Implicit SPH Drag and Dusty Gas Dynamics

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In a multiphase flow such as gas and dust, the time step for numerical integration is controlled by the Courant condition, by the drag between the fluids, and by gravity. If the dust particles are sufficiently small the time step is determined by the drag. Since the primary effect of very large drag is to keep the fluids moving together, and the details of how this is achieved are not important when the drag is very large, it is desirable to treat the drag terms implicitly. For standard grid-based methods this is straightforward, but for particle methods like SPH it appears difficult because the drag appears in the form of pair interactions between particles, and any given particle can interact with \sim 40 neighbours. The idea exploited in this paper is to treat each pair interaction separately. The velocities of the two particles involved are updated implicitly, according to their pair interaction, and the initial velocities of these particles are then replaced by the new velocities. This process is repeated for each pair interaction. Two sweeps over the particles gives satisfactory convergence. In this paper the method is tested first by keeping just the drag terms, then including pressure and drag to test wave propagation, and finally including gravity to consider the fall of a layer of gas in an isothermal atmosphere. The results are in good agreement with theory. The basic idea of working with implicit pair interactions can be extended to other SPH problems. © 1997 Academic Press

1. INTRODUCTION

Particle methods like SPH (smoothed particle hydrodynamics) have several advantages for multiphase flow. For example, in the case of a volcanic eruption, the system can be represented by several fluids each with a resolution which varies in space and time. Thus the billowing cloud of a plinean eruption can be simulated with a resolution length scale which increases as the cloud expands, while denser material falling to the ground can have at the same time a much smaller resolution scale. Appropriate equations for multiphase SPH are given by Monaghan and Kocharyan [6]. They take the form of ordinary differential equations for the motion and properties of interpolation points which can be thought of as particles. Each particle represents a fixed mass of the appropriate fluid. For example, each SPH dust particle represents a large number of real dust particles. The equations are derived from the continuum equations of fluid dynamics using a procedure for interpolation from disordered points. The interpolation depends on kernels, and the resolution depends on a characteristic length scale h which determines the range or spread of the kernel. Each particle can have a different h so that the resolution can differ in both space and time.

These SPH equations have been solved with an explicit method for which the time step is controlled by the Courant condition, the drag term, and gravity [6]. If the dust particles are sufficiently small the time step is determined by the drag. Since the primary effect of very large drag is to keep the fluids moving together and the details of how this is achieved are not important when the drag is very large, it is desirable to treat the drag terms implicitly. For standard grid-based methods this is straightforward because the dust and gas velocities are specified at each grid point. The SPH equations (see below) have a drag term which is in the form of a summation over particles. Since a given SPH particle can have \sim 40 neighbours contributing to its drag, any normal implicit scheme will have matrices which are banded with irregular bands \sim 40 elements wide. A numerical scheme based on solving these matrix equations by a direct method would be impractical.

The idea exploited in this paper is to treat each pair interaction separately. The velocities of the two particles involved is updated implicitly according to their pair interaction, and the initial velocities of these particles are then replaced by the new velocities. This process is repeated for each pair interaction. Two sweeps over the particles gives satisfactory convergence. This idea can be extended to other SPH problems. The method automatically conserves linear and angular momentum.

In the following we assume the reader is familiar with the SPH equations (for a review see [5]). For the case of dusty gas the equations of motion are given by Monaghan and Kocharyan [6], but the subset of the equations required for this paper are reproduced below.

2. EQUATIONS OF MOTION

The Continuity Equation

We start with a reduced version of the equations considered by Valentine and Wohletz [7] based on the work of Harlow and Amsden [2]. The dusty gas is approximated by two interpenetrating fluids which interact by pressure and drag terms. We assume the stress tensor of the dust fluid is negligible. Although it is not necessary, we assume for simplicity that the dust grains do not evaporate and the gas does not condense.

The continuity equations for the gas density $\hat{\rho}_g$ and the dust density $\hat{\rho}_d$ are

$$\frac{d\hat{\rho}_g}{dt} = -\hat{\rho}_g \nabla \cdot (\mathbf{v}_g) \tag{2.1}$$

and

$$\frac{d\hat{\rho}_d}{dt} = -\hat{\rho}_d \nabla \cdot (\mathbf{v}_d), \qquad (2.2)$$

where the mass densities per unit volume $\hat{\rho}$ of the dusty gas are related to actual densities ρ by

$$\hat{\rho}_i = \theta_i \rho_i. \tag{2.3}$$

Here θ is the void fraction which satisfies the condition

$$\theta_g + \theta_d = 1. \tag{2.4}$$

To simplify the SPH equations for the gas and dust *it is convenient to reserve the subscripts a and b for the gas and j and k for the dust SPH particles.* The continuity equations then become

