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SPAM-BASED RECIPES FOR CONTINUUM SIMULATIONS

By William G. Hoover and Carol G. Hoover

IN THE ABSENCE OF IMPORTANT ATOMIC-SCALE EFFECTS, MACROSCOPIC CONTINUUM MECHANICS IS THE METHOD OF CHOICE FOR SIMULATION. IN CONTINUUM MECHANICS THE DENSITY, VELOCITY, PRESSURE, AND SIMILAR FIELD VARIABLES ARE

assumed to vary continuously throughout the space-time region of interest. Undergraduate texts describe the solution of “easy” continuum problems, including the flow of heat in response to imposed thermal boundary conditions and the linear-elastic response of solids to imposed loads. A variety of grid-based approaches work very well for such problems. For more difficult problems, in which the structure under study undergoes extreme shape changes and forms new surfaces while resisting interpenetration at interfaces, more sophisticated and flexible techniques are required.

Smooth Particle Applied Mechanics is such a technique.¹⁻⁶ SPAM provides a versatile approach to simulating many difficult problems in continuum mechanics, such as the breakup of a cavitating fluid and the penetration of one solid by another. SPAM also provides a simple evaluation method for all the continuum variables, as well as the spatial gradients required by the evolution equations. This global evaluation simplifies interpolation, rezoning, and Fourier transformation. Because SPAM is so flexible and easy to program, it should be included in the toolkit of anyone doing simulations.

SPAM

The primary application of SPAM is to the solution of problems in continuum mechanics, where the governing partial differential equations describe the evolution of the mass density ρ , velocity \vec{v} , and energy per unit mass e in terms of gradients of the velocity, pressure tensor \mathbf{P} , and heat-flux vector \vec{Q} :

$$\frac{1}{\rho} \frac{d\rho}{dt} \equiv \dot{\rho} = -\nabla \cdot \vec{v} \quad (1)$$

$$\rho \frac{d\vec{v}}{dt} \equiv \rho \dot{\vec{v}} = -\nabla \cdot \mathbf{P} \quad (2)$$

$$\rho \frac{de}{dt} \equiv \rho \dot{e} = -\mathbf{P} : \nabla \vec{v} - \nabla \cdot \vec{Q} \quad (3)$$

Vectors are denoted by an arrow and tensors are in boldface. If we denote the components of a vector as A_{α} , then the components of the tensor \mathbf{AB} are

$$(\vec{A}\vec{B})_{\alpha\beta} = A_{\alpha}B_{\beta}$$

and

$$(\nabla \vec{A})_{\alpha\beta} = \partial A_{\beta} / \partial x_{\alpha}$$

In D spatial dimensions the notation $\mathbf{P} : \nabla \vec{v}$ in the energy evolution equa-

tion (Equation 3) indicates the sum of D^2 terms of the form $P_{\alpha\beta} \partial v_{\beta} / \partial x_{\alpha}$. These continuum equations are completely general, with \mathbf{P} and \vec{Q} the *co-moving* fluxes of momentum and energy—that is, fluxes measured in a frame moving with the local velocity \vec{v} . The equations apply to gases, liquids, and solids, both near to and far from equilibrium. Flows in systems as diverse as phase-separating fluid mixtures, deforming metals, breaking rocks, and colliding astrophysical bodies can all be treated with SPAM.

Although the dependent variables ρ , \vec{v} , and e are defined throughout space and for a continuously varying time, the solutions of the partial differential equations (Equations 1 through 3) can be made tractable by converting them to ordinary differential equations, spanning space with a grid of points, and computing the time histories for a closely spaced set of discrete times. A low-order Runge-Kutta method is the best choice for the time integration. Until Leon Lucy¹ and Joseph Monaghan² conceived of SPAM in 1977, spatial gradients of the field variables ρ , \vec{v} , and e were typically evaluated on an underlying spatial grid of interpolation points. (Joseph Monaghan of Monash University, Adelaide, Australia, is a prolific and creative exponent of smooth-particle methods. The reader is encouraged to seek out Monaghan’s recent work on the Internet.) Both comoving Lagrangian grids, moving with the material, and stationary Eulerian grids, fixed in space, were

used in this way. In both cases, the spatial derivatives appearing in the continuum equations were approximated as simple finite differences of field-point values at neighboring points. Although this interpolation approach works well for simple problems, it has difficulties with the chaotic irregular flows typified by mixing, penetration, fracture, and turbulence. The distortion of a comoving mesh, the difficulty of following material interfaces, the prevention of overlaps within a fixed mesh, and the smooth implementation of boundary conditions all can cause major headaches.

