Notes

Smoothed Particle Hydrodynamics

IPAM

J. J. Monaghan

School of Mathematical Sciences

Monash University.

email: joe.monaghan@sci.monash.edu.au

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1 Introduction

The idea behind SPH is to replace the equations of fluid dynamics by equations for particles. In effect we replace the continuum equations by a set of particle equations that approximates the continuum and, at the same time, provides a rigorous model of the underlying, and more fundamental, molecular system. There are many particle methods but these notes are concerned with Smoothed Particle Hydrodynamics (SPH) devised by Gingold and Monaghan (1977) and by Lucy (1977). Useful reviews are those of Benz (1990) and Monaghan (1992).

The simplest set of equations are the acceleration and density convergence equations for an ideal gas without dissipation. These are the Euler equations. The acceleration equation is

$$\frac{d\mathbf{v}}{dt} = -\frac{1}{\rho}\nabla P, \tag{1.1}$$

where $\mathbf{v}$ is the velocity, ρ is the density, and P is the pressure. In general P is a function of ρ and the thermal energy, but in the case where there is no dissipation the pressure can be taken as a function of ρ alone. The density or convergence equation (we use this name here because $-\nabla \cdot \mathbf{v}$ is the opposite of divergence)

$$\frac{d\rho}{dt} = -\rho\nabla \cdot \mathbf{v}. \tag{1.2}$$

In these equations d/dt denotes the derivative following the motion (the advection term)

$$\frac{d\mathbf{v}}{dt} = \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla\mathbf{v}. \tag{1.3}$$

The solution of this part of the equations alone is given by the trajectories of the particles (these are the characteristics of the hyperbolic term (1.3). Thus if

$$\frac{dA}{dt} = 0, \tag{1.4}$$

the solution is found by assigning A_j to particle j then moving this particle according to $d\mathbf{r}/dt = \mathbf{v}$. However, we need spatial derivatives to calculate how $\mathbf{v}$ changes. To do this we use an interpolant method.

2 Integral and summation interpolants

We begin with the identity

$$A(\mathbf{r}) = \int A(\mathbf{r}')\delta(\mathbf{r} - \mathbf{r}')\mathbf{dr}', \tag{2.1}$$

where $\delta(\mathbf{r})$ denotes the Dirac delta function and $\mathbf{dr}'$ is an element of volume in the space being considered. Recall

$$\int \delta(\mathbf{r})\mathbf{dr}' = 1. \tag{2.2}$$

Now choose a function W (the kernel) with the following properties.

$$\lim_{h\to 0} W(\mathbf{r}, h) = \delta(\mathbf{r}), \tag{2.3}$$

and is normalised so that

$$\int W(\mathbf{r})\mathbf{dr}' = 1. \tag{2.4}$$

One example i is the Gaussian in one dimension

$$W(x, h) = \frac{1}{h\sqrt{(\pi)}} e^{-x^2/h^2}, \tag{2.5}$$

which is a C^∞ function. Another example in one dimension is the spline defined as follows. If $q = |x|/h < 1$ then

$$W(x, h) = \begin{cases} \frac{1}{h}(\frac{2}{3} - q^2 + \frac{1}{2}q^3), & \text{for } 0 \leq q \leq 1, \\ \frac{1}{6h}(2 - q)^3, & \text{for } 1 \leq q \leq 2, \\ 0, & \text{otherwise} \end{cases} \tag{2.6}$$

otherwise, $W(x, h)$ is zero. This function has continuous second derivaties and compact support.

We replace (2.4) by the integral interpolant

$$A(\mathbf{r})_I = \int A(\mathbf{r}')W(\mathbf{r} - \mathbf{r}', h)\mathbf{dr}' \tag{2.7}$$

Divide the volume of fluid into a set of small volume elements. The element a has mass m_a, density ρ_a, and position $\mathbf{r}_a$. Denote the value of A at particle a by A_a. Then

$$\int \frac{A(\mathbf{r}')}{\rho(\mathbf{r}')}\rho(\mathbf{r}')\mathbf{dr}'. \tag{2.8}$$

An element of mass is $\rho \mathbf{dr}'$. We approximate the integral by a summation over the mass elements. This gives us the summation interpolant

$$A_s(\mathbf{r}) = \sum_b m_b \frac{A_b}{\rho_b} W(\mathbf{r} - \mathbf{r_b}, h), \tag{2.9}$$

where the summation is over all the particles but, in practice, is only over near neighbours because W falls off rapidly with distance. Typically, h is close to the particle spacing, and the kernel W is effectively zero beyond a distance $2h$. In practice we choose kernels which have compact support i.e. they vanish at a finite distance. As an example of the use of kernel estimation suppose A is the density ρ. The interpolation formula then gives the following estimate for the density at a point $\mathbf{r}$

$$\rho(\mathbf{r}) = \sum_b m_b W(\mathbf{r} - \mathbf{r}_b, h), \tag{2.10}$$

which shows how the mass of a set of particles is smoothed to produce the estimated density. The reader who is familiar with the technique of estimating probability densities from sample points (Parzen 1962) will see that our formula for the density is the same with m_b replaced by $1/N$, where N is the number of sample points. The probability algorithm was used by Gingold and Monaghan (1977) as the basis of SPH . Lucy (1977) rediscovered the statistical algorithm and referred to the method as a Monte Carlo method.

If h is constant we can integrate the density estimate to give

$$\int \rho(\mathbf{r})\mathbf{dr} = \sum_b m_b = M, \tag{2.11}$$

which shows that mass is conserved exactly (in the probability case the kernel estimate ensures the total probability = 1). If we allow h to vary, the integral is no longer exactly M but the errors are small because the particles carry their mass unchanged.

2.1 Derivatives

If we take W to be a differentiable function then we can differentiate our estimate of A (2.9) exactly. For example

$$\frac{\partial A}{\partial x} = \sum_b m_b \frac{A_b}{\rho_b} \frac{\partial W}{\partial x}. \tag{2.12}$$

However, this does not vanish exactly when A is constant. Therefore begin with

$$\nabla A = \frac{1}{\Phi} \left(\nabla(A\Phi) - A\nabla\Phi \right). \tag{2.13}$$

Replace each derivative by using the SPH interpolation formula. The gradient of A at the position of particle b is

$$(\nabla A)_a = \frac{1}{\Phi_a} \sum_b \frac{m_b}{\rho_b} \Phi_b (A_b - A_a) \nabla_a W_{ab}, \tag{2.14}$$

where ∇_a means take the gradient with respect to the coordinates of particle a and $W_{ab} = W(\mathbf{r}_a - \mathbf{r}_b, h)$. This form of the gradient vanishes exactly when A is constant. We can apply this to the density convergence equation taking $\Phi = 1$. First estimate the velocity divergence

$$(\nabla \cdot \mathbf{v})_a = \sum_b \frac{m_b}{\rho_b} \mathbf{v}_{ba} \cdot \nabla_a W_{ab}, \tag{2.15}$$

where $\mathbf{v}_{ba} = \mathbf{v}_b - \mathbf{v}_a$. If we take $\Phi = \rho$ we get

$$(\nabla \cdot \mathbf{v})_a = \frac{1}{\rho_a} \sum_b m_b \mathbf{v}_{ba} \cdot \nabla_a W_{ab}. \tag{2.16}$$

The density convergence equation is then either

$$\frac{d\rho_a}{dt} = -\rho_a \sum_b \frac{m_b}{\rho_b} \mathbf{v}_{ba} \cdot \nabla_a W_{ab}, \tag{2.17}$$

or

$$\frac{d\rho_a}{dt} = -\sum_b m_b \mathbf{v}_{ba} \cdot \nabla_a W_{ab}, \tag{2.18}$$

This last equation could be obtained by differentiating the summation interpolant for the density. In problems involving two fluids, for example oil and water, either of these density equations can be used. However, if the density ratio is greater than about 2 it is better to use (2.17).

3 Errors in the Integral Interpolant

We have

$$A_I(x) = \int A(x')W(x - x', h)dx', \tag{3.1}$$

and we assume h is constant. We expand $A(x')$ in a Taylor series about x to get

$$A_I(x) = \int [A(x) + (x' - x)\frac{dA(x)}{dx} + \frac{1}{2}(x' - x)^2 \frac{d^2A(x)}{dx^2} + \ldots] W(x' - x, h) dx'. \tag{3.2}$$

We now assume that $W(q, h)$ is an even function of q.

$$A_I(x) = A(x) + \frac{1}{2}\frac{d^2A(x)}{dx^2} \int (x' - x)^2 W(x' - x, h) dx' \ldots = A(x) + O(h^2). \tag{3.3}$$

which shows that the integral interpolant gives at least second order interpolation provided the function has bounded derivatives up to the second. The interpolation is better if σ is zero when higher order terms must be included in the expansion. The third order term vanishes because of symmetry leaving a possible fourth order term. An example of a higher order kernel is

$$W(x, h) = \frac{1}{h\sqrt{\pi}} \left(\frac{3}{2} - \frac{x^2}{h^2} \right) e^{-x^2/h^2}. \tag{3.4}$$

For this kernel, the integral interpolant is accurate to $O(h^4)$.

