Variational principles for relativistic smoothed particle hydrodynamics

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ABSTRACT

In this paper we show how the equations of motion for the smoothed particle hydrodynamics (SPH) method may be derived from a variational principle for both non-relativistic and relativistic motion when there is no dissipation. Because the SPH density is a function of the coordinates the derivation of the equations of motion through variational principles is simpler than in the continuum case where the density is defined through the continuity equation. In particular, the derivation of the general relativistic equations is more direct and simpler than that of Fock. The symmetry properties of the Lagrangian lead immediately to the familiar additive conservation laws of linear and angular momentum and energy. In addition, we show that there is an approximately conserved quantity which, in the continuum limit, is the circulation.

Key words: relativity - methods: numerical.

1 INTRODUCTION

Approximate equations of motion are better if they incorporate important properties of the original system (for a discussion of this point for Hamiltonian systems see Salmon 1988). These important properties include the conservation laws of momentum and energy and, for barytropic fluids with conservative body forces, the conservation of circulation.

Smoothed particle hydrodynamics (SPH, for a review see Monaghan 1992) is an approximation to the continuum equations of fluid dynamics that can be written in a form which conserves linear and angular momentum. If the external forces are conservative the energy is also conserved. The SPH equations therefore, although approximate, retain these desirable features of the original equations. If the pressure is a function of the density, and there is no dissipation, then the fluid equations have another invariant, the circulation. The circulation invariant is actually an infinite number of invariants because it constrains the circulation around *any* closed path. In the fluid dynamics of either incompressible or barytropic fluids the circulation places a severe constraint on the allowed motion. In astrophysics the circulation is less important because the pressure is usually not a function of the density alone, and dissipation results in changes in the vorticity and the circulation. However, there are examples where the circulation is important. For example when the gas is isothermal or degenerate, or the motion is adiabatic.

It would therefore be desirable if a form of SPH could be found that conserves circulation. However, because SPH is a particle method it is not clear whether a circulation theorem exists or to what extent it is an approximation. For example, the fluid equations are derived from a classical version of molecular dynamics which can in turn be derived from a Lagrangian with the classical additive invariants of momentum and energy. Where then is the circulation theorem hidden, or is it the result of the statistical averaging leading to the continuum equations?

In this paper we establish the conservation laws directly from a Lagrangian and we show how the circulation theorem can be derived. The SPH Lagrangians for the relativistic case can be easily established and with them the equations of motion and the conservation laws. In the case of general relativity the SPH Lagrangian leads to the equations of motion in a manner which is both simpler and more direct than the classic analysis of Fock (1964).

The SPH equations of motion can also be written in Hamiltonian form. Then, because the phase space of the SPH particles is finite the system satisfies Liouville's equation and the Poincaré invariants. The extent to which this Hamiltonian structure can be made the basis of estimate of chaos and the statistical equilibrium of a fluid system without dissipation is not known, but it SPH would seem to provide a transparent formalism for such an investigation.

2 THE NON-RELATIVISTIC LAGRANGIAN

2.1 Equations of motion

The reader is assumed to be familiar with the basic ideas of SPH (see Monaghan 1992 for a review). The Lagrangian for non-relativistic fluid dynamics, with self gravity can be based on Eckart's (1960) Lagrangian

$$L = \int \rho \left[\frac{1}{2} \boldsymbol{v} \cdot \boldsymbol{v} - u(\rho, s) \right] dV,$$
(2.1)

where \boldsymbol{v} is the velocity, ρ is the density, *s* is the entropy and $u(\rho, s)$ is the thermal energy per unit mass. The integration is over the volume. In the SPH formalism the density can be written as a function of the masses of the particles and their coordinates. For particle *b* the density ρ_b is given by

$$\rho_b = \sum_k m_k W(|\mathbf{r}_b - \mathbf{r}_k|), \tag{2.2}$$

where m_k is the mass of particle k, r_k is the coordinate vector of particle k and W is a smoothing kernel. The summation is over all particles although the kernel vanishes beyond a specified distance and only neighbours contribute. It is the fact that the density can be defined as a function of the coordinates, rather than through the equation of continuity, that simplifies the derivation of the equations of motion from a variational principle.

The SPH form of (2.1), generalized to include self gravity, is

$$L = \sum_{b} m_{b} \left[\frac{1}{2} v_{b}^{2} - u(\rho_{b}, s_{b}) + \frac{1}{2} G \sum_{k} \frac{m_{k}}{|\mathbf{r}_{b} - \mathbf{r}_{k}|} \right].$$
(2.3)

with

$$\frac{\mathrm{d}\boldsymbol{r}_b}{\mathrm{d}t} = \boldsymbol{v}_b. \tag{2.4}$$

Lagrange's equations of motion follow from varying the action keeping the entropy of each particle constant. Lagrange's equations for particle a are

$$\frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{\partial L}{\partial \boldsymbol{v}_a} \right) - \frac{\partial L}{\partial \boldsymbol{r}_a} = 0. \tag{2.5}$$

The canonical momentum is

$$\boldsymbol{p}_a = \frac{\partial L}{\partial \boldsymbol{v}_a} = m_a \boldsymbol{v}_a \tag{2.6}$$

and

$$\frac{\partial L}{\partial \boldsymbol{r}_a} = -\sum_b m_b \left(\frac{\partial u_b}{\partial \rho_b}\right)_s \left(\frac{\partial \rho_b}{\partial \boldsymbol{r}_a}\right) - G \sum_b m_b \frac{(\boldsymbol{r}_a - \boldsymbol{r}_b)}{|\boldsymbol{r}_a - \boldsymbol{r}_b|^3}.$$
(2.7)

From equation (2.2)

$$\frac{\partial \rho_b}{\partial r_a} = \sum_k m_k \frac{\partial W_{bk}}{\partial r_a} (\delta_{ba} - \delta_{ka}), \tag{2.8}$$

and from the first law of thermodynamics

$$\left(\frac{\partial u}{\partial \rho}\right)_s = \frac{P}{\rho^2},\tag{2.9}$$

where *P* is the pressure (which can be calculated once the form of $u(\rho, s)$ is given).