SPAM solves the problem of choosing a spatial grid by introducing *smooth particles*, with a finite spatial extent or width. The instantaneous coordinates of the particles define the set of points used to interpolate the field variables' values. The interpolation grid varies continuously as the particles move. This spatial interpolation method is in itself a useful algorithm for smoothing data known on an irregular set of points. To illustrate the interpolation method, consider a 2D space with a set of points (the particle coordinates), all of which have the same mass m and the same weight function $w(r)$. The particle mass density (or probability distribution) can be thought of as spread out in space according to $w(r)$ with a range b characterizing the size of the particles. The sum of all particle contributions to the mass density ρ at a point \vec{r} gives the total density (or probability). We define the mass density as

$$\rho(\vec{r}) \equiv m \sum_j w(|\vec{r} - \vec{r}_j|) \quad (4)$$

where the sum is over all particles within the range b of \vec{r} and m is the particle mass. Note that the form of Equation 4 is similar to the usual expression for the density, but with the usual delta functions replaced by a "smooth" (at least twice differentiable) weight function w . This is the reason the particles are referred to as smooth particles. For a general field variable f , the same procedure of adding all the nearby particle contributions motivates the fundamental definition for $f(\vec{r})$:

$$f(\vec{r})\rho(\vec{r}) \equiv m \sum_j f_j w(|\vec{r} - \vec{r}_j|). \quad (5)$$

At any position \vec{r} , the interpolated value of the field variable $f(\vec{r})$ is given by a weighted average of contributions f_j from nearby particles j within the range b . We emphasize that the discrete particle properties f_j , one for each particle, differ from the continuum of interpolated averages $f(\vec{r})$,

which are defined everywhere, not just at the particle positions \vec{r}_j . In particular, f_j differs from $f(\vec{r} = \vec{r}_j)$ if, as is usual, there are local fluctuations in f .

For reasonable accuracy at manageable cost, the range of the weight function w should be such that the weighted averages include contributions from about 20 particles. Lucy introduced a useful form for $w(r)$:¹

$$w(r < b) = \left(5/\pi b^2\right) \left[1 + 3(r/b)\right] \left[1 - (r/b)\right]^3 \quad (6)$$

where

$$\int_0^b 2\pi r w(r) dr = 1. \quad (7)$$

The normalization of w is chosen to make the representation exact in the limiting case of an infinite number of interpolating particles.

For r just inside the range b , the weight function in Equation 6 vanishes as the cube of the distance to the cutoff, $w(r) \propto (b - r)^3$. Thus w has two continuous derivatives everywhere. Likewise, the first and second spatial derivatives of field-variable sums such as

$$\sum_j f_j w(|\vec{r} - \vec{r}_j|) = f(\vec{r})\rho(\vec{r})$$

have no discontinuities. Such a smooth-particle interpolation method can be applied to molecular dynamics, where the individual particles have kinetic and potential energies. In this case, smooth-particle interpolation provides a twice-differentiable, continuous representation of the two-particle energy functions based on the summed contributions from discrete points. This representation is much more useful than the usual delta-function form.

Continuum equations

The SPAM representation, with two continuous derivatives for the field variables, is the key to solving the continuum equations. Consider ρ_i , the total mass density at the location of particle i . It is given by a special case of the general rule for $\rho(\vec{r})$, with $\vec{r} \rightarrow \vec{r}_i$:

$$\rho_i = \rho(\vec{r}_i) = m \sum_j w(|\vec{r}_i - \vec{r}_j|). \quad (8)$$

Note that the choice of the normalization of w guarantees that the integral over all space, $\iint \rho(x, y) dx dy$, equals the total mass mN , where N is the number of smooth particles.

Not only mass but also momentum and energy are

conserved by SPAM. The latter two conditions follow directly from the smooth-particle version of the continuum evolution equations for velocity and energy. To see this, we use the definition (Equation 5) to find the smooth-particle representation of spatial gradients:

$$\begin{aligned} & \nabla[f(\vec{r})\rho(\vec{r})] \\ &= m\nabla\sum_j f_j w(\vec{r}-\vec{r}_j) \\ &= m\sum_j f_j \nabla w(\vec{r}-\vec{r}_j). \end{aligned} \quad (9)$$

Because the f_j are particle properties rather than spatial averages, the gradient operator affects only the weight function w through its explicit dependence on \vec{r} .

