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Smoothed Particle Magnetohydrodynamics – II. Variational principles and variable smoothing-length terms

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ABSTRACT

In this paper we show how a Lagrangian variational principle can be used to derive the Smoothed Particle Magnetohydrodynamics (SPMHD) equations for ideal Magnetohydrodynamics (MHD). We also consider the effect of a variable smoothing length in the Smoothed Particle Hydrodynamics (SPH) kernels, after which we demonstrate by numerical tests that the consistent treatment of terms relating to the gradient of the smoothing length in the SPMHD equations significantly improves the accuracy of the algorithm. Our results complement those obtained in the companion paper for non-ideal MHD where artificial dissipative terms were included to handle shocks.

Key words: magnetic fields – MHD – methods: numerical.

1 INTRODUCTION

An advantage of deriving numerical algorithms from a variational principle is that conservation laws can be guaranteed. Another advantage is that the algorithms derived from a variational principle are often more stable than other algorithms. For example, in the case of Smoothed Particle Hydrodynamics (SPH, for a review see Monaghan 1992), the density may be determined from the continuity equation, and it proves important for stability to combine the SPH continuity equation with the variational principle to deduce equations of motion. We call such a procedure consistent.

Bonet & Lok (1999) have derived consistent SPH equations for fluids even when non-standard forms of the continuity equation are used. They include the continuity equation as a constraint on Lagrangian density variations. The resulting equations possess very good stability properties when two fluids with very different densities, for example air and water, are in contact. Other, non-consistent, forms of the SPH algorithm, for example with a standard acceleration equation but non-standard continuity equation, exhibit instabilities.

In this paper we show how a Lagrangian variational principle can be used to derive the Smoothed Particle Magnetohydrodynamics (SPMHD) equations for ideal MHD. Variational equations for continuum MHD have been derived by Newcomb (1962) for both the Lagrangian and the Eulerian form of the equations (see also Henyey 1982; Oppeneer 1984; Field 1986). In the Lagrangian form of the equations Newcomb makes use of flux conservation to relate changes in the magnetic field to changes in surface elements. In the present case, where we consider SPH particles, it is not clear how to prescribe such surface elements in a unique way from the particle coordinates. Instead we make use of the induction equation in its Lagrangian form and treat this as a constraint. An alternative, which we do not explore here, is to begin with plasma physics and prescribe the fields in terms of currents. Such an approach would be natural for particle methods [e.g. Particle-In-Cell (PIC)] which have been so effective for plasma physics where the electrons would be treated as one fluid and the ions as another.

The plan of this paper is derive the equations of motion from a standard Lagrangian for SPH particles with either, or both, the continuity and induction equations treated as constraints (Section 3). We then consider the effect of variable smoothing-length in the SPH kernels (Section 4) after which we demonstrate by numerical tests that consistent treatment of the variable smoothing length in the SPH equations significantly improves the accuracy of SPMHD shocks and of wave propagation (Section 6). Our results complement those obtained in the companion paper (Price & Monaghan 2003, hereafter paper I) for non-ideal MHD where artificial dissipative terms were included to handle shocks.

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2 THE LAGRANGIAN

Variational principles for MHD have been discussed by many authors (e.g. Newcomb 1962; Henyey 1982; Oppeneer 1984; Field 1986) and the Lagrangian is given by

$$L = \int \left(\frac{1}{2}\rho \boldsymbol{v}^2 - \rho u - \frac{1}{2\mu_0} B^2 \right) \mathrm{d}V, \tag{1}$$

which is simply the kinetic minus the potential and magnetic energies. The SPH Lagrangian is therefore

$$L_{\rm sph} = \sum_b m_b \left[\frac{1}{2}\boldsymbol{v}_b^2 - u_b(\rho_b, s_b) - \frac{1}{2\mu_0}\frac{B_b^2}{\rho_b} \right]. \tag{2}$$

where we have replaced the integral with a summation and the volume element $\rho\,\mathrm{d}V$ with the mass per SPH particle m. Variational principles for SPH in relativistic and non-relativistic fluid dynamics have been given by Monaghan & Price (2001).

3 SPMHD EQUATIONS

3.1 Equations of motion

3.1.1 Standard formulation

Ideally we would wish to express all the terms in the Lagrangian (2) in terms of the particle coordinates, which would automatically guarantee the conservation of momentum and energy since the equations of motion result from the Euler–Lagrange equations (e.g. Monaghan & Price 2001). The density can be written as a function of the particle coordinates using the usual SPH summation, that is

$$\rho_a = \sum_b m_b W_{ab}, \tag{3}$$

where $W_{ab} = W(\boldsymbol{r}_a - \boldsymbol{r}_b, h)$ is the SPH interpolation kernel. Taking the time derivative of this expression, we have the SPH version of the continuity equation

$$\frac{\mathrm{d}\rho_a}{\mathrm{d}t} = \sum_b m_b(\boldsymbol{v}_a - \boldsymbol{v}_b)\cdot\nabla_a W_{ab}. \tag{4}$$

The internal energy is regarded as a function of the density, where from the first law of thermodynamics we have

$$\left.\frac{\mathrm{d}u}{\mathrm{d}\rho}\right|_s = \frac{P}{\rho^2}. \tag{5}$$

The magnetic field is evolved in SPH according to

$$\frac{\mathrm{d}\boldsymbol{B}_a}{\mathrm{d}t} = \frac{1}{\rho_a}\sum_b m_b[\boldsymbol{B}_a(\boldsymbol{v}_{ab}\cdot\nabla_a W_{ab}) - \boldsymbol{v}_{ab}(\boldsymbol{B}_a\cdot\nabla_a W_{ab})], \tag{6}$$

or equivalently

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\boldsymbol{B}}{\rho}\right)_a = -\frac{1}{\rho_a^2}\sum_b m_b \boldsymbol{v}_{ab}(\boldsymbol{B}_a\cdot\nabla_a W_{ab}) \tag{7}$$

(e.g. Phillips & Monaghan 1985; Monaghan 1992; paper I). We note that these equations represent the correct formulation of the induction equation even in the presence of magnetic monopoles (Janhunen 2000; Dellar 2001).

However, it is not intuitively obvious how the magnetic field $\boldsymbol{B}$ should be related to the particle coordinates, or even that it could be expressed in such a manner [in the SPH context this would imply an expression for $\boldsymbol{B}$ such that taking the time derivative gives (6) or (7), analogous to (3) for the density], though it could be done easily for a plasma with the electrons and ions described by separate sets of SPH particles. We may, however, proceed by introducing constraints on $\boldsymbol{B}$ in a manner similar to that of Bonet & Lok (1999), that is we require

$$\delta \int L \,\mathrm{d}t = \int \delta L \,\mathrm{d}t = 0, \tag{8}$$

where we consider variations with respect to a small change in the particle coordinates $\delta \boldsymbol{r}_a$. We therefore have

$$\delta L = m_a \boldsymbol{v}_a\cdot\delta\boldsymbol{v}_a - \sum_b m_b \left[\left.\frac{\partial u_b}{\partial \rho_b}\right|_s \delta\rho_b + \frac{1}{2\mu_0}\left(\frac{B_b}{\rho_b}\right)^2 \delta\rho_b - \frac{1}{\mu_0}\boldsymbol{B}_b\cdot\delta\left(\frac{\boldsymbol{B}_b}{\rho_b}\right) \right]. \tag{9}$$

