Particle Methods in Astrophysical Fluid Dynamics

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Particle methods play an important role in the study of a wide variety of astrophysical fluid dynamics problems. The different methods currently in use are all variants of the so-called Smoothed Particle Hydrodynamics (SPH) scheme introduced by Lucy and Gingold & Monaghan more than twenty years ago. This paper presents a complete introduction to SPH in its modern form, and discusses some of the main numerical properties of the scheme. In particular, the convergence properties of SPH are studied, as a function of the number of particles \( N \) and the number of interacting neighbors \( N_N \), using a simple analysis based on sound waves. It is shown that consistency of SPH (i.e., convergence towards a physical solution) requires both \( N \to \infty \) and \( N_N \to \infty \), with the smoothing length \( h \to 0 \), i.e., \( N_N/N \to 0 \).

§1. Introduction

Many important problems in modern astrophysics involve fluids moving freely in 3D under the influence of self-gravity and pressure forces. These problems are best approached numerically using a Lagrangian formulation where the fluid system is represented by a large number of particles. The most popular scheme, known as Smoothed Particle Hydrodynamics (SPH), is presented in this paper. The key idea of SPH is to calculate pressure gradient forces by kernel estimation, directly from the particle positions, rather than by finite differencing on a grid. The basic form of SPH was introduced more than twenty years ago by Lucy (1977) and Gingold & Monaghan (1977), who used it to study dynamical fission instabilities in rapidly rotating stars. Since then, a wide variety of astrophysical fluid dynamics processes have been studied numerically in 3D using SPH (see Monaghan 1992 for an overview). These include many stellar interaction processes such as binary star coalescence (e.g., Rasio & Shapiro 1994, 1995; Rasio & Livio 1996; Zhuge et al. 1996; Rosswog et al. 1999) and stellar collisions (e.g., Lai, Rasio, & Shapiro 1993; Lombardi, Rasio, & Shapiro 1996; Bailey & Davies 1999), as well as star formation and planet formation (e.g., Nelson et al. 1998; Burkert et al. 1997), supernova explosions (e.g., Herant & Benz 1992; Garcia-Senz et al. 1998), large-scale cosmological structure formation (e.g., Katz et al. 1996; Shapiro et al. 1996), and galaxy formation (e.g., Katz 1992; Steinmetz 1996).

Because of its Lagrangian nature, SPH presents some clear advantages over more traditional grid-based Eulerian methods for calculations of astrophysical fluid flows. Most importantly, fluid advection, even for objects with a sharply defined surface such as stars, is accomplished without difficulty in SPH, since the particles simply follow their trajectories in the flow. In contrast, to track accurately, for example, the orbital motion of two stars across a large 3D grid, can be quite tricky, and the stellar
surfaces then require a special treatment (to avoid “bleeding”). SPH is also very computationally efficient, since it concentrates the numerical elements (particles) where the fluid is at all times, not wasting any resources on empty regions of space. This is particularly important for processes involving a large dynamic range in densities, such as gravitational collapse and fragmentation. For this reason, with given computational resources, SPH provides higher averaged spatial resolution than grid-based calculations, although Godunov-type schemes such as PPM (the Piecewise-Parabolic Method; see, e.g., Woodward 1986) typically provide better resolution of shock fronts. SPH also makes it easy to track the hydrodynamic ejection of matter to large distances from central dense regions. Sophisticated nested-grid algorithms are often necessary to accomplish the same with grid-based methods (see, e.g., Ruffert 1993). Finally, SPH makes it easy to track the evolution of any passively advected scalar quantity, such as the chemical composition of the fluid (see, e.g., Lombardi et al. 1995, 1996, for an application to the study of hydrodynamic mixing during stellar collisions).

§2. Basic Equations and Properties of the SPH Scheme

2.1. SPH from a Variational Principle

A straightforward derivation of the basic SPH equations can be obtained from a Lagrangian formulation of hydrodynamics (Gingold & Monaghan 1982). Consider for simplicity the adiabatic evolution of an ideal fluid with equation of state

\[ p = A\rho^\gamma, \]  \hspace{1cm} (2.1)

where \( p \) is the pressure, \( \rho \) is the density, \( \gamma \) is the adiabatic exponent, and \( A \) (assumed here to be constant in space and time) is related to the specific entropy \( s \propto \ln A \).

The Euler equations of motion,

\[ \frac{d\vec{v}}{dt} = \frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla)\vec{v} = -\frac{1}{\rho} \nabla p, \]  \hspace{1cm} (2.2)

can be derived from a variational principle with the Lagrangian

\[ L = \int \left\{ \frac{1}{2} \vec{v}^2 - u[\rho(\vec{r})] \right\} \rho d^3x. \]  \hspace{1cm} (2.3)

Here \( u[\rho] = p/[(\gamma - 1)\rho] = A\rho^{\gamma-1}/(\gamma - 1) \) is the specific internal energy of the fluid.

