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Smoothed Particle Hydrodynamics Code Basics

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ABSTRACT

SPH is the shorthand for Smoothed Particle Hydrodynamics. This method is a Lagrangian method which means that it involves following the motion of elements of fluid. These elements have the characteristics of particles and the method is called a particle method. A useful review of SPH (Monaghan 1992) gives the basic technique and how it can be applied to numerous problems relevant to astrophysics. You can get some basic SPH programs from http://www.maths.monash.edu.au/ jjm/sphlect
In the present lecture I will assume that the student has studied this review and therefore understands the basic principles. In today's lecture I plan to approach the equations from a different perspective by using a variational principle.

Key Words : methods: numerical

I. SPH Interpolation

The SPH equations are based on interpolation from particles. The integral interpolant of a field $A(\mathbf{r})$ is defined by

$$A_I(\mathbf{r}) = \int A(\mathbf{r}')W(\mathbf{r}-\mathbf{r}',h)d\tau, \tag{1}$$

where the element of volume is $d\tau$, and W is a kernel which is normalised over the volume

$$\int W(\mathbf{r}-\mathbf{r}',h)d\tau = 1. \tag{2}$$

The form of W is guided by the requirement that

$$\lim_{h\to\infty} W(\mathbf{r}-\mathbf{r}',h) = \delta(\mathbf{r}-\mathbf{r}'). \tag{3}$$

In this limit A_I is the same as the original function $A(\mathbf{r})$. In the following it is convenient to interpret SPH expressions having in mind a gaussian kernel of the form (in one dimension)

$$W(q,h) = \frac{e^{-\frac{q^2}{h^2}}}{\sqrt{\pi h^2}}. \tag{4}$$

The smoothing length h determines the resolution and is proportional to the local particle spacing. It is convenient to choose $W(\mathbf{q},h)$ to be an even function of $\mathbf{q}$. As a consequence, a Taylor series expansion of $A(\mathbf{r}')$ about $\mathbf{r}$ in the integrand of (1) shows that, away from boundaries, the error in $A_I(\mathbf{r})$ is of $O(h^2)$.

The integral interpolant can be approximated by a splitting the fluid into small volume elements $\Delta\tau$ each with mass $\rho\Delta\tau$, where ρ is a representative density for the small fluid element. We can then approximate (1) by the summation interpolant

$$A_S(\mathbf{r}) = \sum_b \frac{m_b}{\rho_b} A(\mathbf{r}_b)W(\mathbf{r}-\mathbf{r}_b), \tag{5}$$

where the summation is over the particles, m_b is the mass of particle b, and ρ_b is the density at particle b at position $\mathbf{r}_b$.

Provided the kernel is a differentiable function (5) gives us an interpolation formula which can be differentiated analytically. In the SPH method, spatial derivatives are exact derivatives of interpolated quantities. Grids are not needed except as a book keeping device to find neighbouring particles.

In the following the subscript S to denote the summation interpolant will be dropped for convenience. Further details of the approximations are given by Monaghan (1992).

As an example of the SPH method the density at particle a is given by replacing A in (4) by ρ. We find

$$\rho_a = \sum_b m_b W_{ab}, \tag{6}$$

where W_{ab} denotes $W(\mathbf{r}_a - \mathbf{r}_b, h)$. This shows that the SPH density is a function of the coordinates which is galilean invariant. In some contexts, it is convenient to integrate the continuity equation

$$\frac{d\rho}{dt} = -\rho\nabla\cdot\mathbf{v}. \tag{7}$$

where d/dt is the derivative following the motion. This equation can be put in SPH form by first writing it as

$$\frac{d\rho}{dt} = -\nabla\cdot\rho\mathbf{v} + \mathbf{v}\cdot\nabla\rho, \tag{8}$$

then, on replacing $\rho\mathbf{v}$ and ρ by their SPH equivalents and taking the gradients, we find

$$\frac{d\rho_a}{dt} = -\sum_b m_b(\mathbf{v}_b - \mathbf{v}_a)\cdot\nabla W_{ab}. \tag{9}$$

It is easy to check that (6) is a solution of (9). However, differential equations have boundary or initial conditions, and it is sometimes useful to use the differential equations with initial, specified densities for the particles. An example would be the simulation of water or metals. For these fluids the typical initial state is constant density. If the summation is used the density is smaller near a free surface and the equation of state for these fluids would give a negative pressure (this is the elastic pressure and it can be negative). It is much better to assign the reference density and integrate the continuity equation.