The Lagrangian variations in density and magnetic field are given by

$$\delta\rho_b = \sum_c m_c\,(\delta\boldsymbol{r}_b - \delta\boldsymbol{r}_c)\cdot\nabla_b W_{bc} \tag{10}$$

$$\delta\left(\frac{\boldsymbol{B}_b}{\rho_b}\right) = \sum_c m_c(\delta\boldsymbol{r}_b - \delta\boldsymbol{r}_c)\frac{\boldsymbol{B}_b}{\rho_b^2}\cdot\nabla_b W_{bc} \tag{11}$$

where we have used (4) and (7) respectively [note that we also recover the following results if we use (6) instead of (7)]. Using (10), (11) and (5) in (9) and rearranging, we find

$$\frac{\delta L}{\delta \boldsymbol{r}_a} = -\sum_b m_b \left[\frac{P_b}{\rho_b^2} \sum_c m_c \nabla_b W_{bc} (\delta_{ba} - \delta_{ca}) \right] - \sum_b m_b \left[\frac{1}{2\mu_0} \left(\frac{\boldsymbol{B}_b}{\rho_b} \right)^2 \nabla_b W_{bc} (\delta_{ba} - \delta_{ca}) \right]$$
$$+ \sum_b m_b \left[\frac{1}{\mu_0} \frac{\boldsymbol{B}_b}{\rho_b^2} \sum_c m_c \frac{\boldsymbol{B}_b}{\rho_b} \cdot \nabla_b W_{bc} (\delta_{ba} - \delta_{ca}) \right], \quad (12)$$

where δ_{ab} refers to the Kronecker delta. Putting this back into (8), integrating the velocity term by parts and simplifying (using $\nabla_a W_{ab} = -\nabla_b W_{ba}$), we obtain

$$\int \left\{ -m_a \frac{\mathrm{d}\boldsymbol{v}_a}{\mathrm{d}t} - \sum_b m_b \left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2} \right) \nabla_a W_{ab} - \sum_b m_b \frac{1}{2\mu_0} \left(\frac{B_a^2}{\rho_a^2} + \frac{B_b^2}{\rho_b^2} \right) \nabla_a W_{ab} \right.$$
$$\left. + \sum_b m_b \frac{1}{\mu_0} \left[\frac{\boldsymbol{B}_a}{\rho_a^2} (\boldsymbol{B}_a \cdot \nabla_a W_{ab}) + \frac{\boldsymbol{B}_b}{\rho_b^2} (\boldsymbol{B}_b \cdot \nabla_a W_{ab}) \right] \right\} \delta \boldsymbol{r}_a \ \mathrm{d}t = 0. \quad (13)$$

The SPH equations of motion are therefore given by

$$\frac{\mathrm{d}v_a^i}{\mathrm{d}t} = \sum_b m_b \left[\left(\frac{S^{ij}}{\rho^2} \right)_a + \left(\frac{S^{ij}}{\rho^2} \right)_b \right] \nabla_a^j W_{ab}, \quad (14)$$

where the stress tensor S^{ij} is defined as

$$S^{ij} \equiv -P\delta^{ij} + \frac{1}{\mu_0} \left(B^i B^j - \frac{1}{2} B^2 \delta^{ij} \right). \quad (15)$$

This form of the magnetic force term conserves linear momentum exactly (angular momentum is discussed in Section 5) but was shown by Phillips & Monaghan (1985) to be unstable in certain regimes (low magnetic β). We resolve this instability by adding a short-range repulsive force to prevent particles from clumping (Monaghan 2000), the implementation of which is described in paper I. We note that the conservative form of the momentum equation was derived using a non-conservative induction equation, which agrees with the treatment of magnetic monopoles suggested by Janhunen (2000) and Dellar (2001).

3.1.2 Alternative formulation

Consistent sets of SPMHD equations may also be derived using alternative forms of the continuity and induction equations. We give an example below since alternative forms of the pressure terms in the momentum equation are often explored in the context of SPH, without alteration of the other equations to make the formalisms self-consistent. We expect that a lack of consistency in the discrete equations will inevitably lead to loss of accuracy in the resulting algorithm. For example, using the continuity equation

$$\frac{\mathrm{d}\rho_a}{\mathrm{d}t} = \rho_a \sum_b m_b \frac{\boldsymbol{v}_{ab}}{\rho_b} \cdot \nabla_a W_{ab}, \quad (16)$$

and the induction equation

$$\frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{\boldsymbol{B}}{\rho} \right)_a = -\frac{1}{\rho_a} \sum_b m_b \frac{\boldsymbol{v}_{ab}}{\rho_b} (\boldsymbol{B}_a \cdot \nabla_a W_{ab}). \quad (17)$$

results in the momentum equation

$$\frac{\mathrm{d}v_a^i}{\mathrm{d}t} = \sum_b m_b \left[\frac{S_a^{ij} + S_b^{ij}}{\rho_a \rho_b} \right] \nabla_a^j W_{ab}. \quad (18)$$

This form of the SPMHD equations also conserves linear momentum exactly and in the hydrodynamic case has been found to give better performance in situations where there are large jumps in density (for example at a water–air interface). The consistent form of the energy equations is given in Section 3.2.3.

3.2 Energy equation

3.2.1 Internal energy

The internal energy equation follows from the use of the first law of thermodynamics, that is

$$\frac{\mathrm{d}u_a}{\mathrm{d}t} = \frac{P_a}{\rho_a^2} \frac{\mathrm{d}\rho_a}{\mathrm{d}t}. \quad (19)$$

Using the standard continuity equation (4) therefore gives

$$\frac{\mathrm{d}u_a}{\mathrm{d}t} = \frac{P_a}{\rho_a^2}\sum_b m_b \boldsymbol{v}_{ab}\cdot\nabla_a W_{ab}. \tag{20}$$

3.2.2 *Total energy*

The Hamiltonian is given by

$$H = \sum_a \boldsymbol{v}_a \cdot \frac{\partial L}{\partial \boldsymbol{v}_a} - L. \tag{21}$$

which represents the conserved total energy of the SPH particles since the Lagrangian does not explicitly depend on the time coordinate. Using (2) we have

$$H = E = \sum_a m_a\left(\frac{1}{2}v_a^2 + u_a + \frac{1}{2}\frac{B_a^2}{\rho_a}\right). \tag{22}$$

Taking the (comoving) time derivative, we have

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \sum_a m_a\left[\boldsymbol{v}_a\cdot\frac{d\boldsymbol{v}_a}{\mathrm{d}t} + \frac{\mathrm{d}u_a}{\mathrm{d}\rho_a}\frac{\mathrm{d}\rho_a}{\mathrm{d}t} + \frac{1}{2}\frac{B_a^2}{\rho_a^2}\frac{\mathrm{d}\rho_a}{\mathrm{d}t} + \boldsymbol{B}_a\cdot\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\boldsymbol{B}_a}{\rho_a}\right)\right], \tag{23}$$

where the first term is specified by use of the momentum equation (14), the second term using the first law of thermodynamics (5) and the continuity equation (4), the third term by the continuity equation (4) and the fourth term by the induction equation (7). Using these equations and simplifying we find

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \sum_a m_a \sum_b m_b\left[\left(\frac{S^{ij}}{\rho^2}\right)_a v_b^i + \left(\frac{S^{ij}}{\rho^2}\right)_b v_a^i\right]\nabla_a^j W_{ab}, \tag{24}$$

such that the total energy per particle is evolved according to

$$\frac{\mathrm{d}\hat{\epsilon}_a}{\mathrm{d}t} = \sum_b m_b\left[\left(\frac{S^{ij}}{\rho^2}\right)_a v_b^i + \left(\frac{S^{ij}}{\rho^2}\right)_b v_a^i\right]\nabla_a^j W_{ab}, \tag{25}$$

where

$$\hat{\epsilon}_a = \frac{1}{2}v_a^2 + u_a + \frac{1}{2}\frac{B_a^2}{\rho_a} \tag{26}$$

is the energy per unit mass.