The basic idea in SPH is to use the discrete representation

\[ L_{SPH} = \sum_{i=1}^{N} m_i \left[ \frac{1}{2} \vec{v}_i^2 - u(\rho_i) \right] \]  \hspace{1cm} (2.4)

for the Lagrangian, where the sum is over a large but discrete number of small fluid elements, or “particles,” covering the volume of the fluid. Here \( m_i \) is the mass and \( \vec{v}_i \) is the velocity of the particle with position \( \vec{r}_i \). For expression (2.4) to become the Lagrangian of a system with a finite number \( N \) of degrees of freedom, we need a
prescription to compute the density $\rho_i$ at the position of any given particle $i$, as a function of the masses and positions of neighboring particles.

In SPH, the density at any position is calculated as the local average

$$\rho(\vec{r}) = \sum_j m_j W(\vec{r} - \vec{r}_j; h), \quad (2.5)$$

where $W(\vec{r}; h)$ is a smoothing kernel of width $\sim h$. Necessary constraints on the kernel $W(\vec{r}; h)$ are that (i) it integrates to unity (consequently the integral of eq. (2.5) over all space automatically gives the total conserved mass of the system), and (ii) it approaches the Dirac delta function $\delta(\vec{r})$ in the limit where $h \to 0$. In practice, smoothing kernels with finite supports are almost always used, so that a finite number $N_N$ of particles around $\vec{r}$ contribute to the estimate of $\rho(\vec{r})$.

Eq. (2.5) gives, in particular, the density in the vicinity of particle $i$ as $\rho_i = \rho(\vec{r}_i)$, and we can now obtain the equations of motion for all the particles. Deriving the Euler-Lagrange equations from $L_{SPH}$ we get

$$\frac{d\vec{v}_i}{dt} = -\sum_j m_j \left( \frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} \right) \nabla_i W_{ij}, \quad (2.6)$$

where $W_{ij} = W(\vec{r}_i - \vec{r}_j; h)$ and we have assumed that the form of $W$ is such that $W_{ij} = W_{ji}$. The expression on the right-hand side of eq. (2.6) is a sum over neighboring particles (within a distance $\sim h$ of $\vec{r}_i$) representing a discrete approximation to the pressure gradient acceleration $[-(1/\rho)\nabla p]_i$ for particle $i$.

The following energy and momentum conservation laws are satisfied exactly by these simple SPH equations of motion:

$$\frac{d}{dt} \left( \sum_{i=1}^{N} m_i \vec{v}_i \right) = 0, \quad (2.7)$$

and

$$\frac{d}{dt} \left( \sum_{i=1}^{N} m_i \left[ \frac{1}{2} v_i^2 + u_i \right] \right) = 0, \quad (2.8)$$

where $u_i = p_i/[(\gamma - 1)\rho_i]$. Note that energy and momentum conservation in this simple version of SPH is independent of the number of particles $N$.

Typically, a full implementation of SPH for astrophysical problems will add to eq. (2.6) a treatment of self-gravity (e.g., using one of the many grid-based or tree-based algorithms developed for $N$-body simulations) and an artificial viscosity term to allow for entropy production in shocks. In addition, we have assumed here that the smoothing length $h$ is constant in time and the same for all particles. In practice, individual and time-varying smoothing lengths $h_i(t)$ are almost always used, so that the local spatial resolution can be adapted to the (time-varying) density of SPH particles (see Nelson & Papaloizou 1994 for a rigorous derivation of the equations of motion from a variational principle in this case). Other derivations of the SPH equations, based on the application of smoothing operators to the fluid equations (and without the use of a variational principle), are also possible (Monaghan 1985; Hernquist & Katz 1989; Monaghan 1992).
2.2. Basic SPH Equations

In this section, we summarize the basic equations for various forms of the SPH scheme currently in use, incorporating gravity, artificial viscosity, and individual smoothing lengths.