4 Errors in the Summation Interpolant

If the particles are equi-spaced then we can easily estimate the errors in the summation interpolant. However, in general, the particles in an SPH calculation will be disordered. The problem sheets give examples of estimating the interpolation errors for equi-spaced particles. These examples shown that provided the kernel is smooth enough (which implies its Fourier Transform decreases rapidly) the errors in estimation are small. Shoenberg (1946) showed that interpolation accuracy could be related to the properties of the Fourier Transform of the interpolating kernel. Smoothness then shows up as rapid decrease of the the Fourier Transform for large k and the order of accuracy shows up in the expansion of the Fourier Transform in powers of k. In particular, if the Fourier transform has a zero of order m at $k = 0$, then the kernel has continuous derivatives up to the $(m - 2)^{th}$.

Shoenberg was concerned with interpolation when the data was noisy. For that reason he wasn't interested in the standard interpolation formula such as those due to Everett or Bessel but rather interpolation with smoothing. In Shoenberg's formalism the interpolation is written in the form

$$f(x) = \sum_j f_j L(x - x_j), \tag{4.5}$$

which has the same as our SPH interpolation. If the points are equi-separated with spacing Δ, as in a table, then the Bessel's interpolation formula with interpolates quadratic functions exactly is given by the following (where $q = |x|/h$.

$$L(x) = \begin{cases} (1-q)(1+\frac{1}{4}q), & \text{for } 0 \le q \le 1 \\ \frac{1}{4}(1-q)(2-q), & \text{for } 1 \le q \le 2. \\ 0, & \text{otherwise} \end{cases} \tag{4.6}$$

The first derivative of this function is not continuous everywhere. When the data is noisy it is an advantage to have smoother interpolating kernels. Shoenberg(1946) constructed a set of basic smoothing functions which he called Cardinal Splines. They can be defined by their Fourier transform. Thus, the spline with continuous (n-2) derivatives, $M_n(x)$ (which is an even function of x) is given by

$$M_n(x) = \int_{-\infty}^{\infty} \left(\frac{\sin \pi k \Delta}{\pi k \Delta} \right)^n \cos{(2\pi k x)} dk. \tag{4.7}$$

These spline kernels all interpolate with errors of $O(h^2)$, but they are smoother as n increases. The M_0 spline gives nearest grid point interpolation. The M_2 spline is:

$$M_2(x) = \begin{cases} 1-q, & \text{for } 0 \le q \le 1 \\ 0, & \text{for } q \ge 1 \end{cases} \tag{4.8}$$

otherwise M_2 is zero. In this, and the following expressions, q denotes $|x|/\Delta$. M_2 gives linear interpolation but its first derivative is discontinuous.

A commonly used kernel is the M_4 kernel (commonly called the cubic spline because it is a piecewise cubic polynomial). It has the form:

$$M_4(x) = \begin{cases} \frac{2}{3} - q^2 + \frac{1}{2}q^3, & \text{for } 0 \le q \le 1 \\ \frac{1}{6}(2-q)^3, & \text{for } 1 \le q \le 2., \\ 0, & \text{for } q > 2. \end{cases} \tag{4.9}$$

The one dimensional SPH kernel associated with $M_4(x)$ is $W(x,h) = \frac{1}{h}M_4(x)$ where now $q = |x|/h$. These kernels have been used for SPH interpolation because they are less sensitive to particle disorder. They are generalised to more dimensions by replacing x by radius r and choosing a normalising constant so that the integral over the space is 1.

4.1 Errors when the particles are disordered

During the course of an SPH calculation the particles become disordered. The exact form of this disorder depends on the dynamics. The errors are much less than a Monte Carlo estimate would suggest. The reason for the smaller errors is that the probability estimates allow fluctuations which are inconsistent with the dynamics. Because the disorder depends on the dynamics it is not possible to make traditional error estimates like those used for finite differences or finite elements. For that reason estimates of SPH calculations have had to depend on comparisons with known solutions, experiments, or by studying how the error varies with particle number for particular calculations (see for example Cleary and Monaghan (1999). These comparisons show that it is possible to achieve very accurate results with SPH. Another reason for the accuracy of SPH despite the disorder is that it is possible to set up SPH calculations so that they conserve important quantities like linear and angular momentum and energy exactly.

5 The SPH acceleration equation

We can convert the acceleration equation for our ideal fluid into SPH form by writing

$$(\nabla P)_a = \sum_b m_b \frac{P_b}{\rho_b} \nabla_a W_{ab}. \tag{5.1}$$

Our first, crude, SPH form of the acceleration equation is then

$$\frac{d\mathbf{v}_a}{dt} = -\frac{1}{\rho_a} \sum_b m_b \frac{P_b}{\rho_b} \nabla_a W_{ab}, \tag{5.2}$$

However, this equation doesn't conserve linear or angular momentum exactly since the force on particle a due to b is not equal and opposite to the force on b due to a or

$$\frac{m_a m_b P_b}{\rho_a \rho_b} \neq \frac{m_a m_b P_a}{\rho_a \rho_b}. \tag{5.3}$$

To write the acceleration equation in a form which conserves linear and angular momentum we make the force term symmetric by noting that

$$\frac{\nabla P}{\rho} = \nabla \left(\frac{P}{\rho} \right) + \frac{P}{\rho^2} \nabla \rho. \tag{5.4}$$

Using the SPH interpolation rules we can write the first term on the right hand side as

$$\nabla \left(\frac{P}{\rho} \right)_a = \sum_b \frac{P_b}{\rho_b^2} \nabla_a W_{ab}, \tag{5.5}$$

and the second term as

$$\frac{P_a}{\rho_a^2} (\nabla \rho)_a = \frac{P_a}{\rho_a^2} \sum_b m_b \nabla_a W_{ab}, \tag{5.6}$$

Combining these we get the acceleration equation

$$\frac{d\mathbf{v}_a}{dt} = - \sum_b m_b \left(\frac{P_b}{\rho_b^2} + \frac{P_a}{\rho_a^2} \right) \nabla_a W_{ab}, \tag{5.7}$$

Assuming that the kernel W_{ab} is a function of $|\mathbf{r_a} - \mathbf{r_b}|$ we can write its gradient in the following form

$$\nabla_a W_{ab} = \mathbf{r}_{ab} F_{ab}, \tag{5.8}$$

where F_{ab} is a scalar function of $|[\mathbf{r_a} - \mathbf{r_b}|$ and $F_{ab} \leq 0$. The force/mass on a due to b is then

$$m_b \left(\frac{P_b}{\rho_b^2} + \frac{P_a}{\rho_a^2} \right) \mathbf{r}_{ab} F_{ab}, \tag{5.9}$$

which shows that the force on a due to b is now equal and opposite to the force on b due to a.

6 The Thermal Energy equation

We get the thermal energy equation from the first law of thermodynamics

$$\begin{aligned} Tds &= du + Pdv && (6.1) \\ &= du - \frac{P}{\rho^2} d\rho && (6.2) \end{aligned}$$

where s is the Entropy, and we have assumed in the last equation that all quantities are per/unit mass. If there is no source of heat we deduce

$$\frac{du}{dt} = \frac{P}{\rho^2} \frac{d\rho}{dt} = - \frac{P}{\rho^2} \nabla \cdot \mathbf{v}. \tag{6.3}$$

We can write this equation in various ways. For example

$$\frac{du}{dt} = \frac{P}{\rho^2} \left(\nabla \cdot (\rho \mathbf{v}) - \mathbf{v} \cdot \nabla \rho \right), \tag{6.4}$$

and, in SPH form for any particle a, this equation becomes

$$\frac{du_a}{dt} = \frac{P_a}{\rho_a^2}\sum_b m_b \mathbf{v}_{ab} \cdot \nabla_a W_{ab}. \tag{6.5}$$

Alternatively, we could make use of one of the forms of $\nabla \cdot \mathbf{v}$ from the previous chapter and deduce the thermal energy equation

$$\frac{du_a}{dt} = \frac{P_a}{\rho_a}\sum_b \frac{m_b}{\rho_b} \mathbf{v}_{ab} \cdot \nabla_a W_{ab}. \tag{6.6}$$

A good general principle when writing SPH equations is to be consistent. For example, if we use a particular expression for $\nabla \cdot \mathbf{v}$ in the continuity equation, we should use the same form in the energy equation.