3.2.3 *Alternative formulation*

For the alternative formulation given in Section 3.1.2 the internal energy equation is given by

$$\frac{\mathrm{d}u_a}{\mathrm{d}t} = \frac{P_a}{\rho_a}\sum_b m_b \frac{\boldsymbol{v}_{ab}}{\rho_b}\cdot\nabla_a W_{ab}, \tag{27}$$

and the total energy equation by

$$\frac{\mathrm{d}\hat{\epsilon}_a}{\mathrm{d}t} = \sum_b m_b\left[\frac{S_a^{ij}v_b^i + S_b^{ij}v_a^i}{\rho_a\rho_b}\right]\nabla_a^j W_{ab}. \tag{28}$$

4 VARIABLE SMOOTHING-LENGTH TERMS

The smoothing length h determines the radius of interaction for each SPH particle. Early SPH simulations used a fixed smoothing length for all particles; however, allowing each particle to have its own associated smoothing length which varies according to local conditions increases the spatial resolution substantially (Hernquist & Katz 1989; Benz 1990). The usual rule is to take

$$h_a \propto \left(\frac{1}{\rho_a}\right)^{(1/\nu)}, \tag{29}$$

where ν is the number of spatial dimensions, although others are possible (Monaghan 2000). Implementing this rule self-consistently is more complicated in SPH since the density ρ_a is itself a function of the smoothing length h_a via the relation (3). The usual rule is to take the time derivative of (29), giving (e.g. Benz 1990)

$$\frac{\mathrm{d}h_a}{\mathrm{d}t} = -\frac{h_a}{\nu\rho_a}\frac{\mathrm{d}\rho}{\mathrm{d}t}, \tag{30}$$

which can then be evolved alongside the other particle quantities.

This rule works well for most practical purposes, and maintains the relation (29) particularly well when the density is updated using the continuity equation (4). However, it has been known for some time that, in order to be fully self-consistent, extra terms involving the derivative of h should be included in the momentum and energy equations (e.g. Nelson 1994; Nelson & Papaloizou 1994; Serna, Alimi & Chieze 1996). Attempts to do this were, however, complicated to implement (Nelson & Papaloizou 1994) and therefore were not generally adopted by the SPH community. Recently Springel & Hernquist (2002) have shown that the so-called ∇h terms can be self-consistently included in the equations of motion and energy using a variational approach. Springel & Hernquist (2002) included the variation of the smoothing length in their variational principle by use of Lagrange multipliers; however, in the context of the discussion given in Section 3 we note that by expressing the smoothing length as a function of ρ we can therefore specify h as a function of the particle coordinates (Monaghan 2002); that is, we have $h = h(\rho)$ where ρ is given by

$$\rho_a = \sum_b m_b W(\boldsymbol{r}_{ab}, h_a). \tag{31}$$

Taking the time derivative, we obtain

$$\frac{\mathrm{d}\rho_a}{\mathrm{d}t} = \frac{1}{\Omega_a} \sum_b m_b \boldsymbol{v}_{ab} \cdot \nabla_a W_{ab}(h_a), \tag{32}$$

where

$$\Omega_a = \left[1 + \frac{\partial h_a}{\partial \rho_a} \sum_c m_c \frac{\partial W_{ab}(h_a)}{\partial h_a} \right]^{-1}. \tag{33}$$

The equations of motion in the hydrodynamic case may then be found using the Euler–Lagrange equations and will automatically conserve linear and angular momentum. The resulting equations are given by (Monaghan 2002; Springel & Hernquist 2002)

$$\frac{\mathrm{d}\boldsymbol{v}_a}{\mathrm{d}t} = -\sum_b m_b \left[\frac{P_a}{\Omega_a \rho_a^2} \nabla_a W_{ab}(h_a) + \frac{P_b}{\Omega_b \rho_b^2} \nabla_a W_{ab}(h_b) \right]. \tag{34}$$

Calculation of the quantities Ω involve a summation over the particles and can be computed alongside the density summation (31). To be fully self-consistent (31) should be solved iteratively to determine both h and ρ self-consistently. In practice this means that an extra pass over the density summation only occurs when the density changes significantly between time-steps. Springel & Hernquist (2002) also suggest using the continuity equation (32) to obtain a better starting approximation for ρ and consequently h. We perform simple fixed-point iterations of the density, using a predicted smoothing length from (30). Having calculated the density by summation, we then compute a new value of the smoothing length h_{new} using (29). The convergence of each particle is then determined according to the criterion

$$\frac{|h_{\mathrm{new}} - h|}{h} < 1.0 \times 10^{-2}. \tag{35}$$

We then iterate until all particles are converged, although for efficiency we do not allow the scheme to continue iterating on the same particle(s). Note that the smoothing length of a particle is only set equal to h_{new} if the density is to be recalculated (this is to ensure that the same smoothing length that was used to calculate the density is used to compute the terms in the other SPMHD equations). The calculated gradient terms (33) may also be used to implement an iteration scheme such as the Newton–Raphson method which converges faster than our simple fixed-point iteration. We also note that in principle only the density on particles which have not converged needs to be recomputed, since the density of each particle is independent of the smoothing length of neighbouring particles. These considerations will be discussed further in the multidimensional context since the cost of iteration is of greater importance in this case.

Since we cannot explicitly write the Lagrangian (2) as a function of the particle coordinates, we cannot explicitly derive the SPMHD equations incorporating a variable smoothing length. We may, however, deduce the form of the terms which should be included by consistency arguments. We start with the SPH induction equation in the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\boldsymbol{B}}{\rho}\right)_a = -\frac{1}{\rho_a^2} \sum_b m_b \boldsymbol{v}_{ab} (\boldsymbol{B}_a \cdot \nabla_a W_{ab}). \tag{36}$$

Expanding the left-hand side, we have

$$\frac{\mathrm{d}\boldsymbol{B}_a}{\mathrm{d}t} = -\frac{1}{\rho_a} \sum_b m_b \boldsymbol{v}_{ab} (\boldsymbol{B}_a \cdot \nabla_a W_{ab}) - \frac{\boldsymbol{B}_a}{\rho_a} \frac{\mathrm{d}\rho_a}{\mathrm{d}t}. \tag{37}$$

If the smoothing length is a given function of the density, then the SPH continuity equation is given by (32), and (37) becomes

$$\frac{\mathrm{d}\boldsymbol{B}_a}{\mathrm{d}t} = -\frac{1}{\rho_a} \sum_b m_b \left\{ \boldsymbol{v}_{ab} (\boldsymbol{B}_a \cdot \nabla_a W_{ab}) - \frac{1}{\Omega_a} \boldsymbol{B}_a [\boldsymbol{v}_{ab} \cdot \nabla_a W_{ab}(h_a)] \right\}. \tag{38}$$

In one dimension, however, these terms must cancel to give $B_x = \mathrm{const.}$, and thus we deduce that the correct form of the induction equation is therefore

$$\frac{\mathrm{d}\boldsymbol{B}_a}{\mathrm{d}t} = -\frac{1}{\Omega_a \rho_a} \sum_b m_b \{ \boldsymbol{v}_{ab} [\boldsymbol{B}_a \cdot \nabla_a W_{ab}(h_a)]. - \boldsymbol{B}_a [\boldsymbol{v}_{ab} \cdot \nabla_a W_{ab}(h_a)] \}, \tag{39}$$

or in the form (36) we would have

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\boldsymbol{B}}{\rho}\right)_a = -\frac{1}{\Omega_a \rho_a^2}\sum_b m_b \boldsymbol{v}_{ab}[\boldsymbol{B}_a \cdot \nabla_a W_{ab}(h_a)]. \tag{40}$$