2.2.1. Density and Pressure

The SPH estimate of the fluid density at \( \vec{r}_i \) is calculated as \( \rho_i = \sum_j m_j W_{ij} \) [cf. eq. (2.5)]. Many recent implementations of SPH use a form for \( W_{ij} \) proposed by Hernquist & Katz (1989),

\[
W_{ij} = \frac{1}{2} \left[ W(|\vec{r}_i - \vec{r}_j|; h_i) + W(|\vec{r}_i - \vec{r}_j|; h_j) \right].
\]  

(2.9)

This choice guarantees symmetric weights \( W_{ij} = W_{ji} \) even between particles \( i \) and \( j \) with different smoothing lengths. For the smoothing kernel \( W(r; h) \), the cubic spline

\[
W(r; h) = \frac{1}{\pi h^3} \begin{cases} 
1 - \frac{3}{4} \left( \frac{r}{h} \right)^2 + \frac{3}{4} \left( \frac{r}{h} \right)^3, & 0 \leq \frac{r}{h} < 1, \\
\frac{1}{4} \left[ 2 - \left( \frac{r}{h} \right) \right]^3, & 1 \leq \frac{r}{h} < 2, \\
0, & \frac{r}{h} \geq 2,
\end{cases}
\]

(2.10)

introduced by Monaghan & Lattanzio (1985) is a common choice. Eq. (2.10) is sometimes called a “second-order accurate” kernel. Indeed, when the true density \( \rho(\vec{r}) \) of the fluid is represented by an appropriate distribution of particle positions, masses, and smoothing lengths, one can show that \( \rho_i = \rho(\vec{r}_i) + O(h_i^2) \) (see, e.g., Monaghan 1985). Spherically symmetric kernels such as that of eq. (2.10) can lead to loss of spatial resolution for highly anisotropic flows (as in, e.g., cosmological pancake-type collapse). Adaptive, anisotropic kernels can be used for those problems (Fulbright et al. 1995; Shapiro et al. 1996; Owen et al. 1998).

Depending on which thermodynamic evolution equation is integrated (see §2.2.4 below), particle \( i \) also carries either the parameter \( u_i \), the internal energy per unit mass in the fluid at \( \vec{r}_i \), or \( A_i \), the entropic variable, a function of the specific entropy in the fluid at \( \vec{r}_i \). Although arbitrary equations of state can be implemented in SPH, here, for simplicity, we consider only polytropic equations of state: the pressure \( p_i \) at \( \vec{r}_i \) is related to the density by

\[
p_i = (\gamma - 1) \rho_i u_i,
\]

(2.11)

or

\[
p_i = A_i \rho_i^{\gamma_i}.
\]

(2.12)

The speed of sound in the fluid at \( \vec{r}_i \) is \( c_i = (\gamma p_i/\rho_i)^{1/2} \).

2.2.2. Dynamical Equations and Gravity

Particle positions are updated either by

\[
\frac{d\vec{r}_i}{dt} = \vec{v}_i,
\]

(2.13)

or the more general XSPH method

\[
\frac{d\vec{r}_i}{dt} = \vec{v}_i + \epsilon \sum_j m_j \frac{\vec{v}_j - \vec{v}_i}{\rho_{ij}} W_{ij}
\]

(2.14)
where $\rho_{ij} = (\rho_i + \rho_j)/2$ and $\epsilon$ is a constant parameter in the range $0 < \epsilon < 1$ (Monaghan 1989). Eq. (2.14), in contrast to eq. (2.13), changes particle positions at a rate closer to the local smoothed velocity. The XSPH method was originally proposed as a way to minimize spurious interparticle penetration across the interface of two colliding fluid streams.

Generalizing eq. (2.6) to account for gravitational forces and artificial viscosity (hereafter AV), the velocity of particle $i$ is updated according to

$$\frac{d\vec{v}_i}{dt} = a_i^{(\text{Grav})} + a_i^{(\text{SPH})}$$

(2.15)

where $a_i^{(\text{Grav})}$ is the gravitational acceleration and

$$a_i^{(\text{SPH})} = -\sum_j m_j \left[ \left( \frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} \right) + \Pi_{ij} \right] \nabla_i W_{ij}.$$  

(2.16)

Various forms for the AV term $\Pi_{ij}$ are discussed below (§2.2.3). The AV ensures that correct jump conditions are satisfied across (smoothed) shock fronts, while the rest of eq. (2.16) represents one of many possible SPH-estimators for the acceleration due to the local pressure gradient (see, e.g., Monaghan 1985).

To provide reasonable accuracy, an SPH code must solve the equations of motion of a large number of particles (typically $N \gg 1000$). This rules out a direct summation method for calculating the gravitational field of the system, unless special purpose hardware such as the GRAPE is used (Steinmetz 1996; Klessen 1997; see the article by Makino in this volume for an update on GRAPE computers). In most implementations of SPH, particle-mesh algorithms (Evrard 1988; Rasio & Shapiro 1992; Couchman et al. 1995) or tree-based algorithms (Hernquist & Katz 1989; Dave et al. 1997) are used to calculate the gravitational accelerations $a_i^{(\text{Grav})}$. Tree-based algorithms perform better for problems involving large dynamic ranges in density, such as star formation and large-scale cosmological simulations. For typical stellar interaction problems, density contrasts rarely exceed a factor $\sim 10^2 - 10^3$ and grid-based algorithms and direct solvers are then generally faster. Tree-based and grid-based algorithms can also be used to calculate lists of nearest neighbors for each particle, exactly as in gravitational N-body simulations.