7 Dispersion

The SPH formulation affects the dispersion relation for small amplitude waves in a gas in one dimension. To sltudy this assume the initial density $\bar{\rho}$ is constant, the domain is infinite, the SPH particles have equal mass and are initially equi-spaced with spacing Δx. For convenience assume that the equation of state is $P = K\rho^2$. If the sound waves have sufficiently small amplitude then we can linearise the equations. Take the position of particle a as

$$x_a = \bar{x}_a + X e^{i(k\bar{x}_a - \omega t)}, \tag{7.1}$$

where $\bar{x}_a$ is the unperturbed position of particle a. The velocity is

$$v_a = V e^{i(k\bar{x}_a - \omega t)}, \tag{7.2}$$

and the density

$$\rho_a = \bar{\rho}_a + D e^{i(k\bar{x}_a - \omega t)}. \tag{7.3}$$

Because $P = K\rho^2$ we do not need to consider the continuity equation to obtain the dispersion relation for the SPH system. The first order perturbation to the acceleration equation gives

$$-i\omega v_a = -2mK\sum_b (\delta x_a - \delta x_b)\frac{d^2 W_{ab}}{d\bar{x}_a^2}, \tag{7.4}$$

where

$$\delta x_a = X e^{i(k\bar{x}_a - \omega t)}. \tag{7.5}$$

Substituting for v_a we get

$$-i\omega V = -2mKX \sum_b \left[1 - e^{ik(\bar{x}_b - \bar{x}_a)}\right] \frac{d^2 W_{ab}}{d\bar{x}_a^2}, \tag{7.6}$$

From the equation for the change in position $dx_a/dt = v_a$ we get

$$-i\omega X = V. \tag{7.7}$$

Substituting this result into the previous equation we get the dispersion relation

$$\omega^2 = 2mK \sum_b \left[1 - e^{ik(\bar{x}_b - \bar{x}_a)}\right] \frac{d^2 W_{ab}}{d\bar{x}_a^2}, \tag{7.8}$$

Because the particles are equi-spaced and the line is infinite we can shift the origin in the summation to $\bar{x}_a$ and measure lengths from this point. We can then write (7.8) as

$$\omega^2 = 2mK \sum_b \left[1 - e^{ik\bar{x}_b}\right] \frac{d^2 W(\bar{x}_b, h)}{d\bar{x}_b^2}. \tag{7.9}$$

If the wavelength is much large than the particle spacing we can replace the summation by an integration according to

$$\sum_{b=-\infty}^{\infty} \left[1 - e^{ik\bar{x}_b}\right] \frac{d^2 W(\bar{x}_b, h)}{d\bar{x}_b^2} \simeq \frac{1}{\Delta x} \int_{-\infty}^{\infty} \left[1 - e^{ikb\Delta x}\right] \frac{\partial^2 W}{\partial b^2} db, \tag{7.10}$$

where we have used the fact that $\bar{x}_b = b\Delta x$ and, for convenience, b is used to denote both the discrete and the continuous variable. Integrating by parts twice we find

$$\sum_{b=-\infty}^{\infty} \left[1 - e^{ik\bar{x}_b}\right] \frac{d^2 W(\bar{x}_b, h)}{d\bar{x}_b^2} \simeq k^2 \int_{-\infty}^{\infty} W e^{ikb\Delta x} db, \tag{7.11}$$

Since we have assumed $P = K\rho^2$ the speed of sound c_s is equal to $2K\rho = 2Km/\Delta x$. We can therefore write the dispersion relation as

$$\omega^2 \simeq c_s^2 k^2 \tilde{W}, \tag{7.12}$$

where $\tilde{W}$ denotes the fourier transform of W

$$\int_{-\infty}^{\infty} W e^{ikb\Delta x} db. \tag{7.13}$$

If the kernel is a Gaussian we can evaluate the integral to get

$$\omega^2 = c_s^2 k^2 e^{-(kh/2)^2}. \tag{7.14}$$

If the $kh \ll 2$ the dispersion relation is a close approximation to the exact form $\omega^2 = c_s^2 k^2$, but as k increases the frequency of the wave calculated using SPH drops below the correct value. The largest allowed value of k is $\pi/\Delta x$ and for this k the error is a maximum. However, it is not the error that is a concern for short wave lengths but rather whether or not the method remains stable. To determine the stability we evaluate the dispersion relation numerically.

Because the term $\frac{d^2W(\bar{x}_b,h)}{dx_b^2}$ in the original dispersion relation is an even function of the coordinates we can write it as

$$\omega^2 = 2mK \sum_b [1 - \cos k\bar{x}_b] \frac{d^2W(\bar{x}_b, h)}{d\bar{x}_b^2}. \tag{7.15}$$

If the system is unstable the fastest growing mode is usually the one with the shortest wavelength (largest k) and this shows up as clumping. We therefore evaluate the dispersion relation for $k = \pi/\Delta x$ and get

$$\omega^2 = 8mK \sum_{j=1}^{\infty} \frac{d^2W(\bar{x}_j, h)}{d\bar{x}_j^2}, \tag{7.16}$$

where the summation is over odd values of j. For the Gaussian kernel we get

$$\omega^2 = \frac{8mK}{h^3\sqrt{\pi}} \sum_{j=1}^{\infty} \left(-2 + \frac{4\bar{x}_j^2}{h^2} \right) e^{-\bar{x}_j^2/h^2}. \tag{7.17}$$

Evaluating the right hand side for $\Delta x \leq h \leq 2\Delta x$, the usual range for SPH calculations we find it is positive, showing that ω is real and the method stable with a Gaussian kernel. In practice the time evolution is approximated by discrete steps and the stability then depends on the scheme used. We will discuss time stepping schemes later.

8 Test with Toy stars

The usual tests in computational gas dynamics involve systems with rigid or periodic boundaries. In this section we consider tests where the system is a finite region of gas held together by a simple force. In this sense, they are like model stars with the gravitational force replaced by another force which is easy to calculate. These systems are therefore called Toy Stars (Monaghan and Price 2004). The force we consider is such that for any two elements of mass the force between them proportional to their separation and along the line of their centres. This force is the simplest many-body force. It was discovered by Newton who pointed out that if two particles attract each other with a linear force then they move as if attracted to the centre of mass of the pair (see Chandrasekhar (1995) for a modern interpretation of Newton's Principia and, in particular, Newton's proposition LXIV which discusses this force).

The simplest version of the Toy star assumes the pressure P is given in terms of the density ρ by $P = K\rho^2$ where K is a constant. This makes the problem analogous to the problem of shallow water motion in paraboloidal basins. There is an extensive literature on this problem including the early papers of Goldsbrough (1930), the seminal papers of Ball (1962, 1963) and the general analysis by Holm (1990) which contains further references.

8.1 The force law in one dimension

Suppose that we have an isolated group of N particles in one dimension interacting with linear forces so that the force on particle j due to particle k is $\nu m_j m_k (x_k - x_j)$. The potential energy is

$$\Phi = \frac{1}{4}\nu \sum_{j=1}^{N}\sum_{k=1}^{N} m_j m_k (x_j - x_k)^2, \tag{8.1}$$

The equation of motion of the j^{th} particle is then

$$m_j \frac{d^2 x_j}{dt^2} = -\nu m_j \sum_k m_k (x_j - x_k). \tag{8.2}$$

However, the centre of mass

$$\frac{\sum_k m_k x_k}{\sum_k m_k}, \tag{8.3}$$

can be chosen as the origin so the equation of motion becomes

$$\frac{d^2 x_j}{dt^2} = -\nu M x_j, \tag{8.4}$$

where M is the total mass. The potential can then be written

$$\Phi = \frac{1}{2}\nu M \sum_j m_j x_j^2, \tag{8.5}$$

The motion of the N-body system is therefore identical to the independent motion of each particle in a harmonic potential. In the following we replace $M\nu$ by Ω^2.

8.2 The equations of motion for a Toy star

The system is one dimensional with velocity v, density ρ, and pressure P. The acceleration equation is

$$\frac{dv}{dt} = -\frac{1}{\rho}\frac{\partial P}{\partial x} - \Omega^2 x, \tag{8.6}$$

We assume the equation of state is

$$P = K\rho^2, \tag{8.7}$$

which makes our equations identical in form to those for the shallow water equations with density replacing the water depth. The acceleration equation is then

$$\frac{dv}{dt} = -2K\frac{\partial \rho}{\partial x} - \Omega^2 x. \tag{8.8}$$

The simplest case to consider is the static model for which the density is given by

$$\rho = \rho_0(1 - x^2/x_e^2). \tag{8.9}$$

The next simplest case is to study the small oscillations about the static model. However, one of the attractive features of the toy star is that we can find an exact stable non linear oscillation. If M, K and Ω are specifed then ρ_0 and therefore x_e can be calculated. To simplify the following equations we use x_e as the unit of length, and we use $1/\Omega$ as the unit of time. The acceleration equation then becomes

$$\frac{dv}{dt} = -\frac{1}{2}\frac{\partial \rho}{\partial x} - x, \tag{8.10}$$

and then the static density $\bar{\rho}$ is

$$\bar{\rho} = 1 - x^2, \tag{8.11}$$

while $P = \rho^2/4$ and $M = 4/3$.