By setting $f \rightarrow \mathbf{f} = (\mathbf{P}/\rho^2)$, we can show that the smooth-particle equations of motion conserve momentum exactly. We first evaluate the divergence of (\mathbf{P}/ρ) in the usual continuum way, following the rules of ordinary calculus:

$$\nabla \cdot (\mathbf{P}/\rho) = -(\mathbf{P}/\rho^2) \cdot \nabla \rho + (1/\rho) \nabla \cdot \mathbf{P}. \quad (10)$$

We can rearrange this identity to provide a useful form of the continuum equation, $\dot{\vec{v}} = -(1/\rho)\nabla \cdot \mathbf{P}$, for the evolution of \vec{v} :

$$\dot{\vec{v}} = \frac{d\vec{v}}{dt} = -(\mathbf{P}/\rho^2) \cdot \nabla \rho - \nabla \cdot (\mathbf{P}/\rho). \quad (11)$$

The two gradients on the right-hand side, $\nabla \rho$ and $\nabla \cdot (\mathbf{P}/\rho)$, can be replaced by simple sums using the smooth-particle gradient representation given in Equation 9:

$$\nabla \rho = m \sum_j \nabla w(\vec{r}-\vec{r}_j) \quad (12a)$$

and

$$\nabla \cdot (\mathbf{P}/\rho) = m \sum_j (\mathbf{P}/\rho^2)_j \cdot \nabla w(\vec{r}-\vec{r}_j). \quad (12b)$$

If we combine the two gradients and replace \vec{r} by \vec{r}_i , we find the smooth-particle form for the acceleration at the position of particle i . This form is the equation of motion for particle i :

$$\begin{aligned} \dot{\vec{v}}_i &= \frac{d\vec{v}_i}{dt} \\ &= -m \sum_j \left[(\mathbf{P}/\rho^2)_i + (\mathbf{P}/\rho^2)_j \right] \cdot \nabla_i w(\vec{r}_i - \vec{r}_j). \end{aligned} \quad (13)$$

It is important to note—as will be emphasized in the following example—that the special case of a scalar pressure P proportional to ρ^2 gives equations of motion isomorphic to those of molecular dynamics, with the weight function w playing the role of a pair potential. Whenever the quotient (\mathbf{P}/ρ^2) varies slowly in space, the smooth-particle continuum dynamics resembles ordinary molecular dynamics.

Even in the most general case of a tensor pressure, the smooth-particle equations of motion conserve momentum exactly. To see this, consider the time variation of the sum of the particle momenta,

$$\frac{d}{dt} \sum m\vec{v} = \sum m\dot{\vec{v}}.$$

Because the contributions of each interacting $\{i, j\}$ pair exactly cancel in this sum, the sum must vanish. Thus the smooth-particle equation of motion (Equation 13) conserves momentum. The reader should be able to verify, using a similar argument, that the continuum energy equations can be written in a smooth-particle form that conserves energy exactly:

$$\begin{aligned} \dot{e}_i &= \frac{de_i}{dt} \\ &= -m \sum_j \left[(\mathbf{P}/\rho^2)_i + (\mathbf{P}/\rho^2)_j \right] \cdot \frac{1}{2} (\vec{v}_j - \vec{v}_i) \nabla_i w(\vec{r}_i - \vec{r}_j) \\ &\quad - m \sum_j \left[(\bar{Q}/\rho^2)_i + (\bar{Q}/\rho^2)_j \right] \cdot \nabla_i w(\vec{r}_i - \vec{r}_j). \end{aligned} \quad (14)$$