2.2.3. Artificial Viscosity

For the AV, a symmetrized version of the form proposed by Monaghan (1989) is often adopted,

$$\Pi_{ij} = -\alpha \mu_{ij} c_{ij} + \beta \mu^2_{ij},$$

(2.17)

where $\alpha$ and $\beta$ are constant parameters, $c_{ij} = (c_i + c_j)/2$ is the average sound speed, and

$$\mu_{ij} = \begin{cases} \frac{(\vec{v}_i - \vec{v}_j) \cdot (\vec{r}_i - \vec{r}_j)}{h_{ij}(\vec{r}_i - \vec{r}_j)^2 / (\eta^2 + h_{ij})} & \text{if } (\vec{v}_i - \vec{v}_j) \cdot (\vec{r}_i - \vec{r}_j) < 0 \\ 0 & \text{if } (\vec{v}_i - \vec{v}_j) \cdot (\vec{r}_i - \vec{r}_j) \geq 0 \end{cases}$$

(2.18)

with $h_{ij} = (h_i + h_j)/2$ and the constant $\eta^2 \sim 10^{-2}$ (introduced to prevent numerical divergences). This form represents a combination of a bulk viscosity (linear in
\( \mu_{ij} \) and a von Neumann-Richtmyer viscosity (quadratic in \( \mu_{ij} \)) for convergent flows \( (\mu_{ij} = 0 \) in regions of divergent flow). The von Neumann-Richtmyer viscosity was initially introduced to suppress particle interpenetration in the presence of strong shocks. For most problems, eq. (2.17) provides an optimal treatment of shocks when \( \alpha \simeq 0.5 \) and \( \beta \simeq 1 \) (Monaghan 1989; Hernquist & Katz 1989; Lombardi et al. 1999).

A well-known problem with the classical AV of eq. (2.17) is that it can generate large amounts of spurious shear viscosity. For this reason, Hernquist & Katz (1989) introduced another form for the AV:

\[
\Pi_{ij} = \begin{cases} 
\frac{q_i}{\rho_i^2} + \frac{q_j}{\rho_j^2} & \text{if } (\vec{v}_i - \vec{v}_j) \cdot (\vec{r}_i - \vec{r}_j) < 0 \\
0 & \text{if } (\vec{v}_i - \vec{v}_j) \cdot (\vec{r}_i - \vec{r}_j) \geq 0
\end{cases},
\]

(2.19)

where

\[
q_i = \begin{cases} 
\alpha \rho_i c_i h_i |\nabla \cdot \vec{v}_i| + \beta \rho_i h_i^2 |\nabla \cdot \vec{v}_i^2| & \text{if } (\nabla \cdot \vec{v})_i < 0 \\
0 & \text{if } (\nabla \cdot \vec{v})_i \geq 0
\end{cases},
\]

(2.20)

and

\[
(\nabla \cdot \vec{v})_i = \frac{1}{\rho_i} \sum_j m_j (\vec{v}_j - \vec{v}_i) \cdot \nabla_i W_{ij}.
\]

(2.21)

Although this form provides a slightly less accurate description of shocks than eq. (2.17), it does exhibit less shear viscosity.

More recently, Balsara (1995) has proposed the AV

\[
\Pi_{ij} = \left( \frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} \right) \left(-\alpha \mu_{ij} + \beta \mu_{ij}^2 \right),
\]

(2.22)

where

\[
\mu_{ij} = \begin{cases} 
\frac{(\vec{v}_i - \vec{v}_j) \cdot (\vec{r}_i - \vec{r}_j)}{h_{ij}(|\vec{r}_i - \vec{r}_j|^2/h_{ij}^2 + \eta^2)} \frac{f_i + f_j}{2c_{ij}} & \text{if } (\vec{v}_i - \vec{v}_j) \cdot (\vec{r}_i - \vec{r}_j) < 0 \\
0 & \text{if } (\vec{v}_i - \vec{v}_j) \cdot (\vec{r}_i - \vec{r}_j) \geq 0
\end{cases}.
\]

(2.23)

Here \( f_i \) is the form function for particle \( i \) defined by

\[
f_i = \frac{|\nabla \cdot \vec{v}_i|}{|\nabla \cdot \vec{v}_i| + |\nabla \times \vec{v}_i| + \eta' c_i / h_i},
\]

(2.24)

where the factor \( \eta' \sim 10^{-4} - 10^{-5} \) prevents numerical divergences, \( (\nabla \cdot \vec{v})_i \) is given by eq. (2.21), and

\[
(\nabla \times \vec{v})_i = \frac{1}{\rho_i} \sum_j m_j (\vec{v}_j - \vec{v}_i) \times \nabla_i W_{ij}.
\]