Using these results Lagrange's equations for particle *a* can be written

$$\frac{\mathrm{d}\boldsymbol{v}_a}{\mathrm{d}t} = -\sum_b m_b \left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2}\right) \nabla_a W_{ab} - G \sum_b m_b \frac{(\boldsymbol{r}_a - \boldsymbol{r}_b)}{|\boldsymbol{r}_a - \boldsymbol{r}_b|^3},\tag{2.10}$$

where ∇_a denotes the gradient taken with respect to the coordinates of particle *a*. W_{ab} denotes $W(|\mathbf{r}_a - \mathbf{r}_b|)$. Equation (2.10) is the SPH

equivalent of

$$\frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} = -\frac{P}{\rho^2}\nabla\rho - \nabla\left(\frac{P}{\rho}\right) - \nabla\Phi,$$

$$= -\frac{1}{\rho}\nabla P - \nabla\Phi,$$
(2.11)
(2.12)

where Φ is the gravitational potential. These results show that Lagrange's equations lead to the standard non-dissipative SPH equations of fluid dynamics. If we had chosen a separate resolution length *h* for each particle then the equation of motion would have been identical to that above except that the gradient of the kernel would have been replaced by

$$\frac{1}{2}(W(|\mathbf{r}_{a} - \mathbf{r}_{b}|, h_{a}) + W(|\mathbf{r}_{a} - \mathbf{r}_{b}|, h_{b})),$$
(2.13)

where the resolution lengths h_a and h_b are shown explicitly. In practice, the resolution length is required to change during the motion. For the present we assume the resolution lengths are constant. The effect of changes in h on the equations of motion is usually small.

2.2 Conservation laws

2.2.1 Additive integrals

The symmetry of the Lagrangian leads immediately to the conservation laws. In particular, in the present case where the entropy is constant, and the summation for the density is invariant to translations and rotations, linear and angular momentum are conserved. For example, if each particle is given an arbitrary infinitesimal translation q, the change in L is

$$\delta L = \sum_{b} \frac{\partial L}{\partial \boldsymbol{r}_{b}} \cdot \boldsymbol{q} = \boldsymbol{q} \cdot \sum_{b} \frac{\partial L}{\partial \boldsymbol{r}_{b}},$$
(2.14)

from which, using Lagrange's equations, the total linear momentum

$$\sum_{b} \frac{\partial L}{\partial \boldsymbol{v}_{b}} = \sum_{b} m_{b} \boldsymbol{v}_{b}, \tag{2.15}$$

is conserved. Other examples are given by Landau & Lifshitz (1976). The invariance of L to a discrete shift in the time shows that the energy

$$E = \sum_{b} \boldsymbol{v}_{b} \cdot \frac{\partial L}{\partial \boldsymbol{v}_{b}} - L \tag{2.16}$$

$$=\sum_{b}m_{b}\left(\frac{1}{2}v_{b}^{2}+u_{b}+\Phi\right).$$
(2.17)

is conserved.

2.2.2 The circulation

The particle system is invariant to other transformations. Consider, for example Fig. 1 which shows a set of particles each with the same mass



Figure 1. A set of particles each with the same mass and entropy and a marked loop.

and entropy and a marked loop. Imagine each particle in the loop being shifted to its neighbour's position (in the same sense around the loop) and given its neighbour's velocity. Since the entropy is constant, nothing has changed, and the Lagrangian is therefore invariant to this transformation.

The changes in L can be approximated by

$$\delta L = \sum_{c} \left(\frac{\partial L}{\partial \boldsymbol{r}_{c}} \cdot \delta \boldsymbol{r}_{c} + \frac{\partial L}{\partial \boldsymbol{v}_{c}} \cdot \delta \boldsymbol{v}_{c} \right), \tag{2.18}$$

where c denotes the label of a particle on the loop. The change in position and velocity are given by

$$\delta \mathbf{r}_c = \mathbf{r}_{c+1} - \mathbf{r}_c, \tag{2.19}$$

and

 $\delta \boldsymbol{v}_c = \boldsymbol{v}_{c+1} - \boldsymbol{v}_c. \tag{2.20}$

Using Lagrange's equations (2.5) we can rewrite (2.18) in the form

$$\sum_{c} m_{c} \left[\frac{\mathrm{d}\boldsymbol{v}_{c}}{\mathrm{d}t} \cdot (\boldsymbol{r}_{c+1} - \boldsymbol{r}_{c}) + \boldsymbol{v}_{c} \cdot (\boldsymbol{v}_{c+1} - \boldsymbol{v}_{c}) \right] = 0,$$
(2.21)

and recalling that the particle masses are assumed identical, we deduce that

$$\frac{\mathrm{d}}{\mathrm{d}t}\sum_{c}\boldsymbol{v}_{c}\cdot(\boldsymbol{r}_{c+1}-\boldsymbol{r}_{c})=0.$$
(2.22)