So far we have not restricted the pressure tensor \mathbf{P} and the heat flux vector \bar{Q} in any way. They can depend upon velocity or temperature gradients, elastic or plastic strains, and the equilibrium values of density and energy. For the simple idealized Euler fluid, with vanishing viscosity and conductivity, the pressure is purely hydrostatic and is a scalar function ($P_{\alpha\beta} = P\delta_{\alpha\beta}$) of density and energy without any viscous or plastic contributions. Smooth-particle formulas for the velocity and temperature gradients needed for the pressure tensor and heat flux vector of nonideal fluids can be derived by using the gradient definition (Equation 9) in a different way. Consider, for example, $\nabla(T\rho) = \rho\nabla T + T\nabla\rho$, or

$$\rho\nabla T = \nabla(T\rho) - T\nabla\rho. \quad (15)$$

The smooth-particle representation of the two gradients in Equation 15 gives

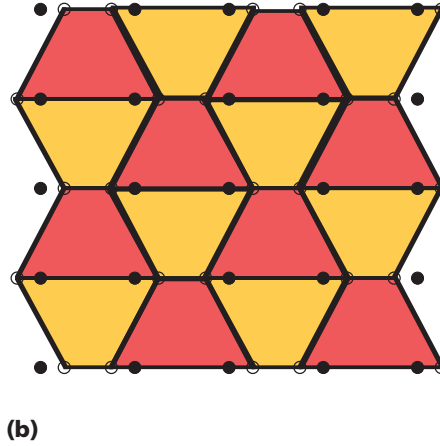
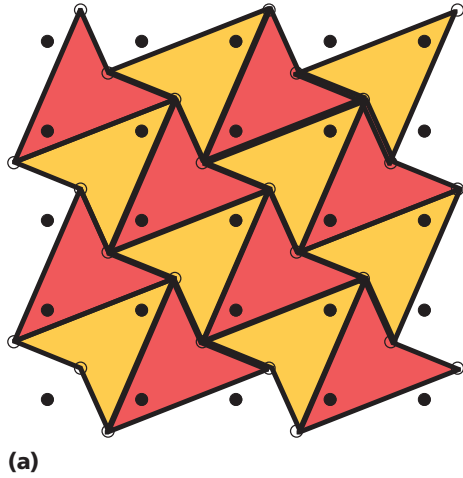


Figure 1. The (a) butterfly and (b) hourglass shear instabilities. In each of the 16 elements shown, the mean shear strain vanishes so that the corresponding deformation has no restoring force.

$$(\rho \nabla T) = m \sum_j T_j \nabla w(|\vec{r} - \vec{r}_j|) - m T_{\vec{r}} \sum_j \nabla w(|\vec{r} - \vec{r}_j|). \quad (16)$$

Equation 16 can be symmetrized by using a mean density, either arithmetic or geometric, for ρ on the left-hand side. The mean density ρ_{ij} is

$$\rho_{ij} = \frac{1}{2}(\rho_i + \rho_j) \text{ or } \rho_{ij} = \sqrt{\rho_i \rho_j}. \quad (17)$$

The corresponding expressions for the velocity and temperature gradients at the position of particle i guarantee that the gradient contributions of each pair of particles are proportional to the corresponding velocity and temperature differences:

$$\nabla \vec{v} \rightarrow (\nabla \vec{v})_i = m \sum_j [\vec{v}_j - \vec{v}_i] \nabla_i w(|\vec{r}_i - \vec{r}_j|) / \rho_{ij} \quad (18)$$

and

$$\nabla T \rightarrow (\nabla T)_i = m \sum_j [T_j - T_i] \nabla_i w(|\vec{r}_i - \vec{r}_j|) / \rho_{ij}. \quad (19)$$

Implementing the simulation

A SPAM simulation can be implemented by the following procedure:

1. Choose initial conditions: positions \vec{r}_i , velocities \vec{v}_i , and energies e_i for each particle i .
2. Compute ρ_i for each particle using Equation 8.
3. Compute the gradients $(\nabla \vec{v})_i$ and $(\nabla T)_i$ for each parti-

cle using Equations 18 and 19. These gradients are generally required for computing the particle values of \mathbf{P}_i and \bar{Q}_i .

4. Compute \mathbf{P}_i and \bar{Q}_i at each particle, using the constitutive relations, which include the equation of state $P(\rho, e)$ or $P(\rho)$ as well as the phenomenological relations governing diffusive, viscous, and conductive flows.
5. Compute \vec{v}_i and \dot{e}_i using Equations 13 and 14, including the pressure tensors and heat flux vectors computed in step 4.
6. Compute new values of \vec{r}_i , \vec{v}_i , and e_i by numerically integrating the differential equations for $d\vec{r}_i/dt = \vec{v}_i$, $d\vec{v}_i/dt$, and de_i/dt .
7. At the end of step 6, return to step 2 until the simulation is completed.

