VARIABLE SMOOTHING LENGTHS AND ENERGY CONSERVATION IN SMOOTHED PARTICLE HYDRODYNAMICS.

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July 13, 2021
Abstract. We present a new formulation of the equations of motion used in smoothed particle hydrodynamics (SPH). The spatial resolution in SPH is determined by the smoothing length, $h$, and it has become common practice for each particle to be given its own adaptive smoothing length, $h_i$. This has the advantage that the dynamic range that may be spatially resolved is greatly increased, but also has the drawback that additional terms which account for the variability of the smoothing lengths should be included in the particle equations of motion in order to satisfy conservation requirements. We refer to these additional terms as $\nabla h$ terms. The difference between our approach and that of previous implementations is that these $\nabla h$ terms have now been included in the equations of motion, whereas they had previously been neglected. This is achieved by defining a functional form for the $h_i$s, that depends on inter–particle distances only, and then deriving the equations of motion using a Hamiltonian formalism.

A number of test calculations, designed to compare the effects of including and ignoring these $\nabla h$ terms, are presented. We find that the inclusion of the $\nabla h$ terms has no detrimental effects on the ability of SPH to model known problems, such as one-dimensional shock–tubes or the adiabatic collapse of cold gas spheres, with reasonable accuracy, and may in some cases lead to improvements in their qualitative outcome. For problems on which SPH has been shown to perform rather badly, because of poor energy conservation, we find that including the $\nabla h$ terms results in a dramatic improvement. In particular, non–conservation of energy during a head on collision between identical polytropes can occur at the level of $\Delta E \approx 10\%$ when the $\nabla h$ terms are neglected. When the $\nabla h$ terms are included, however, then this error reduces to $\Delta E \approx 0.8\%$.

1 Introduction.

Smoothed particle hydrodynamics was introduced in order to study problems in astrophysics involving the motion of compressible fluid masses of arbitrary geometry in three dimensions (Lucy 1977; Gingold & Monaghan 1977). For a recent review see Monaghan (1992), and references therein. Particles are used to represent a sub-set of the fluid elements that arise in the Lagrangian description of a fluid, and because spatial derivatives are calculated analytically from interpolation formulae, rather than on a grid, SPH is by its very nature adaptive and thus well suited to problems in which large density contrasts can occur, such as the fragmentation of self-gravitating gas clouds.

The spatial resolution of SPH is determined by the smoothing length, $h$. In early formulations $h$ was either taken to be constant, or else was a globally time-dependent function of the mean number density of particles in the system. More recently, however, it has become common for each particle to have its own time dependent smoothing length which adapts according to the local number density of particles. Full advantage is then taken of the Lagrangian nature of SPH, and the dynamic range in spatial resolution of the method is dramatically increased. The introduction of time varying smoothing lengths can, however, lead to serious problems with energy conservation in certain situations, as was highlighted in a recent paper by Hernquist (1993). The problem arises from the fact that the use of variable smoothing lengths means that additional terms should appear in the particle equations of motion. Up until recently, these additional terms have been
ignored, and as a consequence the particle equations of motion are no longer conservative.

In a previous paper (Nelson & Papaloizou 1993), using a Hamiltonian formalism, we have derived a set of conservative equations for a barotropic fluid which include terms accounting for the variability of the smoothing lengths. In this paper these equations are generalised for the case of an adiabatic fluid in which the entropy on each particle is conserved. The treatment is then extended to include the effects of viscous dissipation.

By means of simple numerical tests, a comparative study between the newly derived version of SPH and a more standard formulation of the method, including spatially and temporally varying smoothing lengths, is presented. An initial set of calculations is presented, in order to compare the qualitative outcome of different versions of our code when it is used to model known problems, such as one-dimensional Riemann shock-tubes, and the adiabatic collapse of an initially isothermal gas sphere. The inclusion of additional terms in the particle equations of motion are not found to have any detrimental effects on the qualitative outcome of the calculations, and in some cases can lead to improvements as a result of more accurate energy conservation. A second set of test calculations is presented that is specifically designed to test the conservation properties of the SPH algorithm. It is found that errors in the conservation of energy or entropy can occur at the level of \( \approx 10\% \), when the additional \( \nabla h \) terms are neglected, during a head-on collision between identical polytropes. For the same calculation, it is found that these errors are reduced to \( \approx 0.8\% \) when the \( \nabla h \) terms are included.

The basic hydrodynamical and thermodynamical equations of the problem are presented in Section (2). The forms of these equations used in SPH methods are derived and discussed in Section (3). In Section (4), calculations designed to compare the qualitative performance of different versions of the SPH method are described. In Section (5) we describe and discuss the results from calculations designed to test the conservation properties of the different formulations. Calculations designed to test the effect of the \( \nabla h \) terms on the numerical diffusivity of SPH are presented in Section (6). Finally, conclusions are drawn in Section (7), and we present a general discussion on issues arising from our calculations, and on the interpretation of the \( \nabla h \) terms.

## 2 Equations of motion.

The equations of motion for a compressible fluid can be written

\[
\frac{d\rho}{dt} + \rho \nabla \cdot \mathbf{v} = 0 \tag{1}
\]

\[
\frac{d\mathbf{v}}{dt} = -\frac{1}{\rho} \nabla P - \nabla \Phi + \mathbf{S}_{\text{visc}} \tag{2}
\]

\[
\rho \frac{dU}{dt} + P \nabla \cdot \mathbf{v} = \rho \mathcal{H} \tag{3}
\]

where

\[
\frac{d}{dt} \equiv \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla
\]
denotes the convective derivative, \( \rho \) is the density, \( \mathbf{v} \) the velocity, \( P \) the pressure, \( \mathcal{U} \) the internal energy per unit mass, and \( \mathcal{H} \) a term comprising all non-adiabatic heating and cooling rates per unit mass. This set of equations is supplemented by an equation of state, which can be written in the form

\[
P = P(\mathcal{U}, \rho)
\]  

(4)

in which the pressure is written as a function of the internal energy per unit mass and the density, which may be adopted as the two thermodynamic variables defining the state of the fluid.

Alternatively, we may introduce the entropy per unit mass, \( S \), which satisfies the equation

\[
T \frac{dS}{dt} = \mathcal{H}
\]

(5)

where \( T \) is the temperature. The quantities \( T, P, \) and \( \mathcal{U} \) are then expressed as functions of the two thermodynamic variables \( \rho \) and \( S \). We note the thermodynamic relation

\[
T = \frac{\partial \mathcal{U}}{\partial S} \bigg|_\rho.
\]

For the special case considered here of an ideal gas with constant specific heat capacity at constant volume \( c_v \), and constant specific heat ratio \( \gamma \), we have

\[
P = (\gamma - 1)\rho \mathcal{U},
\]

(6)

\[
P = c_v(\gamma - 1)\rho T,
\]

(7)

and

\[
S = c_v \log \left( \frac{T \rho^{1-\gamma}}{\gamma} \right).
\]

(8)

In this case, it is also sometimes convenient to work in terms of the quantity

\[
K = \frac{P}{\rho^{\gamma}}, \quad \text{where}
\]

\[
K = c_v(\gamma - 1) \exp \left( \frac{S}{c_v} \right)
\]

and is sometimes referred to as the entropic function.

### 3 Numerical method.

The above set of equations is solved numerically using SPH (Lucy 1977; Gingold & Monaghan 1977). As described above, SPH uses particles to represent a sub-set of the fluid elements that arise in the Lagrangian description of a fluid. This set of particles is chosen in such a way as to ensure that the particles’ mass distribution maps the fluid density, \( \rho \). By calculating the trajectories of the particles according to the hydrodynamic equations, it is then possible to calculate the properties of the fluid at later times.
3.1 Hydrodynamical equations.

3.1.1 Density.

In order to reduce the statistical fluctuations arising from representing a fluid continuum by a finite set of particles, it is necessary to introduce a smoothing procedure. A smoothed quantity may be defined by the expression

\[ \langle f(r) \rangle = \int f(r') W(|r - r'|, h) d^3r' \]  

(9)

where \( f(r) \) is an arbitrary function, \( W \) is a smoothing kernel, and \( h \) is the smoothing length. For a function \( f(r) \) defined only at a discrete set of points, a Monte Carlo representation of equation (9) may be written

\[ \langle f(r_i) \rangle = \frac{\sum m_j f(r_j) W(|r_i - r_j|, h)}{\rho_j} \]  

(10)

where \( m_j \) is the mass of particle \( j \), and \( \rho_j \) is the density at the location of particle \( j \). If the function \( f(r) \) is chosen to be the density, \( \rho(r) \), then we obtain

\[ \rho(r_i) = \frac{\sum m_j W(|r_i - r_j|, h)}{2} \]  

(11)

where the angled brackets have been dropped for the sake of brevity, with the understanding that smoothed functions are used throughout in SPH.