In SPH simulations it is customary to use a cubic spline (see Monaghan 1992). Other kernels have been considered, especially those which give higher order accuracy for the integral interpolant. These have not had widespread use for two reasons. The first is that the particles become disordered and the summation interpolant may then be a poor approximation to the integral interpolant. The precise form and effect of this disorder depends on the dynamical system being studied. The second is that higher order interpolation requires kernels which change sign. In gas dynamics, especially for strong shocks, these high order kernels can cause undershoots which may produce negative densities. One way to control this is to switch to a low order kernel near the shock and use the high order kernel in regions where the flow is smooth. There has been very little work on this idea.

Another issue with the kernel is that in some simulations the particles can clump. Couchman gets around this by replacing the gradient of the kernel by its maximum (which for the cubic spline is at $2/(3h)$).

In astrophysical applications of SPH the resolution length h is determined by the local density and the resolution varies in space as well as time. In addition, some authors have examined the effect of using kernels with ellipsoidal symmetry to take account of the fact that shock fronts, or other thin structures, require different resolution along and perpendicular to the thin structure. The disadvantage of these kernels is that the system does not then conserve angular momentum.

II. The Lagrangian for compressible flow

The Lagrangian for compressible, non dissipative flow is (Eckart 1960)

$$L = \int \rho\left(\frac{1}{2}v^2 - u(\rho, s)\right) d\tau, \tag{10}$$

where $u(\rho, s)$ is the thermal energy per unit mass which is a function of density ρ and entropy s. The SPH form of (10) is

$$L = \sum_b m_b\left(\frac{1}{2}v_b^2 - u(\rho_b, s_b)\right). \tag{11}$$

where

$$\frac{d\mathbf{r}_a}{dt} = \mathbf{v}_a. \tag{12}$$

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

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \mathbf{v}_a}\right) - \frac{\partial L}{\partial \mathbf{r}_a} = 0, \tag{13}$$

we find

$$\frac{d\mathbf{v}_a}{dt} = -\sum_b m_b\left(\frac{\partial u}{\partial \rho}\right)_s \frac{\partial \rho_b}{\partial \mathbf{r}_a}. \tag{14}$$

Making use of the summation for the density (6), and the first law of thermodynamics, the acceleration equation (14) can be written

$$\frac{d\mathbf{v}_a}{dt} = -\sum_b m_b\left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2}\right)\nabla_a W_{ab}, \tag{15}$$

where where P_a is the pressure of particle a (which can be calculated once the form of $u(\rho, s)$ is given), and ∇_a denotes the gradient taken with respect to the coordinates of particle a. Equation (15) is the SPH equivalent of

$$\frac{d\mathbf{v}}{dt} = -\frac{P}{\rho^2}\nabla\rho - \nabla\left(\frac{P}{\rho}\right), \tag{16}$$

$$= -\frac{1}{\rho}\nabla P, \tag{17}$$

which is the standard equation of motion.

These equations complete the SPH formulation of the equations of motion for a non dissipative fluid. In practice additional viscous terms and external forces such as gravity are included. If the fluid is in a container the container can be represented by boundary forces (Monaghan 1994; Monaghan & Kos 1999).

