

PACS numbers: 46; 68.03.Cd; 62.20.Fe; 46.50. + a; 62.20.Mk

1. What is SPAM?

Molecular dynamics is the numerical solution of the ordinary differential equations of motion for particles governed by given interparticle forces. Continuum mechanics requires solution of the partial differential conservation equations. Smooth particle applied mechanics (SPAM) is the solution of ordinary differential equations of motion for particles which model the behavior of continua governed by the partial-differential macroscopic motion equations along with appropriate constitutive relations. Though the SPAM method originated with the study of astophysical problems [1,2], recent applications have treated flows here on earth. Many examples appear in a book [3].

The basic equations to be solved are the usual macroscopic "Lagrangian" equations describing the flows of mass, momentum, and energy in a comoving frame:

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

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

where the pressure tensor P and the heat flux vector Q obey specified constitutive relations (such as Newton's description of viscous flow or Fourier's description of heat flow). The usual approach to solving these equations is to discretize the underlying continuum with a grid of simply-connected points. The grid-point values are then evolved using second-order finite-difference techniques. Smooth-particle methods simplify this task.

The physical idea behind smooth-particle methods is to imagine finite-mass particles which represent the fluid or solid material of interest. These particles have a "range" or size h. The mass density at *any* point in space (not just those points where the particles are) is defined by the summed-up contributions of all nearby particles within a distance h:

$$\rho(r) \equiv \sum m_i w(|r - r_i|) = \sum m_i w_{ri}\,;$$

$$w(r < h) = (5/\pi h^2)\left(1 - 6\frac{r^2}{h^2} + 8\frac{r^3}{h^3} - 3\frac{r^4}{h^4}\right)$$

$$\rightarrow \int_0^h 2\pi r w(r)\mathrm{d}r \equiv 1.$$

This same density definition can also be applied *at* each particle's location, giving the individual densities $\{\rho_i\}$.

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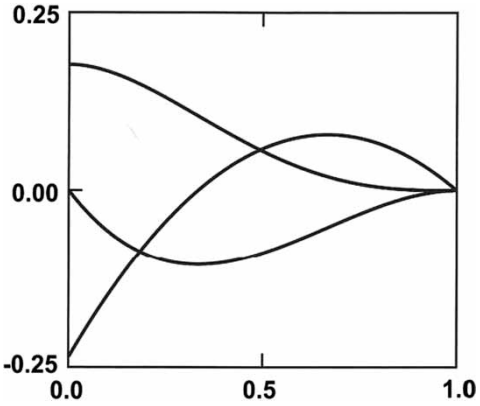

Figure 1. Lucy function and its first two derivatives.

For simplicity, we have given the "weight function" $w(r < h)$ for the two-dimensional case here. The normalizing multipliers corresponding to $(5/\pi h^2)$ would be $(5/4h)$ in one space dimension and $(105/16\pi h^3)$ in three space dimensions. This quartic weight function was introduced by Lucy in 1977 and is the one which we have used in most of our work. The weight function "looks like" a Gaussian function, but has a finite range, so that each particle interacts with only a few others (usually h is chosen so that the "few" are about 20 in number). The derivative of the weight function is a cubic spline (figure 1).

Velocity, energy, the pressure tensor, ..., can be averaged too, using the weight function as a local probability density. Local continuum values of the property $f(r)$ at a field point r are to be calculated by summing up nearby particle contributions $\{f_i\}$:

$$f(r) = \frac{\sum_i m_i f_i w_{ri}}{\sum_i m_i w_{ri}} \leftrightarrow \rho(r) f(r) = \sum_i m_i f_i w_{ri}.$$

To give an idea of the method's accuracy we show in figure 2 the summed-up densities resulting when Lucy's weight function, $w(r < h)$ is applied to regular linear, square, and simple cubic lattices of points in one, two, and three dimensions. For typical choices of h, where the number of particles contributing to the sums is about 20, the errors are less than a percent.

