SPH Code Notes

Choice of Kernel

Following most implementations (and as introduced by Monaghan & Lattanzio 1985), we will employ an interpolation kernel based upon the M_4 B-spline function

$$w(q) = \sigma \begin{cases} \frac{1}{4}(2-q)^3 - (1-q)^3, & 0 \le q < 1 \\ \frac{1}{4}(2-q)^3, & 1 \le q < 2 \\ 0, & q \ge 2 \end{cases} \tag{1}$$

with (obviously) compact support on $q \le 2$. The SPH smoothing kernel is defined in terms of this function as

$$W(|\mathbf{r}_a - \mathbf{r}_b|, h) = W_{ab}(h) = \frac{1}{h^d} w(q), \quad \text{with} \quad q = \frac{|\mathbf{r}_a - \mathbf{r}_b|}{h} \tag{2}$$

and with the normalization condition

$$\int W(r', h) dr' = 1 \tag{3}$$

This condition is satisfied by choosing $\sigma = 2/3, 10/(7\pi), 1/\pi$ for dimensions $D = 1, 2$, and 3. The kernel is always evaluated on the distance between two particles $\mathbf{r}_{ab} = \mathbf{r}_a - \mathbf{r}_b$, and we will define

$$W_{ab}(h) = W(|\mathbf{r}_{ab}|, h) \tag{4}$$

The gradient of this kernel (with respect to $\mathbf{r}$) is then

$$\nabla W(\mathbf{r}, h) = \frac{\mathbf{r}}{h^D} w'(|\mathbf{r}|/h) \tag{5}$$

with

$$w'(q) = \frac{\sigma}{h^2} \begin{cases} -3 + \frac{9}{4}q, & 0 \le q < 1 \\ -\frac{3}{4}(2-q)^2/q, & 1 \le q < 2 \\ 0, & q \ge 2 \end{cases} \tag{6}$$

In writing the SPH equations, we will often make use of the scalar function $F_{ab}(h)$ defined by

$$\nabla W_{ab} = \mathbf{r}_{ab} F_{ab} = \mathbf{r}_{ab} \frac{1}{h^D} w'(|\mathbf{r}_{ab}|, h) \tag{7}$$

Note that $F_{ab} \le 0$. In some treatments, this quantity is defined as $\nabla W_{ab}(h) = \hat{\mathbf{r}}_{ab} F_{ab}(h)$ ($\hat{\mathbf{r}}$ instead of $\mathbf{r}$) – *caveat lector!*

The derivative of W with respect to the smoothing length h is

$$\frac{\partial W_{ab}(h)}{\partial h} = \frac{\sigma}{h^{D+1}} \begin{cases} -D + (3 + \frac{3}{2}D)q^2 - (\frac{9}{4} + \frac{3}{4}D)q^3, & 0 \le q < 1 \\ -2D + (3 + 3D)q - (3 + \frac{3}{2}D)q^2 + (\frac{3}{4} + \frac{1}{4}D)q^3, & 1 \le q < 2 \\ 0, & q \ge 2 \end{cases} \tag{8}$$

Price & Monaghan (2007) give the kernel for the gravitational acceleration as

$$\phi'(r,h) = \frac{1}{r^2}\int\int_0^r W(r',h)r'^2 dr' d\Omega' \tag{9}$$

For the cubic spline with $D = 3$, this is

$$\phi'(r,h) = \begin{cases} \frac{1}{h^2}\left(\frac{4}{3}q - \frac{6}{5}q^3 + \frac{1}{2}q^4\right), & 0 \le q < 1 \\ \frac{1}{h^2}\left(\frac{8}{3}q - 3q^2 + \frac{6}{5}q^3 - \frac{1}{4}q^4 - \frac{1}{15}q^{-2}\right), & 1 \le q < 2 \\ r^{-2}, & q \ge 2 \end{cases} \tag{10}$$

The kernel for the gravitational potential is then

$$\phi(r,h) = \int\left(-\frac{1}{r}\int_0^r W(r',h)r'^2 dr' + \int_0^r W(r',h)r' dr' - \int_0^{R_h} W(r',h)r' dr'\right) d\Omega' \tag{11}$$

where the upper limit of the final integral R_h is the radius of compact support for the chosen kernel. For the cubic spline with $D = 3$, this is

$$\phi(r,h) = \begin{cases} \frac{1}{h}\left(-\frac{7}{5} + \frac{2}{3}q^2 - \frac{3}{10}q^4 + \frac{1}{10}q^5\right), & 0 \le q < 1 \\ \frac{1}{h}\left(-\frac{8}{5} + \frac{4}{3}q^2 - q^3 + \frac{3}{10}q^4 - \frac{1}{30}q^5 + \frac{1}{15}q^{-1}\right), & 1 \le q < 2 \\ -r^{-1}, & q \ge 2 \end{cases} \tag{12}$$