so that

$$C = \sum_{c} \boldsymbol{v}_{c} \cdot (\boldsymbol{r}_{c+1} - \boldsymbol{r}_{c}), \tag{2.23}$$

is conserved to this approximation, for every loop. The conservation is only approximate because the change to the Lagrangian is discrete, and only approximated by the first order terms. However, if the particles are sufficiently close together (2.23) approximates the circulation theorem to arbitrary accuracy. A related argument was used by Feynman (1957) to establish from the invariance of the wave function that circulation should be quantized in quantum fluids. These results are mirrored in Salmon's (1988) analysis of Lagrangian and Hamiltonian methods in fluid mechanics. Salmon (1988), following Bretherton's (1970) work, establishes the conservation laws by appealing to the invariance to particle interchange. However, because their analysis is within the context of the continuum, it is more complicated than the derivation given above.

The system is also invariant to the particles shifting around the loop in the opposite sense. This gives an approximation to the circulation with the opposite sign to that above. If these two are combined (taking account of their signs so we subtract one from the other) we get

$$\frac{d}{dt} \sum_{c} \boldsymbol{v}_{c} \cdot \frac{(\boldsymbol{r}_{c+1} - \boldsymbol{r}_{c-1})}{2} = 0.$$
(2.24)

which is a better approximation to the circulation of the continuous fluid.

The accuracy of the approximate circulation invariant can be estimated easily for simple systems of particles. For example, if there are no forces the velocity is constant and the rate of change of circulation from (2.21) is

$$\sum_{c} \boldsymbol{v}_{c} \cdot (\boldsymbol{v}_{c+1} - \boldsymbol{v}_{c-1}), \tag{2.25}$$

which vanishes on summing around the loop. Another example is the rate of change of C for a set of particles of equal mass on the same circular orbit of radius r about a much more massive object of mass M. It is given by

$$\frac{\mathrm{d}C}{\mathrm{d}t} = \sum_{c} \left[-\frac{GM\boldsymbol{r}_{c}}{r^{3}} \cdot (\boldsymbol{r}_{c+1} - \boldsymbol{r}_{c-1}) + \boldsymbol{v}_{c} \cdot (\boldsymbol{v}_{c+1} - \boldsymbol{v}_{c-1}) \right],\tag{2.26}$$

and this vanishes on summing around the orbit.

If the particles are on an ellipse about the central massive object, then the rate of change of C does not vanish exactly. It is easy to show, however, that the error is second order in the spacing, and approximately third order if the change in spacing from one pair to the next is much less than the spacing.

2.2.3 Liouville's theorem and Poincaré invariants

The equations of motion can easily be written in Hamiltonian form with the Hamiltonian

$$H = \sum_{a} m_a \left(\frac{p_a^2}{2m_a^2} + u_a\right),\tag{2.27}$$

with the canonical momentum p_a defined by (2.6). If there are *n* SPH particles then the phase space has canonical coordinates $r_1, r_2, ..., r_n$ and canonical momenta $p_1, p_2, ..., p_n$. Louiville's theorem then shows that

$$\iint \dots \int d\mathbf{r}_1 \, d\mathbf{r}_2 \dots d\mathbf{r}_n \, d\mathbf{p}_1 \, d\mathbf{p}_2 \dots d\mathbf{p}_n \tag{2.28}$$

is invariant. In (2.28) dr denotes dx dy dz and dp denotes $dp_x dp_y dp_z$ for a three-dimensional Cartesian coordinate system. The Poincaré invariants involving integrals on sub-manifolds, e.g. the integral over a manifold of two dimensions

$$\iint \sum_{a} \mathrm{d}q_a \,\mathrm{d}p_a,\tag{2.29}$$

is invariant. These integral invariants apply to an ensemble of systems. Accordingly, if we set up a dense set of replica SPH systems, the volume in phase space associated with the replica systems will remain invariant. This idea is used as a basis for statistical mechanics and raises the interesting question of the equilibrium state of a non-dissipative fluid, and how that state might be related to the additive invariants and the approximate circulation invariant.

The existence of the Hamiltonian also suggests that the powerful Hamiltonian methods for analysing dynamical systems might be applied to non-dissipative fluids.

2.3 The particle energy equation

The rate of change of total energy per unit mass $\hat{\epsilon}$ can be found easily from the expression for the total energy by writing E as $\sum_{a} m_a \hat{\epsilon}_a$ where

$$\hat{\boldsymbol{\epsilon}} = \frac{1}{2}\boldsymbol{v}^2 + \boldsymbol{u} + \boldsymbol{\Phi}. \tag{2.30}$$

Thus

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \sum_{a} m_a \frac{\mathrm{d}\hat{\epsilon}_a}{\mathrm{d}t} = \sum_{a} m_a \left[\boldsymbol{v}_a \frac{\mathrm{d}\boldsymbol{v}_a}{\mathrm{d}t} + \left(\frac{\partial u_a}{\partial \rho_a}\right)_s \frac{\mathrm{d}\rho_a}{\mathrm{d}t} + \frac{\mathrm{d}\Phi_a}{\mathrm{d}t} \right].$$
(2.31)