III. Conservation Laws

The symmetry of the Lagrangian leads immediately to the conservation laws. In particular, in the present case where the entropy of each particle remains constant, and the summation for the density is invariant to translations and rotations, linear and angular momentum are conserved. In the presence of external forces this is no longer true in general. As a simple example consider the invariance to translations. Let each particle have its position shifted by the arbitrary infinitesimal vector ϵ. The change in the Lagrangian is zero, therefore

$$\delta L = 0 = \sum_a \frac{\partial L}{\partial \mathbf{r}_a} \cdot \epsilon, \tag{18}$$

which becomes

$$\epsilon \cdot \sum_a \frac{\partial L}{\partial \mathbf{r}_a} = 0. \tag{19}$$

But from Lagranges equations we can write this as

$$\epsilon \cdot \frac{d}{dt} \sum_a \frac{\partial L}{\partial \mathbf{v}_a} = 0. \tag{20}$$

Since ϵ is arbitrary, we deduce the conservation of momentum

$$\sum_a \frac{\partial L}{\partial \mathbf{v}_a}. \tag{21}$$

In a similar way we can deduce the conservation of angular momentum. If there is no explicit time dependence in the Lagrangian energy is conserved.

The particle system is invariant to other transformations. Consider, for example figure 1 which shows a set of particles each with the same mass 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 change in L can be approximated by

$$\delta L = \sum_j \left(\frac{\partial L}{\partial \mathbf{r}_j} \cdot \delta \mathbf{r}_j + \frac{\partial L}{\partial \mathbf{v}_j} \cdot \delta \mathbf{v}_j \right), \tag{22}$$

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

$$\delta \mathbf{r}_j = \mathbf{r}_{j+1} - \mathbf{r}_j, \tag{23}$$

and

$$\delta \mathbf{v}_j = \mathbf{v}_{j+1} - \mathbf{v}_j. \tag{24}$$

Using Lagrange's equations (13) we can rewrite (22) in the form

$$\sum_j m_j \left(\frac{d\mathbf{v}_j}{dt} \cdot (\mathbf{r}_{j+1} - \mathbf{r}_j) + \mathbf{v}_j \cdot (\mathbf{v}_{j+1} - \mathbf{v}_j) \right) = 0, \tag{25}$$

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

$$\frac{d}{dt} \sum_j \mathbf{v}_j \cdot (\mathbf{r}_{j+1} - \mathbf{r}_j) = 0. \tag{26}$$

so that

$$C = \sum_j \mathbf{v}_j \cdot (\mathbf{r}_{j+1} - \mathbf{r}_j), \tag{27}$$

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 (26) approximates the circulation theorem to arbitrary accuracy. A related argument was used by Feynman to establish from the invariance of the wave function that circulation should be quantised.

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

$$\frac{d}{dt} \sum_j \mathbf{v}_j \cdot \frac{(\mathbf{r}_{j+1} - \mathbf{r}_{j-1})}{2} = 0. \tag{28}$$

which is a better approximation to the circulation of the continuous fluid. The errors in the discrete approximation to the circulation theorem arise because of the higher order terms in the change to the Lagrangian.

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.

IV. Dissipation

The previous analysis concerns the non dissipative fluid. In standard SPH calculations viscous dissipation is achieved by adding a term of the form (Monaghan 1992; 1997)

$$\Pi_{ab} = -\frac{\sigma_{ab} \mathbf{v}_{ab} \cdot \mathbf{r}_{ab}}{|\mathbf{r}_{ab}|}, \tag{29}$$

to the pressure terms. The quantity σ_{ab} is a positive definite parameter which is invariant to the interchange of a and b. It typically has the form

$$\sigma_{ab} = \frac{\alpha v_{sig}}{\bar{\rho}_{ab}}, \tag{30}$$

where the average density $\bar{\rho}_{ab} = 0.5(\rho_a + \rho_b)$. The signal velocity v_{sig} is given by

$$v_{sig} = c_a + c_b + 2|\mathbf{v_{ab}} \cdot \mathbf{j}|, \tag{31}$$

where $\mathbf{j} = \mathbf{r_a b}/r_{ab}$ and $\mathbf{r}_{ab} = \mathbf{r}_a - \mathbf{r}_b$. The viscosity can be interpreted as an artificial pressure which is positive when the particles are moving together ($\mathbf{v}_{ab} \cdot \mathbf{r}_{ab} < 0$).

