12 Smoothed Particle Hydrodynamics

Smoothed Particle Hydrodynamics (SPH) is a technique for approximating the continuum dynamics of fluids through the use of particles, which may also be viewed as interpolation points. SPH was originally developed in astrophysics. Since then it has found widespread use also in other areas of science and engineering.

The principal idea of SPH is to treat hydrodynamics in a completely mesh-free fashion, in terms of a set of sampling particles. Hydrodynamical equations of motion are then derived for these particles, yielding a quite simple and intuitive formulation of gas dynamics. Moreover, it turns out that the particle representation of SPH has excellent conservation properties. Energy, linear momentum, angular momentum, mass, and entropy (if no artificial viscosity operates) are all simultaneously conserved. In addition, there are no advection errors in SPH, and the scheme is fully Galilean invariant, unlike alternative mesh-based Eulerian techniques. Due to its Lagrangian character, the local resolution of SPH follows the mass flow automatically, a property that is convenient in representing the large density contrasts often encountered in astrophysical problems.

12.1 Kernel Interpolants

At the heart of smoothed particle hydrodynamics lie so-called kernel interpolants. In particular, we use a kernel summation interpolant for estimating the density, which then determines the rest of the basic SPH equations through the variational formalism.

For any field \( F(\mathbf{r}) \), we may define a smoothed interpolated version, \( F_s(\mathbf{r}) \), through a convolution with a kernel \( W(\mathbf{r}, h) \):

\[
F_s(\mathbf{r}) = \int F(\mathbf{r}') W(\mathbf{r} - \mathbf{r}', h) \, d\mathbf{r}'.
\]  

(12.1)

Here \( h \) describes the characteristic width of the kernel, which is normalized to unity and approximates a Dirac \( \delta \)-function in the limit \( h \to 0 \). We further require that the kernel is symmetric and sufficiently smooth to make it at least differentiable twice. One possibility for \( W \) is a Gaussian. However, most current SPH implementations are based on kernels with a finite support. Usually a cubic spline is adopted.
with $W(r, h) = w\left(\frac{r}{h}\right)$, and

$$w_{3D}(q) = \frac{8}{\pi} \begin{cases} 
1 - 6q^2 + 6q^3, & 0 \leq q \leq \frac{1}{2}, \\
2(1 - q)^3, & \frac{1}{2} < q \leq 1, \\
0, & q > 1,
\end{cases}$$

(12.2)

in three-dimensional normalization. Through Taylor expansion, it is easy to see that the kernel interpolant is at least second-order accurate due to the symmetry of the kernel.

![B-Spline Kernel](image)

Suppose now we know the field at a set of points $r_i$, i.e. $F_i = F(r_i)$. The points have an associated mass $m_i$ and density $\rho_i$, such that $\Delta r_i \sim m_i/\rho_i$ is their associated finite volume element. Provided the points sufficiently densely sample the kernel volume, we can approximate the integral in Eqn. (12.1) with the sum

$$F_s(r) \simeq \sum_j \frac{m_j}{\rho_j} F_j W(r - r_j, h).$$

(12.3)

This is effectively a Monte-Carlo integration, except that thanks to the comparatively regular distribution of points encountered in practice, the accuracy is better
than for a random distribution of the sampling points. In particular, for points in one dimension with equal spacing $d$, one can show that for $h = d$ the sum of Eqn. (12.3) provides a second order accurate approximation to the real underlying function. Unfortunately, for the irregular yet somewhat ordered particle configurations encountered in real applications, a formal error analysis is not straightforward. It is clear however, that at the very least one should have $h \geq d$, which translates to a minimum of $\sim 33$ neighbours in 3D.