Using the acceleration equation, the rate of change of the density, and the expression for the gravitational potential energy we find

$$\sum_{a} m_{a} \frac{\mathrm{d}\hat{\epsilon}_{a}}{\mathrm{d}t} = -\sum_{a} \sum_{b} m_{a} m_{b} \left(\frac{P_{a}}{\rho_{a}^{2}} \boldsymbol{v}_{b} + \frac{P_{b}}{\rho_{b}^{2}} \boldsymbol{v}_{a} \right) \nabla_{a} W_{ab} - \sum_{a} \sum_{b} m_{a} m_{b} \frac{G(\boldsymbol{v}_{ab} \cdot \boldsymbol{r}_{ab})}{r_{ab}^{3}}.$$
(2.32)

We can then identify

$$\frac{\mathrm{d}\hat{\boldsymbol{\epsilon}}_{a}}{\mathrm{d}t} = -\sum_{b} m_{b} \left(\frac{P_{a}}{\rho_{a}^{2}} \boldsymbol{v}_{b} + \frac{P_{b}}{\rho_{b}^{2}} \boldsymbol{v}_{a} \right) \nabla_{a} W_{ab} - \sum_{b} m_{b} \frac{G(\boldsymbol{v}_{ab} \cdot \boldsymbol{r}_{ab})}{r_{ab}^{3}}.$$
(2.33)

This expression is the SPH equivalent of

$$\frac{\mathrm{d}\hat{\boldsymbol{\epsilon}}}{\mathrm{d}t} = -\frac{P}{\rho^2} \nabla \cdot (\rho \boldsymbol{v}) - \boldsymbol{v} \cdot \nabla \left(\frac{P}{\rho}\right) + \frac{\mathrm{d}\Phi}{\mathrm{d}t}$$
(2.34)

$$= -\frac{1}{\rho}\nabla \cdot (P\boldsymbol{v}) + \frac{\mathrm{d}\Phi}{\mathrm{d}t},\tag{2.35}$$

which is the usual energy equation.

3 THE SPECIAL RELATIVITY LAGRANGIAN

3.1 Equations of motion

The SPH special relativity equations have been deduced from the continuum relativistic hydrodynamic equations by Chow & Monaghan (1997) using SPH approximations to the spatial derivatives.

It is convenient to consider the fluid as composed of baryons each with the same rest mass m_0 and then scale the energy with m_0c^2 and

the velocity with the speed of light c. We require the relativistic action to be Lorentz invariant and this requires the Lagrangian L to be the integral of a Lorentz invariant quantity over volume. It is easy to guess that the Lagrangian is

$$L = -\int T^{\mu\nu} U_{\mu} U_{\nu} \,\mathrm{d}V,\tag{3.1}$$

where U_{μ} is the four-velocity, and $T^{\mu\nu}$ is the energy-momentum tensor defined by

$$T^{\mu\nu} = (n + nu(n, s) + P)U^{\mu}U^{\nu} + P\eta^{\mu\nu},$$
(3.2)

where *n* is the baryon number density, u(n, s) is the thermal energy per baryon and *P* is the pressure. These quantities are defined in the rest frame of the element of fluid being considered. The metric tensor $\eta^{\mu\nu}$ has signature (-1,1,1,1). The Lagrangian can be simplified to

$$L = -\int n[1 + u(n, s)] \,\mathrm{d}V.$$
(3.3)

The SPH formalism will be set up in a selected frame which we call the computing frame. In this frame the baryon number density is *N* and it is related to *n* according to

$$N = nU^0 = n\gamma = \frac{n}{\sqrt{(1 - v^2)}},$$
(3.4)

where \boldsymbol{v} is the velocity of the fluid relative to the computing frame and γ is the usual Lorentz factor.

The SPH interpolation in the computing frame is based on the integral interpolant

$$A_{I}(\mathbf{r}) = \int A(\mathbf{r}') W(|\mathbf{r} - \mathbf{r}'|) \, \mathrm{d}V', \tag{3.5}$$

where

0

$$\int W(|\mathbf{r} - \mathbf{r}'|) \, \mathrm{d}V' = 1.$$
(3.6)

The integral interpolant (3.5) can be approximated by subdividing the space into small volumes such that the small volume ΔV_b contains $\nu_b = N_b \Delta V_b$ baryons. Replacing the integral by summation over the elements of volume we get the summation interpolant

$$A(\mathbf{r}) = \sum_{b} A_b \frac{\nu_b}{N_b} W(|\mathbf{r} - \mathbf{r}_b|), \tag{3.7}$$

As an example the number density is given by

$$N(\mathbf{r}) = \sum_{b} \nu_b W(|\mathbf{r} - \mathbf{r}_b|), \tag{3.8}$$

and from (3.6)

$$\int N(\mathbf{r}) \,\mathrm{d}V = \sum_{b} \nu_b,\tag{3.9}$$

which shows that the total number of baryons is conserved.

All integrals over a volume can be replaced by summations over the SPH particles. The Lagrangian (3.3) can then be approximated by

$$L = -\sum_{b} \frac{\nu_{b} n_{b}}{N_{b}} (1 + u_{b}), \tag{3.10}$$

$$= -\sum_{b} \nu_b \sqrt{(1 - v_b^2)} (1 + u_b).$$
(3.11)

The relativistic SPH equations can now be obtained from Lagrange's equations. We first need the partial derivatives of *L* with respect to the velocity and to the coordinates. The velocity occurs both in the square root factor in *L* and in *u* through the dependence of the thermal energy on $n = N/\gamma$. We find for particle *a*

$$\frac{\partial L}{\partial \boldsymbol{v}_a} = \nu_a \gamma_a \boldsymbol{v}_a (1+u_a) - \nu_a \sqrt{(1-v_a^2)} \left(\frac{\partial u_a}{\partial \boldsymbol{v}_a}\right)_{s,\boldsymbol{r}}.$$
(3.12)