(2.25)

The form function \( f_i \) acts as a switch, approaching unity in regions of strong compression \( (|\nabla \cdot \vec{v}| \gg |\nabla \times \vec{v}|_i) \) and vanishing in regions of large vorticity \( (|\nabla \times \vec{v}|_i \gg |\nabla \cdot \vec{v}|_i) \). Consequently, this AV has the advantage that dissipation in shear layers is suppressed. Note that since \( (p_i/\rho_i^2 + p_j/\rho_j^2) \simeq 2c_{ij}^2/(\gamma \rho_{ij}) \), eq. (2.22) behaves like eq. (2.17) when \( |\nabla \cdot \vec{v}|_i \gg |\nabla \times \vec{v}|_i \), provided one rescales the \( \alpha \) and \( \beta \) in eq. (2.22) to be a factor of \( \gamma/2 \) times the \( \alpha \) and \( \beta \) in eq. (2.17).
For additional alternative treatments of AV, see the papers by Morris & Monaghan (1997), Shapiro et al. (1996), Selhammar (1997), and Owen et al. (1998).

Note that a physical viscosity can also be added to SPH, for simulations of 3D viscous flows, solving the Navier-Stokes equation (e.g., Flebbe et al. 1994; Watkins et al. 1996).

2.2.4. Thermodynamics

To complete the description of the fluid, either $u_i$ or $A_i$ is evolved according to a discretized version of the first law of thermodynamics. Although various forms of these evolution equations exist, the most commonly used are

\[
\frac{du_i}{dt} = \frac{1}{2} \sum_j m_j \left( \frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} + \Pi_{ij} \right) (\vec{v}_i - \vec{v}_j) \cdot \nabla_i W_{ij}, \tag{2.26}
\]

and

\[
\frac{dA_i}{dt} = \gamma - 1 \frac{1}{2\rho_i^{\gamma-1}} \sum_j m_j \Pi_{ij} (\vec{v}_i - \vec{v}_j) \cdot \nabla_i W_{ij}. \tag{2.27}
\]

We call eq. (2.26) the “SPH energy equation,” while eq. (2.27) is the “SPH entropy equation.” Which equation one should integrate depends upon the problem being treated. Each has its own advantages and disadvantages. Note that the simple forms of eqs. (2.26) and (2.27) neglect terms proportional to the time derivative of $h_i$. Therefore, if we integrate the energy equation, even in the absence of AV, the total entropy of the system will not be strictly conserved if the particle smoothing lengths are allowed to vary in time; if the entropy equation is used to evolve the system, the total entropy is then strictly conserved when $\Pi_{ij} = 0$, but not the total energy (Rasio 1991; Hernquist 1993). Both errors generally decrease as the number of particles $N$ is increased (Rasio 1991), so that for large simulations eqs. (2.26) and (2.27) are usually adequate. For more accurate treatments involving time-dependent smoothing lengths, see Nelson & Papaloizou (1994) and Serna et al. (1996). The energy equation has the advantage that other thermodynamic processes such as heating and cooling (Katz et al. 1996) and nuclear burning (Garcia-Senz et al. 1998) can be incorporated more naturally.

2.2.5. Integration in Time

The results of SPH simulations involving only hydrodynamic forces and gravity do not depend strongly on the particular time-stepping scheme used, as long as the timesteps are short enough to maintain stability and accuracy. A simple second-order, explicit leap-frog scheme is often employed. Implicit schemes must be used when other processes such as heating and cooling are coupled to the dynamics (Katz et al. 1996). A low-order scheme is appropriate for SPH because pressure gradient forces are subject to numerical noise. For stability, the timestep must satisfy a modified Courant condition, with $h_i$ replacing the usual grid separation. For accuracy, the timestep must be a small enough fraction of the dynamical time.

Among the many possible choices for determining the timestep, the prescription proposed by Monaghan (1989) is recommended. This sets

\[
\Delta t = C_N \text{Min}(\Delta t_1, \Delta t_2), \tag{2.28}
\]
where the constant dimensionless Courant number $C_N$ typically satisfies $0.1 < C_N < 0.8$, and where

$$\Delta t_1 = \text{Min}_i \left( \frac{h_i}{\hat{v}_i} \right)^{1/2},$$

$$\Delta t_2 = \text{Min}_i \left( \frac{h_i}{c_i + k (\alpha c_i + \beta \text{Max}_j |\mu_{ij}|)} \right),$$

with $k$ being a constant of order unity. If the Hernquist & Katz AV [eq. (2.19)] is used, the quantity $\text{Max}_j |\mu_{ij}|$ in eq. (2.30) can be replaced by $h_i |\nabla \cdot \vec{v}_i|$ if $(\nabla \cdot \vec{v}_i) < 0$, and by 0 otherwise. By accounting for AV-induced diffusion, the $\alpha$ and $\beta$ terms in the denominator of eq. (2.30) allow for a more efficient use of computational resources than simply using a smaller value of $C_N$.

