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Numerical heat conductivity in smooth particle applied mechanics

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Smooth particle applied mechanics provides a method for solving the basic equations of continuum mechanics, interpolating these equations onto a grid made up of moving particles. The moving particle grid gives rise to a thoroughly artificial numerical heat conductivity, analogous to the numerical viscosities associated with finite-difference schemes. We exploit an isomorphism linking the smooth-particle method to conventional molecular dynamics, and evaluate this numerical heat conductivity. We find that the corresponding thermal diffusivity is comparable in value to the numerical kinematic viscosity, and that neither is described very well by the Enskog theory. [S1063-651X(96)13511-X]

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I. INTRODUCTION

A simple numerical technique for solving the continuum equations, smooth particle applied mechanics SPAM, retains the simplicity and stability of molecular dynamics, but is applicable to macroscopic problems [1–3]. SPAM replaces the partial differential equations of continuum mechanics with simpler, but equivalent, ordinary differential equations for particle motion. The method has been successfully applied to simple thermomechanical problems in fluid mechanics, including the Rayleigh-Bénard instability of a conducting compressible fluid, heated from below in a gravitational field [4]. In the present work we stress an unusual aspect of this particle-based continuum method, a thoroughly artificial numerical heat conductivity analogous to the thermal conductivity of atomistic fluids. Though corresponding numerical viscosities are well-known in finite-difference schemes, numerical heat conductivities have not been discussed previously. These numerical transport coefficients are analogs of the eddy viscosity and eddy conductivity of simple turbulence models [5].

We begin this paper by reviewing the smooth-particle method; then we describe and apply Ashurst's simulation scheme to the measurement of this numerical heat conductivity. We study dense-fluid states with known viscosities and compare our results to the predictions of the Enskog theory [6] and turbulence models. Our conclusions appear in the final section.

II. SMOOTH PARTICLE APPLIED MECHANICS

SPAM is a particle-based interpolation scheme applicable to both fluids and solids. The continuum density, velocity, and energy at any space point are all to be evaluated by summing suitably weighted contributions from nearby moving particles. The contributions of these nearby particles to the sums are proportional to their weighting functions $\{w(r)\}$, where the $\{r\}$ are the distances between the space point and the various nearby particles.

The weighting function $w(r<h)$ is normalized; its integral over all $\mathbf{r}$ is unity. Typically w has a range h on the order of two or three interparticle spacings. The example flows we consider in the present work incorporate the simplest such weight function, Lucy's [2], with a range of 3 and at a number density of unity. Normalized in two space dimensions, the Lucy function is

$$w_{\rm Lucy}(r)=(5/\pi h^2)[1+3(r/h)][1-(r/h)]^3, \quad r<h.$$

The very smooth character of Lucy's weight function is typical of those used in smooth particle simulations. This smoothness property implies that both ∇w and $\nabla\nabla w$ are continuous, guaranteeing the continuities of the first and second spatial derivatives of interpolated continuum variables, such as $\nabla\rho$, $\nabla^2 T$, and $\nabla\cdot\boldsymbol{\sigma}$.

The continuum equation of motion, $\rho\ddot{\mathbf{r}}=\nabla\cdot\boldsymbol{\sigma}$, expresses the acceleration in terms of the divergence of the stress tensor σ. The equivalent smooth-particle form gives the accelerations of individual particles in terms of individual stress tensors and densities, weighted with gradients of the corresponding weight functions. The equation of motion for particle i, for example, includes a sum over all particles $\{j\}$ lying within the range h of particle i:

$$\ddot{\mathbf{r}}_i=m\sum[(\boldsymbol{\sigma}/\rho^2)_i+(\boldsymbol{\sigma}/\rho^2)_j]\cdot\nabla w_{ij}.$$

The simplest possible example problem using this smooth-particle equation of motion describes the flow of an ideal gas with $\boldsymbol{\sigma}\propto\rho^2$. In this case the smooth-particle accelerations, and also the resulting trajectories, are isomorphic to those of molecular dynamics, with w playing the role of a pair potential [7]. Thus the microscopic transport coefficients associated with the corresponding Lucy fluid—which can be estimated from nonequilibrium molecular dynamics, kinetic theory, or equilibrium Green-Kubo theory—must describe

the observed macroscopic diffusive flows of momentum and energy in the smooth-particle representation of the corresponding continuum flow.