$$\frac{d\hat{\rho}_a}{dt} = \sum_b m_b \mathbf{v}_{ab} \cdot \nabla_a W_{ab}$$
(2.5)

for the gas SPH particles and

$$\frac{d\hat{\rho}_j}{dt} = \sum_k m_k \mathbf{v}_{jk} \cdot \nabla_j W_{jk}$$
(2.6)

for the dust SPH particles. In these equations m_j denotes the mass of SPH particle j, with velocity \mathbf{v}_j at position \mathbf{r}_j . The kernel W_{ab} depends on the distance between the particles. Its typical form is similar to a gaussian though here we use the spline-based kernel (for a description of various kernels, see [5]). We use the notation for any vector \mathbf{q} that

$$\mathbf{q}_{aj} = \mathbf{q}_a - \mathbf{q}_j, \tag{2.7}$$

and since we use spherically symmetric kernels we can write

$$\nabla_a W_{aj} = \mathbf{r}_{aj} F_{aj}, \tag{2.8}$$

where F_{aj} is an even function which is ≤ 0 .

Once ρ_j has been found, θ_j can be calculated from (2.3) since ρ_j is constant. θ_a is calculated from the relation (2.4) in the form

$$\theta_a = 1 - \sum_j \frac{m_j}{\hat{\rho}_j} \theta_j W_{aj}, \qquad (2.9)$$

where the summation gives θ_d at the position of gas particle *a*. We can write (2.9) as

$$\theta_a = 1 - \frac{1}{\rho_d} \sum_j m_j W_{aj}, \qquad (2.10)$$

so that, recalling ρ_d is constant,

$$\frac{d\theta_a}{dt} = -\frac{1}{\rho_d} \sum_j m_j \mathbf{v}_{aj} \cdot \mathbf{r}_{aj} F_{aj}.$$
(2.11)

In the tests we use (2.11) rather than (2.10).

The Acceleration Equations

In the absence of viscous effects the acceleration equations for gas and dust are

$$\frac{d\mathbf{v}_g}{dt} = -\frac{\nabla P}{\rho_g} - \frac{K}{\hat{\rho}_g} (\mathbf{v}_g - \mathbf{v}_d) + \tilde{\mathbf{g}}$$
(2.12)

and

$$\frac{d\mathbf{v}_d}{dt} = -\frac{\nabla P}{\rho_d} - \frac{K}{\hat{\rho}_d} (\mathbf{v}_d - \mathbf{v}_g) + \tilde{\mathbf{g}}, \qquad (2.13)$$

where \tilde{g} is the gravitational acceleration. The drag factor K depends on the gas density, the dust θ , and the geometry of the dust grains [7, 4]. For example the drag used by Valentine and Wohletz [7] is

$$K = \frac{\rho_g \theta_d C_D}{r_d} |\mathbf{v}_g - \mathbf{v}_d|, \qquad (2.14)$$

where r_d is the radius of a dust grain (assumed spherical) and C_D depends, in general, on the local Reynolds number calculated from the relative velocity of the grains and the gas and the size of the grains (see [4] for more elaborate drag coefficients).

In order to construct SPH equations which conserve linear and angular momentum it is necessary to write the pressure term in (2.5) in the form

$$\frac{\nabla P}{\rho_d} = \nabla \left(\frac{P\theta_g}{\hat{\rho}_g} \right) + \frac{P\theta_g}{\hat{\rho}_g} \nabla \hat{\rho}_g - \frac{P}{\hat{\rho}} \nabla \theta_g.$$
(2.15)

A simple form for the drag term can be obtained by smoothing with the kernel according to the following integral interpolant

$$K(\mathbf{r})(\mathbf{v}_{g}(\mathbf{r}) - \mathbf{v}_{d}(\mathbf{r})) = \sigma \int K(\mathbf{r}, \mathbf{r}') \left(\frac{\Delta \mathbf{v}' \cdot \Delta \mathbf{r}'}{(\Delta \mathbf{r}')^{2} + \eta^{2}}\right) \Delta \mathbf{r}' \ W(|\mathbf{r} - \mathbf{r}'|) \ \mathbf{d}\mathbf{r}', \quad (2.16)$$

where

 $\Delta \mathbf{v}' = \mathbf{v}_g(\mathbf{r}) - \mathbf{v}_d(\mathbf{r}')$

and

 $\Delta \mathbf{r}' = \mathbf{r} - \mathbf{r}'.$

 η^2 is a clipping constant $\sim 0.001h^2$ which prevents singularities when a gas and a dust particle coincide, and σ is a constant equal to the number of dimensions. The reader familiar with SPH will recognize the integrand of (2.10) as being similar to the term used in the gas viscosity.