To illustrate the smooth-particle method we apply it to a relatively difficult problem, the free expansion of a 2D ideal gas, an Euler fluid with vanishing transport coefficients, into a container four times its original size.^{5,6} The equilibrium isentropic equation of state for such a gas is $P \propto \rho^2$, with the proportionality constant a function of energy only. A conventional fixed-mesh Eulerian grid approach to this problem exhibits catastrophic instabilities unless artificial damping is added. A conventional Lagrangian approach, with its mesh elements moving with the fluid, exhibits two kinds of numerical shear instabilities, the *butterfly* and the *hourglass*, as shown in Figure 1. Both instabilities can be tamed by introducing numerical viscous damping terms to control them, but the programming effort is severe. The smooth-particle method requires no unusual precautions. No catastrophic instabilities can occur, because the particle grid is continually evolving, with the field variables everywhere smooth. Because the system is not heated in any way, and there are

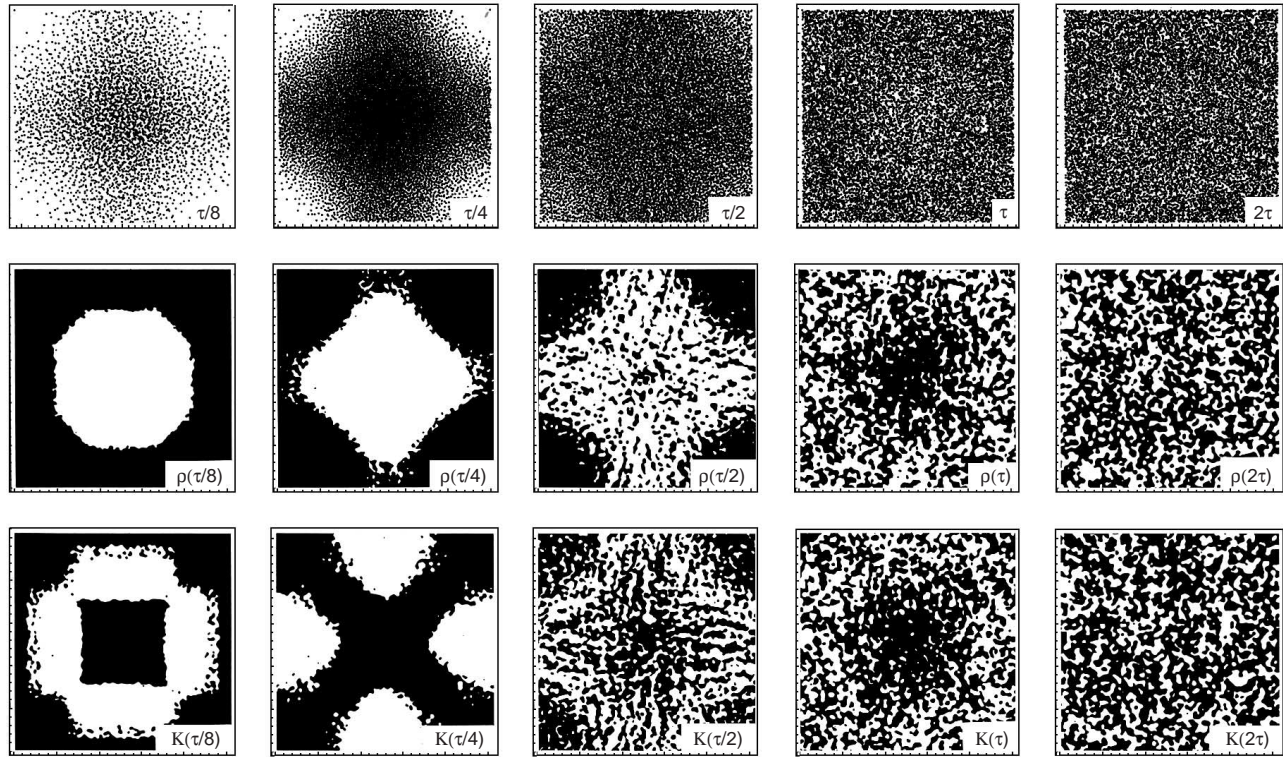


Figure 2. The top row shows snapshots of 16,384 smooth particles undergoing free expansion. The time τ is that required for a sound wave to travel across the system. The second and third rows show contours of density and kinetic energy, respectively. Above-average values are indicated by white; below-average values are indicated by black.

no transport coefficients to increase the entropy above its initial value, it is a challenge to understand the entropy increase that must result, $\Delta S = Nk \ln 4$. The resolution of this problem arises naturally from the SPAM simulations.^{5,6}