Using (39) or (40) and (32) as constraints we may then derive the equations of motion using the variational principle described in Section 3 to give

$$\frac{\mathrm{d}\boldsymbol{v}_a}{\mathrm{d}t} = \sum_b m_b \left[\left(\frac{S^{ij}}{\Omega\rho^2}\right)_a \nabla_a^j W_{ab}(h_a) + \left(\frac{S^{ij}}{\Omega\rho^2}\right)_b \nabla_a^j W_{ab}(h_b)\right]. \tag{41}$$

The total energy equation is given by

$$\frac{\mathrm{d}\hat{\epsilon}_a}{\mathrm{d}t} = \sum_b m_b \left[\left(\frac{S^{ij}}{\Omega\rho^2}\right)_a v_b^i \nabla_a^j W_{ab}(h_a) + \left(\frac{S^{ij}}{\Omega\rho^2}\right)_b v_a^i \nabla_a^j W_{ab}(h_b)\right], \tag{42}$$

whilst the internal energy equation is found using the first law of thermodynamics and (32), that is

$$\frac{\mathrm{d}u_a}{\mathrm{d}t} = \frac{P_a}{\Omega_a \rho_a^2}\sum_b m_b \boldsymbol{v}_{ab} \cdot \nabla_a W_{ab}(h_a). \tag{43}$$

We show in Section 6.1 that including the correction terms for a variable smoothing length in this manner significantly improves the numerical wave speed in the propagation of MHD waves and enables the shock tube problems considered in paper I to be computed with no smoothing of the initial conditions.

5 MOMENTUM CONSERVATION

The equations of motion conserve linear momentum exactly. However, angular momentum is not conserved exactly because the stress force between a pair of particles is not along the line joining them. Returning to (41), and considering motion in two dimensions x and y, the change in angular momentum of the system is given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\sum_a (\boldsymbol{r}_a \times \boldsymbol{v}_a)^z = \sum_a \sum_b m_a m_b \left(\left[\bar{\sigma}_{ab}^{xx} - \bar{\sigma}_{ab}^{yy}\right] y_{ab} x_{ab} + \bar{\sigma}_{ab}^{xy}\left[y_{ab}^2 - x_{ab}^2\right]\right) F_{ab}, \tag{44}$$

where $y_{ab} = y_a - y_b$, $x_{ab} = x_a - x_b$, $\sigma^{ij} = S^{ij}/\Omega\rho^2$ and $\bar{\sigma}_{ab}^{ij} = \sigma_a^{ij} + \sigma_b^{ij}$. We have replaced ∇W_{ab} by $\boldsymbol{r}_{ab} F_{ab}$. It can be seen from (44) that if the stress is isotropic, and proportional to the identity tensor, as is the case for isotropic fluids, the rate of change of angular momentum vanishes. If, however, the stress is not proportional to the identity tensor then the total angular momentum of the system will change. It can be shown that when the summations can be converted to integrals the angular momentum is conserved exactly.

The same problem arises in the case of elastic stresses where the problem is exacerbated by the fact that the particles near the edge of a solid have densities similar to the interior and the particles do not have neighbours exterior to the solid. In this case the conservation of angular momentum is significantly in error. Bonet & Lok (1999) showed, however, that angular momentum could be conserved by altering the gradient of the kernel to a matrix operator. The astrophysical problem could be solved in the same way but we expect the astrophysical conservation to be very much better without changing the kernel, because edges are associated with low density and correspondingly low angular momentum.

6 NUMERICAL TESTS

We demonstrate the usefulness of the variable smoothing-length terms in the MHD case by the simulation of MHD waves and the shock tube problem of Brio & Wu (1988). We find that with the variable smoothing-length terms included it is better to use (40) to update the magnetic field rather than (39) since we find that using (39) can lead to negative thermal energies in the shock tube problem. The results shown use the total energy equation (as in paper I) although similar results are obtained when the thermal energy is integrated.

6.1 MHD waves

The equations of magnetohydrodynamics admit three 'families' of waves, the so-called slow, Alfvén and fast waves (Appendix A). The tests presented here are taken from Dai & Woodward (1998). We consider travelling slow and fast MHD waves propagating in a one-dimensional domain, where the velocity and magnetic field are allowed to vary in three dimensions. We use $\gamma = 5/3$ for the problems considered here. The perturbation in density is applied by perturbing the particles from an initially uniform set-up (since we use equal-mass particles). Details of this perturbation are given in Appendix B and the amplitudes for the other quantities are derived in Appendix A. We leave the artificial dissipation on for this problem, with the switch of Morris & Monaghan (1997) implemented using $K_{\min} = 0.05$ (see paper I for details of this implementation). This is to demonstrate that the switch is effective in turning off the artificial dissipation in the absence of shocks. The variable smoothing-length terms (Section 4) do not affect the wave profiles but inclusion of these terms gives very accurate numerical wave speeds.

The fast wave is shown in Fig. 1, with the dashed line giving the initial conditions. The initial amplitude is 0.55 per cent as in Dai & Woodward (1998). Results are shown at $t = 10$ for five different simulations using 32, 64, 128, 256 and 512 particles in the x-direction. The