The diffusive transport implicit in the Lucy-fluid molecular dynamics, since it represents a macroscopic flow without transport coefficients, describes an additional artificial flow of momentum and energy in addition to those described by the continuum constitutive equations. The extra flows are consequences of the particulate discretization of the continuum. They describe the diffusion of momentum and kinetic energy present in the smooth-particle representation, but absent in the macroscopic constitutive equations. Both types of transport are at least in part artifacts of the extra fluctuations and the discretization inherent in the smooth-particle method. Our numerical work shows that the extra transport of momentum and kinetic energy corresponds to the kinetic parts of the shear viscosity and thermal conductivity of microscopic molecular dynamics.

Momentum fluctuations are conventionally thought of as being transported by "eddy viscosity" in turbulence theories. The transport of fluid kinetic energy is likewise, but less frequently, ascribed to an "eddy conductivity" [5]. Both these phenomenological coefficients can be estimated from kinetic theory, measured by computer simulation, and compared to data taken from turbulent flows. A good understanding of the corresponding particulate transport effects is essential to evaluating the accuracy of the smooth-particle method as applied to fluid flows.

The smooth-particle shear viscosity has recently been measured, for Lucy's pair potential, in two dense-fluid states [8]. The results found depended only slightly on the number of particles and were the same order of magnitude as were guesses based on kinetic-theory arguments. Subsequent accurate evaluation of the low-density kinetic-theory shear viscosity for the Lucy potential gave an accurate interpolation between the low-temperature hard-disk limit [6] and the high-temperature weak-scattering limit [9]:

$$\eta(h)=[0.24(mkT)^{1/2}/h][1+4(kTh^2)^2].$$

In the present work we consider two different temperatures, 0.07 and 0.54, bracketing the maximum value of the Lucy potential, $5/9\pi=0.177$. At the lower of the two dense-fluid temperatures studied in the present work, the low-density kinetic-theory viscosity, 0.055, is ten times less than the measured high-density viscosity, 0.6. At the higher temperature this disagreement is substantially reduced. The two-dimensional kinetic-theory prediction [6] for the thermal conductivity, $\kappa=4\eta k/m$, suggests that the artificial transport of kinetic energy is potentially a significant source of error in smooth-particle simulations of continuum flows. We confirm this idea here by simulating corresponding heat flows, in two dimensions and using the Lucy potential, as described in the following section.

III. NONEQUILIBRIUM HEAT-FLOW SIMULATIONS

Because the Evans-Gillan [10,11] algorithm for heat conductivity seems to be unstable, at least in two dimensions [12], we used the direct method pioneered by Ashurst [13] in his dissertation. Two heat reservoirs, one hot and one cold, bound two symmetric regions filled with Lucy particles. The complete four-region system is periodic in both the horizontal and vertical directions. See Fig. 1 for a typical case with $18\times18=324$ particles in each of the four regions. The number density in all four regions is unity and the range of the Lucy potential is 3. The bulk Lucy particles obey ordinary Newtonian dynamics. The boundaries between the reservoirs and the Newtonian fluid regions are perfectly reflecting walls. Particles can interact without interference across these walls, but on reaching them undergo elastic reflection. The particles contained within the reservoir regions follow constrained equations of motion, $\{\dot{p}=F-\zeta_T p\}$, where the hot and cold friction coefficients $\{\zeta_H,\zeta_C\}$ control the reservoir temperatures through either differential [14,15] "Gaussian" or integral [16,17] "Nosé-Hoover" control. In the latter case the friction coefficient is determined by integral feedback:

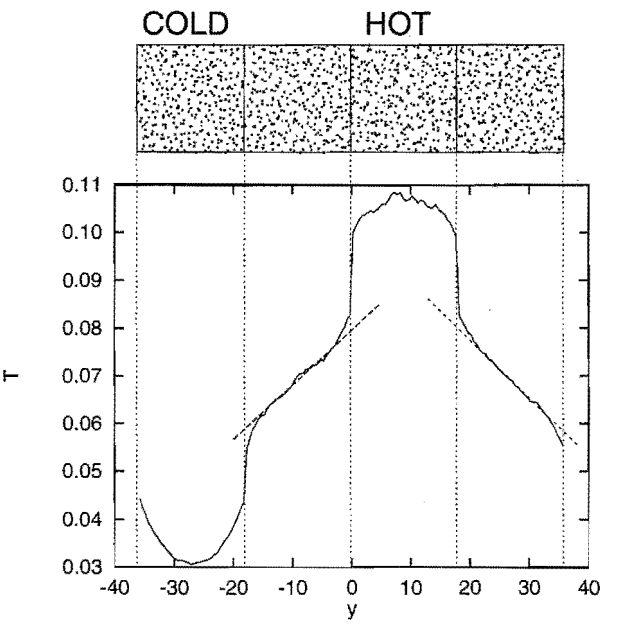

FIG. 1. Typical $4(18\times18)$ geometry for thermal conductivity simulations, with two Newtonian regions of Lucy particles confined between cold and hot reservoir regions. Each of the four regions contains $18\times18=324$ smooth particles. The range of the potential is 3. The top and bottom boundaries are periodic. The vertical boundaries contain perfectly reflecting walls. The horizontal periodic repeat length here is $4\times18=72$. A hot-to-cold temperature ratio of 3 is imposed on the two reservoir regions by Gaussian or Nosé-Hoover thermostat forces $\propto-\zeta p$.

$$\zeta_{\rm NH}=[(K/K_{eq})-1]/\tau^2.$$

We have used the basic geometry of Fig. 1, with a hot-to-cold temperature ratio of 3 and with each region made up of one or more equal squares. In the Nosé-Hoover simulations the thermostat relaxation time τ was chosen such that the combination $K_{eq}\tau^2$ was equal to unity.

To counter thermal fluctuations, relatively large temperature gradients are required in two dimensions. Even so, reducing uncertainties in the average fluxes to a few percent required simulation times of the order of millions of time steps.

TABLE I. The Enskog theory predictions for the thermal conductivity are compared to simulation results using the geometry indicated in Fig. 1. Gaussian and Nosé-Hoover thermostats are indicated by G and N, respectively. The hot-to-cold temperature ratio is 3 in all these simulations, with the mean temperature given in the table. The simulations use Runge-Kutta time steps of 0.01 so that a run length of 10 000 uses a million steps. The uncertainties in the data are of order 5–10 %.

System size	Temperature	Run length	κ	κ_{Enskog}
$4(6\times6)N$	0.07	20000	0.31	0.23
$4(9\times9)N$	0.07	50000	0.50	0.23
$4(9\times9)G$	0.07	30000	0.56	0.23
$4(18\times9)G$	0.07	16000	1.18	0.23
$4(18\times18)G$	0.07	16000	1.23	0.23
$4(27\times18)G$	0.07	30000	1.42	0.23
$4(36\times18)G$	0.07	12000	1.51	0.23
$4(6\times6)N$	0.54	10000	0.90	23
$4(9\times9)N$	0.54	40000	1.0	23
$4(12\times12)N$	0.54	20000	2.3	23
$4(9\times9)G$	0.54	50000	2.0	23
$4(18\times9)G$	0.54	32000	4.8	23
$4(27\times18)G$	0.54	13000	6.2	23
$4(36\times18)G$	0.54	12000	6.8	23

The heat conductivity can be measured in two equivalent ways: either the time-averaged heat flux within the Newtonian sections of the system or the average rate at which heat is introduced into and extracted from those regions can be combined with measured values of the Newtonian temperature gradient. The direct determination of the temperature gradient is complicated by a relatively large temperature discontinuity at the Newton-reservoir walls; see Fig. 1. In our relatively small-scale calculations, with Newtonian sections ranging from 6 to 36 particles in length, wall discontinuities contributed a substantial reduction in the measured interior temperature gradient. The reduction was typically a factor of 3 or 4. Detailed investigation of the temperature profiles, such as the typical case shown in Fig. 1, made it plain that the "bulk" region lying within the range h of the reservoirs has also a strongly nonlinear temperature profile. Accordingly, the region lying within this distance of the reservoirs was excluded in the analysis of all but our smallest-sized systems.

Despite the relatively large fluctuations present here, and characteristic of two-dimensional systems, conductivities accurate within several percent could be obtained for systems of several hundred particles. Results are shown in Table I, along with the simple kinetic-theory predictions. The numerical work confirmed that the potential contribution to the mean heat flux is negligibly small. The lower-temperature data suggest, with considerable uncertainty, an extrapolated heat conductivity of order 2, an order of magnitude larger than the Enskog prediction, but consistent with the known value of the shear viscosity, $\eta=0.6$, and a two-dimensional Prandtl number from kinetic theory, $\Pr=k\eta/(m\kappa)=0.25$. The higher-temperature data are somewhat more size dependent, but suggest an extrapolated conductivity around 8, somewhat less than the Enskog-theory prediction of 23. Despite the considerable uncertainty in the extrapolations, these crude results are sufficient for semiquantitative estimates of artificial momentum and energy flows under conditions similar to those found in real simulations.