The spatial resolution of a calculation is determined by the smoothing length, \( h \). Most implementations of the SPH algorithm employ temporally and spatially variable smoothing lengths in order to increase the dynamic range that can be spatially resolved, and hence take full advantage of the Lagrangian nature of the method. When variable smoothing lengths are employed each particle, \( i \), will have an associated smoothing length \( h_i \). In the standard formulation of SPH, it is then necessary, in order to conserve momentum, to symmetrise expressions such as

\[ W(|r_i - r_j|, h) \equiv W_{ij} \]

with respect to \( i \) and \( j \). In Nelson & Papaloizou (1993) we set, following (Evrard 1988),

\[ h \rightarrow h_{ij} = \frac{h_i + h_j}{2} \]  

(12)

Alternatively one can use the method suggested by Hernquist & Katz (1989) which symmetrises using the replacement

\[ W_{ij} \rightarrow \frac{1}{2} [W(|r_i - r_j|, h_i) + W(|r_i - r_j|, h_j)]. \]  

(13)

For comparison purposes, we have adopted the method of Hernquist & Katz (1989) in this paper. The smoothed density (11) then becomes

\[ \rho(r_i) = \sum_{j=1}^{N} m_j \frac{1}{2} [W(|r_i - r_j|, h_i) + W(|r_i - r_j|, h_j)] \]  

(14)
3.1.2 Equations of motion.

We now have to form equations of motion for each particle. From equation (2) we obtain, denoting quantities associated with particle \( i \) by a subscript \( i \),

\[
m_i \frac{d\mathbf{v}_i}{dt} = \mathbf{F}_{P,i} + \mathbf{F}_{G,i} + \mathbf{S}_{\text{visc},i}.
\]  

(15)

Here we have denoted the forces on particle \( i \) due to pressure, gravity and viscosity by \( \mathbf{F}_{P,i} \), \( \mathbf{F}_{G,i} \), and \( \mathbf{S}_{\text{visc},i} \) respectively.

3.1.3 A conservative system.

In the early formulations of SPH a global smoothing length was used that could be either constant (Lucy 1977), or a function of time by relating it to the mean density of the system (Gingold & Monaghan 1977). In an attempt to increase the dynamic range that can be modelled, later formulations (Evrard 1988; Hernquist & Katz 1989) have replaced the global smoothing length by one with a spatial and temporal dependence, together with an appropriate symmetrisation with respect to particle pairs (see above). This has the consequence that, for barotropic or isentropic systems, the particle equations of motion are no longer conservative as they should be because the forces have not been derived from an appropriate potential function. It has been suggested in the literature (Gingold & Monaghan 1982; Evrard 1988) that effects arising from the variation of the \( h_i \)'s in time and space should be small, although there is no firm evidence to show that these terms may be neglected. This concern is also true for a system in which a time varying, global smoothing length is employed, as shown recently for example by Hernquist (1993), but it is expected that, in general, the effects of non-conservation will be less severe. This is because the time change in the smoothing length, which drives the non-conservation of energy, is attenuated by the fact that it is dependent on the global properties of the system rather than on purely local ones.

In his recent paper, Hernquist (1993) has shown that, under certain circumstances, errors at the \( \approx 10\% \) level can occur in the conservation of either energy or entropy, depending on whether the entropy or energy equations are integrated, when modelling adiabatic flows. These errors were shown to arise as a direct consequence of the use of variable smoothing lengths. In view of this, it is desirable that a conservative formulation for the various terms in the particle equations of motion be derived that can incorporate variable smoothing lengths. This has already been given for the pressure force in a barotropic fluid in Nelson & Papaloizou (1993). Here we generalise the approach to the case of a general adiabatic flow in which there may not be a barotropic equation of state, but in which the entropy of each particle is conserved. We then extend the treatment to include viscosity.

3.1.4 The pressure force.

An inviscid fluid with a barotropic equation of state is a Hamiltonian system, so it is desirable, when modeling such a system, that the particle equations of motion in SPH form a Hamiltonian system also. The thermal contribution to the total energy can be written (see Nelson & Papaloizou, 1993) as
\[ U = \int_V F(\rho) \rho d^3r, \text{ where } \frac{dF}{d\rho} = \frac{P}{\rho^2}. \]

This has the Monte Carlo representation

\[ U = \sum_{k=1}^{N} m_k F(\rho_k). \] (16)

It is then natural to use \( U \) as a potential function for deriving the pressure force on particle \( i \) through

\[ \mathbf{F}_{P,i} = -\frac{\partial U}{\partial \mathbf{r}_i}. \]

The same formulation goes through for an adiabatic system for which the entropy of each particle is conserved. One simply replaces \( F(\rho) \) in the above by the internal energy per unit mass \( U(S, \rho) \) written as a function of the entropy and the density. The Monte Carlo representation for the pressure potential function is then

\[ U = \sum_{k=1}^{N} m_k U_k(S_k, \rho_k), \] (17)

where \( S_k \) denotes the entropy per unit mass for particle \( k \). We remark that the property of \( U \) that is needed is

\[ \left( \frac{\partial U}{\partial \rho} \right)_S = \frac{P}{\rho^2}. \]

For an adiabatic flow \( S_k \) is constant, so that in both the adiabatic and barotropic cases the pressure force on particle \( i \) is found, after differentiating either (16) or (17) and using (14), to be

\[ \mathbf{F}_{P,i} = -\sum_{k=1}^{N} \sum_{j=1}^{N} m_k m_j \left( \frac{P_k}{\rho_k^2} + \frac{P_j}{\rho_j^2} \right) \frac{1}{2 \rho_i} \frac{\partial W(|r_k - r_j|, h_k)}{\partial \mathbf{r}_i} \frac{1}{2 \rho_i} \frac{\partial W(|r_k - r_j|, h_j)}{\partial \mathbf{r}_j} \]

where we adopt the notation \( r_{kj} \equiv r_k - r_j \). The first part of the above pressure force, which does not involve derivatives of the smoothing lengths, is of the usual symmetrised form (Hernquist & Katz 1989). The second part, which involves derivatives of the smoothing lengths, arises because of the spatial and temporal variability of the \( h_i \)s. We shall refer to terms of this type as \( \nabla h \) terms. In order to evaluate the second part, we need to specify the way that the smoothing length depends on the particle coordinates. In order that
the system conserve linear and angular momentum as well as energy, we take the $h_k$ to be functions only of the absolute distances between particles. Here, we shall adopt the prescription given in Nelson & Papaloizou (1993), namely

$$h_k = G_k \left( \sum_{n=1}^{N} \chi_{kn} H_{kn}(|r_k - r_n|) \right) \quad (20)$$

where $G$ and $H$ are arbitrary functions, and $\chi_{kn}$ are arbitrary numbers, being zero when $k = n$. After differentiation of equation (20) with respect to $r_i$, we obtain

$$\frac{\partial h_k}{\partial r_i} = \delta_{ki} G_k' \sum_{n=1}^{N} \left( \chi_{kn} H_k' \frac{r_{kn}}{|r_{kn}|} \right) + G_k' \chi_{ki} H_k' \frac{r_{ik}}{|r_{ik}|}, \quad (21)$$

where a prime denotes differentiation of a function with respect to its argument. By combining equations (19) and (21) we eventually obtain, for the pressure force on particle $i$, the expression

$$F_{P,i} = -\frac{1}{2} \sum_{j=1}^{N} m_i m_j \left( \frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} \right) \left[ \frac{\partial W(r_{ij}, h_i)}{\partial r_i} \bigg|_{h_i, \text{const}} + \frac{\partial W(r_{ij}, h_j)}{\partial r_i} \bigg|_{h_j, \text{const}} \right]$$

$$- \frac{1}{2} \sum_{k=1}^{N} \frac{P_k}{\rho_k^2} G_k' \chi_{ki} H_k' \frac{r_{ik}}{|r_{ik}|} \sum_{j=1}^{N} m_j \frac{\partial W(r_{kj}, h_k)}{\partial h_k}$$

$$- \frac{1}{2} \sum_{k=1}^{N} \frac{P_k}{\rho_k^2} G_k' \chi_{ki} H_k' \frac{r_{ik}}{|r_{ik}|} \sum_{j=1}^{N} m_j \frac{P_j}{\rho_j^2} \frac{\partial W(r_{kj}, h_k)}{\partial h_k}. \quad (22)$$

This form of the pressure force leads to a fully conservative set of equations because it has been derived from either of the potential functions (16) or (17) which are explicit functions of the inter-particle distances only.