2.2.6. Smoothing Lengths and Accuracy

The size of the smoothing lengths is often chosen such that all particles maintain approximately some predetermined number of neighbors $N_N$. Typical values of $N_N$ for 3D work range from about 20 to 100. If a particle interacts with too few neighbors, then the forces on it are sporadic, a poor approximation to the forces on a true fluid element. In general, one finds that, for given physical conditions, the noise level in a calculation always decreases when $N_N$ is increased.

At the other extreme, large neighbor numbers degrade the resolution by requiring unreasonably large smoothing lengths. However, higher accuracy is obtained in SPH calculations only when both the number of particles $N$ and the number of neighbors $N_N$ are increased, with $N$ increasing faster than $N_N$ so that the smoothing lengths $h_i$ decrease. Otherwise (e.g., if $N$ is increased while maintaining $N_N$ constant) the SPH method is inconsistent, i.e., it converges to an unphysical limit (see §3 below). The choice of $N_N$ for a given calculation is therefore dictated by a compromise between an acceptable level of numerical noise and the desired spatial resolution (which is $\propto h \propto N_N^{-1/d}$ in $d$ dimensions) and level of accuracy.

2.3. Test Calculations

A number of numerical studies of the SPH scheme based on test calculations have been published recently. A comprehensive study focusing on stellar interaction problems was presented in Lombardi et al. (1999). In that study, a series of systematic tests were performed to evaluate quantitatively the effects of spurious transport in 3D SPH calculations. In particular, the tests examined particle diffusion, numerical viscosity, and angular momentum transport. The main results can be summarized briefly as follows. Individual SPH particles behave like molecules in a liquid (or a solid for the relaxed configurations often used as initial conditions). Spurious particle diffusion in the “liquid phase” can be characterized by a diffusion coefficient $D$, which is a function of the “temperature,” or level of noise in the system, and the particle density $n$. For simulations with $N_N \approx 50 - 100$, typical noise levels correspond to a Maxwellian distribution of random particle velocities with $v_{rms} \approx 0.05 c_s$, where $c_s$ is the local (physical) speed of sound, leading to a minimal amount of spurious diffusion, with $D \approx 0.005 - 0.02 c_s^{-1/3}$. A single set of values for the AV parameters $\alpha$ and $\beta$ remain nearly optimal in a large number of situations: $\alpha \approx 0.5$, $\beta \approx 1$ for
the classical AV of Monaghan (eq. [2.17]), \( \alpha \simeq \beta \simeq 0.5 \) for the Hernquist & Katz AV (eq. [2.19]), and \( \alpha \simeq \beta \simeq \gamma / 2 \) for the Balsara AV (where \( \gamma \) is the adiabatic index; see eq. [2.22]). However these choices may be modified depending on the goals of the particular application. For instance, if spurious particle mixing is not a concern and only weak shocks (Mach number \( \mathcal{M} \sim 1 - 2 \)) are expected during a calculation, then a smaller value of \( \alpha \) is appropriate. Somewhat larger values for \( \alpha \) and \( \beta \) may be preferable if an accurate treatment of high Mach number shocks (\( \mathcal{M} \gg 1 \)) is required. Both the Hernquist & Katz and Balsara forms introduce relatively small amounts of numerical shear viscosity. Furthermore, both Monaghan’s and Balsara’s AV do well at treating shocks and at limiting the amount of spurious mixing.

Other papers presenting results of more narrowly focused sets of test calculations with SPH include those by Rasio & Shapiro (1992), Navarro & White (1993), Steinmetz & Müller (1993), Shapiro et al. (1996), and Owen et al. (1998). Comparisons between the results of SPH and Eulerian grid-based codes for the same problems have been presented by Davies et al. (1993), Smith et al. (1996), Bate & Burkert (1997), and Sigalotti & Klapp (1997).

§3. Convergence and Consistency

For practical purposes, it is not enough to know that the solution of the SPH equations will converge towards the exact fluid solution of a problem in the limit where \( N \to \infty \) and \( h \to 0 \). We are more interested in knowing how far from the exact solution we can expect to be, for given computational resources. Moreover, since two independent parameters are involved (the total number of particles \( N \) and the smoothing length \( h \)), we would like to know how this limit should be taken. If we wanted to construct a hierarchy of increasingly accurate solutions, how should \( N \) and \( h \) be changed from one calculation to the next? In this section, we try to answer these questions by studying a specific example in detail.