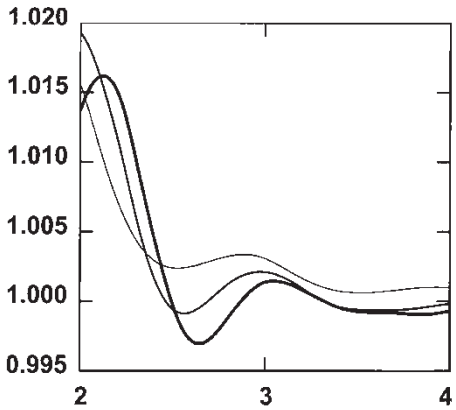

Figure 2. Densities, using Lucy's weight function, of one, two, and three dimensional lattices as functions of h. Line thickness increases with dimensionality.

Solving the continuum equations requires an ongoing evaluation of all the gradients needed for the evolution equations, $\{\nabla v, \nabla \cdot P, \nabla \cdot Q\}$. A fundamental advantage of the particle approach is the simplicity of the gradient operation in SPAM. Apply the gradient operator to the product (ρf):

$$\nabla_r(\rho f) = \nabla_r \sum_i m_i f_i w_{ri} = \sum_i m_i f_i \nabla_r w_{ri}.$$

Because the individual particle properties $\{f_i\}$ do not depend upon r the gradient operation affects only the weight functions $\{w\}$. Any of the continuum field variables can be averaged and differentiated spatially in this way. The typical choices are velocity, internal energy, pressure tensor (or stress), and the heat flux vector. Gradients of these quantities are found by making corresponding choices of the function f.

For a weight function (such as Lucy's) with two continuous derivatives everywhere the gradients defined in this way are continuous in space, so that the righthandsides of the continuum equations all have spatially continuous cubic-spline solutions with this particle method.

A detailed investigation shows that the density definition used in SPAM is exactly consistent with the continuum conservation equation (the "continuity equation"):

$$\dot\rho \equiv -\rho \nabla \cdot v \leftrightarrow (\rho v)_r \equiv \sum_i m_i v_i w_{ri}.$$

Conservation of mass is *exact* in SPAM, as should be expected for a particle method. Further, a SPAM equation of motion, based on the gradient idea just given,

$$m_i \dot v_i = -\sum_j m_i m_j \left[\left(\frac{P}{\rho^2}\right)_i + \left(\frac{P}{\rho^2}\right)_j \right] \cdot \nabla_i w_{ij},$$

can be shown to conserve (linear) momentum exactly. Likewise, a SPAM energy equation with similarly-developed heat flux and work contributions conserves energy exactly too.

The continuum equations for $\{\dot r, \dot v, \dot e\}$ reduce to a set of ordinary differential equations for the evolution of the particle coordinates, velocities, and energies. These ordinary differential equations can conveniently be solved by Runge–Kutta methods, just as are the equations of molecular dynamics. Unlike grid-based continuum methods SPAM has no underlying grid (the particles themselves are the basis for interpolation) to tangle. This frees SPAM of the usual difficulties in describing flows with large-scale deformation.

2. Isomorphisms with molecular dynamics

The similarity of the SPAM motion equations to those of molecular dynamics, is apparent for any thermodynamic internal energy function which depends only upon the

density,

$$e = e(\rho) \rightarrow P = \rho^2(\mathrm{d}e/\mathrm{d}\rho).$$

Consider, for example, the isentropic thermodynamics of a two-dimensional ideal gas:

$$e \propto \rho \rightarrow P \propto \rho^2.$$

The corresponding SPAM equations of motion give simple pair sums:

$$m_i\ddot{r}_i = m_i\dot{v}_i \propto -\sum_j m_i m_j \nabla_i w_{ij},$$

so that the weight function w plays the role of a repulsive pair potential.

A simple macroscopic equation of state, useful for either liquids or solids, furnishes a second example. Suppose that the energy varies quadratically about the stress-free density ρ_0:

$$e \propto (\rho - \rho_0)^2 \rightarrow P \propto (\rho/\rho_0)^3 - (\rho/\rho_0)^2.$$

This equation of state model gives SPAM equations of motion *identical* to those derived from a molecular dynamics particle potential Φ:

$$\Phi = \sum_i \frac{1}{2}(\rho_i - \rho_0)^2; \rho_i \equiv \sum_j m_j w_{ij}.$$

Thus, for simple constitutive relations of this kind, the motion of molecular particles and representative continuum particles are identical ("isomorphic").