The SPH approximation to (2.16) for a gas particle is obtained by replacing the integral by a sum over dust particles. We find

$$\sigma \sum_{j} m_{j} \frac{K_{aj}}{\hat{\rho}_{j}} \left(\frac{\mathbf{v}_{aj} \cdot \mathbf{r}_{aj}}{\mathbf{r}_{ja}^{2} + \eta^{2}} \right) \mathbf{r}_{aj} W_{ja}.$$
(2.17)

If the particles *a* and *j* are approaching $\mathbf{v}_{aj} \cdot \mathbf{r}_{aj} < 0$, and if they are receding, $\mathbf{v}_{aj} \cdot \mathbf{r}_{aj} > 0$. The drag term on approaching particles then acts like a repulsive force and if they are receding it acts like an attractive force. The drag term between any two particles is along their line of centres so the conservation of linear and angular momentum is guaranteed.

The drag coefficient K depends on the gas SPH particle and on the dust SPH particle because it depends on the properties of the gas and dust.

The momentum equation for the gas particle *a* can be written immediately from (2.12), (2.15), and (2.14) using the SPH rules. When doing so we replace $\nabla \theta_g$ by $-\nabla \theta_d$ and estimate this gradient by using a summation over the dust particles. The acceleration of particle *a* is then given by

$$\frac{d\mathbf{v}_{a}}{dt} = -\sum_{b} m_{b} \left(\frac{P_{a}\theta_{a}}{\hat{\rho}_{a}^{2}} + \frac{P_{b}\theta_{b}}{\hat{\rho}_{b}^{2}} + \Pi_{ab} \right) \mathbf{r}_{ab} F_{ab}$$

$$-\sum_{j} m_{j} \frac{P_{a}\theta_{j}}{\hat{\rho}_{a}\hat{\rho}_{j}} \mathbf{r}_{aj} F_{aj}$$

$$-\sigma \sum_{j} m_{j} \frac{K_{aj}}{\hat{\rho}_{a}\hat{\rho}_{j}} \left(\frac{\mathbf{v}_{aj} \cdot \mathbf{r}_{aj}}{\mathbf{r}_{ja}^{2} + \eta^{2}} \right) \mathbf{r}_{aj} W_{ja} + \tilde{\mathbf{g}}_{a}.$$
(2.18)

The momentum equation for the dust particles can be written

$$\frac{d\mathbf{v}_{j}}{dt} = -\theta_{j} \sum_{a} m_{a} \frac{P_{a}}{\hat{\rho}_{j} \hat{\rho}_{a}} \mathbf{r}_{ja} F_{ja}
- \sigma \sum_{a} m_{a} \frac{K_{aj}}{\hat{\rho}_{a} \hat{\rho}_{j}} \left(\frac{\mathbf{v}_{aj} \cdot \mathbf{r}_{aj}}{\mathbf{r}_{ja}^{2} + \eta^{2}} \right) \mathbf{r}_{ja} W_{ja} + \tilde{\mathbf{g}}_{j},$$
(2.19)

where the drag term for the SPH dust particle has been estimated by a summation over the SPH gas particles.

It is easy to show that the momentum equations conserve linear and angular momentum exactly when the kernel W_{ab} is a function of $|\mathbf{r}_{ab}|$.

3. IMPLICIT DRAG

In this section we consider the acceleration produced by pure drag and we assume that all quantities other than the velocity are constant. The acceleration equation for gas particle a is then

$$\frac{d\mathbf{v}_a}{dt} = -\sum_j m_j s_{aj} (\mathbf{v}_{aj} \cdot \mathbf{r}_{aj}) \mathbf{r}_{aj}, \qquad (3.1)$$

and for dust particle *j* the acceleration is given by

$$\frac{d\mathbf{v}_j}{dt} = -\sum_a m_a s_{aj} (\mathbf{v}_{aj} \cdot \mathbf{r}_{aj}) \mathbf{r}_{ja}, \qquad (3.2)$$

where

$$s_{aj} = \sigma \frac{K_{aj}}{\hat{\rho}_a \hat{\rho}_j} \left(\frac{W_{aj}}{\mathbf{r}_{aj}^2 + \eta^2} \right).$$
(3.3)

We now consider the implicit integration of (3.1) and (3.2). For simplicity we begin with a backward Euler (BE) method in which \mathbf{v}_a^0 denotes the initial value of the velocity of particle *a* and \mathbf{v}_a^1 denotes the new value. The time step is δt . The discrete form of (3.1) is then

$$\mathbf{v}_a^1 = \mathbf{v}_a^0 - \delta t \sum_j m_j s_{aj} (\mathbf{v}_{aj}^1 \cdot \mathbf{r}_{aj}) \mathbf{r}_{aj}, \qquad (3.3)$$

and the discrete form of (3.2) is

$$\mathbf{v}_j^1 = \mathbf{v}_j^0 - \delta t \sum_a m_a s_{aj} (\mathbf{v}_{aj}^1 \cdot \mathbf{r}_{aj}) \mathbf{r}_{ja}.$$
(3.4)