Making use of the thermodynamic relations at constant entropy we can write

$$\frac{\partial u_a}{\partial \boldsymbol{v}_a} = \frac{P_a}{n_a^2} \frac{\partial n_a}{\partial \boldsymbol{v}_a}.$$
(3.13)

Using the relation between n and N we find

$$\frac{\partial n_a}{\partial \boldsymbol{v}_a} = -N_a \gamma_a \boldsymbol{v}_a,\tag{3.14}$$

so that the canonical momentum of SPH particle a is

$$\boldsymbol{p}_{a} = \frac{\partial L}{\partial \boldsymbol{v}_{a}} = \nu_{a} \left(1 + u_{a} + \frac{P_{a}}{n_{a}} \right) \gamma_{a} \boldsymbol{v}_{a}. \tag{3.15}$$

For particle a the spatial derivative is

$$\frac{\partial L}{\partial \boldsymbol{r}_a} = -\sum_b \frac{\nu_b}{\gamma_b} \frac{\partial u_b}{\partial \boldsymbol{r}_a},\tag{3.16}$$

and from the thermodynamic relations

$$\frac{\partial u_a}{\partial r_a} = \frac{P_a}{n_a^2} \frac{\partial n_a}{\partial r_a} = \frac{P_b}{\gamma_b n_b^2} \frac{\partial N_b}{\partial r_a}.$$
(3.17)

Analogously to the non-relativistic case we find

$$\frac{\partial L}{\partial \boldsymbol{r}_a} = -\nu_a \sum_b \nu_b \left(\frac{P_a}{N_a^2} + \frac{P_b}{N_b^2} \right) \nabla_a W_{ab}.$$
(3.18)

The Lagrangian equation of motion of particle *a* is therefore

$$\frac{\mathrm{d}\boldsymbol{p}_a}{\mathrm{d}t} = -\nu_a \sum_b \nu_b \left(\frac{P_a}{N_a^2} + \frac{P_b}{N_b^2}\right) \nabla_a W_{ab}.$$
(3.19)

If p_a is replaced by the momentum per baryon $S_a = p_a / \nu_a$ this equation can be written

$$\frac{\mathrm{d}S_a}{\mathrm{d}t} = -\sum_b \nu_b \left(\frac{P_a}{N_a^2} + \frac{P_b}{N_b^2}\right) \nabla_a W_{ab},\tag{3.20}$$

which is the same as the relativistic SPH equation derived from the continuum equations by Chow & Monaghan (1997) and similar in form to the fluid part of the non-relativistic acceleration equation (2.10).

3.2 Special relativistic conservation laws

3.2.1 Additive integrals

As in the non-relativistic case the invariance of the Lagrangian to an arbitrary infinitesimal translation of the system shows that the total momentum

$$\sum_{a} \boldsymbol{p}_{a} = \sum_{a} \nu_{a} \left(1 + u_{a} + \frac{P_{a}}{n_{a}} \right) \gamma_{a} \boldsymbol{v}_{a}, \tag{3.21}$$

is constant. The invariance to a rotations shows that the angular momentum

$$\sum_{a} \boldsymbol{r}_{a} \times \boldsymbol{p}_{a} = \sum_{a} \nu_{a} \left(1 + u_{a} + \frac{P_{a}}{n_{a}} \right) \gamma_{a} \boldsymbol{r}_{a} \times \boldsymbol{v}_{a}, \tag{3.22}$$

is conserved. From the absence of any explicit time dependence the energy E given by

$$E = \sum_{a} \frac{\partial L}{\partial \boldsymbol{v}_{a}} \cdot \boldsymbol{v}_{a} - L \tag{3.23}$$

$$=\sum_{a}\nu_{a}\left(\mathbf{S}_{a}\cdot\boldsymbol{v}_{a}+\frac{1}{\gamma_{a}}(1+u_{a})\right)$$
(3.24)

$$=\sum_{a}\nu_{a}\left[\gamma_{a}\left(1+u_{a}+\frac{P_{a}}{n_{a}}\right)-\frac{P_{a}}{N_{a}}\right],$$
(3.25)

is conserved.

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388 J. J. Monaghan and D. J. Price

3.2.2 The circulation

The argument leading to the approximate circulation theorem follows as before. Assuming each SPH particle contains the same number of baryons we find (using the definition of the momentum per baryon *S* given earlier) that

$$C = \sum_{c} S_{c} \cdot (\mathbf{r}_{c+1} - \mathbf{r}_{c}), \tag{3.26}$$

is invariant. The continuum limit of (3.26) is the special relativistic circulation

$$C = \oint \left(1 + u + \frac{P}{n}\right) \gamma \boldsymbol{v} \cdot d\boldsymbol{r}.$$
(3.27)

3.2.3 Liouville's theorem and Poincaré invariants

Having identified the canonical momentum the Hamiltonian can be written down and the equations of motion can be written in Hamiltonian form. The Hamiltonian is just the energy with γ written in terms of the canonical momentum. From (3.15) we find

$$\gamma^2 = 1 + \frac{\left(\frac{p}{\nu}\right)^2}{\left(1 + u + \frac{p}{n}\right)^2}.$$
(3.28)

As in the non relativistic case Liouville's theorem and the Poincaré invariants can be used to discuss the statistical behaviour of the system.