### 3.1.5 The addition of viscosity.

If dissipative mechanisms are included, then we no longer have a system that is Hamiltonian. However, it is possible to ensure that the net rate of energy input into the system is equal to the time rate of change of the Hamiltonian. The equations derived above for inviscid systems are thus modified so that the energy dissipated through viscosity goes into thermal energy in a consistent manner. For calculations in which artificial viscosity is included, we add an artificial viscous pressure term, $\Pi_{ij}$, (Monaghan & Gingold 1983), in only the leading term of equation (22), not involving $\nabla h$ terms, such that

$$\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} \rightarrow \frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} + \Pi_{ij}.$$
With this addition
\[ \mathbf{F}_{P,i} \rightarrow \mathbf{F}_{P,i} + S_{visc,i}. \]
Where it has been used, we have adopted the artificial viscous pressure given by Monaghan & Gingold (1983) in the form
\[ \Pi_{ij} = \frac{1}{\bar{\rho}_{ij}} \left( -\alpha \mu_{ij} \bar{c}_{ij} + \beta \mu_{ij}^2 \right) \] (23)
where the notation \[ \bar{A}_{ij} = \frac{1}{\tau}(A_i + A_j) \] has been used, \( c \) is the adiabatic sound speed, and
\[ \mu_{ij} = \begin{cases} \bar{h}_{ij} \frac{v_{ij} \cdot r_{ij}}{r_{ij}^2 + \eta^2} & \text{if } v_{ij} \cdot r_{ij} < 0 \\ 0 & \text{otherwise.} \end{cases} \] (24)
Here, the notation \( v_{ij} = (v_i - v_j) \) has been used, and \( \eta^2 = 0.01 \bar{h}_{ij}^2 \) prevents the denominator from vanishing.

### 3.1.6 The entropy equation.

For a representation of the entropy equation (23), we write, for particle \( i \),
\[ \frac{\partial \mathcal{U}_i}{\partial S_i} \bigg|_{\rho_i} \frac{dS_i}{dt} = \mathcal{H}_i. \] (25)
This may be incorporated into a conservative scheme (see below).

### 3.1.7 Conservation of energy.

In the case of either a strictly adiabatic or barotropic inviscid flow, the total energy, \( E \) is conserved. This may be written in the form
\[ E = T_K + U + \Omega. \]
Here
\[ T_K = \frac{1}{2} \sum_{i=1}^{N} m_i |v_i|^2 \]
is the kinetic energy, \( U \) is the potential function representing the thermal energy which we used above to derive the pressure force, and \( \Omega \) represents the gravitational energy. Provided that \( \Omega \) is expressed as a function only of the distances between particles, it may be used to derive the gravitational force.

### 3.1.8 The effect of viscosity.

When viscous terms are included in the equations of motion, and we allow the entropy \( S_i \) associated with particle \( i \) to vary with time, we may derive an equation for \( E \) by taking the scalar product of \( v_i \) with the equation of motion (23) and summing over \( i \), so obtaining...
\[
\frac{dE}{dt} = \sum_{i=1}^{N} m_i \frac{\partial U_i}{\partial S_i} \frac{dS_i}{dt} - \frac{1}{4} \sum_{i=1}^{N} \sum_{j=1}^{N} m_i m_j \Pi_{ij} \frac{v_{ij} \cdot r_{ij}}{|r_{ij}|} \times \\
\left[ \frac{\partial W(r_{ij}, h_i)}{\partial |r_{ij}|} \bigg|_{h_i, \text{const}} + \frac{\partial W(r_{ij}, h_j)}{\partial |r_{ij}|} \bigg|_{h_j, \text{const}} \right] \tag{26}
\]

Here, the second term, involving the double summation, represents the viscous dissipation, which is necessarily positive definite.

If we write equation (25) in the form

\[
\frac{\partial U_i}{\partial S_i} \frac{dS_i}{dt} = H_i = \frac{1}{4} \sum_{j=1}^{N} m_j \Pi_{ij} \frac{v_{ij} \cdot r_{ij}}{|r_{ij}|} \left[ \frac{\partial W(r_{ij}, h_i)}{\partial |r_{ij}|} \bigg|_{h_i, \text{const}} + \frac{\partial W(r_{ij}, h_j)}{\partial |r_{ij}|} \bigg|_{h_j, \text{const}} \right] + L_i, \tag{27}
\]

where the first term on the right hand side represents the heating rate per unit mass due to viscosity and \( L_i \) represents the net non-viscous heating rate per unit mass, then we see that equation (26) becomes

\[
\frac{dE}{dt} = \sum_{j=1}^{N} m_j L_j.
\]

Thus the rate of increase of the total energy is equal to the net non-viscous heating rate as required.

The evolution of the entropic function, \( K \), defined in Section (2), is then given by the expression

\[
\frac{dK(S_i)}{dt} = (\gamma - 1) \frac{\partial U_i}{\partial h_i} \beta^1 \beta^{-\gamma}. \tag{28}
\]

Using the second law of thermodynamics

\[
\frac{dU_i}{dt} = \frac{\partial U_i}{\partial S_i} \frac{dS_i}{dt} + \frac{P_i}{\rho_i^2} \frac{d\rho_i}{dt},
\]

we may derive an equation for the rate of change of the internal energy per unit mass for particle \( i \). Using (27) and differentiating equation (14), this may be written in the form

\[
\frac{dU_i}{dt} = H_i + \frac{1}{2} \left( \frac{P_i}{\rho_i^2} \right) \sum_{j=1}^{N} m_j \frac{v_{ij} \cdot r_{ij}}{|r_{ij}|} \left[ \frac{\partial W(r_{ij}, h_i)}{\partial |r_{ij}|} \bigg|_{h_i, \text{const}} + \frac{\partial W(r_{ij}, h_j)}{\partial |r_{ij}|} \bigg|_{h_j, \text{const}} \right] + \frac{1}{2} \left( \frac{P_i}{\rho_i^2} \right) \sum_{j=1}^{N} m_j \frac{\partial W(r_{ij}, h_i)}{\partial h_i} c_i' \sum_{n=1}^{N} \chi_{in} H'_{in} \frac{v_{in} \cdot r_{in}}{|r_{in}|},
\]

\[
+ \frac{1}{2} \left( \frac{P_i}{\rho_i^2} \right) \sum_{j=1}^{N} m_j \frac{\partial W(r_{ij}, h_j)}{\partial h_j} c_j' \sum_{n=1}^{N} \chi_{jn} H'_{jn} \frac{v_{jn} \cdot r_{jn}}{|r_{jn}|}. \tag{29}
\]

Equation (29) may thus be used as an equivalent alternative to the entropy equation (25).
At this point, we note that the standard method of deriving the SPH equations of motion - i.e. by multiplying the continuum equations by $W$, integrating over the solution domain, and integrating the resulting expressions by parts (see Hernquist & Katz 1989) - will not result in conservative equations of motion when spatially variable smoothing lengths are employed, even if the $\nabla h$ terms that arise from such an approach are included. The reason for this is that, in the standard method, the pressure forces experienced by the particles can be expressed in the form of a sum over pairwise interactions. However, when the smoothing lengths are expressed in terms of inter-particle distances, it is apparent that the pressure force on a particle $i$ can no longer be expressed in the form of a sum of simple pairwise interactions, but simultaneously involves communication with other particles in the system - namely all the particles which contribute to $h_i$, and also those particles in the system that receive a contribution from particle $i$ to the calculation of their own smoothing lengths.

