Smooth-particle boundary conditions

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We study the relative usefulness of static and dynamic boundary conditions as a function of system dimensionality. In one space dimension, *dynamic* boundaries, with the temperatures and velocities of external mirror-image boundary particles linked directly to temperatures and velocities of interior particles, perform qualitatively better than the simpler *static*-mirror-image boundary condition with *fixed* boundary temperatures and velocities. In one space dimension, the Euler-Maclaurin sum formula shows that heat-flux errors with dynamic temperature boundaries vary as h^{-4}, where h is the range of the smooth-particle weight function $w(r<h)$. Geometric effects (lack of a simple sum formula) frustrate a corresponding exact analysis in higher-dimensional problems. We illustrate all of these ideas here for the two-dimensional Rayleigh-Bénard flow.

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I. SMOOTH-PARTICLE SIMULATIONS

Lucy and Monaghan discovered the smooth-particle technique for solving continuum problems in 1977 [1,2]. Their idea was to compute continuum averages of particle properties according to a weight function $w(r<h)$ which is normalized (spatial integral of unity) and has a finite range h. Any continuum property $C(r)$ is an average of nearby particle values:

$$C(r)\equiv\sum C_j w(r-r_j)\Big/\sum w(r-r_j).$$

Likewise, the mass density at any point in space $\rho(r)$ is the sum of contributions from all nearby particles (particles within a distance h):

$$\rho(r)\equiv m\sum w(r-r_j),$$

where each of the particles has a mass m distributed in space according to the weight function w. These averaging ideas, applied to the *partial* differential equations of continuum mechanics, lead directly to sets of *ordinary* differential equations for the time development $\{\dot{r}=v,\dot{v},\dot{e}\}$ of all the particle coordinates, velocities, and energies $\{r,v,e\}$. The smooth-particle equations of motion,

$$\left\{\dot{v}_i=m\sum_j\left[\left(\frac{\sigma}{\rho^2}\right)_i+\left(\frac{\sigma}{\rho^2}\right)_j\right]\cdot\nabla_i w(r_{ij})\right\},$$

look very much similar to the motion equations of molecular dynamics [3,4], but involve the individual particle stress tensors $\{\sigma\}$ in place of the more usual interatomic forces. By using this approach one can solve complex continuum problems with a simple particle technique.

Many of the early applications were devoted to astrophysical problems in which boundary conditions were not important. But continuum problems involving surfaces—penetration, fracture, or heat transfer, for example—require algorithmic implementations of realistic boundary conditions. A simple problem, the formation of convective rolls due to a temperature gradient in a gravitational field (the "Rayleigh-Bénard" problem), is prototypical. Temperature and velocity have specified boundary values on a box containing the fluid under investigation. A "good" boundary algorithm is the one that minimizes the dependence of the results on the number of degrees of freedom used to describe the problem.

We noticed that a simple averaging technique could be applied to smooth-particle simulations, sometimes with relatively small errors (of the order of h^{-4}). It turned out to be possible to demonstrate this result analytically in one dimension. We explain this in the following section. Our further investigations of this idea established that boundary effects are larger, and more complicated, in two space dimensions. This Brief Report summarizes our findings.

II. HEAT TRANSFER IN ONE DIMENSION

The simplest boundary-driven problem is heat transfer between a hot and a cold reservoir. For equally spaced particles with a constant temperature gradient and a constant thermal diffusivity, the simplest versions of the corresponding smooth-particle equations are [5]

$$\left\{ \dot{T}_i \propto -\sum_j [Q_i + Q_j] \frac{dw_{ij}}{dx_i} \right\};$$

$$\left\{ Q_i \propto +\sum_j [T_i - T_j] \frac{dw_{ij}}{dx_i} \right\},$$

where T is temperature and Q is heat flux. The sums and differences on the right-hand sides of these relations guarantee two desirable properties of their solution: (i) energy is conserved exactly and (ii) the heat flux vanishes when all the particle temperatures are identical.

Provided that the range h of the weight function $w(r<h)$ is sufficiently large, a constant temperature gradient should lead to the heat flux from Fourier's law $Q = -\kappa \nabla T$. We arbitrarily choose the proportionality constants equal to unity. We further choose the particle temperatures to correspond to unit temperature gradient, $\{T(x) \equiv x\}$, so that unit thermal diffusivity should give a large-h limiting heat flux of -1. We use a nearest-neighbor particle spacing of unity in the one-dimensional problem, which sets the distance scale. With unit temperature gradient the temperatures of boundary particles "outside" the system take on integer values with $T_n = T_{n-1} + 1$. A numerical evaluation of the heat flux using the one-dimensional form of Lucy's weight function

$$w\left(\tilde{r} = \frac{r}{h} < 1\right) = \frac{5}{4h}(1-\tilde{r})^3(1+3\tilde{r}),$$

gives the results

$$Q_{h=2} = -\frac{15}{16}; \quad Q_{h=3} = -\frac{80}{81}; \quad Q_{h=4} = -\frac{255}{256}$$