Finally, the derivative of the potential with respect to the smoothing length is then

$$\frac{\partial\phi(q)}{\partial h} = -\frac{1}{h^2}\left(h\phi(q) + qh^2\phi'(q)\right) \tag{13}$$

These are used for spline-softened gravity consistent with using the kernel for estimating ρ, as follows.

Density estimation and the smoothing length

The Price & Monaghan (2007) prescription for variable smoothing length is to estimate $\rho(\mathbf{r}_a)$ by the usual summation formula

$$\rho_a = \sum_b m_b W_{ab}(h_a) \tag{14}$$

where there is a smoothing length h_a associated with particle a. The density gradient can then be written as

$$\frac{\partial\rho_b}{\partial\mathbf{r}_a} = \frac{1}{\Omega_b}\sum_c m_c \frac{\partial W_{bc}(h_a)}{\partial\mathbf{r}_a}\left(\delta_{ba} - \delta_{ca}\right) \tag{15}$$

where

$$\Omega_a = 1 - \frac{\partial h_a}{\partial\rho_a}\sum_b m_b \frac{\partial W_{ab}(h_a)}{\partial h_a} \tag{16}$$

is a function of order unity except where the smoothing length h varies rapidly with position.

We would like the smoothing length h to be set so the volume around each particle of radius $2h$ (the radius of support of the kernel) has a volume $V(h)$ containing approximately a fixed number of particles. This is to say we would like h to be determined so that

$$m_a N_{neig} = V(h)\rho_a \tag{17}$$

is approximately true. Let

$$h_a(\rho_a) = \eta \left(\frac{m_a}{\rho_a}\right)^{1/D} \tag{18}$$

so that

$$\rho_a(h_a) = m_a \frac{\eta^D}{h_a^D} \tag{19}$$

The parameter η then gives a scale factor on the smoothing length in terms of the average particle separation. Price & Monaghan (2007) use $\eta = 1.2$, which results in approximately 60 neighbours in three dimensions.

Satisfying Equations (19) and (14), that is to say finding a consistent set of h_a and ρ_a, requires the solution of the non-linear equation

$$f(h_a) = \rho_a(h_a) - \rho_{sum} = 0 \tag{20}$$

for each particle, where ρ_{sum} is given by Equation (14). One can use any root-finding method, but note that, except for the first timestep, you will always have an excellent guess at the solution in the values of h from the previous timestep. This makes the quadratic convergence of Newton's method quite attractive, although the fractal nature of Newton iteration's domain of convergence can be a problem. The derivative of $h(\rho)$ is

$$\frac{\partial h_a(\rho_a)}{\partial \rho_a} = -\frac{h_a}{D\rho_a} \tag{21}$$

and Newton's method becomes the iteration

$$h_a \leftarrow h_a - \frac{f(h_a)}{f'(h_a)} \tag{22}$$

where

$$\begin{aligned} f'(h_a) &= \left(\frac{\partial h_a}{\partial \rho_a}\right)^{-1} - \sum_b m_b \frac{\partial W_{ab}(h_a)}{\partial h_a} \\ &= -\frac{D\rho_a}{h_a}\Omega_a \end{aligned} \tag{23}$$

The determination of h for each particle occurs once per timestep, and can be among the more time-consuming steps in an SPH code.

Derivatives

The divergence of the velocity can be written as

$$\begin{aligned}\nabla \cdot \mathbf{v}_a &= -\sum_b \frac{m_b}{\rho_b}\, \mathbf{v}_{ab} \cdot \nabla W_{ab}(h_a) \\ &= -\sum_b \frac{m_b}{\rho_b}\, \mathbf{v}_{ab} \cdot \mathbf{r}_{ab} F_{ab}(h_a)\end{aligned} \tag{24}$$

Note that, since $F_{ab} \leq 0$, this yields the correct sign of the divergence.

