Chapter 9: Smoothed Particle Hydrodynamics

Oliver Wandel, Roland Speith and Christoph Schäfer

Smoothed Particle Hydrodynamics (SPH) is a numerical method, which was initially introduced to simulate gas flow for astrophysical applications by Lucy in 1977 and independently by Gingold and Monaghan. Nowadays, there are a variety of extensions of this method which allow the modelling of viscous flows, solid bodies, and magnetic fields. There are applications of the scheme in the military field, the automobile industry as well as in the geophysical research areas. Even, some commercial codes feature SPH modules for special purposes or geometries. In computer science, the SPH scheme is used to visualise fluids and brittle bodies. Apart from that, SPH is still used to tackle astrophysical problems by modelling solid bodies or gases, for which the equations of continuum mechanics, hydrodynamics or magnetohydrodynamics (in the presence of magnetic fields) are solved. The main idea of the method is to divide the computational domain into discrete mass packages which move according to the flow. These packages, which are also ofter refered to as (SPH-) particles, carry physical quantities like density, pressure, temperature or internal energy. They construct the moving pillars of the numerical method, which means that at their locations the physical quantities are calculated. In contrast to for example Eulerian finite difference schemes, the SPH method has a Lagrangian nature and the particles move with the flow. Because of this mesh free nature, SPH is suitable to simulate flows in complex geometries with open boundaries. The disadvantages of the SPH method in comparison to other hydrodynamic schemes are a higher computational cost for similar accuracy and spatial resolution, as well as the lack of a mathematical foundation and proof of convergence of the method. Furthermore, the treatment of boundary might be cumbersome.

9.1 Basic formalism

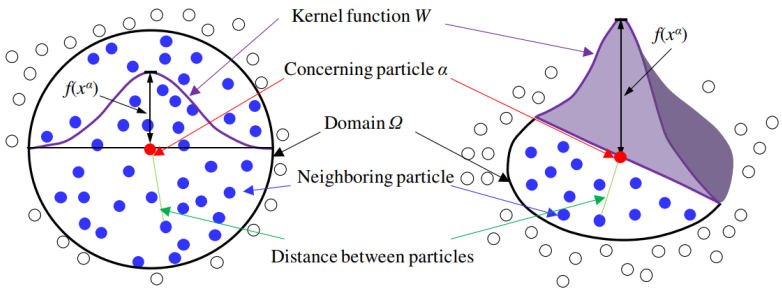

Figure 1: The basic idea of Smoothed Particle Hydrodynamics (Dai et al. 2016).

The basic idea of the SPH scheme is to transform a system of partial differential equations to a system of ordinary differential equations, which can be solved by standard integrators. For this transformation the partial differential equations are approximated in two steps: First, with an average over all spatial field quantities by the help of the convolution with the kernel function and second by a discretisation of this average.

9.1.1 The kernel function convolution

For a position dependent function $f(\mathbf{r})$ we begin with the trivial identity

$$f(\mathbf{r}) = \int_V f(\mathbf{r}')\delta(\mathbf{r} - \mathbf{r}')\mathrm{d}V', \tag{1}$$

where δ denotes Dirac's delta function $\delta(\mathbf{r} - \mathbf{r}')$. This relation motivates as an approximation $\langle f \rangle$ to the function f the following equation

$$\langle f(\mathbf{r}) \rangle = \int_V f(\mathbf{r}')W(\mathbf{r}, \mathbf{r}'; h)\mathrm{d}V', \tag{2}$$

where the integration covers the whole space. The function $W(\mathbf{r}, \mathbf{r}'; h)$ is called kernel function ("kernel") and is the special ingredient of the scheme.
The SPH approach is now to substitute all spatial field quantities $f(\mathbf{r})$ in the equations by the convolution of the kernel function W as following

$$f(\mathbf{r}) \approx \int_V f(\mathbf{r}')\, W(\mathbf{r}, \mathbf{r}'; h)\, \mathrm{d}V'. \tag{3}$$

The kernel function W is an known analytical function, depends on the spatial coordinates $\mathbf{r}$ and $\mathbf{r}'$ and on the parameter h, the so called "smoothing length", which is a measure for the expansion of the kernel function and also gave this numerical method its name.
The kernel function has to fulfill following requirements

- W is normalised
$$\int_V W(\mathbf{r}, \mathbf{r}'; h)\, \mathrm{d}V' = 1,$$
- W approximates the δ function
$$\lim_{h \to 0} W(\mathbf{r}, \mathbf{r}'; h) = \delta(\mathbf{r} - \mathbf{r}'), \tag{4}$$
- W is (at least) once continuously differentiable.

For large values of $\mathbf{r}'$ the kernel function has to go fast enough to zero. Furthermore, for all smoothing lengths h the kernel W should have a distinct maximum at $\mathbf{r} = \mathbf{r}'$ to obtain a certain local character of the averaged function f. This means that $f(\mathbf{r})$ is smoothed out over the space $\sim h^{\mathrm{dim}}$. Normally, a spherically symmetric kernel function is chosen (e.g., the spline kernel, see below), which means that the kernel function depends only on the distance between $\mathbf{r}$ and $\mathbf{r}'$ and not the coordinates themselves anymore (provided that h is independent of the coordinates).
If these conditions are fulfilled, the approximation is of 2nd order in h for any function $f(\mathbf{r})$

$$f(\mathbf{r}) = \int_V f(\mathbf{r}')\, W(|\mathbf{r} - \mathbf{r}'|; h)\, \mathrm{d}V' + O(h^2). \tag{5}$$

For practical purposes, it is convenient to choose a kernel function with compact support, which means that $W = 0$ for $|\mathbf{r} - \mathbf{r}'| > h$.

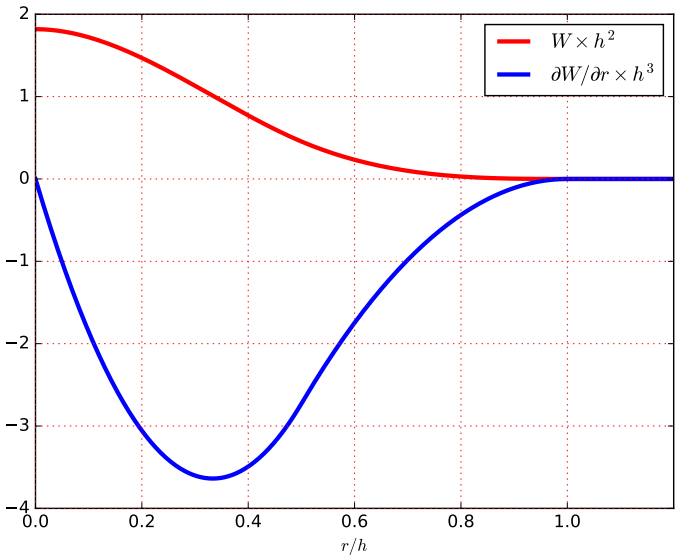

Figure 2: Plot of the symmetrical spline kernel function (6) and its antisymmetric derivative (8).