for weight-function ranges of 2,3, and 4. This suggests the exact result

$$Q(h) = -1 + h^{-4}.$$

In fact, this surprisingly simple result can be derived from the Euler-Maclaurin sum formula [6], which relates the sum over particles to an integral plus Bernoulli-number corrections C_{BN} involving the derivatives of the integrand at the integration end points:

$$\sum xw' = \int_{-h}^{+h} xw'\,dx + C_{\mathrm{BN}} = -1 + h^{-4}.$$

The polynomial form of the weight function guarantees that only a finite number (exactly one in this case) of Bernoulli-number corrections to the integral contribute to the sum of heat fluxes. This very favorable convergence of the particle sum to the continuum flux suggests trying the same technique in two and three space dimensions. We studied next a two-dimensional problem, using the two-dimensional form of Lucy's weight function

$$w\left(\tilde{r} = \frac{r}{h} < 1\right) = \frac{5}{\pi h^2}(1-\tilde{r})^3(1+3\tilde{r}).$$

This Rayleigh-Bénard problem is described in the following section.

III. THE RAYLEIGH-BÉNARD PROBLEM

In our prior investigations of the Rayleigh-Bénard problem [7,8] using smooth particles we used external mirror-image particles at the system boundaries, giving each mirror particle the temperature (T_H or T_C) and velocity ($v=0$) associated with the nearby boundary. This approach leads to flow fields agreeing with accurate continuum solutions within a few percent when the number of particles used is a few thousand. This "static mirror" (with static indicating fixed values of temperature and velocity) is illustrated in the middle of Fig. 1, and is evidently an improvement over using fixed particles to form a boundary layer. The fixed-particle approach appears at the top of the figure. In two dimensions, we typically set the mass and distance scales by choosing particle masses of unity and a mass density of unity. For details, see Refs. [7,8].

Our experience with the one-dimensional heat flow of Sec. II suggested that we instead use dynamic-mirror-image temperatures and velocities which provide the correct temperature and velocity *on* the boundary:

$$(T,v)_{\mathrm{mirror}} + (T,v)_{\mathrm{interior}} \equiv 2(T,v)_{\mathrm{boundary}}.$$

These choices for the mirror properties ensure that the temperature and velocity on the boundary have their prescribed values. This choice for the temperature also implies that the heat fluxes parallel and perpendicular to the boundary satisfy the two relations

$$Q^{\parallel}_{\mathrm{mirror}} + Q^{\parallel}_{\mathrm{interior}} \equiv 0; \quad Q^{\perp}_{\mathrm{mirror}} = Q^{\perp}_{\mathrm{interior}}.$$

The dynamic mirror approach is illustrated at the bottom of Fig. 1.

In the Rayleigh-Bénard problem, convective rolls are driven by applying a temperature gradient across an enclosed system in the presence of a gravitational field. A snapshot of a smooth-particle simulation, using 5000 particles and Lucy's weight function, appears in Fig. 2. Numerical implementations of (i) static and (ii) dynamic-mirror boundary conditions do lead to significantly different results. See Fig. 3. But the difference, illustrated here for the total kinetic energy of the flow field as it approaches the steady-state value, is small with respect to the deviation from an accurate continuum simulation based on a converged square grid. See again Fig. 3 for the comparison.

We conclude that the dramatic improvement in convergence found in one dimension has no simple analog in two space dimensions. We confirmed this conclusion numerically by studying pure conductive heat flow in two space dimensions for a constant temperature gradient, using both square and triangular lattices of fixed particles, but with dynamic-mirror temperatures. Although convergence to the continuum limit occurs smoothly and stably in either case, there is no simple power law dependence of heat flux on the gradient. Oscillations (as a function of h) above and below the correct