The example we consider is the propagation of a linear sound wave in a 1D system. This example is simple enough that the SPH equations can be solved analytically, allowing us to calculate the error present in the SPH solution and to study its behavior as a function of \( N \) and \( h \), as well as other parameters.

The 1D gas is represented by an infinite string of SPH particles. All particles have the same mass \( m \), entropy constant \( A \), and smoothing length \( h \). The adiabatic SPH equations (2.1), (2.6), and (2.13) give

\[
\frac{d^2 x_i}{dt^2} = -mA \sum_j \left( \rho_i^{\gamma-2} + \rho_j^{\gamma-2} \right) W''_{ij},
\]

where \( W''_{ij} = \partial W(x_i - x_j)/\partial x_i \). If the kernel \( W(x) \) is an even function, which we assume, it is clear that the solution \( x_i = ia, \ddot{x}_i = 0 \), for \( i = -\infty, +\infty \), describes an equilibrium. Here \( a \) is the interparticle separation. In practice the system would be represented by a segment of finite length \( L \) with periodic boundary conditions, so that \( a = L/N \) is just a measure of the total number of particles. Throughout the calculation, however, we assume that \( L \gg h \) and \( L \gg \lambda \), where \( \lambda \) is the wavelength,
so that the effects of the boundary conditions can be ignored.

We now perturb the equilibrium, writing

$$x_i = ia + \delta x_i,$$  \hspace{1cm} (3.2)

and

$$\rho_i = \rho_0 + \delta \rho_i,$$  \hspace{1cm} (3.3)

where $\rho_0 = m/a$ is the equilibrium density (in 1D). We expand the density as

$$\rho_i = \rho_0^{-2} + (\gamma - 2)\rho_0^{-3}\delta \rho_i + \ldots,$$  \hspace{1cm} (3.4)

and the kernel as

$$W_{ij} = W((i - j)a) + (\delta x_i - \delta x_j)W'(i - j)a \quad + \quad \frac{1}{2}(\delta x_i - \delta x_j)^2W''((i - j)a) + \ldots,$$  \hspace{1cm} (3.5)

and

$$W'_{ij} = W'(i - j)a + (\delta x_i - \delta x_j)W''((i - j)a) + \ldots.$$  \hspace{1cm} (3.6)

We then linearize the equations of motion (3.1) and find, after some algebra,

$$\frac{d^2 \delta x_i}{dt^2} = -mA\rho_0^{-2}\left[ 2\sum_j (\delta x_i - \delta x_j)W''((i - j)a) + \frac{\gamma - 2}{\rho_0} \sum_j W'(i - j)a \right].$$  \hspace{1cm} (3.7)

The second sum on the right vanishes identically for an even kernel. We now let $\delta x_i \propto \exp[i(kia - \omega t)]$. The first sum in the right hand side of eq. (3.7) becomes

$$2\sum_j (\delta x_i - \delta x_j)W''((i - j)a) = 2\delta x_i \sum_n [1 - \exp(-ikna)] W''(na),$$  \hspace{1cm} (3.8)

where we have defined a new index $n = i - j$. Similarly, using eqs. (2.5) and (3.5) for the density, the third sum becomes

$$(\gamma - 2)\frac{\rho_0}{\rho_i} m \sum_n \sum_m \exp(-ikna) \left[ 1 - \exp(-ikma) \right] W'(na) W'(ma).$$  \hspace{1cm} (3.9)

Combining eqs. (3.7)—(3.9) we find the dispersion relation,

$$\omega^2 = mA\rho_0^{-2}\left[ 2\sum_n [1 - \exp(-ikna)] W''(na) + (\gamma - 2)a \sum_n \sum_m \exp(-ikna) \left[ 1 - \exp(-ikma) \right] W'(na) W'(ma) \right].$$  \hspace{1cm} (3.10)
We are interested in taking two different limits of this equation, and comparing them to the exact dispersion relation, $\omega^2 = k^2 \omega_0^2$, where $c_0 = (\gamma p_0/\rho_0)^{1/2} = (\gamma A\rho_0^{-1})^{1/2}$ is the speed of sound.