In principle, it is not necessary to employ either of the symmetrisation procedures described by equations (12) or (13) when the equations of motion are derived from a Hamiltonian. When the Hamiltonian is formed using either of the so-called gather or scatter formulations (for definition of these terms see Hernquist & Katz 1989), the resulting equations of motion are symmetric and will conserve both momentum and energy. However, the form in which they appear does not allow the artificial viscosity in equation (23) to be incorporated in the usual manner.

### 3.1.9 The smoothing kernel.

The smoothing kernel used is that proposed by Monaghan & Lattanzio (1985), and takes the form

$$W(u, h) = \frac{1}{\pi h^3} \begin{cases} 
1 - \frac{3}{2} \left( \frac{u}{h} \right)^2 + \frac{3}{4} \left( \frac{u}{h} \right)^3 & 0 \leq u/h \leq 1 \\
\frac{1}{4} \left( 2 - \left( \frac{u}{h} \right) \right)^3 & 1 \leq u/h \leq 2 \\
0 & u/h \geq 2
\end{cases}$$

where $u = |\mathbf{r}_i - \mathbf{r}_j|$.

### 3.1.10 Smoothing lengths.

There are two basic requirements that must be met by the method chosen to calculate the individual particle smoothing lengths. Firstly, the smoothing lengths must be explicit functions of the distances between particles, and secondly, the number of particles with which a given particle interacts should be roughly constant. We use a method similar to that suggested by Hernquist & Katz (1989), in order to keep the number of neighbours within $2h_i, N_{TOL}$, constant. Having obtained this list of nearest neighbours, $h_i$ is then defined to be

$$h_i = \frac{1}{2} |\mathbf{r}_i - \mathbf{r}_{imax}|$$

where $\mathbf{r}_{imax}$ is the position vector of particle $i$’s most distant nearest neighbour. In terms of our general functional form for $h_i$ given by equation (20), the functions $G(x) = x$
\( \chi_{in} = \delta_{n,imax} \), and \( H(x) = \frac{1}{2}x \). From equation (22), the pressure force on particle \( i \) then becomes

\[ F_{P,i} = -\frac{1}{2} \sum_{j=1}^{N} m_i m_j \left( \frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} \right) \left[ \frac{\partial W(r_{ij}, h_i)}{\partial r_i} \bigg|_{h_i \text{ constant}} + \frac{\partial W(r_{ij}, h_j)}{\partial r_i} \bigg|_{h_j \text{ constant}} \right] \]

\[ -\frac{1}{4} \sum_{j=1}^{N} m_i m_j \left( \frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} \right) \frac{\partial W(r_{ij}, h_i)}{\partial r_i} \frac{r_{i,imax}}{|r_{i,imax}|} \]

\[ -\frac{1}{4} \sum_{k=1}^{N} m_k \frac{P_k}{\rho_k^2} \delta_{ik} \frac{\partial W(r_{kj}, h_k)}{\partial h_k} \frac{r_{k,imax}}{|r_{k,imax}|} \sum_{j=1}^{N} m_j \frac{P_j}{\rho_j^2} \frac{\partial W(r_{kj}, h_k)}{\partial h_k} \]

and similarly for the equation governing the evolution of the specific thermal energy we obtain from (29) the expression:

\[ \frac{dU_i}{dt} = H_i + \frac{1}{2} \left( \frac{P_i}{\rho_i^2} \right) \sum_{j=1}^{N} m_j \frac{v_{ij} \cdot r_{ij}}{|r_{ij}|} \left[ \frac{\partial W(r_{ij}, h_i)}{\partial r_{ij}} \bigg|_{h_i \text{ constant}} + \frac{\partial W(r_{ij}, h_j)}{\partial r_{ij}} \bigg|_{h_j \text{ constant}} \right] \]

\[ + \frac{1}{4} \left( \frac{P_i}{\rho_i^2} \right) \sum_{j=1}^{N} m_j \frac{\partial W(r_{ij}, h_i)}{\partial h_i} \frac{v_{i,imax} \cdot v_{r,i,imax}}{|r_{i,imax}|} \]

\[ + \frac{1}{4} \left( \frac{P_i}{\rho_i^2} \right) \sum_{j=1}^{N} m_j \frac{r_{j,imax} \cdot v_{j,imax} \frac{\partial W(r_{ij}, h_j)}{\partial h_j}}{|r_{j,imax}|} \]

We note that, in order for the potential function given by equation (14) to be a continuous function of its arguments, the functional form adopted for the \( h_i \)s must be continuous. Consequently, the number of nearest neighbours, \( N_{TOL} \), that determines the value of each \( h_i \) should be strictly constant throughout the calculation, and particle \( imax \) in equation (31) must always be the \( N_{TOL} \)th nearest neighbour. This point is discussed further in Section (5).

We also note that the functional form (31) used to calculate the smoothing lengths introduces additional statistical fluctuations into the pressure forces. From the momentum equation (22) it is apparent that when particle \( i \)'s nearest neighbour, \( imax \), changes its identity as the system evolves in time, fluctuations will arise in the pressure forces experienced by particle \( i \). Technically speaking, the potential function defined by equation (14) is itself continuous, but it has a discontinuity in its first derivative, the magnitude of which is determined by the \( \nabla h \) terms. An alternative method for calculating the smoothing lengths, which reduces these fluctuations, is to first find the \( N_{TOL} \) nearest neighbours and to then calculate \( h_i \) from this list of nearest neighbours according to

\[ h_i = \frac{1}{N_{far}} \sum_{n=1}^{N_{far}} \frac{1}{2} |r_i - r_n| \]

\[ \text{(34)} \]
where the summation is over particle $i$’s $N_{far}$ most distant nearest neighbours. In particular, we have experimented with using $N_{far} = 6$ so that the value of $2h_i$ then becomes equal to the mean distance to particle $i$’s six most distant nearest neighbours. In terms of the general functional form for $h_i$ given by equation (20), the functions $G(x) = x, \chi = \delta_i, H(x) = x/2N_{far}$, where each $i_{far}$ represents one of particle $i$’s $N_{far}$ most distant nearest neighbours.

3.1.11 Gravitational forces.

An implementation of the Barnes-Hut hierarchical tree algorithm (Barnes & Hut 1986; Hernquist 1987) was used in the calculations for which the computation of the force $F_{G,i}$ due to self-gravity was required. The interparticle potential was softened by the method of spline softening (Gingold & Monaghan 1977), with a constant value of the softening length used throughout. When calculating the gravitational force on a given particle $i$, an opening angle of $\theta = 0.6$ (where $\theta = \frac{s}{d}; s =$ size of cell, $d =$ distance to centre of mass of cell), was used for cells whose centre of mass lay outside of the softening radius, with forces being calculated up to quadrupole order. For cells lying within the softening radius, an opening angle of $\theta = 0.3$ was employed, and forces were computed up to monopole order only.

This method of calculation gives an approximation to the gravitational potential in such a way that it is no longer strictly a sum of contributions dependent only on the distances between particles, and this will lead to some small ($\Delta E \lesssim 1\%$) error in the total energy conservation.

3.1.12 Time integration.

The standard second order leap-frog scheme, with the modification proposed by Hernquist & Katz (1989) for estimating time-centred velocities in the viscous pressure term (23), the energy equation (29), and the entropy equation (27), was used. The time step was determined by the expression

$$\delta t = Q \text{Min}_{i}\frac{h_i}{c_i + 1.2(\alpha c_i + \beta \max_j |\mu_{ij}|)}$$

where the factor $Q$ is a numerical constant usually taken to be in the range $Q \approx 0.1 - 0.3$.

4 Numerical tests.

A number of test calculations have been performed using different versions of our SPH code in order to compare their ability to reproduce the solutions for problems that have either been studied using independent numerical techniques, or which have known analytical solutions. The main purpose of this paper, however, is to study the effect of including the $\nabla h$ terms on the conservation of energy, and the emphasis will be on those calculations designed to test conservation properties. Tests have also been performed to explore the possibility that the inclusion of $\nabla h$ terms in the manner described above may lead to increased numerical diffusivity.
4.1 Shock-tube calculations.

Extensive one-dimensional Riemann shock-tube calculations (see Sod 1978; Monaghan & Gingold 1983), have been performed. The initial conditions were:

\[
\begin{align*}
\rho &= 1, & P &= 1, & v &= 0, & \text{for } x < 0; \\
\rho &= 0.25, & P &= 0.1795, & v &= 0, & \text{for } x \geq 0.
\end{align*}
\]  

(36)

Here \(x\) is a cartesian coordinate and the calculations were for an ideal gas with specific heat ratio \(\gamma = 1.4\). The equations integrated were the equation of motion (15) using (32) and the entropy equation (27) with \(L_i = 0\).