3.3 The particle energy equation

In order to deduce the rate of change of energy of each SPH particle we write E as $\sum_{a} \nu_a \hat{\epsilon}_a$ where $\hat{\epsilon}_a$ the energy per baryon of SPH particle *a* is

$$\hat{\epsilon}_a = \gamma_a \left(1 + u_a + \frac{P_a}{n_a} \right) - \frac{P_a}{N_a}.$$
(3.29)

The time derivative can then be found noting first that

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{(1+u_a)}{\gamma_a}\right) = -\mathbf{S}_a \frac{\mathrm{d}\mathbf{v}_a}{\mathrm{d}t} + \frac{P_a}{N_a^2} \frac{\mathrm{d}N_a}{\mathrm{d}t},\tag{3.30}$$

and

$$\frac{\mathrm{d}N_a}{\mathrm{d}t} = \sum_a \nu_a (\boldsymbol{v}_a - \boldsymbol{v}_b) \cdot \nabla_a W_{ab},\tag{3.31}$$

so that

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \sum_{a} \nu_a \frac{\mathrm{d}\hat{\epsilon}_a}{\mathrm{d}t} = -\sum_{a} \sum_{b} \nu_a \nu_b \left(\frac{P_a}{N_a^2} \boldsymbol{v}_b + \frac{P_b}{N_b^2} \boldsymbol{v}_a \right) \cdot \nabla_a W_{ab},\tag{3.32}$$

from which we can deduce that

$$\frac{\mathrm{d}\hat{\boldsymbol{\epsilon}}_a}{\mathrm{d}t} = -\sum_b \nu_b \left(\frac{P_a}{N_a^2} \boldsymbol{v}_b + \frac{P_b}{N_b^2} \boldsymbol{v}_a\right) \cdot \nabla_a W_{ab},\tag{3.33}$$

which agrees with the equation used by Chow & Monaghan (1997) derived from the energy-momentum tensor and using SPH approximations of the spatial derivatives. Because of the symmetry of the gradient of the kernel this equation leads directly to the conservation of energy. The reader will note that (5.10) is the SPH equivalent of

$$\frac{\mathrm{d}\hat{\boldsymbol{\epsilon}}}{\mathrm{d}t} = -\frac{1}{N}\nabla\cdot(\boldsymbol{v}P),\tag{3.34}$$

which is the usual relativistic energy equation for a non-dissipative fluid.

4 THE GENERAL RELATIVITY LAGRANGIAN

4.1 Equations of motion

For convenience we assume that the metric is a specified function of the coordinates, and the task is to determine the Lagrangian for a fluid

moving in that metric. The SPH equations for this case have been given by other authors (Laguna, Miller & Zurek 1993; Siegler & Riffert 2000). Their derivations start with the continuum equations which are then approximated by using SPH interpolation to deduce the SPH equations. As before, our aim is to show that these equations, or their equivalent, can be obtained by using a Lagrangian (or Hamiltonian). In the following Greek indices are summed over (0,1,2,3) while Latin indices are summed over (1,2,3). The subscripts *a*, *b*, and *c* are reserved for particle labels.

The Lagrangian for the fluid is (Fock 1964)

$$L = -\int T^{\mu\nu} U_{\nu} U_{\mu} \sqrt{-g} \,\mathrm{d}V,\tag{4.1}$$

where the four-velocity U^{μ} is defined by

$$U^{\mu} = \frac{\mathrm{d}x^{\mu}}{\mathrm{d}\tau},\tag{4.2}$$

where τ is the proper time. We note

$$\frac{d\tau}{dt} = (-g_{\nu\mu}v^{\mu}v^{\nu})^{\frac{1}{2}}.$$
(4.3)

From the previous relations we can write

$$\frac{dx^{\mu}}{dt} = v^{\mu} = \frac{U^{\mu}}{U^{0}},\tag{4.4}$$

where

$$U^{0} = \frac{\mathrm{d}t}{\mathrm{d}\tau} = (-g_{\nu\mu}v^{\mu}v^{\nu})^{-\frac{1}{2}}.$$
(4.5)

For a perfect fluid the Lagrangian is

$$L = -\int [n + nu(n,s)]\sqrt{-g} \,\mathrm{d}V. \tag{4.6}$$

As before we prefer to work with the number density *n* of baryons with rest mass m_0 , and we scale the energy with m_0c^2 and scale the velocity with the speed of light *c*.

The relativistic number conservation equation (the continuity equation) is

$$\frac{1}{\sqrt{-g}}\frac{\partial}{\partial x^{\nu}}(\sqrt{-g}nU^{\nu}),\tag{4.7}$$

which suggests using the transformed number density

$$N^* = \sqrt{-g}nU^0. \tag{4.8}$$

 N^* is the number density equivalent of the variable D^* of Siegler & Riffert (2000). The number conservation equation then becomes

$$\frac{\partial N^*}{\partial t} + \frac{\partial}{\partial x^i} (N^* v^i) = 0.$$
(4.9)

This equation shows that the total number of baryons

$$\int N^* \,\mathrm{d}V = \int n U^0 \sqrt{-g} \,\mathrm{d}V,\tag{4.10}$$

is conserved.