To solve (3.3) and (3.4) directly would require an expensive inversion of matrices. We achieve the same result by an iterative technique which conserves linear and angular momentum. The idea is to consider one dust–gas particle pair at a time. With this in mind we consider the contribution from a gas and dust pair *a* and *j*. In the following \mathbf{v}^0 will denote the current value of \mathbf{v} rather than the value at the beginning of the time step. The new velocity of particle *a* due to the interaction with particle *j* is

$$\mathbf{v}_a^1 = \mathbf{v}_a^0 - \delta t \, \mathbf{r}_{aj} m_j s_{aj} (\mathbf{v}_{aj}^1 \cdot \mathbf{r}_{aj}), \tag{3.5}$$

and the increment to the velocity of dust SPH particle *j* is

$$\mathbf{v}_j^1 = \mathbf{v}_j^0 - \delta t \, \mathbf{r}_{ja} m_a s_{aj} (\mathbf{v}_{aj}^1 \cdot \mathbf{r}_{aj}). \tag{3.6}$$

These two equations can be solved by subtracting (3.6) from (3.5) and then taking the vector dot product with \mathbf{r}_{aj} . We find

$$\mathbf{v}_{aj}^1 \cdot \mathbf{r}_{aj} = \frac{\mathbf{v}_{aj}^0 \cdot \mathbf{r}_{aj}}{1 + \delta t (m_a + m_j) s_{ja} r_{aj}^2}.$$
(3.7)

On substituting (3.7) into (3.5) we find

$$\mathbf{v}_a^1 = \mathbf{v}_a^0 - \frac{\delta t \, \mathbf{r}_{aj} m_j s_{aj} (\mathbf{v}_{aj}^0 \cdot \mathbf{r}_{aj})}{1 + \delta t (m_a + m_j) s_{ja} r_{aj}^2},\tag{3.8}$$

and the corresponding expression for the dust particle is

$$\mathbf{v}_{j}^{1} = \mathbf{v}_{j}^{0} - \frac{\delta t \, \mathbf{r}_{ja} m_{a} s_{aj} (\mathbf{v}_{aj}^{0} \cdot \mathbf{r}_{aj})}{1 + \delta t (m_{a} + m_{j}) s_{ja} r_{aj}^{2}}.$$
(3.9)

This process conserves linear and angular momentum because the interaction is along the line of centres. When the motion is along the line of centres, or is one-dimensional, and the drag is infinite, the new velocities of a and j are both equal to

$$\frac{m_j \mathbf{v}_j^0 + m_a \mathbf{v}_a^0}{m_j + m_a},\tag{3.10}$$

which is the centre of mass velocity of the pair.

We then replace \mathbf{v}_j^0 by \mathbf{v}_j^1 and \mathbf{v}_a^0 by \mathbf{v}_a^1 and repeat the process for the next pair. It may, for example, be gas particle *a* with a different neighbouring dust particle.

One sweep over all the particles does not give satisfactory convergence when the drag term is very large. Direct analytical calculation of the velocity with alternate and equi-spaced gas and dust particles shows that, after two sweeps with infinite drag, the velocity difference between the dust and gas fluids is reduced by a factor close to 10. This is sufficiently rapid convergence to the state of zero velocity difference. The tests considered below confirm that two sweeps give satisfactory convergence for all cases considered. If *n* sweeps are used the time step in each sweep should be replaced by $\delta t/n$.

In general s_{aj} varies with the physical properties associated with the gas and dust particles and with the magnitude of the velocity difference of the gas and dust. The simplest way to take account of this variation is to evaluate s_{aj} by prediction of the density and void fractions to the midpoint and to use the initial values for the velocity differences in the drag coefficient. These initial values change as each new particle pair is taken into account.

4. MORE ACCURATE TIME STEPPING

The BE scheme is simple and robust but it would be preferable to use a more accurate method. In this section we describe a two-stage method (Peter Tischer, private communication) which has an error which is a factor 50 smaller than the BE scheme.

For a single equation of the form

$$\frac{dy}{dt} = f,\tag{4.1}$$

we denote the current value of y by y^0 , the intermediate value by \tilde{y} , and the final value by y^1 with the same notation for the function f. The time step is δt . The two stages use half-time steps. We denote the half-time step by Δ . The two-stage scheme takes the form of two implicit steps

$$\tilde{y} = y^0 + \Delta(0.6\tilde{f} + 0.4f^0)$$
(4.2)

and then

$$y^{1} = 1.4\tilde{y} - 0.4y^{0} + 0.6\,\Delta f^{1}.$$
(4.3)

If f is $-\lambda y$ and $\beta = \lambda \, \delta t$, then the 2-step algorithm gives

$$y^{1} = \frac{y^{0}(1 - 0.4\beta)}{(1 + 0.3\beta)^{2}} = y^{0}(1 - \beta + 0.51\beta^{2} + \cdots),$$
(4.4)

which can be compared with the exact expansion

$$y^1 = y^0(1 - \beta + 0.50\beta^2 + \cdots).$$
 (4.5)

When these expansions are valid the error of the 2-step scheme is $0.01\beta^2 y^0$. The BE scheme gives

$$y^{1} = \frac{y^{0}}{1+\beta} = y^{0}(1-\beta+\beta^{2}+\cdots)$$
 (4.6)

which has an error 50 times larger than the 2-stage scheme.