8.3 Small amplitude oscillations of a Toy star

We now consider small oscillations of our toy star. We assume v is small and we write the density in the form

$$\rho = \bar{\rho} + \eta. \tag{8.12}$$

If we retain only quantities which are linear in the perturbations the acceleration equation becomes

$$\frac{\partial v}{\partial t} = -\frac{1}{2}\frac{\partial \eta}{\partial x}, \tag{8.13}$$

and the continuity equation becomes

$$\frac{\partial \eta}{\partial t} = -\frac{\partial(\bar{\rho} v)}{\partial x}. \tag{8.14}$$

We let the time variation be $e^{i\omega t}$ and, by combining the equations, the equation for v becomes

$$(1-x^2)\frac{d^2 v}{dx^2} - 4x\frac{dv}{dx} + 2(\omega^2 - 1)v = 0. \tag{8.15}$$

The solutions of this equation are the Gegenbauer polynomials $G_n(x)$. The solution for G_n requires that

$$2(\omega^2 - 1) = n^2 + 3n, \tag{8.16}$$

or

$$\omega^2 = \frac{(n+1)(n+2)}{2}. \tag{8.17}$$

Typical examples of Gegenbauer polynomials are $G_0 = 1$, $G_1 = x$, $G_2 = 3(5x^2 - 1)/2$, and $G_3 = 5(7x^3 - 3x)/2$. Note that the Gegenbauer polynomials rise rapidly near the edge of the Toy Star. The standard normalization is

$$\int_{-1}^{1} G_n^2 (1-x^2) dx = 2\frac{(n+1)(n+2)}{2n+3}. \tag{8.18}$$

Other properties of G_n can be found in books on special functions e.g. Abramowitz and Stegun which is available on the web). The equation for the density perturbation is

$$(1-x^2)\frac{d^2 \eta}{dx^2} - 2x\frac{d\eta}{dx} + 2\omega^2 \eta = 0. \tag{8.19}$$

The solution to this equation are Legendre polynomials P_m. We note that

$$\frac{dP_{m+1}}{dx} = G_m. \tag{8.20}$$

We compare the perturbation solution with the SPH calculation below.

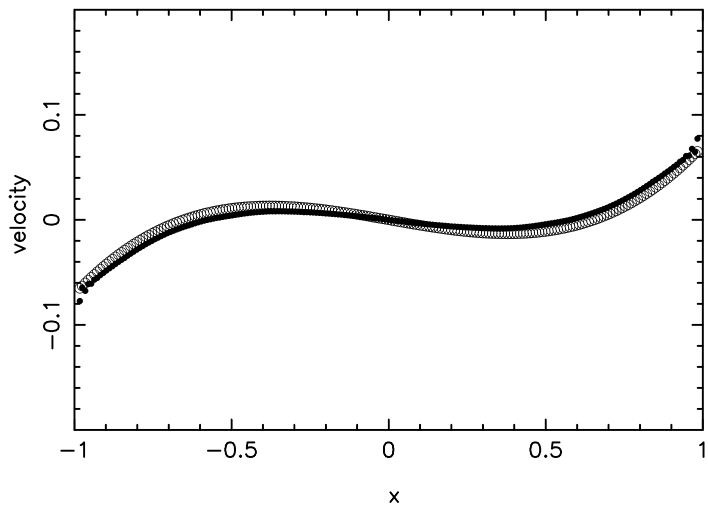

Figure 1: The velocity field for the toy star oscillating with the velocity field in the 3rd mode after 4 periods. The SPH results are shown by the filled symbols and the exact result by the circles.

8.4 SPH results for small oscillations

To simulate the high order oscillations we need enough particles to ensure the resolution length is much smaller than the separation of the nodes. In the present case we use 400 particles. The toy star can be set up with the particles in the static position with initial velocity $v = 0.01 C_s G_n(x)$ and solution $v = 0.01 C_s G_n(x) \cos(\omega t)$, where C_s is the speed of sound (with value $1/\sqrt{2}$ in our scaled units). Correspondingly the expected density perturbation is $\eta = 0.02 C_s \omega P_{n+1} \sin(\omega t)$. Results for other modes are given by Monaghan and Price (2004). These results have been used by Monaghan and Price (2004) to test the SPH algorithm. They find that the frequencies calculated using SPH are in good agreement with theory for the first 20 modes and the oscillations match theory very well over the first 10 oscillation periods. The Toy stars considered here can be extended to 2 and 3 dimensions. In the 3 D case there are no incompressible flow problems which are related to the Toy star.

9 The Lagrangian

The Lagrangian L for the non dissipative motion of a fluid is (Eckart 1960)

$$L = \int \rho \left(\frac{1}{2} v^2 - u(\rho, s) \right) \mathbf{dr}, \tag{9.1}$$

where $\mathbf{v}$ is the velocity, u the thermal energy per unit mass, ρ the density and s is the entropy. We assume the entropy of each element of fluid remains constant though each particle can have a different entropy.

The SPH form of this Lagrangian is

$$L = \sum_b m_b \left(\frac{1}{2} v_b^2 - u(\rho_b, s_b) \right) \tag{9.2}$$

From Lagrange's equations for particle a

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \mathbf{v}_a} \right) - \frac{\partial L}{\partial \mathbf{r}_a} = 0, \tag{9.3}$$

we find

$$\frac{d\mathbf{v}_a}{dt} = - \sum_b m_b \left(\frac{\partial u}{\partial \rho} \right)_s \frac{\partial \rho_b}{\partial \mathbf{r}_a}. \tag{9.4}$$

From the first law of thermodynamics we find

$$\left(\frac{\partial u}{\partial \rho} \right) = \frac{P}{\rho^2}, \tag{9.5}$$

where P_a is the pressure at particle a and, from the SPH summation for the density (but assuming h is constant),

$$\frac{\partial \rho_b}{\partial \mathbf{r}_a} = \sum_c m_c \nabla_b W_{bc} (\delta_{ab} - \delta_{ac}), \tag{9.6}$$

where δ_{ab} is a Kronecker delta, and ∇_a denotes the gradient taken with respect to the coordinates of particle a.

Substituting these results into Lagrange's equation and noting that

$$\frac{\partial L}{\partial \mathbf{v}_b} = m_b \mathbf{v}_b. \tag{9.7}$$

we get

$$\frac{d\mathbf{v}_a}{dt} = - \sum_b m_b \left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2} \right) \nabla_a W_{ab}. \tag{9.8}$$

which agrees with the result we obtained in Lecture 2 using a symmetrized form of the force. As remarked earlier this symmetrized form was discovered from Lagrange's equations. If there is a body force which can be derived from a potential Φ then

$$L = \sum_b m_b \left(\frac{1}{2} v_b^2 - u(\rho_b, s_b) - \Phi \right) \tag{9.9}$$

10 Conservation Laws

The conservation laws of fluid mechanics are intimately related to the invariance properties. These conserved quantities can be found by studying the invariance properties of the Lagrangian.

10.1 Momentum conservation

If the Lagrangian is invariant to a shift in the coordinate system, the momentum is conserved. To see this consider a shift in the coordinate system by the small vector $\mathbf{q}$. In this case the change in $\mathbf{r}$ is $\mathbf{q}$ and the velocity remains unchanged. If L is invariant to this change then the change in L, to first order, is

$$\begin{aligned} \delta L &= \sum_b \frac{\partial L}{\partial \mathbf{r_b}} \cdot \mathbf{q} && (10.1) \\ &= \mathbf{q} \cdot \sum_b \frac{\partial L}{\partial \mathbf{r_b}} && (10.2) \\ &= \mathbf{q} \cdot \frac{d}{dt} \sum_b \frac{\partial L}{\partial \mathbf{v}_b}, && (10.3) \end{aligned}$$

where the last equation follows from Lagrange's equations. Since δL must vanish for arbitrary small $\mathbf{q}$ we conclude that the linear momentum

$$\sum m_b \mathbf{v}_b, \tag{10.4}$$

is conserved.