As suggested by Siegler & Riffert, we can interpolate according to

$$A(\mathbf{r}) = \int A(\mathbf{r}') W(|\mathbf{r} - \mathbf{r}'|) \,\mathrm{d}V,\tag{4.11}$$

where

$$W(|\mathbf{r} - \mathbf{r}'|) \,\mathrm{d}V = 1.$$
 (4.12)

This normalization is over a flat space so that we can use the same kernels as in the non-relativistic calculations. The summation interpolant is

$$A(\mathbf{r}) = \sum_{b} \nu_b \frac{A_b}{N_b^*} W(\mathbf{r} - \mathbf{r}_b), \tag{4.13}$$

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where

$$\nu_b = N_b^* \Delta V_b = n_b U^0 \sqrt{-g_b} \Delta V_b, \tag{4.14}$$

is the number of baryons in the volume $\sqrt{-g}\Delta V_b$.

We can now write the Lagrangian as

$$L = -\int \frac{N^*}{U^0} (1 + u(n, s)) \,\mathrm{d}V,\tag{4.15}$$

and the SPH Lagrangian is then

$$L = -\sum_{b} \nu_b (1 + u_b) X_b^{1/2},$$
(4.16)

where

$$X_a = (-g_{\mu\nu}v^{\mu}v^{\nu})_a.$$
(4.17)

The variational principle involves the variation of the trajectory of particles with constant entropy. The partial derivative of L with respect to v^{i} is straightforward to calculate. Noting

$$\frac{\partial X_a}{\partial v_a^i} = (-2g_{i\mu}v^{\mu})_a,\tag{4.18}$$

and the thermodynamics relation

$$\frac{\partial u_a}{\partial v_a^i} = \frac{P_a}{n_a^2} \frac{\partial n_a}{\partial v_a^i},\tag{4.19}$$

with

$$n = \frac{N^*}{\sqrt{-g}} X^{1/2}.$$
(4.20)

we find

$$\frac{\partial L}{\partial v_a^i} = \frac{\nu_a}{X_a^{1/2}} \left(1 + u_a + \frac{P_a}{n_a} \right) (g_{i\mu} v^{\mu})_a, \tag{4.21}$$

from which we can identify the canonical momentum per baryon of particle a as

$$S_{i(a)} = \frac{1}{X_a^{1/2}} \left(1 + u_a + \frac{P_a}{n_a} \right) (g_{i\mu} v^{\mu})_a.$$
(4.22)

in agreement, in the flat space limit, with the special relativistic canonical momentum deduced earlier. This expression is similar to that of Siegler & Riffert (2000) who use the 3+1 formalism and include an artificial dissipation term.

To complete Lagrange's equations we need the spatial derivative of L. The derivative of the thermal energy is

$$\frac{\partial u_b}{\partial x_a^i} = \frac{P_b}{n_b^2} \frac{\partial n_b}{\partial x_a^i} \tag{4.23}$$

$$=\frac{P_b}{n_b}\left(\frac{1}{N_b^*}\frac{\partial N_b^*}{\partial x_a^i} - \frac{\partial \sqrt{-g_b}}{\partial x_a^i} + \frac{1}{2X_b}\frac{\partial X_b}{\partial x_a^i}\right).$$
(4.24)

Writing N_b^* in SPH interpolant form, and noting that

$$\frac{\partial \sqrt{-g_b}}{\partial x^i} = \left(\frac{1}{2}g^{\mu\nu}\frac{\partial g_{\mu\nu}}{\partial x^i}\right)_b \delta_{ba},\tag{4.25}$$

together with

$$\frac{\partial X}{\partial x^{i}} = -v^{\mu}v^{\nu}\frac{\partial g_{\mu\nu}}{\partial x^{i}} = -XU^{\mu}U^{\nu}\frac{\partial g_{\mu\nu}}{\partial x^{i}},\tag{4.26}$$

the spatial derivative of L can be written

$$\frac{\partial L}{\partial x_a^i} = -\nu_a \sum_b \nu_b \left(\frac{\sqrt{-g_a} P_a}{N_a^{*2}} + \frac{\sqrt{-g_b} P_b}{N_b^{*2}} \right) \frac{\partial W_{ab}}{\partial x_a^i} + \nu_a \frac{\sqrt{-g_a}}{2N_a^*} \left(T^{\mu\nu} \frac{\partial g_{\mu\nu}}{\partial x^i} \right)_a. \tag{4.27}$$

Lagrange's equation of motion then becomes

$$\frac{\mathrm{d}S_{i(a)}}{\mathrm{d}t} = -\sum_{b} \nu_b \left(\frac{\sqrt{-g_a} P_a}{N_a^{*2}} + \frac{\sqrt{-g_b} P_b}{N_b^{*2}} \right) \frac{\partial W_{ab}}{\partial x_a^i} + \frac{\sqrt{-g_a}}{2N_a^*} \left(T^{\mu\nu} \frac{\partial g_{\mu\nu}}{\partial x^i} \right)_a. \tag{4.28}$$

This equation is similar in form to equation (41) of Siegler & Riffert (2000). It is not identical because they include an artificial dissipation, and there is a factor $\sqrt{-g}$ outside the summation. The fluid part of our equation of motion conserves momentum exactly. This is not the case for the Siegler & Riffert equation because their fluid term has not been symmetrized. With the Lagrangian formulation this symmetrization occurs naturally.