We implement this analogously to the BE scheme. For every pair we solve the equations equivalent to (4.2) and (4.3), thereby updating their velocities and setting new initial velocities for the pair.

In place of (3.5) and (3.6) we solve

$$\tilde{\mathbf{v}}_a = \mathbf{v}_a^0 - \Delta \mathbf{r}_{aj} m_j s_{aj} (0.6 \tilde{\mathbf{v}}_{aj} \cdot \mathbf{r}_{aj} + 0.4 \mathbf{v}_{aj}^0 \cdot \mathbf{r}_{aj})$$
(4.7)

$$\tilde{\mathbf{v}}_{j} = \mathbf{v}_{j}^{0} - \Delta \mathbf{r}_{ja} m_{a} s_{aj} (0.6 \tilde{\mathbf{v}}_{aj} \cdot \mathbf{r}_{aj} + 0.4 \mathbf{v}_{ja}^{0} \cdot \mathbf{r}_{ja});$$
(4.8)

then

$$\mathbf{v}_a^1 = 1.4\tilde{\mathbf{v}}_a - 0.4\mathbf{v}_a^0 - 0.6\,\Delta\mathbf{r}_{aj}m_js_{aj}(\mathbf{v}_{aj}^1\cdot\mathbf{r}_{aj}) \tag{4.9}$$

and

$$\mathbf{v}_i^1 = 1.4 \widetilde{\mathbf{v}}_i - 0.4 \mathbf{v}_i^0 - 0.6 \,\Delta \mathbf{r}_{ia} m_a s_{ai} (\mathbf{v}_{ai}^1 \cdot \mathbf{r}_{ai}). \tag{4.10}$$

We solve these equations analogously to those for the BE method. That is, we subtract (4.8) from (4.7) and solve for $\tilde{\mathbf{v}}_{aj} \cdot \mathbf{r}_{aj}$, after which the $\tilde{\mathbf{v}}_a$ and $\tilde{\mathbf{v}}_j$ can be found. Equations (4.9) and (4.10) are then solved in the same way. We then sweep over all particles. As before two complete sweeps give satisfactory convergence. If *n* sweeps are used Δ should be replaced by Δ/n , that is $0.5 \delta t/n$.

5. TESTS WITH DRAG ONLY

In these tests we work with uniform densities in one dimension. For that reason each particle has the same *h*. Since the densities and void fraction are kept constant, the only variables we need to consider are the velocity and position. The particles have mass $m = \hat{\rho} \Delta p$, where Δp is the initial particle spacing. We use the cubic spline kernel [5].

For a given step we first shift the particles to the midpoint using the current velocities. The two sweeps of the implicit scheme are then carried out. This gives the velocities at the end of the step. The particles are then shifted to their positions at the end of the step using a half step with the new velocity. The particle stepping is therefore a trapezoidal rule.

One Dust Particle

The first test is for one dust particle moving through a uniform array of gas particles. Although this test is artificial because the density of the dust fluid is not properly defined, it allows us to test that the code reproduces the correct drag forces and determines whether, and with what accuracy, the implicit scheme converges.

The case shown here is for a dust particle with $\rho_d = 0.01$ and $\theta_d = 0.1$ and 50 gas SPH particles with $\rho_g = 1.0$ and $\theta_g = 0.9$. The particles lie between [-1, 1] with spacing 0.04 and h = 0.06. The dust particle is placed at the centre of the configuration. The initial velocity of the dust particle is 1.0 and the gas particles are at rest. Because the mass of the dust particle is much smaller than the mass of any gas particle the velocities of the gas particles remain extremely small compared to the initial velocity of the dust particle. We choose $\delta t = 0.003$.

t/δt	K = .01			K = 0.1			K = 1.0		
	Exact	А	В	Exact	А	В	Exact	А	В
1	0.970	0.970	0.945	0.736	0.737	0.577	0.047	0.047	0.011
3	0.912	0.913	0.845	0.399	0.401	0.192	0.000	0.005	0.000
5	0.858	0.858	0.755	0.216	0.218	0.064	0.000	0.004	0.000
7	0.807	0.807	0.676	0.117	0.118	0.022			
15	0.632	0.632	0.433	0.010	0.019	0.000			

 TABLE I

 The Velocity of a Single Dust Particle with Initial Value 1.0

Note. Results under A are for the 2-step scheme. Results under B are for the Backward Euler.