Importantly, we see that the estimate for $F_s(r)$ is defined everywhere (not only at the underlying points), and is differentiable thanks to the differentiability of the kernel, albeit with a considerably higher interpolation error for the derivative. Moreover, if we set $F(r) = \rho(r)$, we obtain

$$\rho_s(r) \simeq \sum_j m_j W(r - r_j, h),$$

yielding a density estimate just based on the particle coordinates and their masses. In general, the smoothing length can be made variable in space, $h = h(r, t)$, to account for variations in the sampling density. This adaptivity is one of the key advantages of SPH and is essentially always used in practice. There are two options to introduce the variability of $h$ into Eqn. (12.4). One is by adopting $W(r - r_j, h(r))$ as kernel, which corresponds to the so-called ‘scatter’ approach. It has the advantage that the volume integral of the smoothed field recovers the total mass, $\int \rho_s(r) \, dr = \sum_i m_i$. On the other hand, the so-called ‘gather’ approach, where we use $W(r - r_j, h(r_i))$ as kernel in Eqn. (12.4), requires only knowledge of the smoothing length $h_i$ for estimating the density of particle $i$, which leads to computationally convenient expressions when the variation of the smoothing length is consistently included in the SPH equations of motion. Since the density is only needed at the coordinates of the particles and the total mass is conserved anyway (since it is tied to the particles), it is not important that the volume integral of the gather form of $\rho_s(r)$ exactly equals the total mass.

In the following we drop the subscript $s$ for indicating the smoothed field, and adopt as SPH estimate of the density of particle $i$ the expression

$$\rho_i = \sum_{j=1}^N m_j W(r_i - r_j, h_i).$$

It is clear now why kernels with a finite support are preferred. They allow the summation to be restricted to the $N_{\text{ngb}}$ neighbors that lie within the spherical region of radius $2h$ around the target point $r_i$, corresponding to a computational cost of order $O(N_{\text{ngb}}N)$ for the full density estimate. Normally this number $N_{\text{ngb}}$ of neighbors within the support of the kernel is approximately (or exactly) kept constant by choosing the $h_i$ appropriately. $N_{\text{ngb}}$ hence represents an important parameter of the SPH method and needs to be made large enough to provide sufficient sampling of the kernel volumes. Kernels like the Gaussian on the other hand would require a
summation over all particles $N$ for every target particle, resulting in a $O(N^2)$ scaling of the computational cost.

If SPH was really a Monte-Carlo method, the accuracy expected from the interpolation errors of the density estimate would be rather problematic. But the errors are much smaller because the particles do not sample the fluid in a Poissonian fashion. Instead, their distances tend to equilibrate due to the pressure forces, which makes the interpolation errors much smaller. Yet, they remain a significant source of error in SPH and are ultimately the primary origin of the noise inherent in SPH results.

Even though we have based most of the above discussion on the density, the general kernel interpolation technique can also be applied to other fields, and to the construction of differential operators. For example, we may write down a smoothed velocity field and take its derivative to estimate the local velocity divergence, yielding:

$$\left(\nabla \cdot \mathbf{v}\right)_i = \sum_j \frac{m_j}{\rho_j} \mathbf{v}_j \cdot \nabla_i W(r_i - r_j, h).$$

(12.6)

However, an alternative estimate can be obtained by considering the identity $\rho \nabla \cdot \mathbf{v} = \nabla (\rho \mathbf{v}) - \mathbf{v} \cdot \nabla \rho$, and computing kernel estimates for the two terms on the right hand side independently. Their difference then yields

$$\left(\nabla \cdot \mathbf{v}\right)_i = \frac{1}{\rho_i} \sum_j m_j (\mathbf{v}_j - \mathbf{v}_i) \cdot \nabla_i W(r_i - r_j, h).$$

(12.7)

This pair-wise formulation turns out to be more accurate in practice. In particular, it has the advantage of always providing a vanishing velocity divergence if all particle velocities are equal.

### 12.2 Variational Derivation of SPH

The Euler equations for inviscid gas dynamics in Lagrangian (comoving) form are given by

$$\frac{d\rho}{dt} + \rho \nabla \cdot \mathbf{v} = 0,$$

(12.8)

$$\frac{d\mathbf{v}}{dt} + \frac{\nabla P}{\rho} = 0,$$

(12.9)

$$\frac{du}{dt} + \frac{P}{\rho} \nabla \cdot \mathbf{v} = 0,$$

(12.10)

where $\frac{d/dt = \partial/\partial t + \mathbf{v} \cdot \nabla}$ is the convective derivative. This system of partial differential equations expresses conservation of mass, momentum and energy. Eckart (1960) has shown that the Euler equations for an inviscid ideal gas follow from the Lagrangian

$$L = \int \rho \left(\frac{\mathbf{v}^2}{2} - u\right) \, dV.$$  

(12.11)
This opens up an interesting route for obtaining discretized equations of motion for gas dynamics. Instead of working with the continuum equations directly and trying to heuristically work out a set of accurate difference formulas, one can discretize the Lagrangian and then derive SPH equations of motion by applying the variational principals of classical mechanics. Using a Lagrangian also immediately guarantees certain conservation laws and retains the geometric structure imposed by Hamiltonian dynamics on phase space.