4.2 General relativistic conservation laws

4.2.1 Additive integrals

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In general, with an arbitrary metric, momentum is not conserved. It is conserved when the field equations are solved as part of the calculation. If the metric terms have rotational symmetry then the angular momentum about the axis of symmetry is conserved. Provided the metric does not have explicit time dependence the energy

$$E = \sum_{a} v_a^i \frac{\partial L}{\partial v_a^i} - L \tag{4.29}$$

$$=\sum_{a} \left[v_a^i S_{i(a)} + (1+u_a) X_a^{1/2} \right]$$
(4.30)

$$=\sum_{a} \frac{\nu_{a}}{X_{a}^{1/2}} \left[\left(1 + u_{a} + \frac{P_{a}}{n_{a}} \right) g_{i\mu} v^{\mu} v^{i} + X_{a} (1 + u_{a}) \right]$$
(4.31)

is conserved.

Introducing an energy per baryon $\hat{\epsilon}$, the total energy can be written as $\sum \nu_a \hat{\epsilon}_a$, where

$$\hat{\epsilon}_a = \frac{1}{X_a^{1/2}} \left[\left(1 + u_a + \frac{P_a}{n_a} \right) g_{i\mu} v^{\mu} v^i + X_a (1 + u_a) \right]$$
(4.32)

The energy per baryon is equivalent to the expression $(\alpha E - \beta^i S_i)$ introduced by Siegler & Riffert (2000).

The energy equation per particle can be obtained as before by taking the rate of change of E with time and identifying the rate of change of $\hat{\epsilon}$ in terms of the other physical quantities. The first step gives

$$\frac{dE}{dt} = \sum_{a} \nu_a \frac{d\hat{\epsilon}_a}{dt} = \sum_{a} \nu_a \left\{ \nu_a^i \frac{dS_{i(a)}}{dt} + S_{i(a)} \frac{d\nu_a^i}{dt} + \frac{d}{dt} [X_a^{1/2}(1+u_a)] \right\}.$$
(4.33)

We can write the last term as

$$\frac{\mathrm{d}}{\mathrm{d}t}(X^{1/2}(1+u)) = -\frac{X^{1/2}}{2n}T^{\mu\nu}\frac{\mathrm{d}g_{\mu\nu}}{\mathrm{d}t} + \frac{P\sqrt{-g}}{N^{*2}}\frac{\mathrm{d}N^*}{\mathrm{d}t},\tag{4.34}$$

and the rate of change of N^* can be found from the SPH interpolant for N^* . Combining these results we find

$$\frac{\mathrm{d}\hat{\epsilon}_a}{\mathrm{d}t} = -\sum_b \nu_b \left(\frac{\sqrt{-g_a} P_a}{N_a^{*2}} v_b^i + \frac{\sqrt{-g_b} P_b}{N_b^{*2}} v_a^i \right) \frac{\partial W_{ab}}{\partial x_a^i} - \frac{\sqrt{-g_a}}{2N_a^{*2}} \left(T^{\mu\nu} \frac{\partial g_{\mu\nu}}{\partial t} \right)_a. \tag{4.35}$$

This expression for the energy is similar to that of Siegler & Riffert (2000, equation 43). It differs from their result because of the symmetrized form of the pressure terms.

4.2.2 The circulation

The argument leading to the approximate circulation conservation follows as before. We now find that the SPH equivalent is that

$$C = \sum_{c} S_c \cdot (\mathbf{r}_{c+1} - \mathbf{r}_c), \tag{4.36}$$

where $S \cdot r$ denotes $S_i x^i$, is approximately constant. In the continuum limit this result agrees with Taub (1978).

4.2.3 Liouville's theorem and Poincaré invariants

Because we have a particle Lagranian and associated canonical momentum it is possible to write the equations of motion in Hamiltonian form. In the phase space defined for the coordinates and momenta of the SPH particles, Liouville's theorem and the Poincaré invariants hold.

5 CONCLUSION AND DISCUSSION

In this paper we have shown that the SPH equations for an ideal fluid can be deduced from a Lagrangian. The derivation is straightforward and hinges on the fact that in the SPH method the density is a function of the coordinates. The existence of the Lagrangian enables us to deduce the conservation laws including an approximation to the circulation which becomes the usual circulation in the continuum limit. These results suggest that much of the success of SPH can be attributed to the fact that it preserves many of the properties of an ideal fluid. Of course, in many astrophysical applications, dissipation occurs and the equations can no longer be derived from a Lagrangian. However, this does not make it any less desirable to have equations for numerical work which, in the absence of dissipation, preserve important properties of the original equations.

In addition to the use of SPH for numerical work, the formalism allows us to write down Hamiltonian equations in a particularly simple way. This leads to questions regarding the chaotic motion and statistical equilibrium of the system. Can we predict when it will be chaotic and, given the additive integrals of the motion and the approximate circulation invariant, can we predict the equilibrium state of the nondissipative fluid?

In our discussion we have not included the field equations in the Lagrangian except in the non-relativistic case where we have assumed the field is due to self gravity. In that case the potential is known as a function of the particle coordinates. We could have included a term which, when varied gave an SPH approximation to Poisson's equation for the gravitational potential but that is not the preferred form for computations. For that reason we have not included it. In the non-relativistic case the astrophysically significant field is usually the gravitational field and, if relativistic speeds are generated, the fields must be computed from the full GR field equations. In our discussion we have assumed the gravitational field is known and not affected by the motion of the fluid, a valid approximation for fluid of relatively low total mass orbiting beyond the event horizon of a black hole. A discussion of the other significant field, the magnetic field, will be considered elsewhere.

The Lagrangian for the relativistic gravitational field is well known and it may be added to the fluid Lagrangian we have considered and the variation with respect to the metric coefficients then gives the usual Einstein field equations. There is nothing new in this and for that reason we have not included these terms in our discussion of variational principles.

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