The spline kernel

In the literature, the most commonly used kernel function W is a cubic spline kernel given by

$$W(\tilde{r};h) = \frac{\sigma}{h^d}\begin{cases} (6\,(\tilde{r}/h)^3 - 6\,(\tilde{r}/h)^2 + 1) & \text{for} \quad 0 \le \tilde{r}/h < \frac{1}{2} \\ 2\,(1-\tilde{r}/h)^3 & \text{for} \quad \frac{1}{2} \le \tilde{r}/h \le 1 \\ 0 & \text{for} \quad \tilde{r}/h > 1 \end{cases} \tag{6}$$

with $\tilde{r} := |\mathbf{r} - \mathbf{r}'|$, the dimension d and the normalisation constant

$$\sigma = \begin{cases} \frac{4}{3} & \text{in 1D} \\ \frac{40}{7\pi} & \text{in 2D} \\ \frac{8}{\pi} & \text{in 3D} \end{cases}. \tag{7}$$

The derivative of the spline kernel is given by

$$\frac{\partial W(\tilde{r};h)}{\partial \tilde{r}} = \frac{6\,\sigma}{h^{d+1}}\begin{cases} (3\,(\tilde{r}/h)^2 - 2\,(\tilde{r}/h)) & \text{for} \quad 0 \le \tilde{r}/h < \frac{1}{2} \\ -(1-\tilde{r}/h)^2 & \text{for} \quad \frac{1}{2} \le \tilde{r}/h \le 1 \\ 0 & \text{for} \quad \tilde{r}/h > 1 \end{cases}. \tag{8}$$

The kernel function and its derivative in 2D are shown in figure 2.
The following applies

$$\nabla W(|\mathbf{r} - \mathbf{r}'|;h) = \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|}\frac{\partial W(\tilde{r};h)}{\partial \tilde{r}} \quad \text{and} \tag{9}$$

$$\nabla W(|\mathbf{r} - \mathbf{r}'|;h) = -\nabla' W(|\mathbf{r} - \mathbf{r}'|;h) \quad . \tag{10}$$

9.1.2 Spatial derivatives

The calculation of spatial derivatives can now be accomplished by transferring the derivatives to the kernel function by partial integration as follows

$$\begin{aligned}\nabla f(\mathbf{r}) &\overset{(3)}{\approx} \int_V \nabla' f(\mathbf{r}\,') \, W(|\mathbf{r} - \mathbf{r}\,'|; h) \, \mathrm{d}V' \\ &\overset{\text{P.I.}}{=} -\int_V f(\mathbf{r}\,') \, \nabla' W(|\mathbf{r} - \mathbf{r}\,'|; h) \, \mathrm{d}V' + \int_{\partial V} f(\mathbf{r}') W(|\mathbf{r} - \mathbf{r}\,'|; h) \hat{\mathbf{n}} \mathrm{d}S \\ &\overset{(10)}{=} \int_V f(\mathbf{r}\,') \, \nabla W(|\mathbf{r} - \mathbf{r}\,'|; h) \, \mathrm{d}V', \end{aligned} \tag{11}$$

where ∂V is the boundary of V and $\hat{\mathbf{n}}\mathrm{d}S$ is the area element with the normal vector. Since the kernel function vanishes on the boundary by design, the integral over the surface vanishes as well.

9.1.3 Discretisation

In the second step, the convolution integral (3) is approximated by a discrete sum, in which all function values are calculated at the positions of the SPH particles. Even though the kernel function W is analytically known, the function f itself is in most cases only numerically given at discrete positions (e.g., the velocity or the density). In the particle method SPH, the function values are only known at the positions of the particles and they can be distributed over the whole space without any fixed order and furthermore change their positions continuously. The positions of the particles are now used as supporting points for the numerical integration of the convolution of the kernel function (similar to a Monte-Carlo integration).
The positions r_j with $j = 1 \ldots N$ for the N given SPH particles have the known function values $f(\mathbf{r}_j)$ at their individual positions. With these, we define the particle number density n

$$n(\mathbf{r}) := \sum_{j=1}^{N} \delta(\mathbf{r} - \mathbf{r}_j). \tag{12}$$

With the characteristics of the kernel function equation (4) it holds

$$\lim_{h\to 0} \langle n(\mathbf{r}') \rangle = \lim_{h\to 0} \sum_{j=1}^{N} W(\mathbf{r}', \mathbf{r}_j; h) = n(\mathbf{r}'). \tag{13}$$

This means, the expression $n(\mathbf{r}')/\langle n(\mathbf{r}') \rangle$ is an approximation of 1. Therefore, we can multiply the equations for the convolution of the function f (3) and the convolution of the spatial derivatives (11) with this expression and eventually get for the approximation of the function f following discrete form

$$\langle f(\mathbf{r}) \rangle = \sum_{j=1}^{N} \frac{f(\mathbf{r}_j)}{\left\langle n(\mathbf{r}_j) \right\rangle} W(\mathbf{r}, \mathbf{r}_j; h). \tag{14}$$

This equation is valid for arbitrary positions $\mathbf{r}$. The special case for which the approximation of f is calculated at the particle position $\mathbf{r}_i$ leads to following equation

$$\langle f(\mathbf{r}_i) \rangle = \sum_{j=1}^{N} \frac{f(\mathbf{r}_j)}{\left\langle n(\mathbf{r}_j) \right\rangle} W(\mathbf{r}_i, \mathbf{r}_j; h). \tag{15}$$

Another crucial simplification is gained by the introduction of particle masses m_j with the definition

$$m_j := \frac{\varrho(\mathbf{r}_j)}{\left\langle n(\mathbf{r}_j) \right\rangle}, \tag{16}$$

from the particle number density n and the mass density ϱ. With the assumption of a spherically symmetric kernel function, we can now write equation (15) as follows

$$f(\mathbf{r}_i) \approx \sum_{j=1}^{N} \frac{m_j}{\varrho(\mathbf{r}_j)} f(\mathbf{r}_j)\, W(|\mathbf{r}_i - \mathbf{r}_j|; h). \tag{17}$$