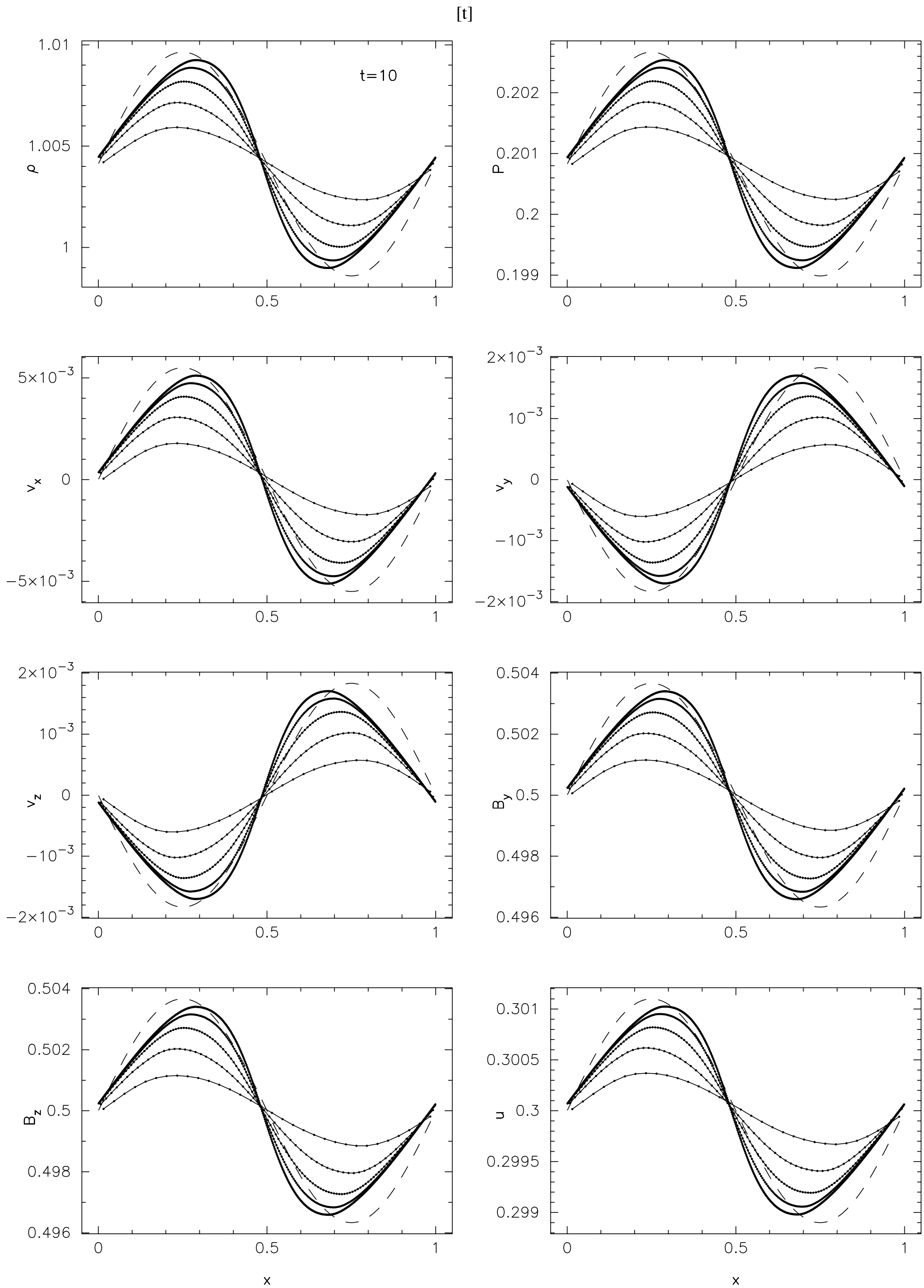

Figure 1. Results for the one-dimensional travelling fast wave problem. Initial conditions are indicated by the dashed line. Results are presented after 10 periods for simulations with 32, 64, 128, 256 and 512 particles. The fast wave speed in the gas is very close to unity which is accurately reproduced by the SPMHD solution (i.e. the numerical solution is in phase with the initial conditions). The artificial dissipation is turned on but uses the switch of Morris & Monaghan (1997) which dramatically reduces its effects away from shocks. The wave is steepened slightly by non-linear effects.

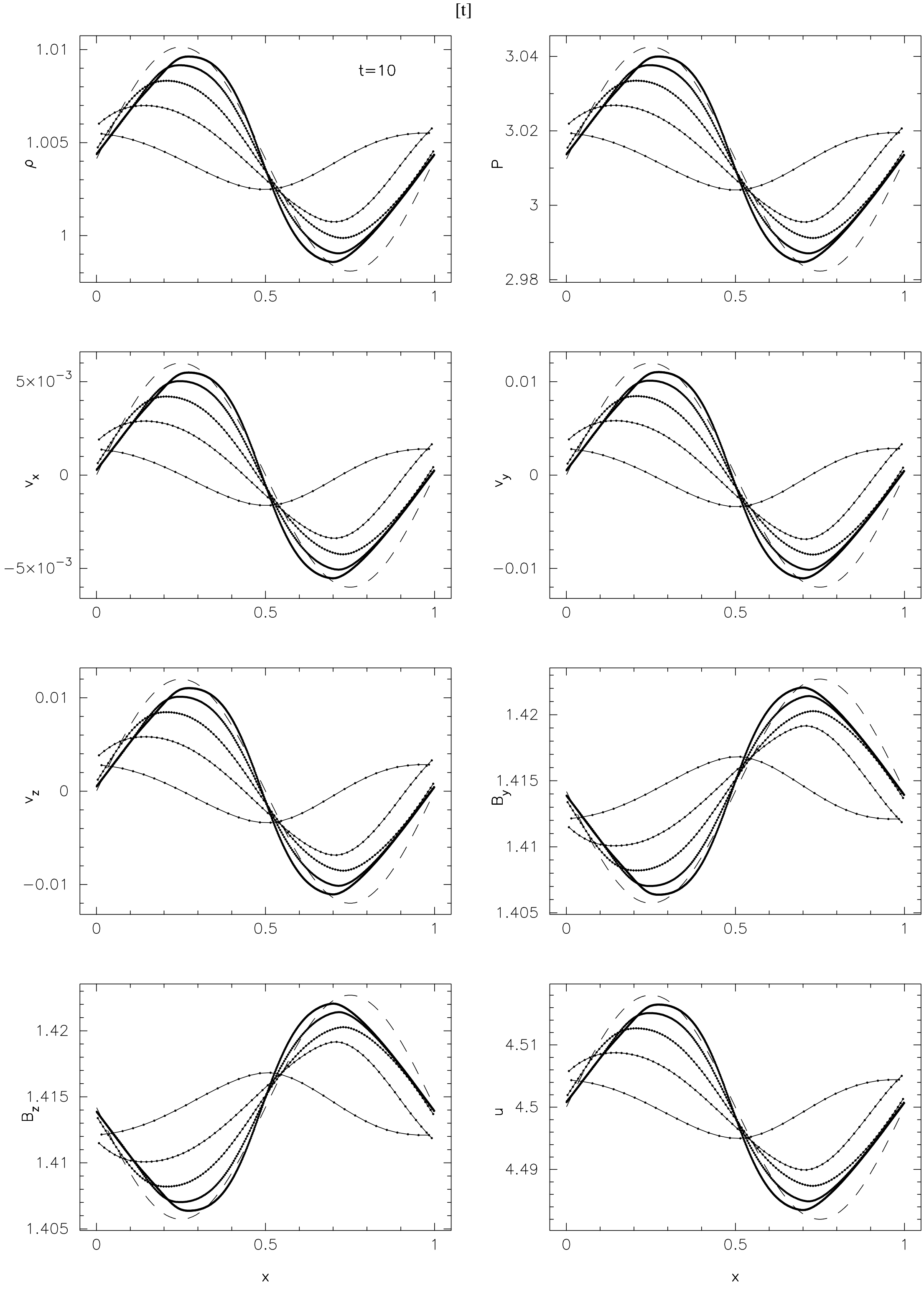

Figure 2. Results for the one-dimensional travelling slow wave problem. Initial conditions are indicated by the dashed line and results are presented after 10 periods for simulations with 32, 64, 128, 256 and 512 particles. The slow wave speed in the gas is very close to unity, such that the numerical solution at $t = 10$ should be in phase with the initial conditions. This is well represented by the SPMHD solution for the higher-resolution runs. The artificial dissipation is turned on but uses the switch of Morris & Monaghan (1997) which dramatically reduces its effects away from shocks. The wave is steepened slightly by non-linear effects.