The first limit of interest is the long wavelength limit, which corresponds to $a/\lambda \to 0$. This is equivalent to the limit of a large number of particles, $N \to \infty$. In taking this limit, we do not assume anything about the ratio $h/a$, so that the number of neighbors $N_N$ remains arbitrary. Taking the $k \to 0$ limit of eq. (3.10) and defining $c_{SPH}^2 \equiv \omega^2/k^2$ we get

$$c_{SPH}^2 = \frac{2}{\gamma} \frac{(a/h)^2}{\gamma} \sum_{n>0} n^2 w''[n(a/h)] + 4 \frac{\gamma - 2}{\gamma} \left( \frac{a}{h} \right)^4 \left( \sum_{n>0} n w'[n(a/h)] \right)^2.$$  (3.11)

The three relevant parameters in this expression are the dimensionless form of the kernel, $w(\xi) \equiv hW(h\xi)$, the ratio $h/a \propto N_N$, and the adiabatic exponent $\gamma$. It is easy to see from eq. (3.11) that $w(\xi)$ should be twice differentiable and that the correct physical result is then recovered only in the limit where $N_N \to \infty$. One implication, which is of great practical importance, is that the combined limit $N \to \infty$ and $h \to 0$ should not be constructed by letting the number of particles increase while keeping $N_N$ constant. Taking the limit in this way results in an inconsistent scheme, one which does converge, but not towards the correct result. Instead, both $N_N$ and $N$ should be increased, with $N$ increasing faster than $N_N$ so that $h \to 0$ in the process. In addition, it is easy to show (e.g., by evaluating eq. (3.11) for different spline kernels of increasing order) that the convergence is faster when a smoother kernel is used. Therefore, for given computational resources, increasing the smoothness of the kernel can improve the accuracy of the results. Note also that the convergence is faster for larger values of the adiabatic exponent $\gamma$, i.e., for more incompressible fluids.

The other limit of interest for eq. (3.10) is when the ratio $h/a \to \infty$, which corresponds to the limit of a large number of neighbors, $N_N \to \infty$. In this limit, all the sums in eq. (3.10) can be replaced by integrals, using the substitution $\sum_n(\ldots) \to \int(\ldots)dx/a$, with $x = na$. After some algebra we find,

$$c_{SPH}^2 = \frac{2}{\gamma} \int_{-\infty}^{+\infty} \cos kx W(x)dx + (1 - \frac{2}{\gamma})\left( \int_{-\infty}^{+\infty} \cos kx W(x)dx \right)^2.$$  (3.12)

Note that this expression is valid for any $k$, since we did not take the long wavelength limit.

Finally, we can combine both limits by taking the $k \to 0$ limit of eq. (3.12), which gives

$$c_{SPH}^2 = 1 - \frac{\gamma - 1}{\gamma} k^2 \int_{-\infty}^{+\infty} x^2 W(x)dx + O(k^4).$$  (3.13)

This equation demonstrates explicitly the consistency of the scheme in the limit $(N, N_N) \to \infty$ and $h \to 0$. The leading term of the error is, in general, $O(k^2)$. The only exceptions are when $\gamma = 1$ (the isothermal case) and when $W(x)$ is such that the

\footnote{Monaghan (1989) performed a similar calculation but considered only, for simplicity, the isothermal case. This led him to conclude, incorrectly, that the leading error term in the dispersion relation was in general $O(k^6)$ (cf. his eq. [3.11]).}
integral in eq. (3.13) vanishes. This would require the kernel to be nonpositive. An example of a 1D kernel having this property is the $W_4$ kernel of Monaghan (1985):

$$W_4(x; h) = \frac{1}{h} \left\{ \begin{array}{ll} 1 - \frac{5}{2} \left( \frac{x}{h} \right)^2 + \frac{3}{2} \left( \frac{x}{h} \right)^3, & 0 \leq \frac{x}{h} < 1; \\ \frac{1}{2} \left( 1 - \frac{x}{h} \right) \left( 2 - \frac{x}{h} \right)^2, & 1 \leq \frac{x}{h} < 2; \\ 0, & \text{otherwise.} \end{array} \right. $$

(3.14)

This kernel is negative over the interval $1 < x/h < 2$ and has a continuous first derivative. Naturally, one should be careful when using such a kernel in SPH, since physical quantities such as pressure and density are no longer guaranteed to remain positive.

We conclude by summarizing some of our key results:

(a) Higher accuracy is obtained in SPH calculations when both the number of particles $N$ and the number of neighbors $N_N$ are increased, with $N$ increasing faster than $N_N$ so that the smoothing length $h$ decreases.

(b) A number of neighbors $N_N \gg 1$ must be maintained at all times for a calculation to be meaningful.

(c) The SPH scheme is consistent in the limit where $N \to \infty$, $N_N \to \infty$, and $h \to 0$.

(d) Convergence can be accelerated significantly by increasing the smoothness of the kernel.

These results were obtained here on the basis of a particularly simple example, but we expect them to be applicable in general. In particular, it is easy to apply this analysis to other forms of the SPH scheme (e.g., using eq. [2.14] instead of eq. [2.13]), or to extend it to more than one dimension, which allows a study of spurious anisotropy effects (Kalogera & Rasio 1999).

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