Here $\mathbf{r}_j$ is the position of the particle j, m_j is the (predetermined) mass and $\varrho(\mathbf{r}_j)$ the density at the position of this particle. The abbreviations $f_j := f(\mathbf{r}_j)$, $\varrho_j := \varrho(\mathbf{r}_j)$, $W_{ij}(h) := W(|\mathbf{r}_i - \mathbf{r}_j|; h)$ et cetera will be used. With this, one can write the discrete approximation in a more compact form

$$f_i = \sum_{j=1}^{N} \frac{m_j}{\varrho_j} f_j W_{ij}. \tag{18}$$

Using the same procedure for the spatial derivatives, we get the following approximation

$$\nabla_i f(\mathbf{r}_i) \approx \sum_{j=1}^{N} \frac{m_j}{\varrho_j} f_j\, \nabla_i W_{ij}(h). \tag{19}$$

Using the SPH algorithm, we can eliminate all unknown spatial derivatives and transform them to know spatial derivatives of the kernel function and the field quantities at the particles' locations. The error of the convolution of the kernel function is of the order of $O(h^2)$. However, in general the error from the discretisation can not be given by a closed expression and is hard to estimate. The distribution of the SPH particles obviously plays a greater role to express the error of the discretisation. During a simulation it is generally possible to check if the constraint

$$\sum_{j=1}^{N} \frac{m_j}{\varrho_j} W_{ij}(h) \stackrel{!}{=} 1 \tag{20}$$

is fulfilled for all particles i. In practice, it is necessary to run simulations with varying number of particles and different values for the smoothing length to show convergence.

9.2 The hydrodynamic equations in SPH formalism

With the above presented formalism, we are now in the position to convert any partial differential equations into ordinary differential equations. In the following, we will apply the SPH scheme to solve the equations of hydrodynamics and transform them into a system of equations for discrete (particle) quantities and their time derivatives. However, the SPH representation of these equations are not unique and many different formulations are identical in the order of the scheme. Different representations have been used in the literature and often, the best representation can only be found by trial and error.

The representations that ensure the conservation of momentum and energy on the particle level are generelly preferred. These representations are symmetrical in respect to particle exchange, c.f. the force from particle i on j has the same absolute value as the force from j on i but in opposite direction.

For the Euler equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{v} = -\frac{1}{\varrho}\nabla p \tag{21}$$

the direct SPH representation reads

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{v}_i = -\frac{1}{\varrho_i}\sum_{j=1}^{N} \frac{m_j}{\varrho_j} p_j \nabla_i W_{ij}(h). \tag{22}$$

Potentially the force of particle i on particle j would not be identical to the force of particle j on i, which would directly violate the conservation of momentum. Hence, the more suitable and symmetric representation

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{v}_i = -\sum_{j=1}^{N} m_j \frac{p_j + p_i}{\varrho_i \varrho_j} \nabla_i W_{ij}(h). \tag{23}$$

which also conserves momentum is preferred. Equation (23) is a special case of different possible representations which originated from following fundamental consideration. It is

$$\frac{1}{\varrho}\nabla p = \frac{\varrho^{\lambda-2}}{\varrho^{\lambda-2}}\frac{\nabla p}{\varrho} = \frac{1}{\varrho^{2-\lambda}}\nabla\left(\frac{p}{\varrho^{\lambda-1}}\right) + \frac{p}{\varrho^{\lambda}}\nabla\left(\frac{1}{\varrho^{1-\lambda}}\right). \tag{24}$$

Converting this equation into SPH, we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{v}_i = -\sum_{j=1}^{N} m_j \left[\frac{p_j}{\varrho_i^{2-\lambda}\varrho_j^{\lambda}} + \frac{p_i}{\varrho_i^{\lambda}\varrho_j^{2-\lambda}}\right] \nabla_i W_{ij}(h), \tag{25}$$

and with $\lambda = 1$ equation (23). Alternatively, with $\lambda = 2$ we obtain another quite often applied SPH representation of the Euler equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{v}_i = -\sum_{j=1}^{N} m_j \left[\frac{p_j}{\varrho_j^2} + \frac{p_i}{\varrho_i^2}\right] \nabla_i W_{ij}(h). \tag{26}$$

The calculation of the density ϱ_i is a special issue. Using equation (17) with $f = \varrho$, we obtain

$$\varrho_i = \sum_{j=1}^{N} m_j \, W_{ij}(h). \tag{27}$$

Hence, the density can be calculated immediately from the particle distribution. The continuity equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\varrho = -\varrho \nabla \cdot \mathbf{v} \tag{28}$$

does not need to be integrated. For some applications, however, it is superior to integrate the continuity equation, especially when simulating liquids or solid bodies. The SPH representation of the continuity equation is given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\varrho_i = -\sum_{j=1}^{N} m_j \mathbf{v}_j \cdot \nabla_i W_{ij}(h). \tag{29}$$

This representation has the disadvantage that if all particles move with the same velocity $\mathbf{v}_i$, the change in the density does not necessarily vanish. Again, in the order of the scheme, it is possible to find a representation that avoids this problem. A typical trick for the derivation of this alternative presentation is to insert a 1. In the order of the method it holds

$$\langle \nabla_i f_i \rangle = \left\langle \frac{\varrho_i}{\varrho_i} \nabla_i f_i \right\rangle = \left\langle \frac{1}{\varrho_i} \left[\nabla_i (\varrho_i f_i) - f_i \nabla_i \varrho_i \right] \right\rangle \tag{30}$$

$$= \frac{1}{\varrho_i} \sum_{j=1}^{N} \frac{m_j}{\varrho_j} (\varrho_j f_j) \nabla_i W_{ij}(h) - \frac{f_i}{\varrho_i} \sum_{j=1}^{N} \frac{m_j}{\varrho_j} \varrho_j \nabla_i W_{ij}(h) \tag{31}$$

$$= \sum_{j=1}^{N} \frac{m_j}{\varrho_i} (f_j - f_i) \nabla_i W_{ij}(h). \tag{32}$$