The relatively long-range nature of the Lucy potential is responsible for the insensitivity of density, pressure, and potential energy $\Phi=\Sigma\phi_{ij}$ to temperature [8]. As a consequence, the thermal part of the pressure for the Lucy potential corresponds closely to that of the ideal gas law, $V\Delta P=Nk\Delta T$. The potential contribution to the pressure, though much greater [9] is almost temperature independent:

$$(PV)_\Phi=-(1/2)\sum \mathbf{r}_{ij}\cdot\nabla w_{ij}\doteq[N(N-1)/2V]\int w d\mathbf{r}$$

$$\equiv N(N-1)/2V.$$

Accordingly, the remaining thermal pressure of the Enskog theory, $P_{\text{thermal}}=T(\partial P/\partial T)_v$ is nearly equal to the thermal part of the Lucy pressure:

$$P_K=NkT/V\doteq T(\partial P/\partial T)_v .$$

The Enskog-theory transport coefficient is therefore nearly equal to the low-density (ideal-gas) kinetic-theory prediction:

$$\kappa_{\text{Enskog}}\doteq 4(k/m)\,\eta_{\text{Enskog}}\doteq[(k^3T/m)^{1/2}/h][1+4(kTh^2)^2].$$

In describing our numerical results we choose the volume per particle, the particle mass, and Boltzmann's constant all equal to unity. The normalization of the Lucy function also fixes the unit of energy, $(9\pi/5)w_{\text{Lucy}}(0)$. At our lower temperature of 0.07, the simulations suggested a heat conductivity several times larger than the Enskog prediction and relatively close to the Prandtl value, $\kappa=4\eta k/m$. Thus, at low temperature, corresponding to slow hydrodynamic flows, the numerical transport of kinetic energy is relatively important. At the higher temperature, 0.54, the Enskog viscosity, 6, is lower than the direct simulation value, 12. Our estimate for the high-temperature smooth-particle conductivity, 8, is substantially less than the kinetic-theory Enskog conductivity prediction, 23. See Table I.

Evidently Enskog's approximate dense-fluid theory, or equivalently, kinetic theory, though far from quantitative, produces correct order-of-magnitude estimates for the transport of momentum and heat for weak soft potentials, like Lucy's. A conclusive study of still higher temperatures would certainly require much larger, and correspondingly more expensive, studies, because the mean free path estimated from simple kinetic theory already greatly exceeds the interparticle spacing at the higher of the two temperatures studied here.

IV. SUMMARY

We find that the intrinsic numerical thermal diffusivity associated with the smooth-particle representation of a continuum is the same order of magnitude as the numerical kinematic viscosity, at both low and high temperatures. Thus both momentum and kinetic energy diffuse, artificially, at comparable rates. These two diffusion coefficients correspond, in a qualitative way, to the transport coefficients used in phenomenological turbulence models to describe the transfer of momentum and energy by turbulent eddies. The conditions studied here in our simulations correspond to those for which SPAM is a useful numerical approach to nonequilibrium flows [4,8]. In such SPAM simulations there are two different contributions to the kinetic-theory "temperature." First, particles interact with neighbors within a circle or sphere of radius h. The root-mean-square speed in such a region differs from the mean speed by terms of order $h^2\nabla^2 v$, where v is the hydrodynamic flow velocity. In addition, the SPAM particles exhibit intrinsic velocity fluctuations. Both effects need to be taken into account in order to estimate the artificial energy transport due to the numerical conductivity characterized here.

The numerical conductivity in SPAM, equal to the kinetic heat transport in the corresponding molecular dynamics simulations, is certainly not given quantitatively by the Enskog theory. The relative strengths of viscosity and conductivity are conventionally expressed as the Prandtl number, $\mathrm{Pr}=(\eta/m)(c_v/\kappa)$. For the Lucy fluid at low temperature the Prandtl number is not far from the kinetic-theory Enskog value, 0.25. At high temperature, Pr appears to be much larger, of order unity. This (two-dimensional) result is not at all inconsistent with (three-dimensional) estimates of eddy Prandtl numbers for real turbulent flows [5]. Though the simulations carried out here are based on an isomorphism strictly valid only for a special ideal gas, with $P\propto\rho^2$, it is likely that closely similar conclusions will hold in any flow simulation with pressure and density varying slowly in space.

The numerical conductivities found here fail to explain the large shockwave widths found for the Lucy fluid. In part, those paradoxical results motivated the present work. An explanation of the (two-dimensional) shockwave problem, including an understanding of the long times required for the equilibration of the longitudinal and transverse temperatures, awaits the completion of very-large-scale massively parallel shockwave simulations now undergoing development at the Livermore Laboratory.

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