The exact solution for the velocity v_j of the dust particle, assuming the gas particles remain at rest, is

$$v_i(t) = v_i(0)e^{-t/\tau},$$
(5.1)

where $\tau = \hat{\rho}_i / K = 0.001 / K$ for this configuration.

In Table I we show the results for K = 0.01, 0.1, and 1.0 with both the BE integration (B) and the two-stage integration (A). For the first two values of K the time step is much less than τ and we expect the results of the backward Euler method to be reasonably accurate. However, for K = 1.0 this is no longer the case and the BE results are seriously in error. Nevertheless, the implicit BE integration gives the physically sensible result of rapid slowing down. It is clear that the two-stage integrator is much more accurate than the BE method.

These results confirm that the algorithm correctly reproduces the drag term and the iterative solution of the implicit equations is accurate.

Two Streams

In the next test an initially uniform stream of dust particles with velocity 0.5 moves through an initially uniform stream of gas particles with velocity 1.5. The dust and gas particles have equal density ($\rho = 1.0$) and equal void fraction with $\hat{\rho} = 0.5$. The spacing and time step (0.003) are as before. The backward Euler (BE) method requires a time step $\ll 0.5/K$ for reasonable accuracy and the explicit Euler requires a time step $\ll 0.5/K$ for stability.

In Fig. 1 we show results for the case K = 10 and the BE integrator. Successive frames show the particle velocities for time steps 1, 3, 7, and 15. The particle velocities smoothly converge to the expected value of 1.0, except near the edges where some particles move away from their neighbours. This is to be expected. In Fig. 2 we show the results for K = 1000. In this case the explicit Euler scheme requires a time step 6 times smaller than the one we use. With the scheme described in the text the convergence is excellent. The two-stage integrator gives similar results, but the accuracy is always much higher.

6. COMBINING PRESSURE, GRAVITY, AND DRAG

Because the focus of this paper is on the implicit technique for the drag we only consider a simple isothermal gas and the thermal energy equation is not integrated. This is a good approximation for many industrial applications.

To integrate the equations over a single step we use a predictor corrector to take into account the effects of pressure, viscosity, and gravity and combine this with the implicit drag calculations. At the start of the step we have the rate of change of density (R), the rate of change of void fraction (T), and the current values of velocity \mathbf{v}^0 , density ρ^0 , void fraction θ^0 , and position x^0 . We also have the contribution to the force/mass due to the pressure and viscous forces \mathbf{f}^0 .

Step 1

We shift to the midpoint according to

$$\mathbf{v}^{1/2} = \mathbf{v}^0 + \frac{1}{2} \,\delta t (\mathbf{f}^0 + \mathbf{\tilde{g}}),$$

$$\mathbf{r}^{1/2} = \mathbf{r}^0 + \frac{1}{2} \,\delta t \,\mathbf{v}^0,$$

$$\hat{\rho}^{1/2} = \hat{\rho}^0 + \frac{1}{2} \,\delta t \,R^0,$$

$$\theta^{1/2} = \theta^0 + \frac{1}{2} \,\delta t \,T^0,$$

where the last equation only applies to the gas particles because θ_d is calculated from $\hat{\rho}_d$ and the constant ρ_d . With these midpoint values we call a routine to calculate **f** at the midpoint. The value of **v** at the end of the step due to the effects of pressure, viscosity, and gravity is then given by

$$\mathbf{v}' = \mathbf{v}^0 + \delta t (\mathbf{f}^{1/2} + \mathbf{\tilde{g}}).$$

The drag coefficient can be calculated from these midpoint quantities.

Step 2

With \mathbf{v}' as the initial velocity we include the effects of the drag with the twostage, two-sweep integrator. This gives the final velocity \mathbf{v}^1 . We then call a routine to calculate the rate of change of density and void fraction using this velocity. The density and void fraction are then integrated to the end of the step using a trapezoidal rule,

$$\hat{\rho}^{1} = \hat{\rho}^{0} + \frac{1}{2} \,\delta t \,R^{1},$$

$$\theta^{1} = \theta^{0} + \frac{1}{2} \,\delta t \,T^{1},$$

$$\mathbf{r}^{1} = \mathbf{r}^{0} + \frac{1}{2} \,\delta t \,\mathbf{v}^{1}.$$

If the density and void fractions are calculated by summation then appropriate routines can be called after the positions are projected to the midpoint.



FIG. 1. A one-dimensional, pure drag simulation with a stream of dust SPH particles with speed 0.5 moving through gas SPH particles with speed 1.5. The dust and gas have equal density and equal void fraction. The drag coefficient K = 10. The four frames are for 1, 3, 7, and 15 timesteps. The circle symbols denote gas SPH particles and the dots the dust SPH particles.