This representation has the tremendous advantage that the derivative of a constant function f perfectly vanishes. For the continuity equation, a good SPH presentation is given by

$$\frac{\mathrm{d}}{\mathrm{d}t} \varrho_i = - \sum_{j=1}^{N} m_j (\mathbf{v}_j - \mathbf{v}_i) \cdot \nabla_i W_{ij}(h). \tag{33}$$

Since the particles move with the velocity $\mathbf{v}$ of the flow, the time evolution of the particles' locations is given by

$$\frac{\mathrm{d}\mathbf{r}_i}{\mathrm{d}t} = \mathbf{v}_i. \tag{34}$$

To close the system of equations, an additional equation of state (eos) that relates the thermodynamical quantities pressure, density and internal energy is required. The equation of state can immediately be used as an algebraic equation (in this case polytropic) given by

$$p_i = \varrho_0 \varrho_i^{\gamma}. \tag{35}$$

Together with the eos, the discretised system of equations is complete, the equations (23), (27), (34) and (35) describe the system entirely.
If the equation of state depends on the temperature, we additionally solve the equation for the conservation of the specific internal energy

$$\frac{\mathrm{d}}{\mathrm{d}t} \varepsilon = - \frac{p}{\varrho} \nabla \cdot \mathbf{v}. \tag{36}$$

It is important to apply the same SPH representation for the energy equation as for the Euler equation. The direct application of the SPH method for equation (36) leads to

$$\frac{\mathrm{d}}{\mathrm{d}t} \varepsilon_i = - \sum_{j=1}^{N} m_j \frac{p_i}{\varrho_i \varrho_j} \mathbf{v}_j \cdot \nabla_i W_{ij}(h). \tag{37}$$

Using the same conversion as for the continuity equation it also follows

$$\frac{\mathrm{d}}{\mathrm{d}t} \varepsilon_i = \sum_{j=1}^{N} m_j \frac{p_i}{\varrho_i \varrho_j} (\mathbf{v}_i - \mathbf{v}_j) \cdot \nabla_i W_{ij}(h). \tag{38}$$

Using the relation

$$- \frac{p}{\varrho} \nabla \mathbf{v} = \frac{1}{\varrho} \left[\mathbf{v} \cdot \nabla p - \nabla \cdot (p \mathbf{v}) \right], \tag{39}$$

we get the following representation

$$\frac{\mathrm{d}}{\mathrm{d}t}\varepsilon_i = \sum_{j=1}^{N} m_j \frac{p_j}{\varrho_i \varrho_j} (\mathbf{v}_i - \mathbf{v}_j) \cdot \nabla_i W_{ij}(h). \tag{40}$$

We can average the two equations (38) and (40) and obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\varepsilon_i = \frac{1}{2} \sum_{j=1}^{N} m_j \frac{p_i + p_j}{\varrho_i \varrho_j} (\mathbf{v}_i - \mathbf{v}_j) \cdot \nabla_i W_{ij}(h). \tag{41}$$

This form has to be used if the Euler equation is solved using representation (23). Solving the Euler equation in the discretised form (26), the equivalent discretised form of the energy equation reads

$$\frac{\mathrm{d}}{\mathrm{d}t}\varepsilon_i = \frac{1}{2} \sum_{j=1}^{N} m_j \left[\frac{p_i}{\varrho_i^2} + \frac{p_j}{\varrho_j^2} \right] (\mathbf{v}_i - \mathbf{v}_j) \cdot \nabla_i W_{ij}(h). \tag{42}$$

9.3 Description of the whole algorithm

A complete SPH simulation is divided into three parts:

1. the creation of the initial distribution,
2. the time integration (the actual simulation), and
3. the analysis of the resulting particle distribution.

9.3.1 Initial distribution

The creation of the initial distribution is important since it defines the physical problem, which is supposed to be simulated. For this, one has to find a particle distribution for a given density and flow field, which describes this initial flow as good as possible. However, there are no methods for 2D and 3D, which guarantee an optimal distribution. Furthermore, many problems are far from well defined. There are two possible strategies: All particles have the same mass and the density differences are adjusted using the particle positions, or the particles are evenly distributed over the space and the density differences are modelled using different particle masses. Other than that, there are all possible mixed forms.

9.3.2 Time integration

In most SPH codes, a slightly modified version of the leapfrog integrator is used. The acceleration $\mathbf{a}(t) := \mathrm{d}\mathbf{v}_i/\mathrm{d}t$ is calculated for every particle i at the time t using (23). The SPH density (27) has to be calculated in advance for every particle at this certain time. To know the position, as well as the velocity of a specific particle starting with the time t at every full timestep $t + \Delta t$, the following steps

will be done

$$\begin{aligned} & & \text{calculate} \quad \mathbf{a}(t) \\ \mathbf{v}(t+\Delta t/2) &= \mathbf{v}(t) + \frac{\Delta t}{2}\mathbf{a}(t) \\ \mathbf{r}(t+\Delta t/2) &= \mathbf{r}(t) + \frac{\Delta t}{2}\mathbf{v}(t) \\ & \rightarrow \quad \text{calculate} \quad \mathbf{a}(t+\Delta t/2) \\ \mathbf{v}(t+\Delta t) &= \mathbf{v}(t) + \Delta t\, \mathbf{a}(t+\Delta t/2) \\ \mathbf{r}(t+\Delta t) &= \mathbf{r}(t+\Delta t/2) + \frac{\Delta t}{2}\mathbf{v}(t+\Delta t). \end{aligned}$$

The time derivative of the acceleration (the jerk) $\dot{\mathbf{a}}$ can not be easily determined anymore as for example in N-body simulations. The timestep Δt is therefore calculated using the particle velocities and the smoothing length h as follows

$$\Delta t = \eta\, h / \max_{i=1\ldots N}(\mathbf{v}_i). \tag{43}$$

If initially all velocities $\mathbf{v}_i$ are 0, then $\Delta t = \eta^2$ is chosen.

9.3.3 Analysis

In the analysis of the resulting particle distribution, the calculated physical parameters at the particle positions give indications about the flow in the continuum. The type of analysis strongly depends on the problem and may be also time consuming.

9.4 Additions

9.4.1 Boundary effects

In simulations with constant smoothing lengths, the particles at the boundaries have less interaction partners than particles that are at least one smoothing length away from the boundary (see Figure 4). If the density of the particles are directly calculated using the kernel sum (27), the boundary particles automatically have a lower density than their neighbours, even if they have the same mass. This leads to undesirable effects like density gradients and consequently possible pressure gradients and non vanishing forces. Hence, especially for simulations of solid bodies with homogeneous densities, the continuity equation of the form (33) has to be solved, to ensure that the density of boundary particles is calculated correctly.