We start by discretizing the Lagrangian in terms of fluid particles of mass $m_i$, yielding

$$L_{\text{SPH}} = \sum_i \left( \frac{1}{2} m_i v_i^2 - m_i u_i \right), \quad (12.12)$$

where it has been assumed that the thermal energy per unit mass of a particle can be expressed through an entropic function $A_i$ of the particle, which simply labels its specific thermodynamic entropy. The pressure of the particles is

$$P_i = A_i \rho_i^\gamma = (\gamma - 1) \rho_i u_i, \quad (12.13)$$

where $\gamma$ is the adiabatic index. Note that for isentropic flow (i.e. in the absence of shocks, and without mixing or thermal conduction) we expect the $A_i$ to be constant. We hence define $u_i$, the thermal energy per unit mass, in terms of the density estimate as

$$u_i(\rho_i) = A_i \frac{\rho_i^{\gamma - 1}}{\gamma - 1}. \quad (12.14)$$

This raises the question of how the smoothing lengths $h_i$ needed for estimating $\rho_i$ should be determined. As we discussed above, we would like to ensure adaptive kernel sizes, meaning that the number of points in the kernel should be approximately constant. In much of the older SPH literature, the number of neighbours was allowed to vary within some (small) range around a target number. Sometimes the smoothing length itself was evolved with a differential equation in time, exploiting the continuity relation and the expectation that $\rho h^3$ should be approximately constant. In case the number of neighbours outside the kernel happened to fall outside the allowed range, $h$ was suitably readjusted, at the price of some errors in energy conservation.

A better method is to require that the mass in the kernel volume should be constant, viz.

$$\rho_i h_i^3 = \text{const} \quad (12.15)$$

for three dimensions. Since $\rho_i = \rho_i(r_1, r_2, \ldots, r_N, h_i)$ is only a function of the particle coordinates and of $h_i$, this equation implicitly defines the function $h_i = h_i(r_1, r_2, \ldots, r_N)$ in terms of the particle coordinates.

We can then proceed to derive the equations of motion from

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{r}_i} - \frac{\partial L}{\partial r_i} = 0. \quad (12.16)$$
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This first gives

$$m_i \frac{dv_i}{dt} = - \sum_{j=1}^{N} m_j \frac{P_j}{\rho_j^2} \frac{\partial \rho_i}{\partial r_i},$$

(12.17)

where the derivative $\partial \rho_j/\partial r_i$ stands for the total variation of the density with respect to the coordinate $r_i$, including any variation of $h_j$ this may entail. We can hence write

$$\frac{\partial \rho_j}{\partial r_i} = \nabla_i \rho_j + \frac{\partial \rho_j}{\partial h_j} \frac{\partial h_j}{\partial r_i},$$

(12.18)

where the smoothing length is kept constant in the first derivative on the right hand side (in our notation, the Nabla operator $\nabla_i = \partial/\partial r_i$ means differentiation with respect to $r_i$ holding the smoothing lengths constant). On the other hand, differentiation of $\rho_j h_j^3 = \text{const}$ with respect to $r_i$ yields

$$\frac{\partial \rho_j}{\partial h_j} \frac{\partial h_j}{\partial r_i} \left[ 1 + 3 \frac{\rho_j}{h_j} \left( \frac{\partial \rho_j}{\partial h_j} \right)^{-1} \right] = -\nabla_i \rho_j.$$

(12.19)

Combining equations (12.18) and (12.19) we then find

$$\frac{\partial \rho_j}{\partial r_i} = \left( 1 + \frac{h_j}{3 \rho_j} \frac{\partial \rho_j}{\partial h_j} \right)^{-1} \nabla_i \rho_j.$$

(12.20)