7. FURTHER TESTS

In the following tests we examine the algorithm's ability to simulate waves and the fall of a layer of dust in an isothermal atmosphere.

Waves

The dispersion relation for waves propagating through a dusty gas gives complex solutions, except when the drag is zero or infinite when the phase speed is real and nondispersive. When the drag is zero the speed of wave propagation c is given by



FIG. 1—Continued

$$c^2 = c_0^2 \left(1 + \frac{\theta_d \rho_g}{\theta_g \rho_d} \right),\tag{7.1}$$

and when the drag is infinite,

$$c^2 = \frac{c_0^2}{\theta_g(\theta_g + \theta_d \rho_d/\rho_g)},\tag{7.2}$$

where c_0 is the speed of sound in the gas alone. Numerous tests confirm that our algorithm correctly reproduces the theory. For example, Fig. 3 shows the velocity



FIG. 2. As for Fig. 1, except K = 1000. Note the rapid transition to uniform velocity.

for a disturbance set up in a uniform dusty gas. The parameters of the gas are $\theta_g = 0.9$, $\rho_g = 1$, $\rho_d = 100$, and K = 500. The initial density and void fractions are constant. The velocity perturbation takes the form

$$v = 0.05c_0 e^{-x^2/d^2},\tag{7.3}$$

where $d = 10 \Delta x$, where Δx is the spacing between particles of the same type and we take $c_0 = 1$ and time step $\delta t = 0.3h/c_0$. We use 100 particles in the domain. The value of K is effectively infinite and the theoretical speed of wave propagation is 0.707. The SPH calculation gives 0.712 with variations of 1% depending on the ratio of h to the particle spacing (for the results of Fig. 3 we take $h = 1.3 \Delta x$).



The Fall of a Layer of Dust

In this test we consider the fall of a layer of dust through gas. If the gas is at rest under gravity the dust layer, initially at rest, will accelerate until the drag arising from the velocity difference between dust and gas balances gravity and the dust layer moves with constant velocity. The relevant equations are well known but they can be derived easily and they are given below.

If the configuration is in a steady state and the system is one-dimensional, (2.12) and (2.13) become

$$\frac{1}{\rho_g} \frac{\partial P}{\partial x} = -\tilde{g} - \frac{K\Delta V}{\theta_g \rho_g} \tag{7.4}$$



FIG. 3. An initial gaussian velocity perturbation has split into two disturbances, one propagating to the left and one to the right. The drag factor is sufficiently large to keep the dust and gas moving together. Further details are given in the text.

and

$$\frac{1}{\rho_d} \frac{\partial P}{\partial x} = -\tilde{g} + \frac{K \Delta V}{\theta_d \rho_d},\tag{7.5}$$

where $\Delta V = (v_g - v_d)$ and we assume K is constant. We can solve these equations for the pressure gradient and the velocity difference. We find

$$\Delta V = -\frac{\tilde{g}(\rho_g - \rho_d)\theta_g\theta_d}{K}$$
(7.6)

and

$$\frac{\partial P}{\partial x} = -\tilde{g}(\hat{\rho}_g + \hat{\rho}_d). \tag{7.7}$$

In the tests to be described the gas is assumed to be isothermal with $P = c^2 \rho_g$. The initial gas density is chosen to be the equilibrium density under gravity (neglecting the dust). The initial density is therefore given by

$$\rho_g = \rho(0) e^{-\tilde{g}x/c^2}, \tag{7.8}$$

where $\rho(0)$ is the density at x = 0.

We now consider a layer of dust placed in the isothermal atmosphere. The layer descends under gravity, eventually moving at constant velocity with the drag balancing gravity. If we neglect the time and space variations of ρ_g in the gas continuity equation and recall that ρ_d is constant, the continuity equations for gas and dust can be converted into equations for θ_g and θ_d . Adding these we find

$$\theta_d v_d + \theta_g v_d = F(t), \tag{7.9}$$

where F(t) is an arbitrary function of t. We assume the boundaries are rigid so that the boundary velocities are zero and then F vanishes everywhere. Making use of this result, and the previous expression for ΔV , we can solve for v_d and v_g . We find

$$v_g = -\frac{\tilde{g}(\rho_g - \rho_d)\theta_d^2 \theta_g}{K}$$
(7.10)

and

$$v_d = \frac{\tilde{g}(\rho_g - \rho_d)\theta_g^2 \theta_d}{K}.$$
(7.11)

A more complete analysis of sedimentation was given by Kynch [3] and used by Andrews and O'Rourke [1]. They show that θ_d is given approximately by the equation

$$\frac{\partial \theta_d}{\partial t} + \Delta V (2\theta_d - 1) \frac{\partial \theta_d}{\partial x} = 0.$$
(7.12)

At any point the advection velocity is therefore $\Delta V(2\theta_d - 1)$. Because $\theta_d \ll 1$ the layer of dust moves with speed $\sim \Delta V$, as we found earlier. At the front of the layer θ_d increases linearly from zero to the constant value $\hat{\theta}_d$ in the layer in a distance $2 \Delta V \hat{\theta}_d t$. At the rear of the layer, θ_d drops discontinuously to zero. This discontinuity is a kinematic shock, where the dust particles which might fall behind find themselves in a region of lower θ_d and speed up.