9.4.2 Artificial viscosity

In SPH it is not possible to describe the appearances of shocks in an ideal fluid with solely non viscous equations, since in the shock front kinetic energy is dissipated into heat. Because of the discretisation, the appearance of unphysical artefacts like oscillations can also occur during hydrodynamic simulations.
In order to damp such oscillations and to avoid numerical artifacts, additional terms are included into the equations of motion and energy conservation equations. These purely numerical terms have the form of an additional pressure and prevent the mutual penetration of the particles. Because of their properties, they are normally called “artificial viscosity”.

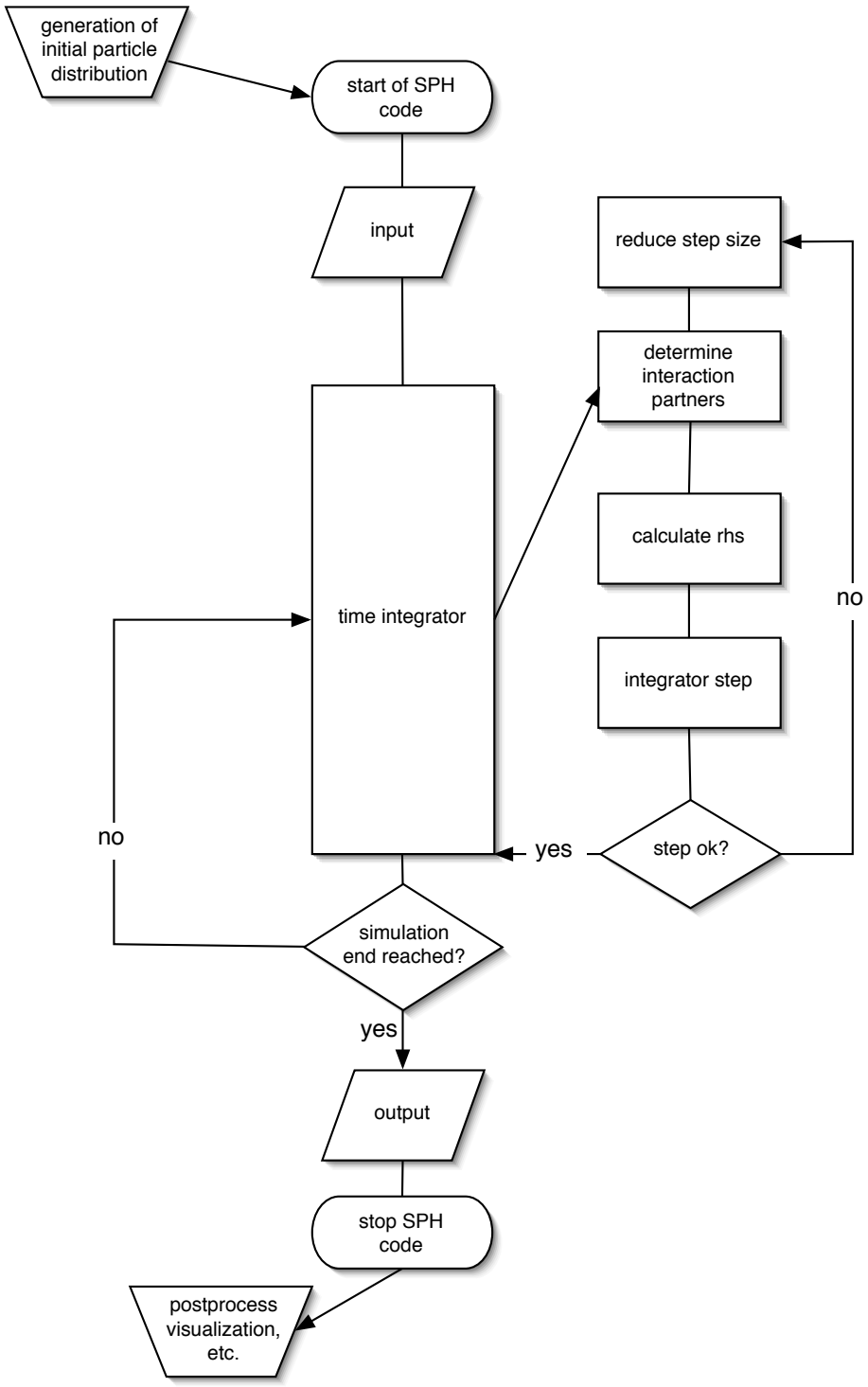

Figure 3: Flow diagram of a SPH simulation.

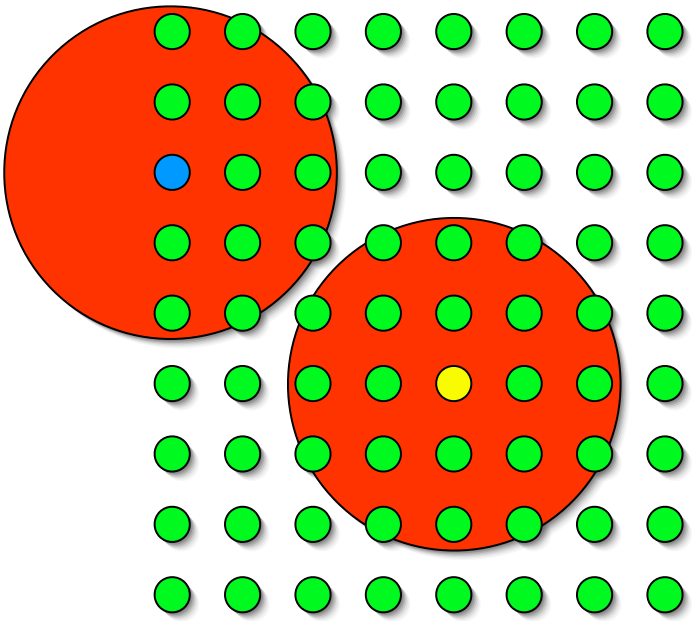

Figure 4: During simulations with a constant smoothing length the particles at the simulation boundary have less interaction partners that particles in the middle of the simulation area.