Suppose now that L is invariant to a rotation of the coordinate system through a small angle ϕ about an axis in the direction $\mathbf{k}$. In this case the change in the coordinate is $\delta \mathbf{r} = \phi \mathbf{k} \times \mathbf{r}$ and the change in the velocity is $\delta \mathbf{v} = \phi \mathbf{k} \times \mathbf{v}$. The resulting change in L

is then

$$\delta L = \sum_b \left(\frac{\partial L}{\partial \mathbf{r_b}} \cdot \delta \mathbf{r} + \frac{\partial L}{\partial \mathbf{v_b}} \cdot \delta \mathbf{v} \right). \tag{10.5}$$

If we use Lagrange's equation and note that

$$\delta \mathbf{v} = \frac{d}{dt} \delta \mathbf{r}, \tag{10.6}$$

we can write

$$\delta L = \frac{d}{dt} \sum_b \frac{\partial L}{\partial \mathbf{v}_b} \cdot \delta \mathbf{r}_b \tag{10.7}$$

$$= \phi \mathbf{k} \cdot \frac{d}{dt} \sum_b \mathbf{r}_b \times \frac{\partial L}{\partial \mathbf{v}_b}. \tag{10.8}$$

But δL must vanish for arbitrary small $\phi \mathbf{k}$. We therefore conclude that

$$\sum_b \mathbf{r}_b \times \frac{\partial L}{\partial \mathbf{v}_b} = \sum_b m_b \mathbf{r}_b \times \mathbf{v}_b, \tag{10.9}$$

is constant. This quantity is the angular momentum.

10.2 Circulation

Imagine a necklace of particles like those illustrated in figure 2. If the particles have the same entropy (so the necklace lies in a constant entropy surface) then nothing will change if each particle is shifted to its neighbour's positions always moving in the same sense around the necklace. The the dynamics should therefore be unchanged.

If the particles on the necklace are denoted by ℓ the change in position and velocity of the ℓth particle will be $(\mathbf{r}_{\ell+1} - \mathbf{r}_\ell)$ and $(\mathbf{v}_{\ell+1} - \mathbf{v}_\ell)$ respectively. The first order change in L is

$$\delta L = \sum_\ell \left(\frac{\partial L}{\partial \mathbf{r}_\ell} \cdot \delta \mathbf{r}_\ell + \frac{\partial L}{\partial \mathbf{v}_\ell} \cdot \delta \mathbf{v}_\ell \right). \tag{10.10}$$

where the summation only applies to the particles around the necklace. Using the previous expressions for $\delta \mathbf{r}$ and $\delta \mathbf{v}$ together with Lagrange's equations results in

$$\delta L = \frac{d}{dt} \sum_\ell \mathbf{v}_\ell \cdot (\mathbf{r}_{\ell+1} - \mathbf{r}_\ell) = 0, \tag{10.11}$$

and we deduce that

$$C = \sum_j \mathbf{v}_\ell \cdot (\mathbf{r}_{\ell+1} - \mathbf{r}_\ell), \tag{10.12}$$

is constant and this is true regardless of the necklace in the constant entropy surface. This result is a discrete version of the conservation of circulation of Kelvin's theorem (Lamb 1932) which states that for a fluid which has no dissipation, and the pressure is a function of the density, the circulation

$$C_K = \int \mathbf{v} \cdot \mathbf{dr}, \tag{10.13}$$

is constant. The integration is around any closed loop. Therefore, by contrast with the conservation of momentum, the circulation invariant is really an infinite number of invariants, one for each loop. Our result is, in general, only approximate because the changes in position and velocity to get from one place in the necklace to its neighbour are discrete whereas exact conservation is only true when infinitesimal transformations are relevant. We get the same result, but with opposite sign, by going around the necklace in the opposite sense. Combine the two and take account of sign shows that

$$\frac{1}{2}\sum_\ell \mathbf{v}_\ell \cdot (\mathbf{r}_{\ell+1} - \mathbf{r}_{\ell-1}), \tag{10.14}$$

which is a more accurate estimate of the circulation.

Now consider the case where the particle entropies vary. The shift of particle ℓ will require a change in its entropy when it gets to the neighbouring position on the necklace. δL contains the following entropy term

$$\sum_\ell \frac{\partial L}{\partial s}\delta s = -\sum_\ell \left(\frac{\partial u}{\partial s}\right)_\rho \delta s = -\sum_\ell T_\ell (s_{\ell+1} - s_\ell). \tag{10.15}$$

where T is the temperature. If, following Eckart (1960), we define a quantity κ by

$$\frac{d\kappa}{dt} = T, \tag{10.16}$$

the extra term can be written, recalling that the entropy of each particle is constant, as

$$-\frac{d}{dt}\sum_\ell \kappa_\ell (s_{\ell+1} - s_\ell). \tag{10.17}$$

As before we can take advantage of the fact that we can go around the necklace in either direction, to write this as

$$-\frac{1}{2}\frac{d}{dt}\sum_\ell \kappa_\ell (s_{\ell+1} - s_{\ell-1}). \tag{10.18}$$

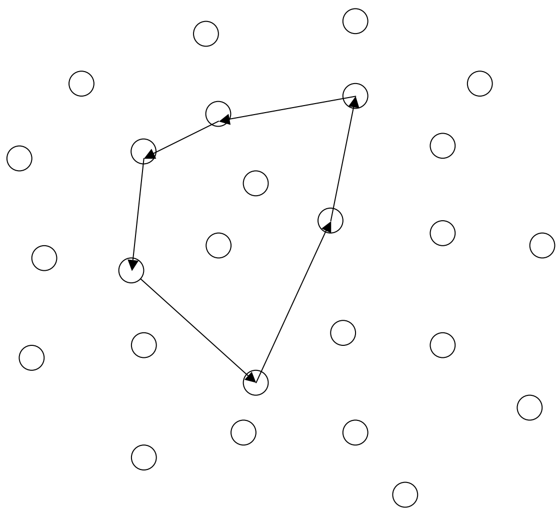

Figure 2: The necklace transformation.

From the fact that δL should vanish for the necklace transformation we infer the conservation of

$$\frac{1}{2}\sum_{\ell} \mathbf{v}_{\ell} \cdot (\mathbf{r}_{\ell+1} - \mathbf{r}_{\ell-1}) - \frac{1}{2}\sum_{\ell} \kappa_{\ell}(s_{\ell+1} - s_{\ell-1}), \tag{10.19}$$

where the second term may be called the thermodynamic circulation. The continuum limit of this conserved quantity is

$$C = \oint \mathbf{v} \cdot \mathbf{dr} - \oint \kappa ds. \tag{10.20}$$

The quantity κ is montonically increasing. Therefore, if we consider C for a loop that involves particles with different entropies, the thermal contribution will force the normal velocity based circulation to change continually. This suggests that such systems can become unstable quite easily.

11 The Lagrangian with constraints

Suppose we use SPH density convergence equation as

$$\frac{d\rho_a}{dt} = -\rho_a \sum_b \frac{m_b}{\rho_b} \mathbf{v}_{ab} \cdot \nabla_a W_{ab}. \tag{11.21}$$

Suppose now we want to use L. If we go back to the original action principle it requires that the action

$$S = \int L dt, \tag{11.22}$$

is stationary for arbitrary and infinitesimal variations $\delta\mathbf{r}$ in the coordinates and corresponding variations $\delta\mathbf{v}$ in the velocities. These variations are related by

$$\frac{d\delta\mathbf{r}}{dt} = \delta\mathbf{v}. \tag{11.23}$$

Suppose then that the only non zero variation is $\delta\mathbf{r}_a$. The first order change in S is

$$\delta S = \int \left(m_a \mathbf{v}_a \cdot \delta\mathbf{v}_a - \sum_b m_b \frac{\partial u(\rho_b, s)}{\partial \rho_b} \frac{\delta\rho_b}{\delta\mathbf{r}_a} \cdot \delta\mathbf{r}_a \right) dt, \tag{11.24}$$

where

$$\frac{\delta\rho_b}{\delta\mathbf{r}_a}, \tag{11.25}$$

denotes the Lagrangian change in ρ_b when the position of particle a changes by $\delta \mathbf{r}_a$at time t. From (4.24) we get

$$\delta \rho_b = -\rho_b \sum_c \frac{m_c}{\rho_c} (\delta \mathbf{r}_b - \delta \mathbf{r}_c) \cdot \nabla_b W_{bc}, \tag{11.26}$$

and therefore

$$\frac{\delta \rho_b}{\delta \mathbf{r}_a} = -\rho_b \sum_c \frac{m_c}{\rho_c} (\delta_{ab} - \delta_{ac}) \nabla_b W_{bc}, \tag{11.27}$$

where δ_{ab} is the Kronecker delta which is 1 if a equals b and zero otherwise. If we substitute this expression into the integral for δS, we find

$$\delta S = \int (m_a \mathbf{v}_a \cdot \delta \mathbf{v}_a - m_a \sum_b m_b \frac{(P_a + P_b)}{\rho_a \rho_b} \nabla_a W_{ab} \cdot \delta \mathbf{r}_a) dt. \tag{11.28}$$

If we now integrate the velocity term by parts recalling that $d(\delta \mathbf{r})/dt = \delta \mathbf{v}$, we get

$$\delta S = m_a \int \left(-\frac{d\mathbf{v}_a}{dt} - \sum_b m_b \frac{(P_a + P_b)}{\rho_a \rho_b} \nabla_a W_{ab} \right) \cdot \delta \mathbf{r}_a dt. \tag{11.29}$$

Since this must vanish for arbitrary $\delta \mathbf{r}_a$ we conclude that

$$\frac{d\mathbf{v}_a}{dt} = -\sum_b m_b \frac{(P_a + P_b)}{\rho_a \rho_b} \nabla_a W_{ab}. \tag{11.30}$$

This is the acceleration equation that is consistent with the continuity equation (11.21). The Lagrangian basis for this choice of the SPH acceleration equation was first pointed out by Bonet and his colleagues.