Using

$$\nabla_i \rho_j = m_i \nabla_i W_{ij}(h_j) + \delta_{ij} \sum_{k=1}^{N} m_k \nabla_i W_{ki}(h_i),$$

(12.21)

we finally obtain the equations of motion

$$\frac{dv_i}{dt} = - \sum_{j=1}^{N} m_j \left[ f_i \frac{P_j}{\rho_j^2} \nabla_i W_{ij}(h_i) + f_j \frac{P_j}{\rho_j^2} \nabla_i W_{ij}(h_j) \right],$$

(12.22)

where the $f_i$ are defined by

$$f_i = \left[ 1 + \frac{h_i}{3 \rho_i} \frac{\partial \rho_i}{\partial h_i} \right]^{-1},$$

(12.23)

and the abbreviation $W_{ij}(h) = W(|r_i - r_j|, h)$ has been used. Note that the correction factors $f_i$ can be easily calculated alongside the density estimate, all that is required is an additional summation to get $\partial \rho_i/\partial r_i$ for each particle. This quantity is in fact also useful to get the correct smoothing radii by iteratively solving $\rho_i h_i^3 = \text{const}$ with a Newton-Raphson iteration.

The equations of motion (12.22) for inviscid hydrodynamics are remarkably simple. In essence, we have transformed a complicated system of partial differential equations into a much simpler set of ordinary differential equations. Furthermore, we only have to solve the momentum equation explicitly. The mass conservation
12.3 Artificial Viscosity

equation as well as the total energy equation (and hence the thermal energy equation) are already taken care of, because the particle masses and their specific entropies stay constant for reversible gas dynamics. However, later we will introduce an artificial viscosity that is needed to allow a treatment of shocks. This will introduce additional terms in the equation of motion and requires the time integration of one thermodynamic quantity per particle, which can either be chosen as entropy or thermal energy. Indeed, the above formulation can also be equivalently expressed in terms of thermal energy instead of entropy. This follows by taking the time derivative of Eqn. (12.14), which first yields

\[
\frac{du_i}{dt} = \frac{P_i}{\rho_i^2} \sum_j v_j \cdot \frac{\partial \rho_i}{\partial r_j}.
\]  

(12.24)

Using equations (12.20) and (12.21) then gives the evolution of the thermal energy as

\[
\frac{du_i}{dt} = f_i \frac{P_i}{\rho_i^2} \sum_j m_j (v_i - v_j) \cdot \nabla W_{ij}(h_i),
\]  

(12.25)

which needs to be integrated along the equation of motion if one wants to use the thermal energy as independent thermodynamic variable. There is no difference however to using the entropy; the two are completely equivalent in the variational formulation.

Note that the above formulation readily fulfills the conservation laws of energy, momentum and angular momentum. This can be shown based on the discretized form of the equations, but it is also manifest due to the symmetries of the Lagrangian that was used as a starting point. The absence of an explicit time dependence gives the energy conservation, the translational invariance implies momentum conservation, and the rotational invariance gives angular momentum conservation.

12.3 Artificial Viscosity

Even when starting from perfectly smooth initial conditions, the gas dynamics described by the Euler equations may readily produce true discontinuities in the form of shock waves and contact discontinuities. At such fronts the differential form of the Euler equations breaks down, and their integral form (equivalent to the conservation laws) needs to be used. At a shock front, this yields the Rankine-Hugoniot jump conditions that relate the upstream and downstream states of the fluid. These relations show that the specific entropy of the gas always increases at a shock front, implying that in the shock layer itself the gas dynamics can no longer be described as inviscid. In turn, this also implies that the discretized SPH equations we derived above can not correctly describe a shock, simply because they keep the entropy strictly constant.

One thus must allow for a modification of the dynamics at shocks and somehow introduce the necessary dissipation. This is usually accomplished in SPH by an artificial viscosity. Its purpose is to dissipate kinetic energy into heat and to produce
entropy in the process. The usual approach is to parameterize the artificial viscosity in terms of a friction force that damps the relative motion of particles. Through the viscosity, the shock is broadened into a resolvable layer, something that makes a description of the dynamics everywhere in terms of the differential form possible. It may seem a daunting task though to somehow tune the strength of the artificial viscosity such that just the right amount of entropy is generated in a shock. Fortunately, this is however relatively unproblematic. Provided the viscosity is introduced into the dynamics in a conservative fashion, the conservation laws themselves ensure that the right amount of dissipation occurs at a shock front.