To the discretised Euler equation (23), following term

$$\left.\frac{\mathrm{d}\mathbf{v}_i}{\mathrm{d}t}\right|_{\text{art.visc.}} = -\sum_{j=1}^{N} m_j \Pi_{ij} \nabla_i W_{ij}(h) \tag{44}$$

is added. The artificial viscosity term Π_{ij} does not vanish only for approaching particles. It has the following form

$$\Pi_{ij} = \begin{cases} \dfrac{-\alpha \bar{c}_{ij} \mu_{ij} + \beta \mu_{ij}^2}{\bar{\varrho}_{ij}} & \text{for} \quad (\mathbf{v}_i - \mathbf{v}_j)\cdot(\mathbf{r}_i - \mathbf{r}_j) < 0 \\ 0 & \text{for} \quad (\mathbf{v}_i - \mathbf{v}_j)\cdot(\mathbf{r}_i - \mathbf{r}_j) \geq 0 \end{cases} . \tag{45}$$

Here α and β are free parameters (with standard values $\alpha = 1$ and $\beta = 2$). Furthermore, $\bar{c}_{ij} = (c_i + c_j)/2$ and $\bar{\varrho}_{ij} = (\varrho_i + \varrho_j)/2$ are the averages of the sound speed and the density. The term μ_{ij} is an approximation to the velocity divergence and reads

$$\mu_{ij} := \frac{h(\mathbf{v}_i - \mathbf{v}_j)\cdot(\mathbf{r}_i - \mathbf{r}_j)}{(\mathbf{r}_i - \mathbf{r}_j)^2 + \epsilon h^2}, \tag{46}$$

where the additional term ϵh^2 prevents the divergence for small particle distances $|\mathbf{r}_i - \mathbf{r}_j|$. The sound speed c_i is calculated using the relation (in this example the polytropic equation of state is used)

$$c^2 = \frac{\partial p}{\partial \varrho} = \gamma \varrho_0 \varrho^{\gamma - 1}. \tag{47}$$

The additional pressure term from the artificial viscosity has to be taken into account also in the energy equation. The artificial pressure term yields the following expression that needs to be added to

equation (41)

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\varepsilon_i\right|_{\text{art.visc.}} = \frac{1}{2}\sum_{j=1}^{N} m_j \Pi_{ij}(\mathbf{v}_i - \mathbf{v}_j)\cdot\nabla_i W_{ij}(h). \tag{48}$$

9.4.3 Interaction search

If a compact kernel function W is used in the computations, the particles interact only with particles in distances closer than the smoothing length h. In general, the SPH sums run over all other particles which results in a $O(N^2)$ algorithm. Since we know that only neighbouring particles contribute to the kernel sums, it is more efficient to generate a list of interacting particles and run the sums only over interacting pairs. This can reduce the computational costs to $O(N \log N)$. Two different approaches to find the interacting particles are normally applied: The interaction partner search with the help of a grid and the search with the help of a hierarchical tree.

The search with the help of a grid. At first, the particles are sorted into a helping grid. The grid covers the whole computational domain and ideally has an edge length of one smoothing length. When the particles are sorted into the grid, the interaction partner search for particle i requires only to search in the neighbouring grid cells of its grid cell, the ones that are within the smoothing length. The following steps are performed

- Determine the dimensions of the simulation area $\mathbf{x}_{\min}, \mathbf{x}_{\max}$.
- Divide the simulation area into N_c cells, so that the length of a cell equals the smoothing length h (see Figure 5).
- Sort all particles i into this helping grid. Normally, a linked-list for each grid cell is used: a cell has a pointer onto the first particle in this cell. Particle 1 has then a pointer to particle 2, particle 2 on particle 3 and so on.

The search using a tree. The search with the help of an hierarchical tree is numerically a bit more expensive and is mainly used for cases in which the particles are already sorted into a so called Barnes-Hut Tree (BH tree). BH trees are used in simulations to calculate self gravity. As a by-product, all interaction partners for a particle can be determined in an elegant way by doing a "tree walk". This also leads to a $O(N \log N)$ scheme. The following steps are performed to build the tree structure

- Determine the dimension of the simulation area $\mathbf{x}_{\min}, \mathbf{x}_{\max}$. This is the geometry of the root node of the tree (size).
- Sort the first particle into the tree.
- Sort the next particles into the tree with following algorithm
  1. Determine the node of the particle using the position of the particle. If there is already another particle inside the node, divide this node into 2^{DIM} children with half the size and sort the new particle, as well as the already present particle, into the newly formed children. If both particles are still inside the same child, divide them further until both particles end up in different children.
  2. Take the next, unsorted particle and go to point 1.

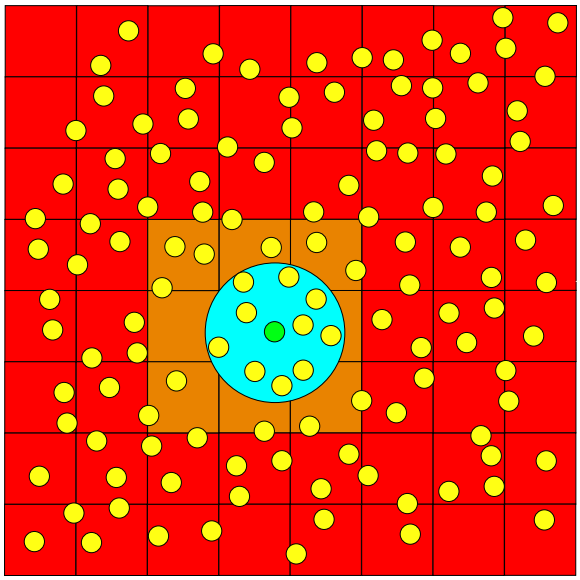

Figure 5: The interaction partner search with the help of a grid. Ideally the cell size equals the smoothing length h. Now, for the calculation of the interaction partners of particle i (here in green) only the cells direcly next to its cell have to be searched (orange). The computational cost of the search algorithm is $O(N \log N)$ in comparison to the N^2 algorithm of the direct search.