12 Resolution varying in space and time

In the SPH formulation the density of particle a can be written

$$\rho_a = \sum_b m_b W_{ab}(h_a). \tag{12.1}$$

In many SPH simulations h_a is chosen so that a particle a has a specified number of neighbours. However, to retain the Lagrangian formulations we need to specify h as a function of the coordinates, and this is most easily done by assuming h_a is a function of ρ_a which we denote by $H(\rho_a)$ or H_a. In many astrophysical calculations $H_a \propto (1/\rho_a^{1/d})$

where the number of dimensions is d, but a more general function could be used. For example, to prevent arbitarily large h when ρ becomes very small we could choose

$$H_a = \frac{A}{1 + B\rho_a^{1/d}},$$

where A and B are constants. Furthermore, while the usual practice is to estimate ρ_a at a given time using the value of h_a from a previous time, it would be possible to calculate ρ_a with h_a a function of ρ_a. From Lagrange's equations for particle a we find

$$\frac{d\mathbf{v}_a}{dt} = -\sum_b m_b \left(\frac{\partial u}{\partial \rho}\right)_s \frac{\partial \rho_b}{\partial \mathbf{r}_a} \tag{12.2}$$

From (5.1)

$$\frac{\partial \rho_b}{\partial \mathbf{r}_a} = \sum_c m_c \nabla_a W_{ac}(h_a)\delta_{ab} - m_a \nabla_b W_{ab}(h_b) + \sum_c m_c \frac{\partial W_{bc}}{\partial h_b}\frac{\partial h_b}{\partial \mathbf{r}_a}, \tag{12.3}$$

which we can write as

$$\Omega_b \frac{\partial \rho_b}{\partial \mathbf{r}_a} = \sum_c m_c \nabla_a W_{ac}(h_a)\delta_{ab} - m_a \nabla_b W_{ab}(h_b), \tag{12.4}$$

where the gradient of W_{ab} is taken keeping h constant and

$$\Omega_b = 1 - H_b' \sum_c m_c \frac{\partial W_{bc}(h_b)}{\partial h_b}. \tag{12.5}$$

Here H_b' denotes $\partial H_b/\partial \rho_b$. If the density variation is smooth then $\Omega = 1 + O(h^2)$. Using the first law of thermodynamics the acceleration equation becomes

$$\frac{d\mathbf{v}_a}{dt} = -\sum_b m_b \left(\frac{P_a}{\Omega_a \rho_a^2}\nabla_a W_{ab}(h_a) + \frac{P_b}{\Omega_b \rho_b^2}\nabla_a W_{ab}(h_b)\right). \tag{12.6}$$

This equation conserves linear and angular momentum as we expect from the symmetry of the Lagrangian.

13 Heat conduction and Matter diffusion

The previous sections have been concerned with constant entropy dynamics. In this section we consider the diffusion of heat and matter . The equations describing these diffusion processes are parabolic equations which involve second derivatives of spatially varying quantities such as temperature. In an SPH simulation the particles become disordered and calculating second derivatives by differentiating the interpolation formula often results in unacceptable errors and may not guarantee that entropy increases in isolated systems. We describe a different method which does not have these problems.

14 Heat conduction

The heat conduction equation is

$$\frac{du}{dt} = \frac{1}{\rho}\nabla(\kappa\nabla T), \tag{14.7}$$

where u is the thermal energy per unit mass, T is the absolute temperature, ρ the density, κ the coefficient of thermal conductivity (which in general varies in space), and d/dt is the derivative following the motion. For simplicity we assume that du can be replaced by $\mathcal{C}_p dT$ where $\mathcal{C}_p$ is the specific heat at constant pressure. We will assume that $\mathcal{C}_p$ is constant. The heat conduction equation then takes the form

$$\mathcal{C}_p\frac{dT}{dt} = \frac{1}{\rho}\nabla(\kappa\nabla T), \tag{14.8}$$

14.1 Derivatives from integrals

Consider the integral

$$\int \left(\kappa(x) + \kappa(x')\right)\left(T(\mathbf{r}') - T(\mathbf{r})\right)\frac{(\mathbf{r}-\mathbf{r}')\cdot\nabla W(\mathbf{r}-\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|^2}\mathbf{dr}', \tag{14.1}$$

where $\mathbf{dr}'$ denotes a volume element. For convenience we set $\mathbf{q}F(|\mathbf{q}|) = \nabla W(\mathbf{q}, h)$, and we note that $F \leq 0$. The integral then becomes

$$\int \left(\kappa(x) + \kappa(x')\right)\left(T(\mathbf{r}') - T(\mathbf{r})\right)F\mathbf{dr}'. \tag{14.2}$$

If we expand the functions of $\mathbf{r}'$ about $\mathbf{r}$, and keep the dominant terms, the integral reduces to $-\nabla\cdot(\kappa\nabla T)$. In making this approximation the reader will note that, for example in two dimensions, integrals like

$$\int \left(\frac{\partial^2 T}{\partial x^2}(x-x')^2 + \frac{\partial^2 T}{\partial y^2}(y-y')^2\right)F\mathbf{dr}' \tag{14.3}$$

occur. From symmetry in a two dimensional space we can equate the integrals as follows

$$\int (x-x')^2 F(|\mathbf{r}-\mathbf{r}'|)\mathbf{dr}' = \int (y-y')^2 F(|\mathbf{r}-\mathbf{r}'|)\mathbf{dr}' = \frac{1}{2}\int (\mathbf{r}-\mathbf{r}')^2 F(|\mathbf{r}-\mathbf{r}'|)\mathbf{dr}'. \quad (14.4)$$

Substituting these results into the expression (5.4) it becomes

$$\frac{1}{2}\nabla^2 T \int (\mathbf{r}-\mathbf{r}')^2 F(|\mathbf{r}-\mathbf{r}'|)\mathbf{dr}'. \quad (14.5)$$

If we define $\mathbf{q} = \mathbf{r}' - \mathbf{r}$, and make use of the definition of $F(|\mathbf{q}|)$ we can write the integral in the previous expression as

$$\int \mathbf{q}\cdot\nabla_q W(\mathbf{q},h)\mathbf{dq} = -\int W\nabla\cdot\mathbf{q}\mathbf{dq} = -d, \quad (14.6)$$

where d is the number of dimensions which in this case is 2 which cancels the 1/2 from the series expansion. In 3 dimensions a similar cancellation occurs. If we now write the integral using the usual rule for integral interpolants we find that the heat conduction equation becomes

$$\mathcal{C}_{p,a}\frac{dT_a}{dt} = \sum_b m_b \frac{(\kappa_a+\kappa_b)(T_a-T_b)}{\rho_a\rho_b}F_{ab}. \quad (14.7)$$

The errors in the integral formulation is $O(h^2)$, but there are further errors due to approximating the integral by a summation. This form of the heat conduction equation guarantees that if a particle b has a higher temperature than particle a it will give a positive contribution to the rate of change of temperature of particle a.