The continuity equation

$$\frac{D\rho_a}{Dt} = -\rho \nabla \cdot \mathbf{v} \tag{25}$$

thus becomes

$$\frac{D\rho_a}{Dt} = \frac{1}{\Omega_a} \sum_b m_b \mathbf{v}_{ab} \cdot \mathbf{r}_{ab}\, F_{ab} \tag{26}$$

or

$$\frac{D\rho_a}{Dt} = \frac{\rho_a}{\Omega_a} \sum_b \frac{m_b}{\rho_b}\, \mathbf{v}_{ab} \cdot \mathbf{r}_{ab}\, F_{ab} \tag{27}$$

The second expression is alleged to behave somewhat better where the density gradient is large. Note, however, that we will not be solving the continuity equation explicitly but rather be determining the density by summation via Equation (24).

Another useful quantity is the second derivative or Laplacian. The Laplacian of the internal energy density is employed in the artificial conductivity switch (see below), and the Laplacian forms the basis for including diffusive phenomena in the SPH model. The expression most commonly employed comes from Monaghan:

$$\begin{aligned}\nabla^2 u_a &= 2 \sum_b \frac{m_b}{\rho_b} (u_a - u_b) \frac{\nabla W_{ab}}{|\mathbf{r}_{ab}|} \\ &= 2 \sum_b \frac{m_b}{\rho_b} (u_a - u_b) F_{ab}\end{aligned} \tag{28}$$

We will write the acceleration of the particles as

$$\begin{aligned}\frac{D\mathbf{v}_a}{Dt} &= -\sum_b m_b \left(\frac{P_a}{\Omega_a \rho_a^2} \nabla W_{ab}(h_a) + \frac{P_b}{\Omega_b \rho_b^2} \nabla W_{ab}(h_b) + \Pi_{ab} \overline{\nabla W_{ab}} \right) + \mathbf{g}_a \\ &= -\sum_b m_b \left(\frac{P_a}{\Omega_a \rho_a^2} F_{ab}(h_a) + \frac{P_b}{\Omega_b \rho_b^2} F_{ab}(h_b) + \Pi_{ab} \overline{F_{ab}} \right) \mathbf{r}_{ab} + \mathbf{g}_a\end{aligned} \tag{29}$$

where $\mathbf{g}_a$ is the acceleration from body forces (*e.g.* gravity) on particle a, $\overline{F_{ab}} = \frac{1}{2}\left(F_{ab}(h_a) + F_{ab}(h_b)\right)$, and Π_{ab} is the artificial viscosity. The most commonly-used form for artificial viscosity is

$$\Pi_{ab} = -\frac{\alpha v_{sig} (\mathbf{v}_{ab} \cdot \mathbf{r}_{ab})}{\bar{\rho}_{ab} |\mathbf{r}_{ab}|} \tag{30}$$

where the signal speed is

$$v_{sig} = \begin{cases} \frac{1}{2}\left(c_{s,a} + c_{s,b} - \beta \mathbf{v}_{ab}\cdot\hat{\mathbf{r}}_{ab}\right), & \mathbf{v}_{ab}\cdot\hat{\mathbf{r}}_{ab} \le 0 \\ 0, & \text{else} \end{cases} \tag{31}$$

Monaghan (1997) gives one SPH form of the time derivative of the specific (total) energy $e = \frac{1}{2}v^2 + u$. Ignoring dissipation it is

$$\frac{De_a}{Dt} = -\sum_b m_b \left(\frac{P_a}{\Omega_a \rho_a^2}\mathbf{v}_b \cdot \nabla W_{ab}(h_a) + \frac{P_b}{\Omega_b \rho_b^2}\mathbf{v}_a \cdot \nabla W_{ab}(h_b) \right) + \frac{D\phi_a}{Dt} \tag{32}$$

(note that the P's and the $\mathbf{v}$'s have opposite indices).

Monaghan (1997) adds a dissipative term analogous to the viscosity as

$$\Upsilon_{ab} = -\frac{\alpha v_{sig}(e_a^* - e_b^*)}{\bar{\rho}_{ab}|\mathbf{r}_{ab}|}\mathbf{r}_{ab} \tag{33}$$

where, instead of the total energy per particle, only that part of the kinetic energy arising from motion along the line between particles a and b is included to ensure positive definiteness of the dissipation:

$$e_a^* = \frac{1}{2}(\mathbf{v}_a \cdot \hat{\mathbf{r}}_{ab})^2 + u_a \tag{34}$$