For the free-expansion problem, it is straightforward to choose the initial particle coordinates (a square grid is fine). By introducing small random offsets—equivalent to small initial random particle velocities—the square symmetry of the grid can be broken. In the simulations, we choose the smooth-particle mass and initial density both equal to unity and use the isentropic equation of state

$$P = \frac{1}{2} \rho^2.$$

With these choices the equation of motion (Equation 13) becomes

$$\dot{\vec{v}}_i = - \sum_j \nabla_i w(|\vec{r}_i - \vec{r}_j|). \quad (20)$$

Equation 20 is the smooth-particle representation of an Euler fluid with the polytropic equation of state $P \propto \rho^2$. The weight function w plays the role of a pair potential, and the

heat flux vector \vec{Q} vanishes. Thus the smooth-particle representation of a special ideal gas isentropic gives particle trajectories identical to those of molecular dynamics. The reader should be able to show that the continuity equation (Equation 1) and the energy equation (Equation 14) both lead to the same result:

$$\frac{\dot{\rho}_i}{\rho_i} = \frac{\dot{e}_i}{e_i} = \sum_j (\vec{v}_i - \vec{v}_j) \cdot \nabla_i w(|\vec{r}_i - \vec{r}_j|). \quad (21)$$

Because these two continuum equations are simultaneously satisfied by the density definition (Equation 4), we do not need to integrate the energy equation. Figure 2 shows snapshots of the particle motion during the free-expansion simulation. The underlying equations of motion have simple cubic forces derived from the weight function given in Equation 6. The range h of the weight function w was chosen to be equal to six times the initial square-lattice nearest-neighbor spacing of unity. The density contours—equivalent to internal energy contours—and the kinetic energy contours shown in Figure 2 were computed with the smooth-particle definitions. The smooth-particle approach captures velocity fluctuations in the flow, through the difference of $\langle v \rangle^2$ and $\langle v^2 \rangle$ at each point.