14.2 Does the Entropy increase?

Assuming there are no other processes operating we can write the change of s_a (s denotes entropy/mass) as

$$T_a\frac{ds_a}{dt} = \frac{dQ}{dt} = \sum_b m_b \frac{(\kappa_a+\kappa_b)(T_a-T_b)}{\rho_a\rho_b}F_{ab}, \quad (14.1)$$

where Q denotes the heat per unit mass. Multiplying by m_a and summing gives the change in the total entropy

$$\frac{dS}{dt} = \sum_a m_a\frac{ds_a}{dt} = \sum_a\sum_b m_a m_b \frac{(\kappa_a+\kappa_b)(T_a-T_b)}{\rho_a\rho_b T_a}F_{ab}. \quad (14.2)$$

In the summation we can interchange the dummy suffices a and b . If this is added to the original summation , compensating by a factor 1/2 , we get

$$\frac{dS}{dt} = \sum_a m_a \frac{ds_a}{dt} = \frac{1}{2} \sum_a \sum_b m_a m_b \frac{(\kappa_a + \kappa_b)}{\rho_a \rho_b} \left[(T_a - T_b) \left(\frac{1}{T_a} - \frac{1}{T_b} \right) \right] F_{ab}. \tag{14.3}$$

The factor is square brackets is ≤ 0 and since F_{ab} is also ≤ 0, the terms in the summation are all positive. The entropy therefore increases as a result of heat conduction regardless of the positions and temperatures of the particles. This form of the heat conduction equation conserves thermal energy. Cleary and Monaghan (1999) show that when the thermal conductivity is discontinuous or sharply varying it is better to replace

$$\kappa_a + \kappa_b, \tag{14.4}$$

by

$$\frac{4\kappa_a \kappa_b}{\kappa_a + \kappa_b}. \tag{14.5}$$

As a result SPH simulations of two or more fluids in contact do not need any special interface boundary condition for heat conduction

14.3 An example with discontinuous thermal conductivity

A simple application of the SPH algorithm is to calculate the temperature conduction in a composite one dimensional medium. In figure 1 we show the temperature distance variation when the density and specific heats are the same, but the thermal conductivity for $x < 0$ is 1.0 and for $x \geq 0$ is 10.0. The temperature at the end points is fixed. At $x = -1$ the temperature is 0.1 and at $x = 1.0$ the temperature is 1. The results are shown after 100 times steps (using a predictor corrector time stepping scheme Cleary and Monaghan 1999). The continuous line shows the exact results (taken from Carslaw and Jaeger (1990) and the symbols show the SPH results. The agreement is clearly very good. A similar formulation can be used for matter diffusion.

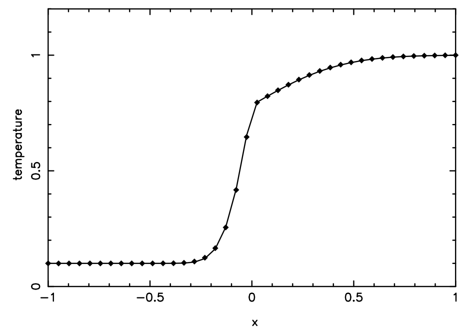

Figure 3: The temperature distance variation in a composite one dimensional system, where the thermal conductivity on the right is 10 times that on the left, and the left and right boundaries are kept at constant temperature.

15 Viscosity

The viscous SPH acceleration equation is (Gingold and Monaghan 1983)

$$\frac{dv_a}{dt} = -\sum_b m_b \left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2} + \Pi_{ab} \right) \frac{\partial}{\partial x_a} W_{ab}, \tag{15.1}$$

where Π_{ab} is the SPH viscous dissipation term

$$\Pi_{ab} = -\left(\frac{\bar{h}_{ab} \mathbf{v}_{ab} \cdot \mathbf{r}_{ab}}{\bar{\rho}_{ab}(r_{ab}^2 + \eta^2)} \right) (\alpha \bar{c}_{ab} - \beta \mu_{ab}) \, . \tag{15.2}$$

where

$$\mu_{ab} = \frac{\bar{h}_{ab} \mathbf{v}_{ab} \cdot \mathbf{r}_{ab}}{r_{ab}^2 + \eta^2}. \tag{15.3}$$

Good results have been obtained with the choice $\alpha = 1$ and $\beta = 2$. Another form of the viscosity for shock problems can be found using ideas from Riemann solvers as a guide. This viscosity uses

$$\Pi_{ab} = -\frac{K v_{sig}(a,b) \mathbf{v}_{ab} \cdot \mathbf{r}_{ab}}{\bar{\rho}_{ab} |\mathbf{r}_{ab}|} \tag{15.4}$$

where K is a constant (typically 0.5) and $v_{sig}(a,b)$ is a signal velocity (Monaghan 1997). This signal velocity automatically includes a term equivalent to the β term in the previous viscosity.

15.1 Invariance properties

A fundamental property of the non relativistic fluid dynamical equations is that they are Galilean invariant. That is, if we shift to a coordinate frame moving with constant velocity $\mathbf{V}$ the equations should be unchanged. This is the case for Π_{ab} because it involves differences of velocity and the shift to the new frame simply replaces $\mathbf{v}_a$ by $\mathbf{v}_a - \mathbf{V}$ and $\mathbf{v}_b$ is replaced in the same way. The difference $\mathbf{v}_{ab}$ is unchanged. Similarly if we shift the origin of the coordinate system to $\mathbf{R}$ the equations are unchanged.

If the fluid is rigidly rotating $\mathbf{v}_a = \Omega \times \mathbf{r}_a$, where Ω is the angular velocity. Substitution into Π_{ab} shows that the viscous term disappears in this case as expected.

15.2 Effective pressure and viscosity

If particles a and b are approaching each other

$$\mathbf{v}_{ab} \cdot \mathbf{r}_{ab} \leq 0, \tag{15.5}$$

and $\Pi_{ab} \geq 0$ and the contribution to the pressure terms is positive. The viscosity therefore acts to slow down approaching particles. The reverse happens for receding particles. If we take the dot product of the acceleration equation with $\mathbf{v}_a$, followed by multiplying by m_a and summing to get

$$\sum_a m_a \mathbf{v}_a \cdot \frac{d\mathbf{v}_a}{dt} = -\sum_a \sum_b m_a m_b \left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2} + \Pi_{ab} \right) \mathbf{v}_a \cdot \nabla_a W_{ab}. \tag{15.6}$$

The left hand side is the rate of change of total kinetic energy so the right hand side must be minus the rate of change of total thermal energy. By interchanging a and b on the right hand side and combining the result with the original right hand side (compensating by a factor 1/2) show that the thermal energy equation is

$$\frac{du_a}{dt} = \frac{P_a}{\rho_a^2} \sum_b m_b \mathbf{v}_{ab} \cdot \nabla_a W_{ab} + \frac{1}{2} \sum_a m_a \sum_b m_b \Pi_{ab} \mathbf{v}_{ab} \cdot \nabla_a W_{ab}., \tag{15.7}$$

It is easy to show that the the viscous dissipation increases the thermal energy and increases the entropy.

16 Applications to shock and rarefaction problems

16.1 Rarefaction waves

The first case we consider is the rarefaction wave. This can be set up by placing SPH particles in the region $-0.5 \leq x \leq 0.5$. The separation Δx is uniform and the density $\rho = 1$. For this example we use 200 particles and set $\gamma = 1.4$, and the initial $h = 1.5 * \Delta x$, and the thermal energy/mass to be 2. We integrate the SPH acceleration, continuity and thermal energy equation. The viscosity is turned off for the rarefaction wave. In figure 4 we show the velocity field for $x \geq 0$. The exact velocity field in the wave is a linear function of x shown by the solid line. The SPH velocity is very close to a linear function, and the slope is within ∼2 percent of the exact slope.

16.2 The Sod shock tube

We now consider the shock tube used by Sod (1978). The system is one dimensional with uniform conditions one each side of a diaphragm which breaks at $t = 0$. To the left of the diagphragm ($x < 0$) the conditions are $\rho, P, v, \gamma = 1.0,\ 1.0,\ 0.0,\ 1.4$ and to the right (0.125, 0.1, 0.0, 1.4). The evolved system consists of (from the left), the undisturbed original conditions, a rarefaction, a contact discontinuity and a shock. Between the shock and the rarefaction the pressure and velocity are constant. The density and thermal energy change discontinuously at the contact discontinuity.

We use the viscosity (15.2) with $\alpha = 1$ and $\beta = 2$. Because the density changes we can choose to have the particles equispaced or equi-mass, or some other combination. For the present simulations we use equi-mass particles with spacing $\Delta x = 0.005$ on the far right hand side and spacing 0.125 this on the far left hand side. The mass of each particle is then $\rho_{\Delta} x = 0.000625$. Because there is an initial discontinuity in all the properties other than the velocity, and because SPH is based on smoothing, we smooth the density and thermal energy at the interface. This means that to be consistent with the particles having constant mass and the density being smoothed we must smooth the spacing.