What is more problematic is to devise the viscosity such that it is only active when there is really a shock present. If it also operates outside of shocks, even if only at a weak level, the dynamics may begin to deviate from that of an ideal gas.

The viscous force is most often added to the equation of motion as

\[
\frac{dv_i}{dt} \mid_{\text{visc}} = - \sum_{j=1}^{N} m_j \Pi_{ij} \nabla_i W_{ij},
\]

(12.26)

where \( W_{ij} = \frac{1}{2} [W_{ij}(h_i) + W_{ij}(h_j)] \)

(12.27)

denotes a symmetrized kernel, which some researchers prefer to define as \( W_{ij} = W_{ij}([h_i + h_j]/2) \). Provided the viscosity factor \( \Pi_{ij} \) is symmetric in \( i \) and \( j \), the viscous force between any pair of interacting particles will be antisymmetric and along the line joining the particles. Hence linear momentum and angular momentum are still preserved. In order to conserve total energy, we need to compensate the work done against the viscous force in the thermal reservoir, described either in terms of entropy,

\[
\frac{dA_i}{dt} \mid_{\text{visc}} = \frac{1}{2} \gamma - \frac{1}{\rho_i^{\gamma-1}} \sum_{j=1}^{N} m_j \Pi_{ij} v_{ij} \cdot \nabla_i W_{ij},
\]

(12.28)

or in terms of thermal energy per unit mass,

\[
\frac{du_i}{dt} \mid_{\text{visc}} = \frac{1}{2} \sum_{j=1}^{N} m_j \Pi_{ij} v_{ij} \cdot \nabla_i W_{ij},
\]

(12.29)

where \( v_{ij} = v_i - v_j \). There is substantial freedom in the detailed parametrization of the viscosity \( \Pi_{ij} \). The most commonly used formulation of the viscosity is

\[
\Pi_{ij} = \begin{cases} 
-\alpha c_{ij} \mu_{ij} + \beta \mu_{ij}^2 / \rho_{ij} & \text{if } v_{ij} \cdot r_{ij} < 0 \\
0 & \text{otherwise},
\end{cases}
\]

(12.30)

with

\[
\mu_{ij} = \frac{h_{ij} v_{ij} \cdot r_{ij}}{|r_{ij}|^2 + c h_{ij}^2}.
\]

(12.31)
Here \( h_{ij} \) and \( \rho_{ij} \) denote arithmetic means of the corresponding quantities for the two particles \( i \) and \( j \), with \( c_{ij} \) giving the mean sound speed, whereas \( r_{ij} \equiv r_i - r_j \). The strength of the viscosity is regulated by the parameters \( \alpha \) and \( \beta \), with typical values in the range \( \alpha \simeq 0.5 - 1.0 \) and the frequent choice of \( \beta = 2 \alpha \). The parameter \( \epsilon \simeq 0.01 \) is introduced to protect against singularities if two particles happen to get very close.

In this form, the artificial viscosity is basically a combination of a bulk and a von Neumann-Richtmyer viscosity. Historically, the quadratic term in \( \mu_{ij} \) has been added to the original Monaghan-Gingold form to prevent particle penetration in high Mach number shocks. Note that the viscosity only acts for particles that rapidly approach each other, hence the entropy production is always positive definite. Also, the viscosity vanishes for solid-body rotation, but not for pure shear flows. To cure this problem in shear flows, Balsara (1995) suggested adding a correction factor to the viscosity, reducing its strength when the shear is strong. This can be achieved by multiplying \( \Pi_{ij} \) with a prefactor \( (f_{AV}^i + f_{AV}^j)/2 \), where the factors

\[
f_{AV}^i = \frac{|\nabla \cdot \mathbf{v}_i|}{|\nabla \cdot \mathbf{v}_i| + |\nabla \times \mathbf{v}_i|},
\]

are meant to measure the rate of local compression in relation to the strength of the local shear (estimated with formulas such as Eqn. 12.7).