The acceleration equation (15) now becomes

$$\frac{d\mathbf{v}_a}{dt} = -\sum_b m_b \left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2} - \frac{\epsilon}{2} \frac{(\hat{\mathbf{v}}_b - \hat{\mathbf{v}}_a)^2}{\bar{\rho}_{ab}} + \Pi_{ab} \right) \nabla_a W_{ab}. \tag{32}$$

Angular and linear momentum are conserved because the viscous force is along the line joining the centres of the SPH particles.

The viscosity term is excellent near shocks but diffuses vorticity and angular momentum strongly. To avoid this one technique is due to Balsara and involves multiplying the viscosity term by a factor

$$\frac{|\nabla \cdot \mathbf{v}|}{(|\nabla \cdot \mathbf{v}| + |\nabla \times \mathbf{v}|}. \tag{33}$$

Another method for reducing the viscosity away from shocks is due to Morris and Monaghan (1997). They give each particle its own α and allow the α to change according to a simple differential equation.

$$\frac{d\alpha}{dt} = -\frac{(\alpha - \alpha_0)}{\tau} + S, \tag{34}$$

where $\tau \sim h/c_s$, S is a source term proportional to $|\nabla \cdot \mathbf{v}|$, and α_0 is a reference value taken as ~ 0.1 by Morris and Monaghan. The idea is to have $\alpha \sim 1$ near shocks but smaller $\alpha \sim 0.1$ away from shocks. If smoothed velocities are used it appears to be possible to have $\alpha \sim 0.01$ in regions of smooth flow. Many astrophysicists now use an alpha for each particle and find that it improves their results significantly.

V. Various Applications

(a) Astrophysics

I will just list the authors without references. You can check these at web sites. I apologise in advance to to the very large number of people left off this list.

Accretion disks Murray (leicester U.K), Molteni (Italy)

Stellar collisions Benz (Bern), Sills and Rosswog (Leicester)

Galaxies (Hernquist, Barnes)

Cosmology (Katz, Walmsley and Bond)

Relativity (Siegler and Ruffert, Chow and Monaghan)

Star Formation (Bates, Bonnell)

Planetesimal collisions (Benz and Asphaug)

(b) Non Astrophysics Applications

There are numerous applications of SPH to problems outside astrophysics. These applications often allow comparisons against experiment and they show that SPH gives very good results in flow problems which cannot be tackled successfully by other methods.

(c) Water Waves

The dynamics of waves can be studied with SPH by using an equation of state which approximates the elastic properties of water and ensures that the density remains nearly constant (Monaghan 1994). Typically

$$P = \frac{\rho_0 c_s^2}{\gamma}\left(\left(\frac{\rho}{\rho_0}\right)^\gamma - 1\right), \tag{35}$$

where the speed of sound c_s is chosen to be ~ 10 times the largest speeds expected in the flow. In addition the boundaries can be modelled using particles (real or ghost). Examples are the simulations of solitary waves on coastlines (Monaghan and Kos 1999) and the simulation of gravity currents (Monaghan, Cas, Kos & Hallworth 1999).

(d) Impact problems

A solid body hitting water is considered to be a very difficult problem. With SPH it can be handled very simply. An example is the motion produced by a box falling vertically into water (Monaghan and Kos 2000). The agreement with experiment is good. Another example is fluid motion produced by a weighted box running down a curved slope into a tank. Comparison with experiment again produces good agreement. These results show that even in complicated fluid dynamical problems quite different to those in astrophysics SPH can reproduce the experimental results. Applications in progress include the dynamics of a dam initiated by a seismic wave.

(e) Elasticity and Fragmentation

Benz and Asphaug initiated the application of SPH to problems involving elastic materials and brittle fracture. Standard SPH has a benign instability for elastic materials. It arises because the elastic pressure can be negative and the SPH particles clump. However, this problem can be eliminated (see for example Monaghan 2000). In the work of Benz and Asphaug the brittle materials fragmented before the tensile instability developed. The application considered by Benz and Asphaug was to the collision of planetesimals. There are numerous applications in geology. Think of earthquakes, and the sudden change in a volcano as the magma chamber beneath collapses.

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