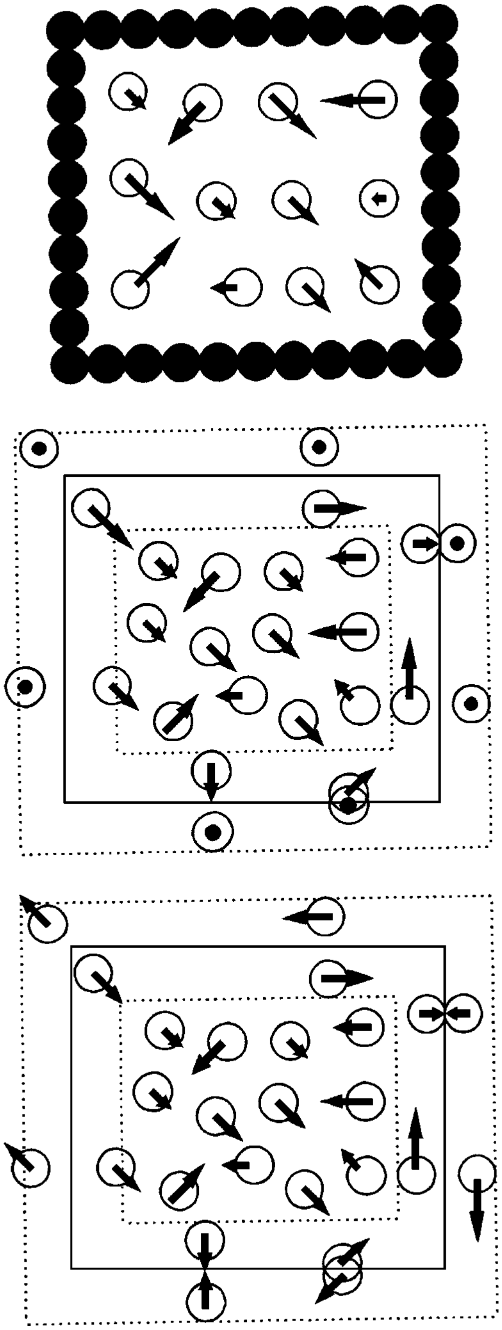

FIG. 1. Three types of smooth-particle boundary conditions. At the top the boundary particles are fixed, as are also their temperatures and velocities. In the middle static view, the moving mirror exterior particles have temperatures and velocities corresponding to fixed boundary values. In the bottom dynamic view, the moving mirror exterior particles have instantaneous temperatures and velocities, providing correct averages when combined with corresponding interior particles.

continuum result can be observed. We checked that a weight function with *three* vanishing derivatives at h,

$$w\left(\tilde{r}=\frac{r}{h}<1\right)_{2D}=\frac{7}{\pi h^2}(1-\tilde{r})^4(1+4\tilde{r}),$$

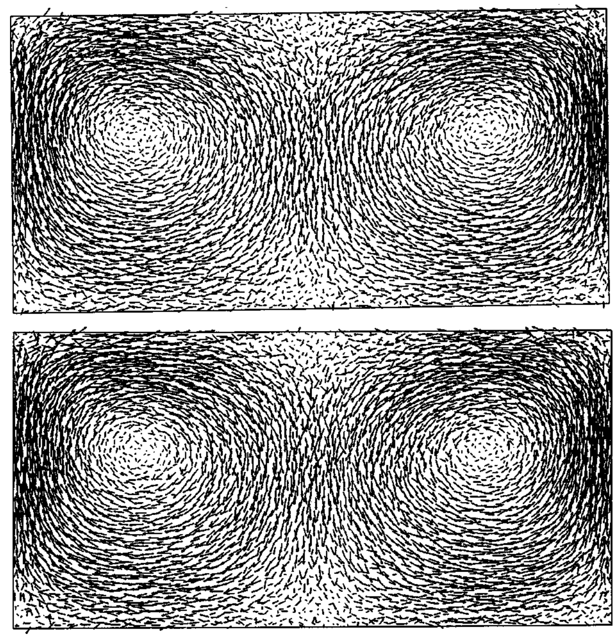

FIG. 2. The Rayleigh-Bénard flow for 5000 smooth particles. The simulation corresponds to the exterior static-boundary mirrors (above) though an illustration with exterior dynamic-boundary mirrors (below) looks almost the same. The aspect ratio of the syatem is 2. For details, see Ref. [7].

rather than just the two given by Lucy's form, made no qualitative change to these results.

IV. CONCLUSIONS

Despite the advantages of the dynamic-mirror boundaries, the deviations of fluid flow fields in two dimensions are not significantly improved over those obtained by using static-mirror boundary conditions. Our investigation of simple

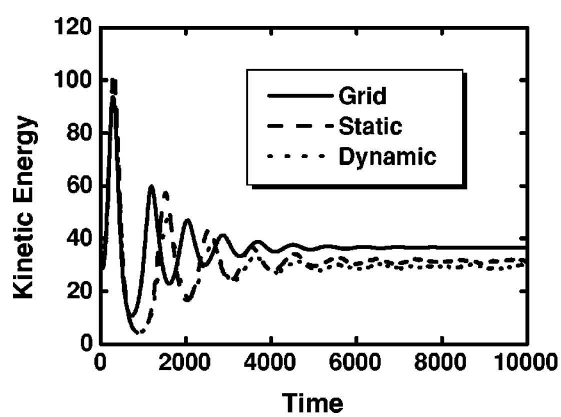

FIG. 3. Time history of the kinetic energy for a Rayleigh-Bénard flow. The solid line is an accurate grid-based solution of the continuum equations of motion. The dashed and dotted lines correspond to the exterior static-boundary mirror particles and the exterior dynamic-boundary mirror particles described in the text. Reduced units for kinetic energy and time are used, as is explained in Refs. [7,8].

heat-flow problems in two dimensions suggests that there is no analog of the simple Euler-Maclaurin sum formula responsible for the enhanced convergence of dynamic mirrors in one space dimension. More complicated mesh-dependent weight functions could conceivably improve convergence. We leave such speculation for others to investigate.

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