3. Stability of condensed phases, liquid and solid

Continuum mechanics ordinarily ignores surface tension (justifiable as a negligible surface/volume effect). In a grid-free method like SPAM surface tension must somehow be included to encourage liquids, for instance, to assume a spherical shape in the absence of external forces. Figure 3 shows the tendency of SPAM particles to form stringlike structure when surface tension is absent. One way to incorporate surface tension in SPAM, is to add a "surface potential" sensitive to density gradients:

$$\Phi_{\mathrm{Surface}} \propto \sum_i (\nabla\rho)_i^2.$$

This idea has been applied successfully to liquid-phase simulations, controlling the formation of string structures (in two dimensions) and sheet structures (in three) [4].

Solids, in addition to maintaining stable stress-free surfaces, must also maintain their *shapes* (for stresses less than the yield stress). This need requires the stability of some solid-phase particle arrangement in SPAM. Investigation, with simple equations of state $P = P(\rho)$ shows that regular lattices are typically (but not always) unstable with the SPAM motion equations [3]. To provide shear strength a potential sensitive to the symmetry in the vicinity of a particle needs to be used. In two space dimensions the "invariant-curvature" potential is:

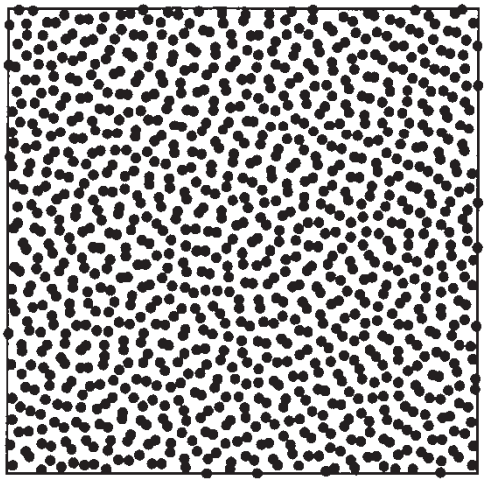

Figure 3. Relaxed periodic structure, showing string tendencies, with $h = 3.5$. Density deviations for this structure are of order 0.00001.

$$\Phi_{\mathrm{Strength}} \propto (\rho_{xx} - \rho_{yy})^2 + 4\rho_{xy}^2;$$

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

It vanishes for a regular lattice, and can stabilize such a lattice by providing a nonvanishing shear modulus.

4. Applications

To demonstrate the usefulness of the surface and strength potentials in stabilizing fluid and solid SPAM simulations we have carried out a wide range of exploratory simulations [3,4]. These only scratch the surface of an interesting and useful research area. Stabilizing material interfaces (to prevent interpenetration of colliding materials) is an allied and important research area [5].

Here we display results from two prototypical problem areas. Figures 4 and 5 show initial and evolving snapshots of a quasistatic tension test with SPAM. The strength in this simulation is provided by an elastic–plastic equation of state. Figure 6 illustrates a ball-plate penetration problems carried out with a hybrid "SPAM-like" version of molecular dynamics—the strength potential is added to the simple $\sum(\rho_i - \rho_0)^2$ potential. Figure 7 shows a more conventional finite-element simulation of a similar problem, using Dyna3D [6]. These examples illustrate

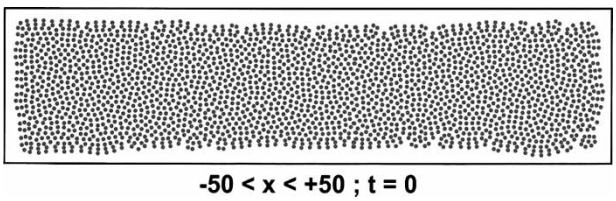

Figure 4. Relaxed initial structure for the tension test. 2304 smooth particles.