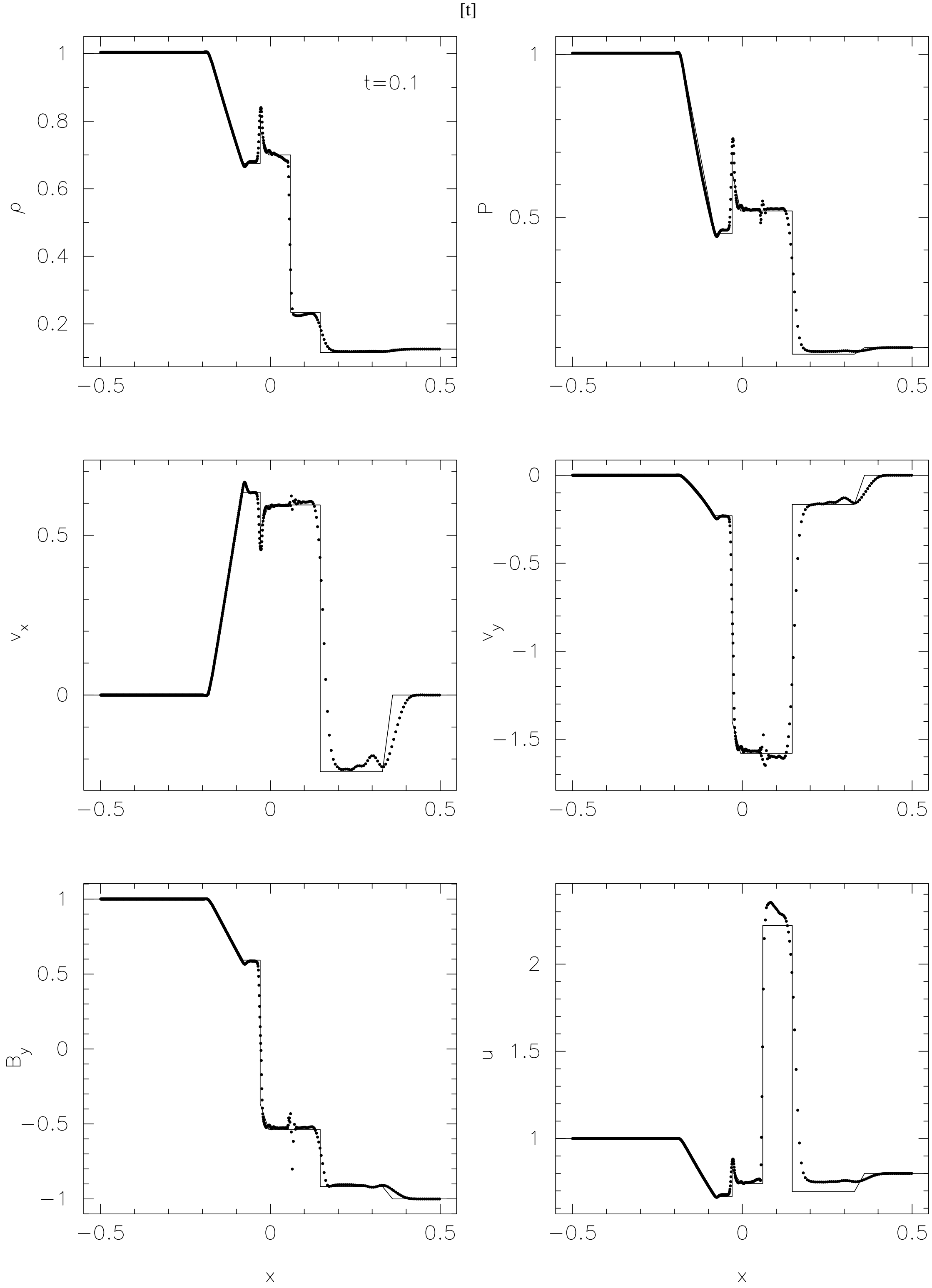

Figure 3. Results of the shock tube test of Brio & Wu (1988) with no smoothing of the initial conditions. Initial conditions to the left of the origin are given by $(\rho, P, v_x, v_y, B_y) = [1, 1, 0, 0, 1]$ and to the right by $(\rho, P, v_x, v_y, B_y) = [0.125, 0.1, 0, 0, -1]$ with $B_x = 0.75$ and $\gamma = 2.0$. Profiles of density, pressure, v_x, v_y, transverse magnetic field and thermal energy are shown at time $t = 0.1$ and may be compared with the numerical solution from Balsara (1998) given by the solid line. In this case the density summation, total energy equation and the induction equation using $\boldsymbol{B}/\rho$ have been used, incorporating the variable smoothing-length terms.

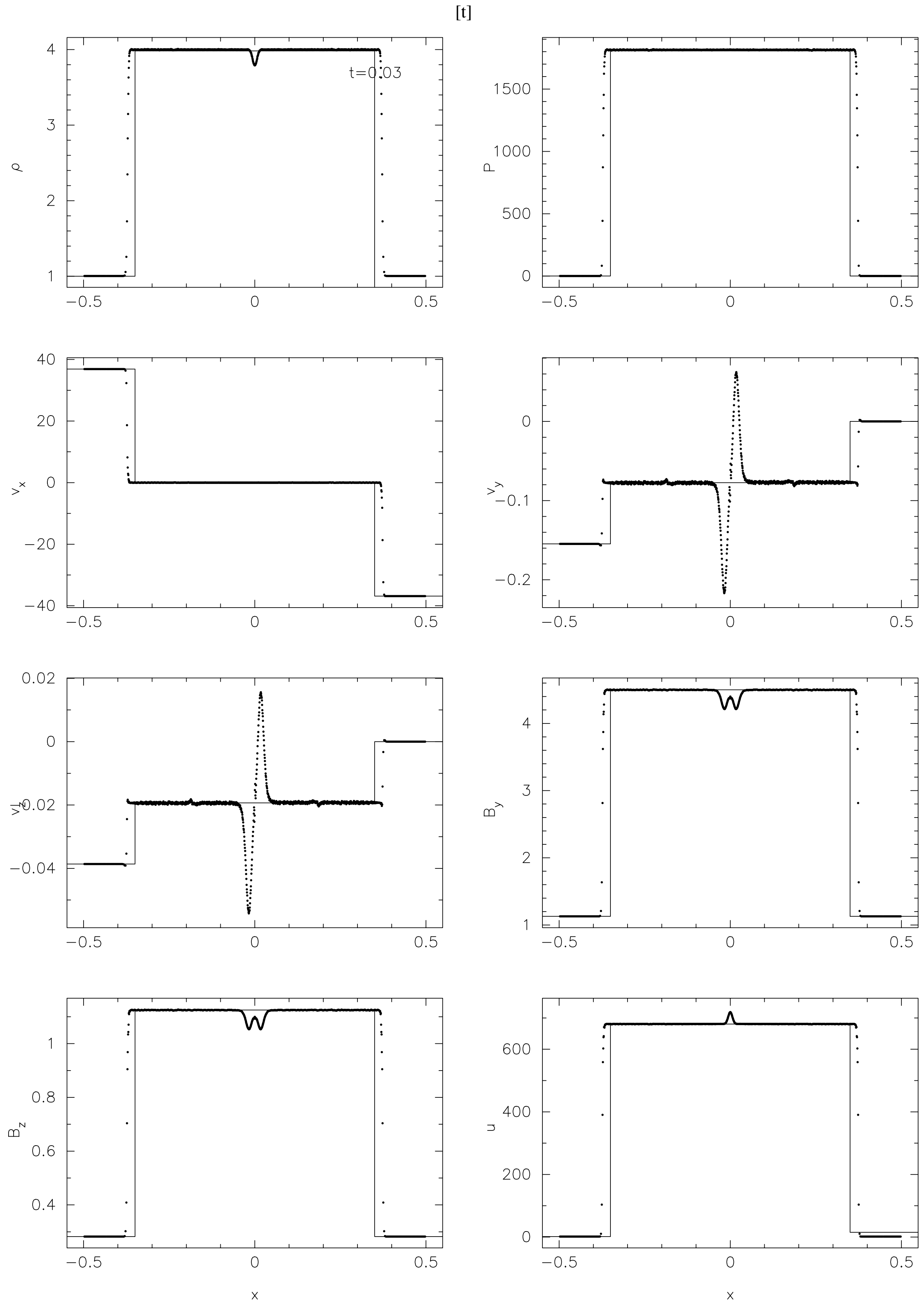

Figure 4. Results of the MHD shock tube test with initial conditions to the left of the shock given by $(\rho, P, v_x, v_y, v_z, B_y, B_z) = [1, 1, 36.87, -0.155, -0.0386, 4/(4\pi)^{1/2}, 1/(4\pi)^{1/2}]$ and to the right by $(\rho, P, v_x, v_y, v_z, B_y, B_z) = [1, 1, -36.87, 0, 0, 4/(4\pi)^{1/2}, 1/(4\pi)^{1/2}]$ with $B_x = 4.0/(4\pi)^{1/2}$ and $\gamma = 5/3$. Results are shown at time $t = 0.03$ and compare extremely well with the exact solution given by Dai & Woodward (1994) (solid line). The overshoots in density, pressure and magnetic field observed in paper I are no longer present due to our self-consistent inclusion of terms relating to the gradient of the smoothing length.