In figure 5 we show the exact and SPH velocity variation with distance x. The exact post-shock velocity is 0.926. The SPH value is 0.921, an error of 0.5 percent. The

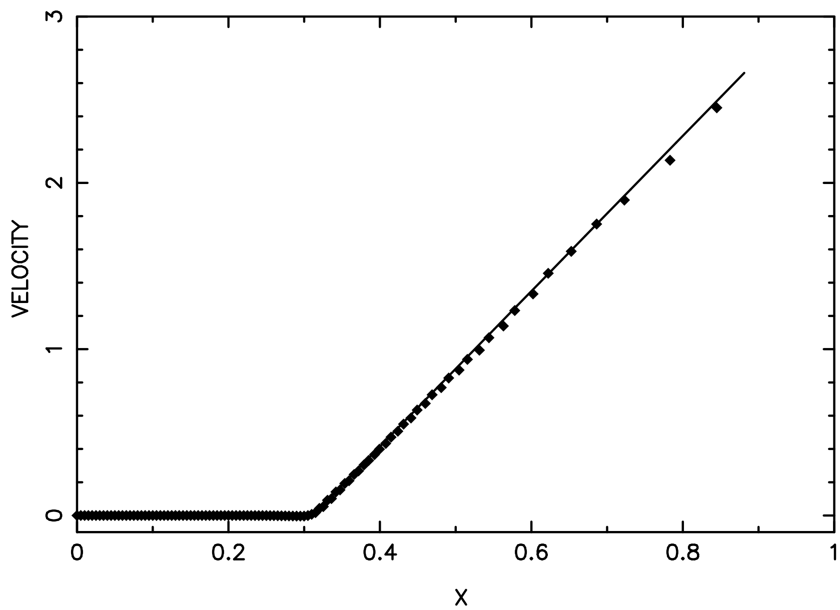

Figure 4: The velocity field for the one dimensional rarefaction waves from the expansion of uniform gas initially in the region $-0.5 \leq x \leq 0.5$. We show the results for the right half $x \geq 0$.The exact velocity field is shown by the solid line and the SPH results by the solid diamonds

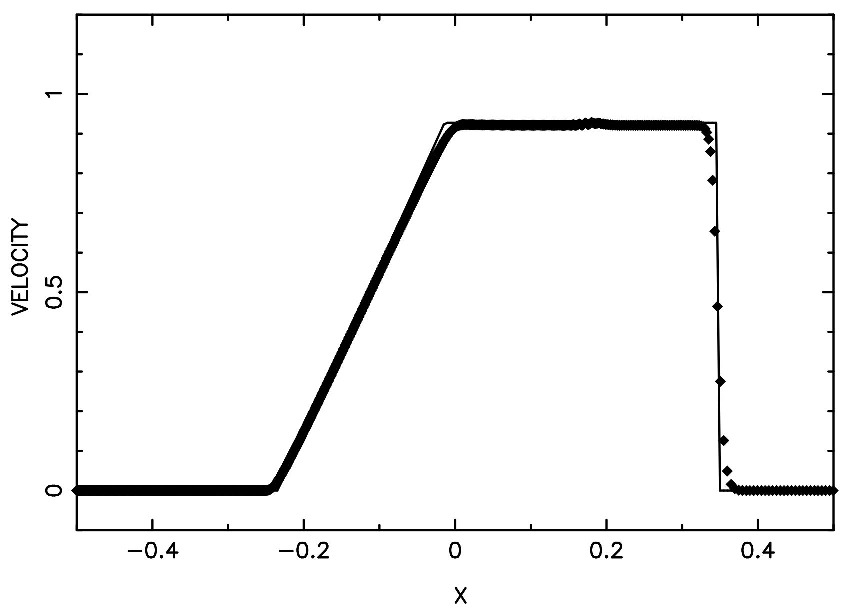

Figure 5: The velocity in the Sod shock tube problem. Note the slight deviation in the velocity associated with the small perturbation to the pressure at the contact discontinuity.

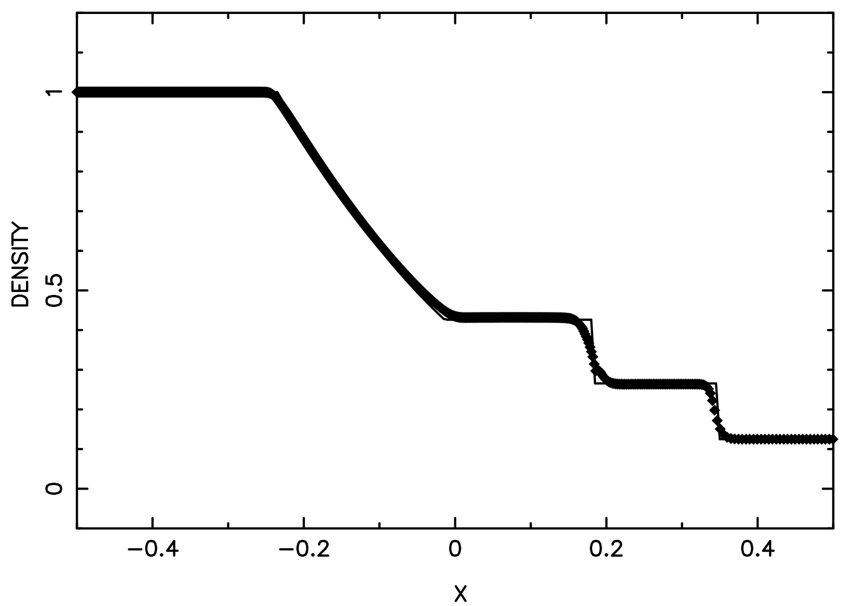

Figure 6: The density in the Sod shock tube problem.

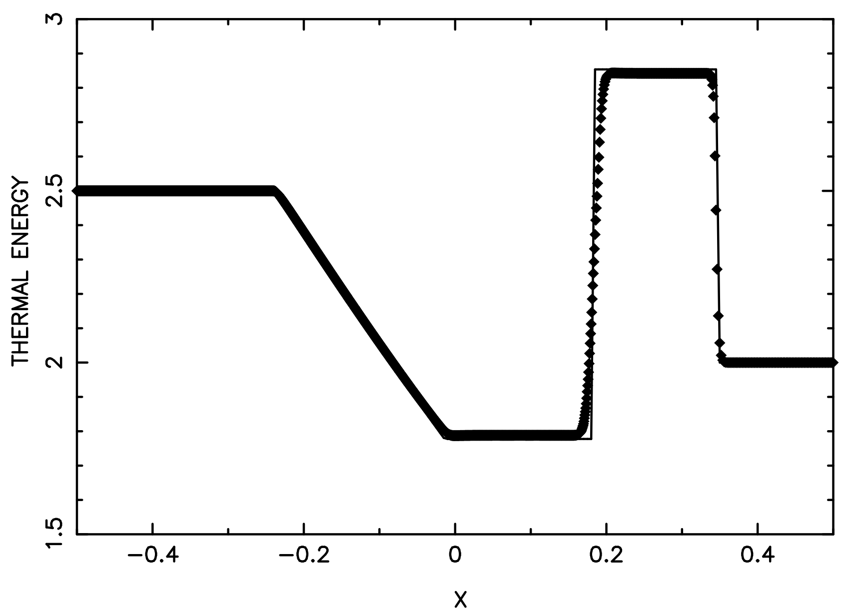

Figure 7: The thermal energy in the Sod shock tube with particle spacing on the right of the diaphragm 0.002. The exact run of thermal energy with distance is shown by the solid line. The solid diamonds are the SPH results. Note the sharpening in the SPH profiles compared with the previous figure.

small bump in the velocity is to an unwanted change in the pressure across the contact discontinuity. The shock front is spread over several particle spacings, but because h and the spacing change across the shock the shock front is 3 of the particle spacings on the low density side. The variation of h with distance is shown in figure 6. In figure 6 we show the exact and SPH density ρ. The density between the contact discontinuity and the shock front is 0.263 to be compared with the exact value of 0.265. In figure 7 we show the thermal energy. All of these results are very satisfactory though, for the resolution used the results are not as accurate as those from finely tuned Riemann solvers. In this lecture we have only considered an SPH viscosity suitable for shocks. In many problems we want to mimic physical viscosities. To do this we can make use of the previous viscosity but note that the effective kinematic viscosity is $\alpha h c_s/6$ in two dimensions (but the numerical coefficient depends on the kernel). We can then write

$$\Pi_{ab} = -\frac{12\mu_a \mu_b}{\rho_a \rho_b(\mu_a + \mu_b)} \frac{\mathbf{v}_{ab} \cdot \mathbf{r}_{ab}}{|\mathbf{r}_{ab}|} \tag{16.8}$$

where $\mu = \nu\rho$. This form of the viscosity has been used by Cleary to model more than one fluid with large differences in viscosity.

Other SPH viscosity calculations are described by Morris et al. (1997) and Chaniotis et al. (2002).

17 References

All the SPH references are available on separate sheets.