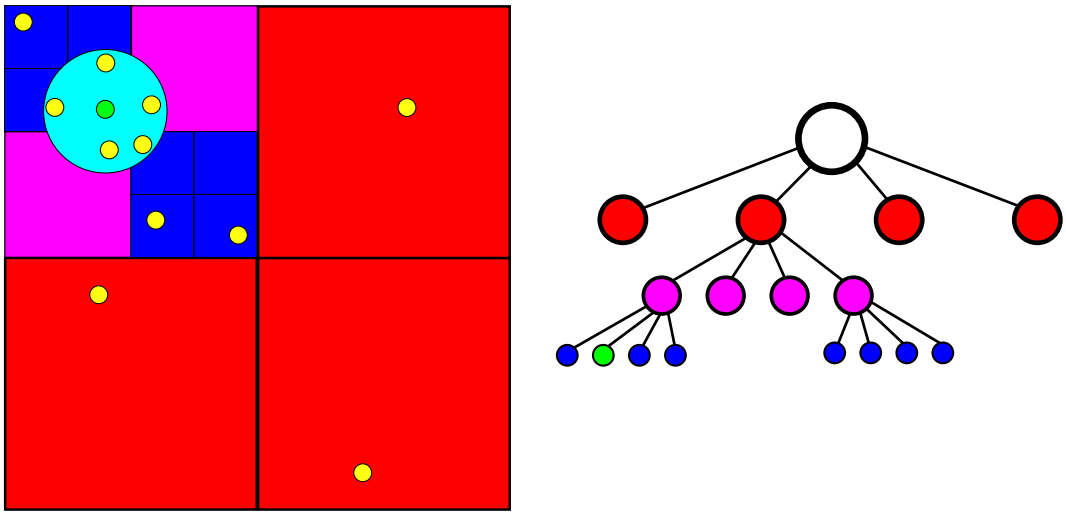

Figure 6: The interaction partner search using a Barnes-Hut tree. In this example a 2D tree. The tree consists of the so called root node (white). The root node has four children (red), one of them with another four children (pink). Two of these pink nodes have again four children (blue). In total there are three red leaves, two pink leaves and six blue leaves, in sum eleven particles. To determine the interaction partners of the green particle, only the nodes which cut the light blue circle have to be searched.

- After all particles are sorted using this algorithm, the leaves of the tree are the SPH particles.

The interaction partner search with the generated BH tree is performed in the following way: For each particle i do a tree walk.

- Start with the root node.
- Search all children of this node which cut the area around particle i with the smoothing length. If the investigated node is a leaf, calculate the distance of the SPH particle in this leaf to particle i and test for interaction.
- If the investigated node is a leaf, calculate the distance of the SPH particle in this leaf to particle i and test for interaction.
- If the investigated node is not a leaf, search all children of this node using the same method.

In the end, the cost of the interaction partner search for the grid and the tree is $O(N \log N)$ with the difference, that the construction of the grid and the sorting of the particles into the grid are computationally cheaper than the construction of a BH tree. In practice, for simulations including self gravity, the interaction partner search is accomplished with a tree and for all other cases with the grid algorithm.

9.4.4 Variable smoothing length

In principle, the SPH algorithm does not require that all particles have the same smoothing length or even that a particle's smoothing length is constant. For physically correct results it is of most importance that the interactions are symmetric, which means that if particle i interacts with particle j, then particle j also has to interact with particle i. Apart from this, each particle can have an individual, time dependent smoothing length. So, instead of a fixed smoothing length, a fixed number of interaction partners can also be used. This mainly has the advantage for simulations with strongly varying length scales like collapse simulations or simulations that include strong expansions, for which the average distance between SPH particles steadily decreases or increases. Furthermore, other than the particle number, the smoothing length significantly determines the accuracy of the SPH method and the spatial resolution. Both extreme cases (i) all particles are inside one smoothing length and (ii) particles have no interaction partner prevent physically reasonable statements regarding the results of the simulation. In addition, the minimal representable density in the simulation depends on the smoothing length. The density for particles without interaction partners (the so called self density) is given by

$$\varrho_i = \sum_{j=1}^{1} m_j W_{ij}(h) = m_i W_{ii}(h). \tag{49}$$

Since $W_{ii} \sim 1/h_i^d$, with the dimension d, the presentable density range can be increased by using a larger smoothing length.
Since in these simulations the smoothing length is not constant anymore, additional terms proportional to ∇h occur in the SPH equations. These terms are generally neglected.
Another possibility of variable smoothing is to couple the change of the smoothing length to the change of the density. This way, the change of the smoothing length is dynamically fitted to the change of the length scale. For this, an additional differential equation for the smoothing length is solved. Naturally, we want to have a constant number of interactions N_i for each particle i, which is

preferably the same for all particles. Using the correlation between the mass density and the number particle density $\varrho_i \sim n_i$ and with $n_i \approx N_i/V_i$, where $V_i \sim h^d$ is a measure for the volume of particle i, the relation for a constant N_i is given by

$$\frac{h}{h_0} = \left[\frac{\varrho_0}{\varrho}\right]^{\frac{1}{d}}, \tag{50}$$

with the initial density ϱ_0 and the initial smoothing length h_0. Unfortunately, the knowledge of the smoothing length is needed to calculate the density. Calculating the total time derivative of equation (50) it follows

$$\frac{\mathrm{d}}{\mathrm{d}t}h = -\frac{1}{d}\frac{h}{\varrho}\frac{\mathrm{d}}{\mathrm{d}t}\varrho. \tag{51}$$

Using the continuity equation (28) it follows

$$\frac{\mathrm{d}}{\mathrm{d}t}h = \frac{1}{d}h\nabla\cdot\mathbf{v}. \tag{52}$$

This equation is an additional partial differential equation for the smoothing length. The SPH presentation is following

$$\frac{\mathrm{d}}{\mathrm{d}t}h_i = \frac{1}{d}\frac{h_i}{\varrho_i}\sum_{j=1}^{N} m_j(\mathbf{v}_j - \mathbf{v}_i)\cdot\nabla W_{ij}(h). \tag{53}$$

9.4.5 Parallelisation

Parallelised SPH codes for computer clusters with distributed memory have the difficulty of perfectly balancing the load over all nodes. If for example there are a lot of particles in a simulation with a constant smoothing length on only one node, the whole calculation time is dominated by the calculation time of this node only and the parallelisation is broken. In comparison to grid codes, for which often a perfect load balancing is achieved by an equally distributed simulation domain (domain decomposition), the distribution of the particles onto the different nodes of the cluster is not trivial. Particles with only a few interactions have a smaller computing time than particles with a lot of neighbours. However, if variable smoothing is used and each particle has the same number of interactions, the load balancing might be achieved effortless by distributing the particles homogeneously on all nodes.