Plots of the density, pressure, velocity field, and entropic function \(K\), are shown in Figs. (1.a - 1.d) for the case when the \(\nabla h\) terms were neglected, and in Figs. (2.a - 2.d) for the case when the \(\nabla h\) terms were included. In both cases shown, 400 equal mass particles were distributed in the range \(-0.6 \leq x \leq 0.6\) so as to satisfy equation (36). The smoothing lengths were allowed to vary in both space and time, with the number of nearest neighbours being fixed at \(N_{TOL} = 4\), using a renormalised, one-dimensional version of the smoothing kernel (30). This corresponds to \(\approx 32\) neighbours for a spherical kernel in three-dimensions. For the calculations presented here, the artificial viscosity parameters in equation (23) were chosen to be \(\alpha = 1\), \(\beta = 1\), \(\eta^2 = 0.01\), and the time-step was calculated using equation (35) with \(Q = 0.2\).

The results shown in both Figs. (1.) and (2.) are almost identical in form, and show a satisfactory agreement with the analytical solution. The shock front located between \(x = 0.2 - 0.25\) is broadened over a range in \(x\) of \(\approx 2\eta_i\), with the contact discontinuity, positioned at \(x \approx 0.1\) having a similar width. The slight overshoot in the density and pressure at \(x \approx -0.2\) appears to be due to the fact that the values of the smoothing lengths become smaller at this point in order to satisfy the constraint that the number of nearest neighbours be constant. This effect was seen to decrease when the number of nearest neighbours \(N_{TOL}\) was increased, though this also had the effect of broadening the shock front.

4.2 Gravitational collapse of cold gas sphere.

The adiabatic collapse of an initially isothermal gas sphere has been calculated using different versions of our code in order to test the qualitative effects of including the \(\nabla h\) terms in a three-dimensional calculation. The initial conditions were chosen to match those of Evrard (1988) and Hernquist & Katz (1989) so as to facilitate comparison with their P3MSPH and TREESPH codes respectively, and with a finite-difference code (Thomas 1987).

Following Evrard (1988), the initial state is an ideal gas sphere of radius \(R\) and mass \(M_T\), with a density profile given by

\[
\rho = \frac{M_T}{2\pi R^2} \frac{1}{r},
\]

(37)

where \(r\) is the usual spherical polar radius. The initial conditions were set up by placing the particles on a uniform grid which was then stretched to achieve the required density distribution. Initially, the gas sphere was isothermal, with specific thermal energy \(u = 0.05GM_T/R\). The ratio of the specific heats is \(\gamma = 5/3\).
As in Evrard (1988), the scales used in presenting the results are: density, \( \rho_* = 3M_T/4\pi R^3 \); energy, \( u_* = GM_T/R \); pressure, \( P_* = \rho_* u_* \); and velocity, \( v_* = (GM_T/R)^{1/2} \). Time is shown in units of the free-fall time at the initial outer radius, \( t_* = (\pi^2/8G)^{1/2} R^{3/2} M_T^{-1/2} \). The equations integrated were the equation of motion (15) using (32), and the entropy equation (27) with \( \mathcal{L}_i = 0 \). The results for the calculation in which the \( \nabla h \) terms were neglected are shown in Figs. (3. - 6.), and those for which the \( \nabla h \) terms were included are shown in Figs. (7. - 10.). The gas sphere begins to collapse due to the low value of the internal energy, and as it does so the ratio of the thermal to the gravitational energy increases since \( \gamma > 4/3 \). At later times, a central bounce occurs and a shock wave propagates outwards through the collapsing sphere, with the system converting most of its kinetic energy into thermal energy between times \( t \approx 0.8t_* \) and \( t \approx 1.2t_* \). Eventually, the sphere tends towards an approximate equilibrium configuration with \( U \approx -\Omega/2 \).

Both of the calculations displayed in Figs. (3. - 6.) and Figs. (7. - 10.) show excellent agreement with the SPH calculations of Evrard (1988), and those of Hernquist & Katz (1989). Particularly encouraging is the good agreement found between our calculations and the results obtained by Evrard (1988) using a one-dimensional finite difference code containing 250 zones (Thomas 1987). The strength and position of the shock at time \( t = 0.8t_* \) is well represented by our calculations, and the thermal energy profile behind the shock shows the slow rise with radius displayed by the one-dimensional model. Similarly, the velocity profiles from our calculations, shown in Fig. (6.) and Fig. (10.), indicate good general agreement with those of the one-dimensional calculation, though there is a larger scatter in these results than in those for the density and pressure caused largely by non-synchronous evolution of the system at different angular positions around the sphere.

When comparing the results of our two SPH calculations, small differences may be observed. Firstly, the results for the case in which the \( \nabla h \) terms were included appear to suffer from a slightly larger scatter than the results from the calculation in which the \( \nabla h \) terms were neglected. This ‘noise’ appears to be due to the functional form, (31), adopted for calculating the \( h_i \), which, as described in Section (3.1.10), introduces increased statistical fluctuations into the pressure forces. However, the overall effect of these increased fluctuations appears to be small. Closer inspection of the results shows that including the \( \nabla h \) terms actually leads to improvements in the performance of the code due to energy being conserved more accurately. For example, at time \( t = 1.2t_* \), the sharp peak and drop in the thermal energy located at \( r \approx 0.6R \) in Evrard’s one-dimensional calculation is more apparent in our results if \( \nabla h \) terms are included than if they are neglected. Consequently, the corresponding feature in the pressure profile is also more accurately represented. Energy was conserved to a level of \( \approx 1.0\% \) when \( \nabla h \) terms were included, and to a level of \( \approx 4.3\% \) when neglected.

The calculation was repeated using the energy equation (33) with the \( \nabla h \) terms being both included and neglected, respectively. As expected, the qualitative outcome of these calculations were almost identical to their equivalent calculations displayed in Figs. (3. - 10.) in which the entropy equation (27) was integrated. If the \( \nabla h \) terms are neglected, then no apparent qualitative improvement in the results is obtained by using the thermal energy equation (33) - which leads to conservation of total energy but not entropy, instead of the entropy equation (27) - which leads to the conservation of entropy but not energy. The calculation was also performed using the functional form for the \( h_i \) given by equation...
with $N_{far} = 6$, and $N_{TOL}$ taking the value $50 \pm 1$. In this case the $\nabla h$ terms were included, and the entropy equation (27) was integrated. The results were almost identical to those shown in Figs. (7.) - (10.), except that the level of scatter was reduced slightly. Energy was conserved to a level of $\approx 0.6\%$.

Obviously, the inclusion of $\nabla h$ terms does not alter the ability of SPH to reproduce the salient features present in the problems studied thus far, and can in fact improve the qualitative outcome of the calculations.

5 Conservation of energy.

Two different sets of test calculations were performed in order to test the energy conservation properties of different versions of our code. These were collision calculations between identical polytropes, including the effects of self-gravity and artificial viscosity, and the free expansion of non self-gravitating polytropes in which the effects of viscosity were ignored.

5.1 Colliding polytropes.

Numerical calculations of collisions between identical $n = 3/2$ polytropes have been performed. Equilibrium polytropes, each consisting of $N = 2085$ particles, were set-up by evolving an initially uniform gaseous sphere in the presence of damping until a stationary state was achieved (Lucy 1977; Goodman & Hernquist 1991). Rather than being allowed to collide after free falling from a distance, the two identical polytropes were placed adjacent to one another with their surfaces just in contact. The polytropes were then given the free-fall velocities that they would have if they had started from a state of rest, with an initial separation between their centres equal to six times their diameter. This procedure was followed in order to reduce the computational costs.

Collision calculations for six different versions of our code were performed, the details of which are summarised in Table 1. In these calculations the equations integrated were the equation of motion (15) using (32), and either the entropy equation (27) or the internal energy equation (33). In all cases $\mathcal{L}_t = 0$. A typical time sequence is shown in Fig. (11.), and the evolution of the total energy for a number of the calculations described in Table 1. are shown in Fig. (12.). For all the calculations presented, a value of $Q = 0.2$ was used in equation (35) to determine the time step, and the artificial viscosity parameters in equation (23) were $\alpha = 0.5$, $\beta = 1$.