In some studies, alternative forms of viscosity have been tested. For example, Monaghan (1997) proposed a modified form of the viscosity which can be written as

\[
\Pi_{ij} = -\frac{\alpha}{2} \frac{v_{ij}^{\text{sig}} w_{ij}}{\rho_{ij}},
\]

where \( v_{ij}^{\text{sig}} = [c_i + c_j - 3w_{ij}] \) is an estimate of the signal velocity between two particles \( i \) and \( j \), and \( w_{ij} = \mathbf{v}_{ij} \cdot \frac{\mathbf{r}_{ij}}{|\mathbf{r}_{ij}|} \) is the relative velocity projected onto the separation vector.

In attempting to reduce the numerical viscosity of SPH in regions away from shocks, several studies have recently advanced the idea of keeping the functional form of the artificial viscosity, but making the viscosity strength parameter \( \alpha \) variable in time. Adopting \( \beta = 2 \alpha \), one may evolve the parameter \( \alpha \) individually for each particle with an equation such as

\[
\frac{d\alpha_i}{dt} = -\frac{\alpha_i - \alpha_{\text{max}}}{\tau_i} + S_i,
\]

where \( S_i \) is some source function meant to ramp up the viscosity rapidly if a shock is detected, while the first term lets the viscosity exponentially decay again to a prescribed minimum value \( \alpha_{\text{min}} \) on a timescale \( \tau_i \). So far, simple source functions like \( S_i = \max[-(\nabla \cdot \mathbf{v})_i, 0] \) and timescales \( \tau_i \simeq h_i/c_i \) have been explored and the viscosity \( \alpha_i \) has often also been prevented from becoming higher than some prescribed maximum value \( \alpha_{\text{max}} \). It is clear that the success of such a variable \( \alpha \) scheme depends critically on an appropriate source function. The form above can still not
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distinguish purely adiabatic compression from that in a shock, so is not completely free of creating unwanted viscosity.

12.4 Advantages and disadvantages of SPH

Smoothed particle hydrodynamics is a remarkably versatile and simple approach for numerical fluid dynamics. The ease with which it can provide a large dynamic range in spatial resolution and density, as well as an automatically adaptive resolution, are unmatched in Eulerian methods. At the same time, SPH has excellent conservation properties, not only for energy and linear momentum, but also for angular momentum. The latter is not automatically guaranteed in Eulerian codes, even though it is usually fulfilled at an acceptable level for well-resolved flows. When coupled to self-gravity, SPH conserves the total energy exactly, which is again not manifestly true in most mesh-based approaches to hydrodynamics. Finally, SPH is Galilean-invariant and free of any errors from advection alone, which is another advantage compared to Eulerian mesh-based approaches.

Thanks to its completely mesh-free nature, SPH can easily deal with complicated geometric settings and large regions of space that are completely devoid of particles. Implementations of SPH in a numerical code tend to be comparatively simple and transparent. At the same time, the scheme is characterized by remarkable robustness. For example, negative densities or negative temperatures, sometimes a problem in mesh-based codes, can not occur in SPH by construction. Although shock waves are broadened in SPH, the properties of the post-shock flow are correct.

The main disadvantage of SPH is its limited accuracy in multi-dimensional flows. One source of noise originates in the approximation of local kernel interpolants through discrete sums over a small set of nearest neighbours. While in 1D the consequences of this noise tend to be reasonably benign, particle motion in multiple dimensions has a much higher degree of freedom. Here the mutually repulsive forces of pressurized neighbouring particle pairs do not easily cancel in all dimensions simultaneously, especially not given the errors of the discretized kernel interpolants. As a result, some ‘jitter’ in the particle motions readily develops, giving rise to velocity noise up to a few percent of the local sound speed. This noise seriously messes up the accuracy that can be reached with the technique, especially for subsonic flow, and also leads to a slow convergence rate.

Particularly problematic in SPH are fluid instabilities across contact discontinuities, such as Kelvin-Helmholtz instabilities. These are usually found to be suppressed in their growth. Another generic problem is that the artificial viscosity is operating at some level also outside of shocks, giving the numerical model a relatively high numerical viscosity, which limits the Reynolds numbers that can be easily reached with SPH.