To test these theoretical predictions we consider a one-dimensional atmosphere with c = 10, $\theta_g = 0.999$, and $\theta_d = 0.001$ within the dust layer, $\rho_g = 1$ at x = 0, and $\rho_d = 1000$. The gas lies in $0 \le x \le 1$, and the dust layer initially occupies $0.6 \le x \le 0.8$. The drag K = 10 and $\tilde{g} = 10$. For these parameters ΔV is 1.0 and the velocity of the gas within the dust layer is negligible. In the simulations we use 100 SPH gas particles and 25 SPH dust particles.

In Fig. 4 we show the initial density of the gas and the layer of dust. The dust accelerates from zero initial velocity and rapidly reaches a near steady state. In Fig. 5 we show the velocity of the gas and dust when t is 0.433. The relative velocity is close to the theoretical value of 1.0 and the gas velocity (after subtracting 1.0 which was added for convenience in graphing) is close to zero. The gas velocity, although small, is larger than predicted by a few percentages, but this is due to the initial state not being in exact equilibrium. In Fig. 6 we show the density when t is 0.433. It can be seen that the layer is moving as a unit with a discontinuous drop in density at the front and the rear, in agreement with the approximate theory. The kink of 4% in the density at the rear is associated with the kinematic shock. In Fig. 7 we show a closeup of the density when t is 0.161. The density gradient can be seen to change within the layer of dust. The gradient changes from the isothermal atmosphere value of 0.1 to 0.22, compared with the theoretical value of 0.20 deduced from the pressure gradient (7.7).



FIG. 4. The density of the gas and dust at time 0.166 when the layer of dust descends in an isothermal atmosphere.

The reader will have noted that the drag factor is not very large and the courant time step is actually much smaller than the time step required by the drag, but this is necessary to allow the layer of gas to descend perceptibly, relative to the gas. The good agreement between the SPH results and theory shows that the algorithm is able to work very satisfactorily with a discontinuous layer and with small void fractions.

9. DISCUSSION AND CONCLUSIONS

The iterative implicit method described in this paper converges rapidly and, when combined with the predictor corrector for the gas dynamics, gives good results. The



FIG. 5. The velocity of the gas and dust at time 0.433. Note that 1.0 has been added to the actual velocities so that the true gas velocity is close to zero and the true dust velocity is close to -1.



FIG. 6. The density of gas and dust at time 0.433.

generalisation to multiphase problems in two and three dimensions is straightforward because all the SPH equations are in vector form. In practice the applications are complicated by the need to use dust particles with a range of sizes and densities and the boundary interactions that occur in industrial problems.

The simplest approach to simulating a dust phase consisting of a variety of dust particles is to use a fluid for each type of dust particle. Provided the number of dust fluids is not large this is a practical solution to the problem. In the SPH simulation each dust fluid would be simulated by a set of SPH dust particles. Details of these applications will be given elsewhere.

It is natural to enquire if the implicit method could be used for pure gas dynamics and therefore used for other problems, for example those involving low Mach



FIG. 7. A closeup of the gas and dust density at time 0.161. This shows the change of density and therefore the pressure gradient within the dust layer, in accordance with theory.

number flow, or low Reynolds number flow, or those involving heat conduction with high thermal conductivity. In all these cases the SPH form of the equations involves pair interactions. For example, in low Mach number flow, the interaction occurs in the acceleration equation and the continuity equation. It would be possible to solve for the contribution of the pair to the velocity and density (and, therefore, pressure), but some care is clearly needed because in the acceleration equation the usual SPH form of the pressure gradient produces a sum of pressure terms. This would mean a substantial shift to the velocity of each particle every time a pair interaction was taken into account. A better method would be to first subtract an estimated pressure and work on this is in progress. In the case of pure thermal conduction in the limit of infinite thermal conductivity and constant specific heat, the implicit rule means that for each pair of particles the temperature is replaced by their average temperature. The iteration to the steady state is then slow and some improvement must be found before the implicit method is practical for this problem. The same considerations apply to low Reynolds number flow. Each of these cases, therefore, presents interesting computational problems which have not been solved, but the solutions will have a large payoff and they appear to be within our grasp.

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