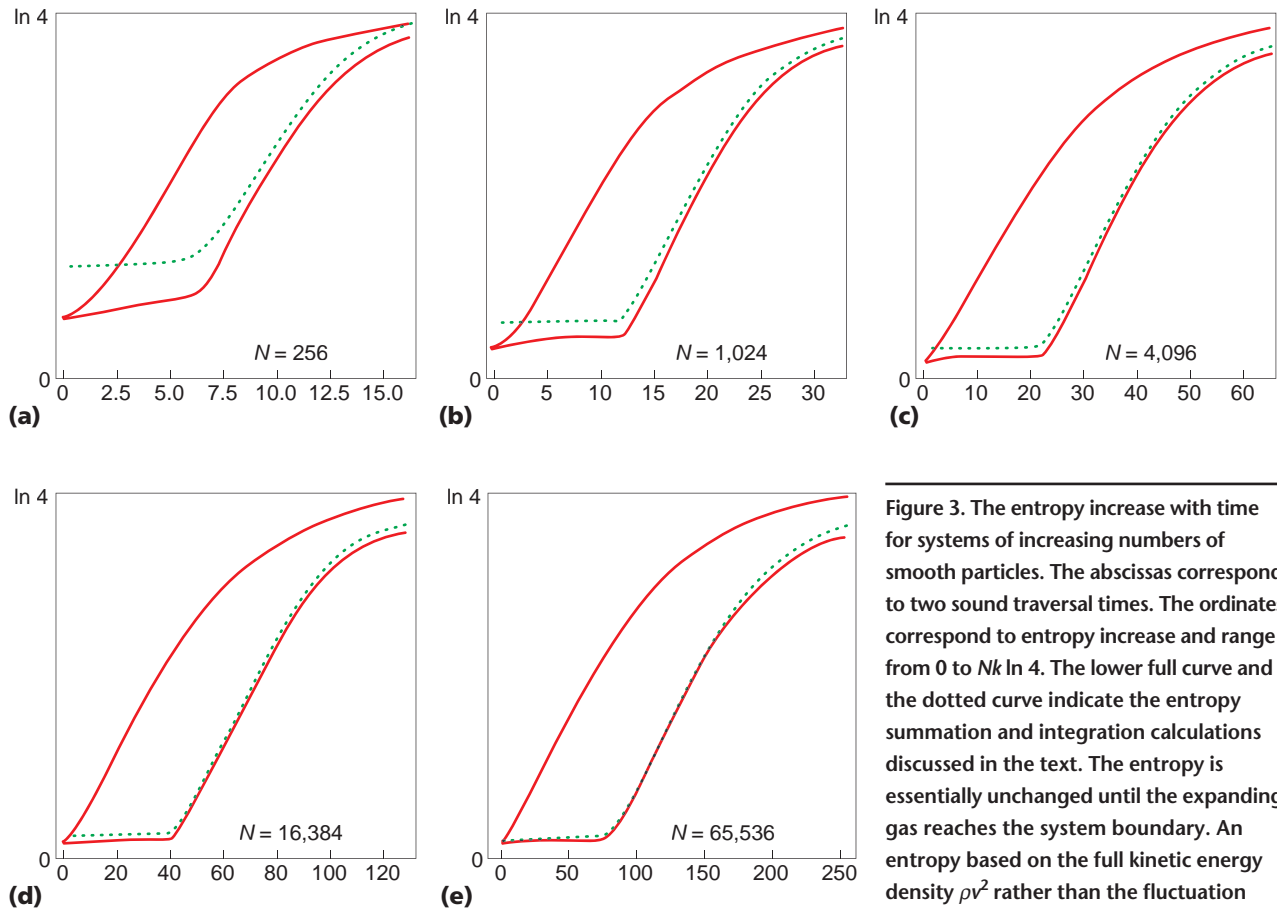


Figure 3. The entropy increase with time for systems of increasing numbers of smooth particles. The abscissas correspond to two sound traversal times. The ordinates correspond to entropy increase and range from 0 to $Nk \ln 4$. The lower full curve and the dotted curve indicate the entropy summation and integration calculations discussed in the text. The entropy is essentially unchanged until the expanding gas reaches the system boundary. An entropy based on the full kinetic energy density ρv^2 rather than the fluctuation leads to a substantial error and is shown in the upper full curve.

The velocity fluctuations are crucial to an understanding of the entropy increase in this problem. In equilibrium s , the entropy density (per unit volume) for a 2D ideal gas is equal to $-k(\rho/m) \ln(e/\rho)$, where k is Boltzmann's constant. In the nonequilibrium case considered here, the local velocity fluctuations, relative to the mean flow, must be included in the local internal energy. The smooth-particle approach gives these fluctuations—absent in the usual grid-based approaches—at every point. The nonequilibrium entropy density, including this local kinetic energy density due to fluctuations, is^{5,6}

$$s = -k(\rho/m) \ln \left[\left(e + \frac{1}{2} \langle (v - \langle v \rangle)^2 \rangle \right) / \rho \right]. \quad (22)$$

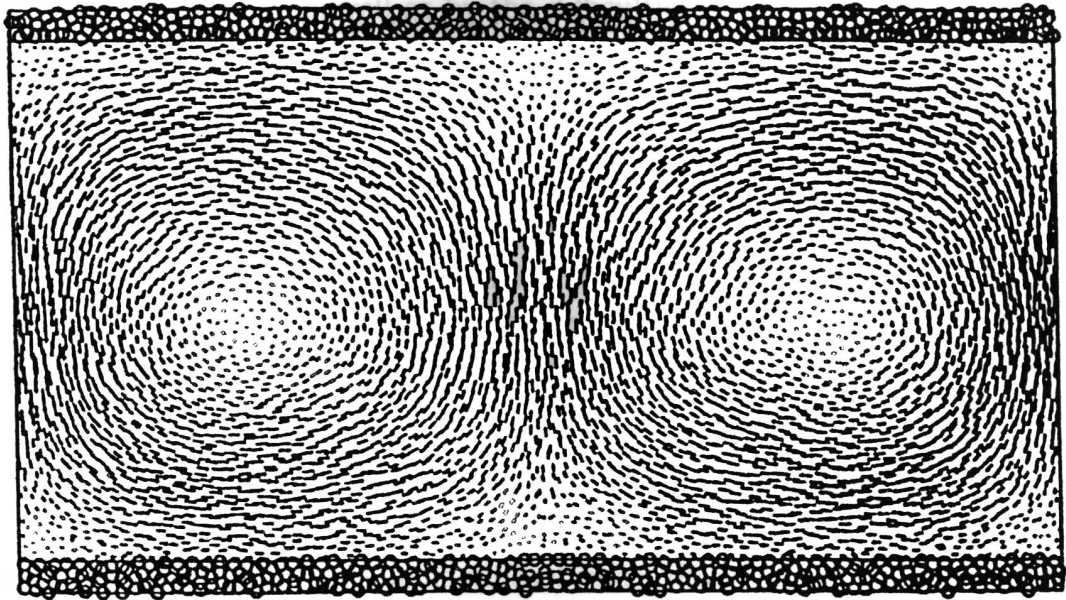
The total entropy for the smooth particles can be evaluated in either of two ways: by integrating this expression over a regular grid spanning the system, or by summing up the individual particle contributions. The two methods agree quite well (see Figure 3). In only a little more than the time required for sound to travel across the system, both the resulting integral and the corresponding sum reproduce the