As the polytropes collide, a shock forms at the interface converting most of the kinetic energy into thermal energy. A period of rapid re-expansion then occurs due to the presence of large pressure gradients in the fluid, but because the system remains bound, the resulting single polytrope undergoes quadrupole oscillations which damp out as the system tends towards an equilibrium state.

5.1.1 $\nabla h$ terms neglected.

From the results for the evolution of the total energy shown in Fig. (12.), it is obvious that large differences exist between the results for the two calculations in which the $\nabla h$ terms
were neglected. It appears that the total energy is conserved with reasonable accuracy (at the \( \approx 2\% \) level) if the energy equation (33) is integrated, whereas errors at the level of \( \approx 10\% \) are incurred if the entropy equation (27) is integrated. These errors largely occur between the times \( t = 0.1 \) and \( t = 0.3 \) during the initial compression and rapid re-expansion phase. However, the apparent improvement in the conservation of energy obtained by integrating the energy equation is somewhat illusory since entropy is no longer conserved (Hernquist 1993). This is because neglecting the \( \nabla h \) terms in both (32) and (33) is consistent with conservation of total energy but is inconsistent with the correct equation for the entropy. We have performed further calculations that show that the errors incurred in the conservation of the total energy when integrating equation (33) are largely due to the use of velocities that are not properly time-centred and from the use of a tree-code to compute the self-gravity of the fluid. Also, calculation \( C4 \) in Table 1. was repeated using a value for \( Q \) in equation (35) of \( Q = 0.03 \). Violations in energy conservation still occurred at the level of 9.75\%, implying that non-conservation is not induced by time-stepping errors, but is instead due to a physical change of the energy in the system introduced by the time variation of the smoothing lengths.

5.1.2 \( \nabla h \) terms included.

It is apparent from Fig. (12.) that the inclusion of \( \nabla h \) terms results in a dramatic improvement in the conservation of total energy. The entropy equation (27) was integrated for all runs displayed in Fig. (12.) in which the \( \nabla h \) terms were included. As mentioned in Section (3.1.10), by allowing the value of \( N_{TOL} \) to vary from a single, fixed value, temporal discontinuities are introduced into the potential energy of the system, and energy is no longer exactly conserved. This point is illustrated by our results, which show the conservation of total energy slowly degrade as the value of \( N_{TOL} \) is allowed to vary from \( N_{TOL} = 50 \) to \( N_{TOL} = 50 \pm 1 \), and \( N_{TOL} = 50 \pm 2 \) respectively. However, even with \( N_{TOL} \) varying by \( \pm 2 \), the errors incurred are still relatively small (\( \approx 3\% \)), and for less violent scenarios are almost negligible. Computational advantage is gained by allowing \( N_{TOL} \) to vary slightly about some fixed value rather than maintaining constancy. Any method used to estimate the \( h_i \)'s at the beginning of a time step has a greater chance of satisfying the demand that the number of nearest neighbours lies within a small range about some value, rather than being equal to a single, specific value. Therefore, the estimated \( h_i \)'s have to be adjusted less often and the execution speed of the code is increased. Errors incurred in the conservation of energy for the run in which \( N_{TOL} \) took a single value (i.e. \( N_{TOL} = 50 \)), were due to residual discretisation errors, and the use of a tree-code to compute gravitational forces.

The collision calculation was also performed by including the \( \nabla h \) terms and integrating the thermal energy equation (33). Although we do not display the results from this calculation in Fig. (12.), because integrating either of the equations (27) or (33) is formally equivalent when \( \nabla h \) terms are included, we found that the evolution of the total energy was very similar to the case in which equation (33) was integrated and the \( \nabla h \) terms were neglected, as should be expected. The deviation from perfect energy conservation in this case is again due to the use of velocities that were not properly time-centred in equation (33), and the use of a tree-code.
5.1.3 Timing tests.

The CPU time per time step was monitored for a number of collision calculations in order to estimate the increase in computation time arising from the inclusion of the $\nabla h$ terms. The results are presented in Table 2. The two parameters that were varied were the number of nearest neighbours within $2h_i$, $N_{\text{TOL}}$, and the functional form used to calculate the smoothing lengths, which was either equation (31) or equation (34). A total of 4170 particles were used in each of the calculations. As mentioned in Section (5.1.2), allowing the value of $N_{\text{TOL}}$ to vary about some value, 50 say, leads to a more efficient code, since less time is spent trying to iterate $2h_i$ towards a value such that it exactly encloses the $50^{th}$ nearest neighbour. It is apparent from Table 3 that the inclusion of the extra $\nabla h$ terms leads to only a small ($<\sim 10\%$) increase in the computational overhead when equation (31) is used to calculate the smoothing lengths. When equation (34) is used, with $N_{\text{far}} = 6$, then the computational expense is greater, due to it being necessary to find the positions of the six most distant nearest neighbours from which the $h_i$s are then calculated. However, a rather naive sorting algorithm was used to perform this task, so we expect to be able to decrease the computational requirements with a more sophisticated approach in future calculations. All calculations shown in Table 3 were performed on a SUN IPX workstation, operating at 33MHz with 16 Mbytes of core storage.

5.2 Expanding polytropes.

In order to test the different forms of the SPH algorithm under less extreme conditions, and in the absence of gravitational and viscous effects, a series of test calculations were performed on the free expansion of gaseous polytropes. An $n = 3/2$ equilibrium polytrope, consisting of $N = 4945$ particles, was set up in the manner previously described in Section (5.1). At time $t = 0$, the self-gravity was switched off. As expected, the absence of pressure at the surface boundary causes a rarefaction wave to propagate through the polytrope which expands freely into space, with the thermal energy being converted into the kinetic energy of the fluid’s bulk motion. Artificial viscosity was neglected, though relation (35) was used to calculate the time step, with $\alpha = 0.5$, $\beta = 1.\, ,\, Q = 0.05$.

A number of free-expansion calculations were performed, with the run parameters being summarised in Table 3. The variation of the total energy in the system as a function of time is plotted in Fig. (13.) for a number of the runs described in Table 3. Although the free expansion of a non self-gravitating polytrope is a considerably less violent phenomenon than the collision between two identical polytropes, a similar trend is seen to occur in the results for the conservation of total energy, though the discrepancies are less marked.

5.2.1 $\nabla h$ terms neglected.

From Fig. (13.) it is obvious that once again the use of the energy equation (33) rather than the entropy equation (27) results in energy being conserved to a higher degree of accuracy when $\nabla h$ terms are not included. If the energy equation is integrated then errors incurred in the conservation of the total energy are small, and mainly arise from the
fact that the velocities used in equation (33) are not correctly time-centred. In this case, however, it can be shown that entropy is not conserved. Errors at the level of $\approx 1.5\%$ arise if the entropy equation (27) is used instead of (33). This is because the total energy is not conserved if time varying smoothing lengths are used and the $\nabla h$ terms are neglected when modeling strictly adiabatic flows. Thus, errors of comparable magnitude are incurred in the conservation of different fundamental properties of the fluid when variable smoothing lengths are employed, depending on whether one chooses to integrate the entropy equation (27) or the energy equation (33). We note that the time period during which most of the energy was lost from the system in calculation $E3$ (see Table 3.), i.e. $t = 0.0 - t = 0.2$, corresponds to $\approx 1200$ time steps in our simulations, and represents the point when more than $99.5\%$ of the initial thermal energy in the system has been converted in to kinetic energy - implying that non-conservation is not largely due to time stepping errors.

5.2.2 $\nabla h$ terms included.

It is apparent from Fig. (13.) that the inclusion of the $\nabla h$ terms results in much improved energy conservation. If the value of $N_{TOL}$ is kept constant, and the entropy equation is used, then energy is conserved almost exactly, with the remaining deviation being due to residual discretisation errors. If $N_{TOL}$ is allowed to vary slightly about a fixed value (i.e. $N_{TOL} = 50 \pm 2$), then small errors ($\approx 0.15\%$) occur, which are substantially smaller than the errors resulting from integrating the entropy equation and neglecting the $\nabla h$ terms. When equation (33) is integrated instead of equation (27), then small errors, the evolution of which are similar to those from calculation $E6$ in Table 3., are incurred (see run $E5$ in Table 3.). We do not present the results from this calculation in Fig. (13.) for similar reasons to those given in Section (5.1.2).