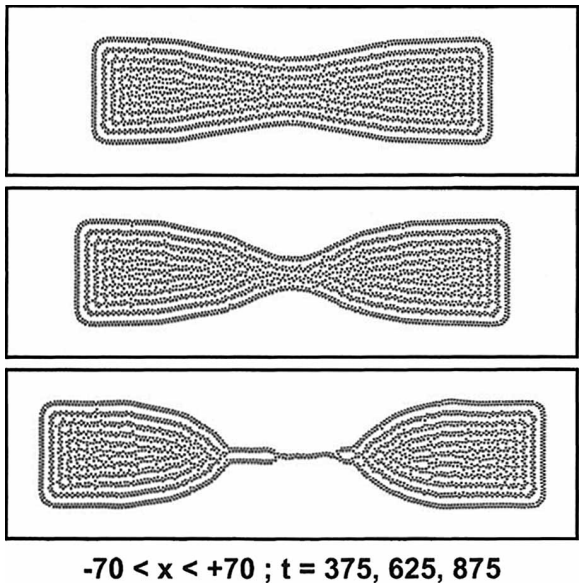

Figure 5. Tension test using SPAM together with a pair core potential discouraging particle overlaps.

prototypical flow and fracture problems, which can be solved with SPAM. Intercomparisons of simulations using different computational approaches are fertile research areas.

In a University setting it is appropriate to stress that a particular advantage of SPAM is pedagogical. Students can solve hard problems in continuum mechanics with relatively short (a few hundred lines) computer programs. Changes are easily made. Results are easily obtained. The procedure is transparent. We think that much of the future of particle methods lies in the direction of solving problems in continuum mechanics.

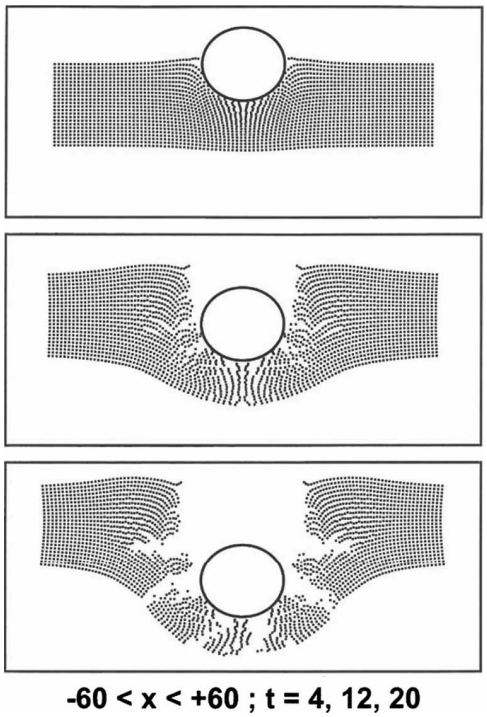

Figure 6. Ball-plate problem with SPAM. Penetration can be achieved when the ball energy exceeds the binding energy of the plate material.

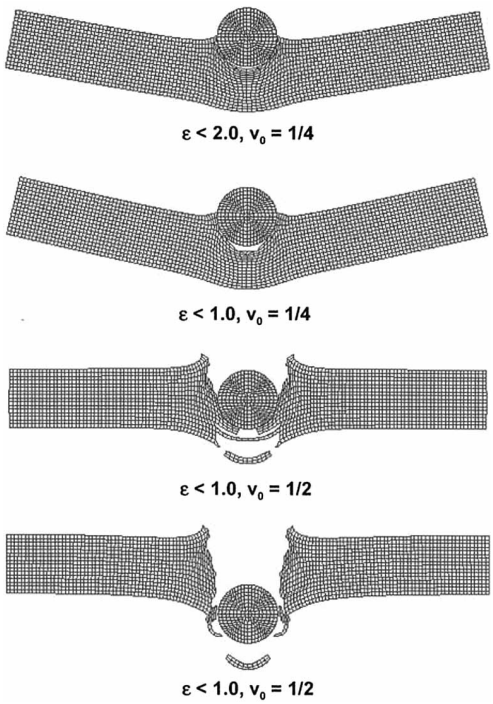

Figure 7. Ball-plate problem with the finite-element code Dyna3D. Finite elements shown here fail at a specified value of the plastic strain.

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