properties of the gas are set such that the fast wave speed is very close to unity, meaning that the solution at $t = 10$ should be in phase with the initial conditions. Fig. 1 demonstrates that this is accurately reproduced by the SPMHD algorithm. The effects of the small amount of dissipation present can be seen in the amount of damping present in the solutions. The small amount of steepening observed in the wave profiles is due to non-linear effects and agrees with the results presented by Dai & Woodward (1998).

The slow MHD wave is shown in Fig. 2, again with the dashed line giving the initial conditions. The perturbation amplitude is 0.6 per cent as in Dai & Woodward (1998). Results are again shown at $t = 10$ at resolutions of 32, 64, 128, 256 and 512 particles. In this case the properties of the gas are set such that the slow wave speed in the medium is very close to unity, again meaning that the solution at $t = 10$ should be in phase with the initial conditions. We see in Fig. 2 that this is reproduced by the SPMHD solution for the higher-resolution runs. The artificial dissipation is again turned on using the switch and a minimum of $K_{\min} = 0.05$. The wave is slightly overdamped in this case since we construct the artificial dissipation using the fastest wave speed (cf. paper I) which in this case is approximately three times the wave propagation speed.

6.2 Shock tube

As an additional example of the advantages of the consistent smoothing-length evolution and the variable smoothing-length terms we recalculate the shock tube test of Brio & Wu (1988) from paper I. In this case, however, we apply no smoothing whatsoever to the initial conditions and calculate the solution using the density summation (31), the total energy equation (42) and the induction equation (40). As in paper I we set up the problem using approximately 800 equal-mass particles in the domain $x = [-0.5, 0.5]$. Conditions to the left of the shock are given by $(\rho, P, v_x, v_y, B_y) = [1, 1, 0, 0, 1]$ and to the right by $(\rho, P, v_x, v_y, B_y) = [0.125, 0.1, 0, 0, -1]$ with $B_x = 0.75$ and $\gamma = 2.0$. The results are shown in Fig. 3 at time $t = 0.1$ and may be compared with the numerical solution from Balsara (1998) given by the solid line. The results may also be compared with Fig. 2 in paper I. The non-smoothed initial conditions result in a small starting error at the contact discontinuity and a small overshoot at the end of the rarefaction wave; however, the compound wave in particular is significantly less spread out than in the results given in paper I. The consistent update of the smoothing length discussed in Section 4 results in some extra iterations of the density (for most of the simulation two passes over the density summation are used).

As a final example we also recompute the shock tube test shown in Fig. 7 of paper I. The initial conditions to the left of the shock are given by $(\rho, P, v_x, v_y, v_z, B_y, B_z) = [1, 1, 36.87, -0.155, -0.0386, 4/(4\pi)^{1/2}, 1/(4\pi)^{1/2}]$ and to the right by $(\rho, P, v_x, v_y, v_z, B_y, B_z) = [1, 1, -36.87, 0, 0, 4/(4\pi)^{1/2}, 1/(4\pi)^{1/2}]$ with $B_x = 4.0/(4\pi)^{1/2}$ and $\gamma = 5/3$, resulting in two extremely strong fast shocks which propagate away from the origin. The resolution varies from 400 to 1286 particles throughout the simulation due to the inflow boundary conditions. Results are shown in Fig. 4 at time $t = 0.03$ and compare extremely well with the exact solution given by Dai & Woodward (1994) (solid lines). In paper I the post-shock density and transverse magnetic field components were observed to overshoot the exact solution. In Fig. 4 we observe that these effects are no longer present when the variable smoothing-length terms are self-consistently accounted for.

7 SUMMARY

In summary, we have shown that

(i) The equations of motion and energy for SPMHD can be derived from a variational principle using the continuity and induction equations as constraints. This demonstrates that the equation set is consistent and the resulting equations conserve linear momentum and energy exactly. In the MHD case this also demonstrates that the treatment of source terms proportional to $\nabla \cdot \boldsymbol{B}$ is consistent, as discussed in paper I with reference to Janhunen (2000) and Dellar (2001).

(ii) The correction terms for a variable smoothing length may be derived naturally from a variational approach. Accounting for these terms is shown to improve the accuracy of SPH wave propagation.

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REFERENCES

Balsara D. S., 1998, ApJS, 116, 133
Benz W., 1990, in Buchler J. R., ed., The numerical modelling of non-linear stellar pulsations. Kluwer, Dordrecht, p. 269
Bonet J., Lok T.-S. L., 1999, Comput. Meth. Appl. Mech. Eng., 180, 97
Brio M., Wu C. C., 1988, J. Comp. Phys., 75, 400
Dai W., Woodward P. R., 1994, J. Comp. Phys., 115, 485
Dai W., Woodward P. R., 1998, ApJ, 494, 317
Dellar P. J., 2001, J. Comp. Phys., 172, 392
Field G., 1986, in Epstein R., Feldman W., eds, AIP Conf. Proc. 144, Magnetospheric Phenomena in Astrophysics. Am. Inst. Phys., Woodbury, NY, p. 324
Henyey F. S., 1982, Phys. Rev. A, 26, 480
Hernquist L., Katz N., 1989, ApJS, 70, 419

Janhunen P., 2000, J. Comp. Phys., 160, 649
Monaghan J. J., 1992, Ann. Rev. Astron. Astrophys., 30, 543
Monaghan J. J., 2000, J. Comp. Phys., 159, 290
Monaghan J. J., 2002, MNRAS, 335, 843
Monaghan J. J., Price D. J., 2001, MNRAS, 328, 381
Morris J. P., Monaghan J. J., 1997, J. Comp. Phys., 136, 41
Nelson R., 1994, Mem. Soc. Astron. Ital., 65, 1161
Nelson R. P., Papaloizou J. C. B., 1994, MNRAS, 270, 1
Newcomb W. A., 1962, Nucl. Fusion Suppl., 2, 451
Oppeneer P. M., 1984, Phys. Lett. A, 104, 207
Phillips G. J., Monaghan J. J., 1985, MNRAS, 216, 883
Price D. J., Monaghan J. J., 2003, MNRAS, accepted (Paper I)
Serna A., Alimi J.-M., Chieze J.-P., 1996, ApJ, 461, 884
Springel V., Hernquist L., 2002, MNRAS, 333, 649

APPENDIX A: LINEAR WAVES IN MHD

In this section we describe the set-up used for the MHD waves described in Section 6.1. The MHD equations in continuum form may be written as