expected increase of the entropy as predicted from statistical mechanics, $\Delta S = Nk \ln 4$.

The results shown in Figures 2 and 3 were computed with periodic boundary conditions. Mirror boundary conditions, applied as illustrated in Figure 4, are another possibility and lead to very similar results. With mirror boundaries, each particle near, but inside, the boundary (within the range b) produces an image particle outside the boundary, to which boundary values of velocity and energy per unit mass can be attributed. The treatment of problems in which the location of the boundary is unknown (as in the surf near a beach or the formation of a crack or tear) is a challenging research area for smooth particles. Now that parallel processing with thousands of processors is a reality, some of the difficulties in treating boundaries are being alleviated by more computer power.

Although the example discussed here involves identical particles with equal masses and the same weight function, there are circumstances that justify the extra work of a more general treatment.² It is relatively easy to use a position-dependent particle size, with b depending upon the local density. A more sophisticated treatment introduces ellip-

Figure 4. Mirror boundaries are shown at the top and bottom of this fluid convection simulation. Each bulk particle within the range h of the top or bottom boundary is mirrored by an image particle, outside the bulk system. The velocities and energies of the mirror particles are all specified by the boundary conditions that, along with gravity, drive the flow.



soidal particles, with the principal-axis lengths depending on the density gradient.

An underlying set of smooth particles makes it possible to evaluate field variables on a regular grid, not just at the particle locations. This flexibility is particularly advantageous if a rectangular mesh is required, as is the case for some graphics programs and for computing fast Fourier transforms of the field variables.

Rezoning can be accomplished easily with smooth particles. In the event that more detail is required in a particular region, a particle can be replaced by two or more smaller ones, choosing the new masses, velocities, and energies so as to conserve mass, momentum, and energy. Similarly, if a region has too many particles, two can be combined into a more massive and energetic single particle. The method can be extended in many ways to treat special situations. Chemical reactions can be introduced. Electromagnetic fields can be included by using tree techniques to evaluate the effect of long-range forces. As is usually the case, the major advances in numerical simulation methods have resulted from the desire to simulate challenging problems. \square

Acknowledgments

Work at Lawrence Livermore National Laboratory, under the Department of Energy's auspices, was supported by University of California Contract W-7405-Eng-48. Our colleagues Harald Posch (Univ. of Vienna), Vic Castillo (LLNL), and Peter Raboin (LLNL) deserve special thanks.

Suggestions for Further Study

1. In one dimension Lucy's¹ choice of the weight function, $w(x) = c[1 + 3|x/h|][1 - |x/h|]^3$, is nonzero over the interval $|x| < h$. Find the value of the normalization constant c . Use this weight function to simulate the twofold expansion problem in one dimension. The free expansion problem of a 1D ideal gas, with $p = pe = \rho^3/3$, should give an entropy increase of $Nk \ln 2$ for a twofold expansion.
2. Plot ∇w and $\nabla^2 w$ in one, two, and three dimensions, where w is given by Equation 6 in the main text. Note the similarities of the derivatives to derivatives of a Gaussian function.
3. Consider a 1D system (with equally spaced particles) and a 2D system (using a square particle grid), and find the maximum and minimum values of the density using Lucy's choice of w with 10 equally spaced choices of the range $1.5 \leq h \leq 6.0$. Note that the fluctuations in the density can be made relatively small by using modest values of the range.
4. Simulate the fourfold expansion problem using 100 smooth particles expanding from an area of 25 to an area of 100. How would the elapsed computer time vary with the number of particles? What is the maximum number of particles that could be considered with a petaflops computer (10^{15} floating-point operations per second)?

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