6 Statistical fluctuations and numerical diffusivity.

This last series of test calculations is concerned with the increased statistical fluctuations resulting from the inclusion of the $\nabla h$ terms, and in particular the functional form, (31), adopted for calculating the $h_i$s. In order to examine the importance of this effect, two test calculations were carried out.

6.1 Pressure force fluctuations.

Firstly, the pressure forces on a random sub-set of the particles were monitored throughout the free expansion of an $n = 3/2$ polytrope. An illustrative selection from these results are presented, that represent the forces experienced by the particle as a function of time in the $x$, $y$, and $z$ directions respectively. Fig. (14.a) shows the forces experienced during a calculation for which the $\nabla h$ terms were neglected, with the entropy equation being integrated, and Fig. (14.b) shows the forces on the same particle during a calculation in which the $\nabla h$ terms were included and equation (33) was used to calculate the smoothing lengths. A similar calculation was also performed, with the smoothing lengths being calculated according to the relation (34), and $N_{far} = 6$. The results from this calculation are presented in Fig. (14.c)
It is apparent from Fig. (14.b) that the use of equation (31) does lead to increased statistical fluctuations in the pressure forces experienced by the particles. These fluctuations, however, are generally not large relative to the absolute value of the overall pressure forces, and are found to decrease for increasing numbers of particles. The results shown in Fig. (14.c) show that it is possible to more or less remove these excess statistical fluctuations by simply increasing the number of particles contributing to the functional form used to calculate the smoothing lengths. The fact that the contribution of only a small number of particles \(N_{\text{far}} = 6\) is required to reduce the pressure force fluctuations adds weight to the argument that the \(\nabla h\) terms should be regarded as essentially being correction terms. Up to now, however, we have not in general used equation (34) to calculate the smoothing lengths since the optimal method for implementing this relation has yet to be found. Finding the furthest \(N_{\text{far}}\) nearest neighbours for each particle is a non trivial computational problem when efficiency is an important consideration.

### 6.2 Numerical diffusion.

Calculations of oscillating \(n = 3/2\) polytropes were performed in order to examine whether the increased statistical fluctuations have the effect of increasing the numerical diffusivity of SPH. These used \(N_{\text{TOL}} = 50 \pm 1\). At time \(t = 0\), oscillations were initiated in an equilibrium polytrope, consisting of \(N = 4945\) particles, by imposing an homologous contraction. The results are presented in Fig. (15.) which, when moving from top to bottom in each panel, shows the time dependence of the thermal energy, kinetic energy, total energy, and gravitational potential energy. Fig. (15.a) shows the time sequence for a calculation in which the \(\nabla h\) terms were included and equation (31) was used to calculate the smoothing lengths, and Fig. (15.b) displays the oscillations for a similar calculation in which the \(\nabla h\) terms were neglected. In both of these calculations, a small amount \((\alpha = 0.1, \beta = 0.)\) of artificial viscosity was used in order to stabilise the time integration scheme, though the dissipated kinetic energy was not converted into thermal energy. Instead, the energy removed by the viscosity was simply allowed to leave the system, thus the polytropic equation of state was adopted throughout.

In both calculations, the period of oscillation is accurate to within a few per cent of that expected from analytical considerations (see Cox 1980). Contrary to initial expectations, however, it is found that the oscillations damp out more quickly if the \(\nabla h\) terms are not included in the calculations, since the improved energy conservation gained by including the \(\nabla h\) terms more than off-sets any detrimental effects due to increased fluctuations in the pressure forces. If the amplitude of the oscillations is measured by the height of the thermal energy curves in Figs. (15.a) and (15.b), then the oscillations damp by \(\approx 35\%\) if the \(\nabla h\) terms are included, and by \(\approx 58\%\) if the \(\nabla h\) terms are ignored, after thirteen oscillation periods.

### 7 Discussion and conclusions.

A reformulation of the SPH equations of motion that contain terms accounting for the local variability of the smoothing lengths has been presented. In a previous paper (Nelson & Papaloizou 1993) a set of conservative equations for a barotropic fluid were derived. In
this current paper the derivation was generalised to adiabatic fluids in which the entropy on each particle is conserved, and then extended in a self-consistent manner to incorporate the effects of viscous heating. Other non-adiabatic effects such as molecular cooling and radiative diffusion may be easily incorporated in a similar way, ensuring that the net rate of change of energy in the system due to such processes is equal to the time rate of change of the system Hamiltonian.

The initial set of numerical tests presented here were designed to allow a direct comparison between a standard formulation of SPH employing spatially and temporally varying smoothing lengths, and our formulation of SPH in which the so-called $\nabla h$ terms are included. It is apparent from the results of these calculations that the inclusion of the $\nabla h$ terms has no detrimental effects on the ability of the algorithm to reproduce, with reasonable accuracy, the qualitative and quantitative features of known problems. In fact, owing to the improved energy conservation, it is found that certain features of the adiabatic collapse of a cold gas sphere are more accurately modeled when the $\nabla h$ terms are included.

The advantages of including the $\nabla h$ terms in SPH are, however, most starkly brought to light by the numerical calculations specifically designed to test the conservation of energy. It is obvious from Figs. (12.) and (13.) that including the $\nabla h$ terms leads to a dramatic improvement in conservation properties when the entropy equation (27) is integrated. Although total energy is formally conserved when the internal energy equation (33) is used and the $\nabla h$ terms are neglected in equations (32) and (33), it is simple to show that entropy is no longer conserved when modeling adiabatic flows (e.g. Hernquist 1993). If the $\nabla h$ terms are included, however, then equations (27) and (33) can be shown to be strictly equivalent, leading to the conservation of entropy and energy in both cases. Computational advantage may be obtained by choosing to integrate the entropy equation (27) since the use of velocities that are not properly time-centred in (27) still results in excellent energy conservation throughout the bulk of the flow. Test calculations summarised in Table 3. imply that the problem of non-conservation is not due to gravitational, viscous, or discretisation effects, but is due to the time variability of the $h_i$s driving the evolution of the total energy.

Up until now, discussions concerning $\nabla h$ terms have tended to view the role of these additional terms as providing information about the local spatial variability of the smoothing lengths with respect to one another. However, once a functional form for the smoothing lengths has been defined in terms of inter-particle distances, as in equation (20), this interpretation appears not to be correct. Instead, it is apparent from equation (22) that the $\nabla h$ terms provide information about the way $\nabla W(r_{ij}, h_i)$ changes when we make changes to $h_i$, independently of the way in which changes are made to the smoothing lengths of neighbouring particles. Thus, it is no longer obvious that one may justify neglecting $\nabla h$ terms on the grounds that local spatial variations of the smoothing lengths are likely to be small because quantities do not vary greatly over the scale of the $h_i$s. Instead, the $\nabla h$ terms are accounting for the local time variability of the smoothing lengths, as the particles change their relative positions, and as such can only be neglected when the time scale over which the smoothing lengths vary appreciably is longer than both the dynamical time scale, and the time period over which the integration is performed. This is often not the case in calculations performed with SPH such as the collapse of gas clouds, or stellar
collisions. It is for the above reasons that the calculation performed by Hernquist (1993) in which each particle was given its own individual smoothing length, which was not allowed to vary in time, showed no substantial errors in energy conservation. $\nabla h$ terms should not arise in such a situation, since, in the Lagrangian sense, the smoothing lengths are not then functions of the particle positions/spatial coordinates.