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\rho\nabla\cdot\boldsymbol{v} \quad \text{(A1)}$$

$$\frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} = -\frac{\nabla P}{\rho} - \frac{\boldsymbol{B}\times(\nabla\times\boldsymbol{B})}{\mu_0\rho} \quad \text{(A2)}$$

$$\frac{\mathrm{d}\boldsymbol{B}}{\mathrm{d}t} = (\boldsymbol{B}\cdot\nabla)\boldsymbol{v} - \boldsymbol{B}(\nabla\cdot\boldsymbol{v}) \quad \text{(A3)}$$

together with the divergence constraint $\nabla\cdot\boldsymbol{B} = 0$. We perturb according to

$$\rho = \rho_0 + \delta\rho$$
$$\boldsymbol{v} = \boldsymbol{v}$$
$$\boldsymbol{B} = \boldsymbol{B}_0 + \delta\boldsymbol{B}$$
$$\delta P = c_s^2\delta\rho \quad \text{(A4)}$$

where $c_s^2 = \gamma P_0/\rho_0$ is the sound speed. Considering only linear terms, the perturbed equations are therefore given by

$$\frac{\mathrm{d}(\delta\rho)}{\mathrm{d}t} = -\rho_0(\nabla\cdot\boldsymbol{v}) \quad \text{(A5)}$$

$$\frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} = -c_s^2\frac{\nabla(\delta\rho)}{\rho_0} - \frac{\boldsymbol{B}_0\times(\nabla\times\delta\boldsymbol{B})}{\mu_0\rho_0} \quad \text{(A6)}$$

$$\frac{\mathrm{d}(\delta\boldsymbol{B})}{\mathrm{d}t} = (\boldsymbol{B}_0\cdot\nabla)\boldsymbol{v} - \boldsymbol{B}_0(\nabla\cdot\boldsymbol{v}). \quad \text{(A7)}$$

Specifying the perturbation according to

$$\delta\rho = D\mathrm{e}^{\mathrm{i}(\boldsymbol{k}\cdot x-\omega t)}$$
$$\boldsymbol{v} = \boldsymbol{v}\mathrm{e}^{\mathrm{i}(\boldsymbol{k}\cdot x-\omega t)}$$
$$\delta\boldsymbol{B} = \boldsymbol{b}\mathrm{e}^{\mathrm{i}(\boldsymbol{k}\cdot x-\omega t)} \quad \text{(A8)}$$

we have

$$-\omega D = -\rho_0(\boldsymbol{v}\cdot\boldsymbol{k}) \quad \text{(A9)}$$

$$-\omega\boldsymbol{v} = -c_s^2\frac{D\boldsymbol{k}}{\rho_0} - \frac{1}{\mu_0\rho_0}\left[(\boldsymbol{B}_0\cdot\boldsymbol{b})\boldsymbol{k} - (\boldsymbol{B}_0\cdot\boldsymbol{k})\boldsymbol{b}\right] \quad \text{(A10)}$$

$$-\omega\boldsymbol{b} = (\boldsymbol{B}_0\cdot\boldsymbol{k})\boldsymbol{v} - \boldsymbol{B}_0(\boldsymbol{k}\cdot\boldsymbol{v}). \quad \text{(A11)}$$

Considering only waves in the x-direction (i.e. $\boldsymbol{k} = [k_x, 0, 0]$), defining the wave speed $v = \omega/k$ and using (A9) to eliminate D, equation (A10) gives

$$v_x\left(v - \frac{c_s^2}{v}\right) = \left(\frac{B_{y0}b_y + B_{z0}b_z}{\mu_0\rho_0}\right) \quad \text{(A12)}$$

$$vv_y = -\frac{B_{x0}b_y}{\mu_0\rho_0} \quad \text{(A13)}$$

$$vv_z = -\frac{B_{x0}b_z}{\mu_0\rho_0} \quad \text{(A14)}$$

where $b_x = 0$ since $\nabla \cdot \boldsymbol{B} = 0$. Using these in (A11) we have

$$vb_y = -B_{x0}v_y + B_{y0}v_x \tag{A15}$$

$$vb_z = -B_{x0}v_z + B_{z0}v_x. \tag{A16}$$

We can therefore solve for the perturbation amplitudes v_x, v_y, v_z, b_y and b_z in terms of the amplitude of the density perturbation D and the wave speed v. We find

$$v_x = \frac{vD}{\rho} \tag{A17}$$

$$v_y\left(v^2 - \frac{B_x^2}{\mu_0\rho}\right) = \frac{B_x B_y}{\mu_0\rho}v_x \tag{A18}$$

$$v_z\left(v^2 - \frac{B_x^2}{\mu_0\rho}\right) = \frac{B_x B_z}{\mu_0\rho}v_x \tag{A19}$$

$$b_y\left(v^2 - \frac{B_x^2}{\mu_0\rho}\right) = vB_y v_x \tag{A20}$$

$$b_z\left(v^2 - \frac{B_x^2}{\mu_0\rho}\right) = vB_z v_x \tag{A21}$$

where we have dropped the subscript 0. The wave speed v is found by eliminating these quantities from (A12), giving

$$\frac{v_x}{\left(v^2 - B_x^2/\mu_0\rho\right)}\left[v^4 - v^2\left(c_s^2 + \frac{B_x^2 + B_y^2 + B_z^2}{\mu_0\rho}\right) + \frac{c_s^2 B_x^2}{\mu_0\rho}\right] = 0, \tag{A22}$$

which reveals the three wave types in MHD. The Alfvén waves are those with

$$v^2 = \frac{B_x^2}{\mu_0\rho}. \tag{A23}$$

These are transverse waves which travel along the field lines. The term in square brackets in (A22) gives a quartic for v (or a quadratic for v^2), with roots

$$v^2 = \frac{1}{2}\left[\left(c_s^2 + \frac{B_x^2 + B_y^2 + B_z^2}{\mu_0\rho}\right) \pm \sqrt{\left(c_s^2 + \frac{B_x^2 + B_y^2 + B_z^2}{\mu_0\rho}\right)^2 - 4\frac{c_s^2 B_x^2}{\mu_0\rho}}\right], \tag{A24}$$

which are the fast (+) and slow (−) magnetosonic waves.

APPENDIX B: DENSITY PERTURBATION IN SPH

The perturbation in density is applied by perturbing the particles from an initially uniform set-up. We consider the one-dimensional perturbation

$$\rho = \rho_0[1 + A\sin(kx)], \tag{B1}$$

where $A = D/\rho_0$ is the perturbation amplitude. The cumulative total mass in the x-direction is given by

$$\begin{aligned} M(x) &= \rho_0 \int [1 + A\sin(kx)]\,\mathrm{d}x \\ &= \rho_0[x - A\cos(kx)]_0^x, \end{aligned} \tag{B2}$$

such that the cumulative mass at any given point as a fraction of the total mass is given by

$$\frac{M(x)}{M(x_{\max})}. \tag{B3}$$

For equal-mass particles distributed in $x = [0, x_{\max}]$ the cumulative mass fraction at particle a is given by $x_a/x_{\max}$ such that the particle position may be calculated using

$$\frac{x_a}{x_{\max}} = \frac{M(x_a)}{M(x_{\max})}. \tag{B4}$$

Substituting the expression for $M(x)$ we have the following equation for the particle position:

$$\frac{x_a}{x_{\rm max}} - \frac{x_a - A\cos(kx_a)}{[x_{\rm max} - {\rm A}\cos(kx_{\rm max})]} = 0, \tag{B5}$$

which we solve iteratively using a simple Newton–Raphson root-finder. With the uniform particle distribution as the initial conditions this converges in one or two iterations.

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