The energy equation becomes

$$\frac{De_a}{Dt} = -\sum_b m_b \left(\frac{P_a}{\Omega_a \rho_a^2}\mathbf{v}_b \cdot \nabla W_{ab}(h_a) + \frac{P_b}{\Omega_b \rho_b^2}\mathbf{v}_a \cdot \nabla W_{ab}(h_b) + \Upsilon_{ab}\cdot\nabla\overline{W_{ab}} \right) + \frac{D\phi_a}{Dt} \tag{35}$$

The dissipation term in De/Dt can then be decomposed as

$$-\sum_b m_b \frac{\alpha v_{sig}}{\bar{\rho}_{ab}}\ \frac{1}{2}(\mathbf{v}_{ab}\cdot\hat{\mathbf{r}}_{ab})^2\ |\mathbf{r}_{ab}|\overline{F_{ab}} - \sum_b m_b \frac{\alpha v_{sig}}{\bar{\rho}_{ab}}(u_a - u_b)|\mathbf{r}_{ab}|\overline{F_{ab}} \tag{36}$$

The first sum is just the dissipation due to the artificial viscosity

$$\sum_b m_b \frac{1}{2}\Pi_{ab}(\mathbf{v}_{ab}\cdot\hat{\mathbf{r}}_{ab})|\mathbf{r}_{ab}|\overline{F_{ab}} \tag{37}$$

Since v_{sig} is non-zero only for $\mathbf{v}_{ab}\cdot\hat{\mathbf{r}}_{ab} \le 0$ and v_{sig} is positive definite, we have $\Pi_{ab} \ge 0$. Since $F_{ab} \le 0$, this term is always greater or equal to zero: viscous dissipation always produces heat.

The second sum represents thermal diffusion. Since in the present case this diffusion is added artificially, there is no reason why the thermal diffusivity should be the same as the viscosity. Price (2008) proposed defining a new signal velocity and coefficient, writing the second sum as

$$\sum_b m_b \frac{\alpha_u v_{sig,u}(u_a - u_b)}{\bar{\rho}_{ab}}|\mathbf{r}_{ab}|\overline{F_{ab}} \tag{38}$$

Note that, if $u_a > u_b$, since $F_{ab} \le 0$ heat flows out of particle a. Price proposed using the thermal diffusion signal velocity

$$v_{sig,u} = \left[\frac{|P_a - P_b|}{\bar{\rho}_{ab}}\right]^2 \tag{39}$$

which acts to equalize the pressure across contact discontinuities. The final expression for the total energy derivative is then

$$\begin{aligned}\frac{De_a}{Dt} = &-\sum_b m_b \left[\frac{P_a}{\Omega_a \rho_a^2}\mathbf{v}_a \cdot \mathbf{r}_{ab} F_{ab}(h_a) + \frac{P_b}{\Omega_b \rho_b^2}\mathbf{v}_b \cdot \mathbf{r}_{ab} F_{ab}(h_b)\right] \\ &\sum_b m_b \left[\frac{1}{2}\Pi_{ab}(\mathbf{v}_{ab}\cdot\hat{\mathbf{r}}_{ab}) + \frac{\alpha_u v_{sig,u}(u_a - u_b)}{\bar{\rho}_{ab}}\right] |\mathbf{r}_{ab}|\overline{F_{ab}} \\ &+ \frac{D\phi_a}{Dt}\end{aligned} \tag{40}$$

To obtain an expression for the rate of change of specific internal energy u, we start by differentiating e to yield

$$\frac{Du}{Dt} = \frac{De}{Dt} - \mathbf{v}\cdot\frac{D\mathbf{v}}{Dt} \tag{41}$$

and then use equations (29) and (40) to obtain

$$\frac{Du_a}{Dt} = \frac{P_a}{\Omega_a \rho_a^2}\sum_b m_b \mathbf{v}_{ab}\cdot\mathbf{r}_{ab} F_{ab}(h_a) + \sum_b m_b \left[\frac{1}{2}\Pi_{ab}(\mathbf{v}_{ab}\cdot\hat{\mathbf{r}}_{ab}) + \frac{\alpha_u v_{sig,u}(u_a - u_b)}{\bar{\rho}_{ab}}\right] |\mathbf{r}_{ab}|\overline{F_{ab}} \tag{42}$$

Of course we need only solve either one form of these two energy equations. For flows with very large ratios of kinetic energy to thermal energy, it is often advantageous to solve for the thermal energy separately; determining the internal energy by subtracting off the kinetic energy is otherwise subject to significant round-off error. In these cases, the ability to solve for the internal energy separately is often a significant advantage of finite-difference methods (such as SPH) over methods which depend upon a Riemann solution which consider only the conserved total energy.