Finally, although it is relatively simple to derive a set of conservative equations from the Hamiltonian in SPH, taking into account the variability of the smoothing lengths, the practical problem of defining a functional form for the $h_i$s still remains. An important consideration is computational expense. If too many particles are allowed to contribute to the calculation of the smoothing lengths then the scheme becomes too costly in terms of CPU time. In order to avoid this problem, we have allowed only one particle to contribute to each $h_i$, as in equation (31), for most of the calculations in this paper. At first glance this approach seems a little dangerous because additional fluctuations are then introduced into the pressure forces. In fact, by inspecting equation (32) one might expect the $\nabla h$ terms to be of the same order as the usual force term, in which case the fluctuations would be very large. However, the quantity $\partial W/\partial h$ has a change of sign, with $\partial W/\partial h < 0$ if $0 < u/h < 1$, and $\partial W/\partial h > 0$ for $1 < u/h < 2$. This leads to a process of self-cancellation, resulting in a much more diminished contribution from the $\nabla h$ terms than one may have initially expected. A problem may still exist for particles that do not play the role of $i_{\text{max}}$ for other particles in the system, or for particles that play the role of $i_{\text{max}}$ for too many particles. In such a situation, the $\nabla h$ contribution to the pressure force becomes either uni-directional, or else is of large magnitude due to the additive nature of these terms. For a purely random distribution of particles, it would be expected that such a situation might occur quite regularly. In practice, however, it seems that the system undergoes a process of relaxation in which correlations are set up between the particles, so that such occurrences are reduced to a few rogue incidents that have little effect on the overall evolution of the system. This is akin to the process described by Monaghan (1988) in order to explain why error estimates based on Monte-Carlo theory are larger that those observed in practice from SPH calculations. The test calculations presented in Section (6) show that in general these fluctuations are indeed small, and do not lead to an increase in the numerical diffusivity of SPH. In fact, the inclusion of $\nabla h$ terms reduces the numerical diffusion in an oscillating polytrope due to improved energy conservation. However, we would still advise caution when using the functional form (31) for calculating the smoothing lengths, and suggest that any effects that may arise from its use be studied on a case by case basis. Should the increased pressure force fluctuations become a cause for concern, then one can easily increase the number of particles contributing to the $h_i$s through equation (34), though at the cost of increased CPU time and more complicated book-keeping. However, it seems from Fig. (14.c) that only a small number of particles ($\approx 6$) are required to all but remove the excess fluctuations.

Acknowledgements. We thank David Balding, Mark Beaumont, and Diana Pallant of the QMWC Statistics group for generously allowing us extensive use of their computer facilities. This work was supported by the SERC QMW rolling theory grant (GR/H/09454). RN is supported by an SERC studentship.
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Table 1: Colliding Polytropes.

| Run | ∇h terms | Equation | $N_{TOL}$ | $E$- deviation (%) |
|-----|----------|----------|-----------|--------------------|
| $C_1$ | Included | Entropy | 50 | 0.8% |
| $C_2$ | Included | Entropy | 50 ± 1 | 2.3% |
| $C_3$ | Included | Entropy | 50 ± 2 | 3.2% |
| $C_4$ | Excluded | Entropy | 50 ± 2 | 9.8% |
| $C_5$ | Included | Energy | 50 ± 2 | 1.8% |
| $C_6$ | Excluded | Energy | 50 ± 2 | 2.1% |
Table 2: Expanding Polytropes.

| Run | \( \nabla h \) terms | Equation | \( N_{TOL} \) | \( E^- \) deviation (%) |
|-----|-----------------|----------|---------------|------------------|
| E1  | Included        | Entropy  | 50            | 0.01%            |
| E2  | Included        | Entropy  | 50 ± 2        | 0.15%            |
| E3  | Excluded        | Entropy  | 50 ± 2        | 1.48%            |
| E4  | Excluded        | Entropy  | 50            | 1.48%            |
| E5  | Included        | Energy   | 50 ± 2        | 0.13%            |
| E6  | Excluded        | Energy   | 50 ± 2        | 0.13%            |
Table 3: Timing Tests for Colliding Polytropes: N=4170

| $\nabla h$ terms | $h_1$-eqn | $N_{TOL}$ | Time/t-step(s) |
|----------------|-----------|-----------|----------------|
| Included        | 31        | 50        | 95             |
| Included        | 31        | 50 ± 1    | 81             |
| Included        | 31        | 50 ± 2    | 78             |
| Excluded        | 31        | 50 ± 2    | 72             |
| Included        | 34        | 50 ± 1    | 95             |
| Included        | 34        | 50 ± 2    | 87             |
Table Captions.

**Table 1.** Results from colliding polytropes. Column(2) identifies whether the $\nabla h$ terms were included, column(3) whether the entropy or internal energy equation was integrated. Column(4) gives the number of nearest neighbours within $2h_i$, and column(5) the percentage deviation from perfect energy conservation.

**Table 2.** Results of timing tests performed for calculations of colliding polytropes. Column (1) indicates whether $\nabla h$ terms were included. Column (2) describes which equation, (31) or (34), was used to calculate smoothing lengths. The values taken for $N_{TOL}$ are given in column (3), and the CPU per time step, measured in seconds, is given in column (4).

**Table 3.** Results from expanding polytropes. Column(2) identifies whether the $\nabla h$ terms were included, column(3) whether the entropy or internal energy equation was integrated. Column(4) gives the number of nearest neighbours within $2h_i$, $N_{TOL}$, and column(5) the percentage deviation from perfect energy conservation.
Figure Captions.

Figure 1. (a) Density, (b) pressure, (c) velocity, (d) entropic profiles in a one-dimensional shock tube, using artificial viscosity defined by equation (23). Analytical solution is shown by dashed lines. In this case the $\nabla h$ terms were neglected.

Figure 2. (a) Density, (b) pressure, (c) velocity, (d) entropic profiles in a one-dimensional shock tube, using artificial viscosity defined by equation (23). In this case the $\nabla h$ terms were included.

Figure 3. Density profile during adiabatic collapse of a gas sphere, initially having an isothermal energy distribution and a $1/r$ density profile. Following Evrard (1988), density is measured in units of $\rho_\ast = 3M_T/4\pi R^2$, where $R$ is initial radius and $M_T$ is total mass. Dimensionless time, normalised to free-fall time at outer radius, is shown in top right corner of each frame. In this case $\nabla h$ terms were neglected.

Figure 4. Thermal energy distribution, normalised to $u_\ast = GM_T/R$, during adiabatic collapse of gaseous sphere. Dimensionless time is shown in top right corner of each frame. $\nabla h$ terms were neglected.

Figure 5. Pressure during adiabatic collapse of gas sphere, normalised to $P_\ast = \rho_\ast u_\ast$. Dimensionless time is shown at top right corner of each frame. $\nabla h$ terms were neglected.

Figure 6. Radial velocity profiles during collapse of gas sphere described in text, normalised to $v_\ast = (GM_T/R)^{(1/2)}$. Dimensionless time is shown in top left corner of each frame. $\nabla h$ terms were neglected.

Figure 7. Same as Fig. 3, except that $\nabla h$ terms were included.

Figure 8. Same as Fig. 4, except that $\nabla h$ terms were included.

Figure 9. Same as Fig. 5, except that $\nabla h$ terms were included.

Figure 10. Same as Fig. 6, except that $\nabla h$ terms were included.

Figure 11. Head on collision between identical $n = 3/2$ polytropes, each containing 2085 particles. Time is indicated at the top right corner of each panel, measured in computational units. Initial velocities and set-up is described in the text.

Figure 12. Evolution of total energy in simulations of head on collisions between identical $n = 3/2$ polytropes. The calculations represented in above figure correspond to the following runs listed in Table 1: $C1$ – Solid line; $C2$ – Dashed line; $C3$ – Dot-dash-dotted line; $C4$ – Dotted line; $C6$ – Dash-dot-dot-dot-dashed line. Units are in computational units.

Figure 13. Evolution of total energy in simulations of freely expanding polytropes in absence of gravity and viscosity. Units are in computational units. The calculations represented correspond to the following runs listed in Table 2: $E1$ – Solid line; $E2$ – Dashed line; $E3$ – Dash-dot-dashed line; $E6$ – Dotted line.
**Figure 14.** The graphs represent the pressure force, experienced as a function of time, by a single particle during free expansion of an $n = 3/2$ polytrope. (a) $\nabla h$ terms are not included in equations of motion. (b) $\nabla h$ terms are included and smoothing lengths are calculated according to equation (31). (c) $\nabla h$ terms are included and smoothing lengths are calculated according to equation (34), with $N_{far} = 6$. Units are in computational units.

**Figure 15.** The graphs represent the various energies, as functions of time, during the normal mode oscillations of an $n = 3/2$ polytrope. In each panel, the line styles representing each of the various energies are: dashed - thermal energy; dotted - kinetic energy; solid - total energy (including energy dissipated by viscosity); dash-dot-dashed - gravitational potential energy. Units are in computational units. (a). $\nabla h$ terms included. (b). $\nabla h$ terms neglected.