Note that for purely isentropic flows (constant specific entropy s), we need not solve an energy equation at all. In this case the pressure is a function of the density alone, $P = K\rho^\gamma$, where $K \propto e^s$. Such a flow cannot have dissipation (even of the artificial kind), of course. Another option is to solve for the evolution of the entropy constant K.

Switches

We need to be able to add dissipation to SPH in order to model phenomena such as shocks. At the same time, at least in astrophysics, we wish to keep the dissipation in smooth parts of the flow as small as possible. Thus we not only need the expressions above for viscous dissipation, we also need a mechanism for turning on this dissipation only where needed; this has come to be known in SPH as a "switch".

Both the α and α_u coefficients employed above can be determined on a per-particle basis and integrated in time according to

$$\frac{d\alpha}{dt} = \mathbf{S} - \frac{\alpha - \alpha_{min}}{\tau}, \qquad \tau = \frac{h}{\sigma c_s} \tag{43}$$

The goal is to choose a quantity S which becomes large near features in the flow which require dissipation but which is elsewhere small, allowing the α coefficients to decay smoothly to their minimum values. Typical values for σ and α_{min} are about 0.1;

The traditional source term for artificial viscosity is based on the convergence (opposite of divergence!) of the flow:

$$\mathbf{S} = \max(0, -\nabla \cdot \mathbf{v}) \tag{44}$$

The recommended switch for conductivity is

$$\mathbf{S}_u = 0.1\, h\, \nabla^2 u \tag{45}$$

which increases conductivity where there are strong gradients in internal energy such as at a contact discontinuity (with constant pressure and different densities).

Cullen & Dehnen (2010) suggest a different form for the viscosity switch which should be explored further.

Gravity

Price & Monaghan (2007) suggest softening the gravitational acceleration with the same smoothing kernel used for the hydrodynamics. Using the gravitational force kernel defined in Equation (9) the gravitational acceleration becomes

$$\mathbf{g}_a = -G \sum_b m_b\, \overline{\phi'_{ab}}\, \hat{\mathbf{r}}_{ab} - \frac{G}{2} \sum_b m_b \left(\frac{\zeta_a}{\Omega_a} F_{ab}(h_a) + \frac{\zeta_b}{\Omega_b} F_{ab}(h_b) \right) \mathbf{r}_{ab} \tag{46}$$

with $\overline{\phi'_{ab}} = \frac{1}{2}(\phi'_{ab}(h_a) + \phi'_{ab}(h_b))$ and

$$\zeta_a = -\frac{h_a}{D\rho_a} \sum_b \frac{\partial \phi_{ab}(h_a)}{\partial h_a} \tag{47}$$

Time Stepping

The Courant-limited timestep is given by the expression

$$\Delta_i t = C\, h_i \left[h_i |\nabla \cdot \mathbf{v}_i| + c_i + 1.2\, (\alpha c_i + \beta h_i |\nabla \cdot \mathbf{v}_i|) \right]^{-1} \tag{48}$$

where the term involving β in the denominator is included only when $\nabla \cdot \mathbf{v} < 0$ and where the CFL limit is $C \leq 0.5$ for stability. One must also limit the timestep for accuracy in the gravitational force, for example $\Delta t_i = \epsilon\, h_i / \sqrt{a_i}$.

A full leapfrog timestep then proceeds as follows:

1. Determine the timestep by finding the global minimum of Δt_i, using the values for the sound speed and velocity divergence found in the previous timestep.
2. Advance the positions half a timestep.
3. Determine a predicted velocity by advancing it a half-timestep using the previous values of the acceleration
4. Determine the smoothing length, density, and velocity divergence.
5. Compute the derivative of the energy using the predicted velocities (the positions are already at the half-timestep).

6. Advance the energy the half-timestep
7. Compute the acceleration, including the gravitational acceleration if desired.
8. Advance the velocity a full timestep using the total acceleration.
9. Recompute the time derivative of the energy, now using the new velocities
10. Advance the energy half a timestep

Since the leapfrog method is not "self-starting," at the first step we must obtain positions at the half-step:

1. Find the timestep as above, this time computing the sound speed and velocity divergence from the initial conditions.
2. Compute the total acceleration.
3. Advance the positions as
$$x^{1/2} = x^0 + \frac{1}{2}v^0\ \Delta t + \frac{1}{4}a^0\ \Delta t^2$$
4. and now continue from step 3, above

References

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