9.4.6 Second spatial derivatives in the SPH scheme, the diffusion equation

Consider the radiant flux $\mathbf{F}$

$$\mathbf{F} = -K\nabla T, \tag{54}$$

with the temperature T and the conductivity K. The additional term in the energy equation (36) for a fluid with $\varepsilon = c_v T$ is given by

$$\varrho c_v \frac{\mathrm{d}}{\mathrm{d}t}T = -\nabla\cdot\mathbf{F}. \tag{55}$$

To calculate the change in temperature we need a SPH representation for the second spatial derivative. The first possibility is to first calculate the heat flow $\mathbf{F}$ for all particles. With $\mathbf{F} = -K\nabla T$ follows the SPH equation

$$\mathbf{F}_i = -K\varrho_i\sum_{j=1}^{N} m_j\left[\frac{T_i}{\varrho_i^2} + \frac{T_j}{\varrho_j^2}\right]\nabla_i W_{ij}(h), \tag{56}$$

an alternative could be

$$\mathbf{F}_i = -K\frac{1}{\varrho_i}\sum_{j=1}^{N} m_j \left[T_j - T_i\right] \nabla_i W_{ij}(h). \tag{57}$$

As soon as the flux for all particles i has been calculated, the temperature change at all particle positions can be calculated using a second SPH sum

$$\varrho_i c_v \frac{\mathrm{d}}{\mathrm{d}t} T_i = -\varrho_i \sum_{j=1}^{N} m_j \left[\frac{\mathbf{F}_i}{\varrho_i^2} + \frac{\mathbf{F}_j}{\varrho_j^2}\right] \cdot \nabla_i W_{ij}(h), \tag{58}$$

or again with the alternative representation

$$\varrho_i c_v \frac{\mathrm{d}}{\mathrm{d}t} T_i = -\frac{1}{\varrho_i} \sum_{j=1}^{N} m_j \left[\mathbf{F}_j - \mathbf{F}_i\right] \cdot \nabla_i W_{ij}(h). \tag{59}$$

Unfortunately, this ansatz leads to unstable behaviour when using compact, symmetric kernel functions. The results are highly sensitive with regard to the particle distribution and produce too noisy results. Hence, we will use another possibility to calculate an approximation of the second spatial derivative with the SPH method, which uses only the first derivative of the kernel function. The heat equation in a homogeneous medium simplifies to

$$\frac{\partial T}{\partial t} = K\nabla^2 T, \tag{60}$$

with the constant diffusion coefficient K. We will limit the next part to the one dimensional heat equation in a homogeneous medium

$$\frac{\partial T}{\partial t} = \frac{\mathrm{d}}{\mathrm{d}t} T = K\frac{\partial^2 T}{\partial x^2} = K\frac{\mathrm{d}^2 T}{\mathrm{d}x^2}. \tag{61}$$

An approximation for the second derivative using a symmetric kernel function $W(x, x', h)$ is given by

$$\frac{\mathrm{d}^2 T}{\mathrm{d}x^2} = 2\int \frac{T(x) - T(x')}{x - x'} \frac{\mathrm{d}W(x, x', h)}{\mathrm{d}x} \mathrm{d}x'. \tag{62}$$

This can be shown as follows: Consider the Taylor series of $T(x)$ around x'

$$T(x) - T(x') = (x - x')\frac{\mathrm{d}T}{\mathrm{d}x} + \frac{1}{2}(x - x')^2 \frac{\mathrm{d}^2 T}{\mathrm{d}x^2} + O((x - x')^3). \tag{63}$$

Insert (63) into (62) and neglect the terms of order $O((x - x')^3)$, which yields

$$2\int \frac{\mathrm{d}T}{\mathrm{d}x} \frac{\mathrm{d}W(x, x', h)}{\mathrm{d}x} \mathrm{d}x' + 2\int \frac{1}{2}\frac{\mathrm{d}^2 T}{\mathrm{d}x^2}(x - x') \frac{\mathrm{d}W(x, x', h)}{\mathrm{d}x} \mathrm{d}x' \tag{64}$$

$$= 0 + \frac{\mathrm{d}^2 T}{\mathrm{d}x^2} \int (x - x') \frac{\mathrm{d}W(x, x', h)}{\mathrm{d}x} \mathrm{d}x' \tag{65}$$

$$\overset{\text{P.I.}}{=} 0 + \frac{\mathrm{d}^2 T}{\mathrm{d}x^2}. \tag{66}$$

The discretised form of equation (62) is given by

$$\frac{\mathrm{d}^2 T_i}{\mathrm{d}x^2} = 2 \sum_{j=1}^{N} \frac{m_j}{\varrho_j} \frac{T_i - T_j}{x_i - x_j} \frac{\mathrm{d}W_{ij}(h)}{\mathrm{d}x_i}. \tag{67}$$

The same procedure in three dimensions, using a spherically symmetric kernel function, leads to following approximation

$$\nabla^2 T(\mathbf{r}) = 2 \int \left[T(\mathbf{r}) - T(\mathbf{r}')\right] \frac{(\mathbf{r} - \mathbf{r}') \cdot \nabla W}{|\mathbf{r} - \mathbf{r}'|^2} \mathrm{d}V', \tag{68}$$

with the SPH representation

$$\nabla^2 T_i = 2 \sum_{j=1}^{N} \frac{m_j}{\varrho_j} \left[T_i - T_j\right] \frac{(\mathbf{r}_i - \mathbf{r}_j) \cdot \nabla_i W_{ij}(h)}{\left|\mathbf{r}_i - \mathbf{r}_j\right|^2}. \tag{69}$$

The proof is analogue to the procedure in one dimension: Taylor series of $T(\mathbf{r})$ around $\mathbf{r}'$

$$T(\mathbf{r}) - T(\mathbf{r}') = (\mathbf{r} - \mathbf{r}')^\alpha \frac{\partial T}{\partial x^\alpha} + \frac{1}{2}(\mathbf{r} - \mathbf{r}')^\alpha (\mathbf{r} - \mathbf{r}')^\beta \frac{\partial^2 T}{\partial x^\alpha \partial x^\beta} + O((\mathbf{r} - \mathbf{r}')^3), \tag{70}$$

inserting into (68) and neglecting the terms of order $O((\mathbf{r} - \mathbf{r}')^3)$ yields

$$\frac{\partial T}{\partial x^\alpha} \int (\mathbf{r} - \mathbf{r}')^\alpha \frac{(\mathbf{r} - \mathbf{r}') \cdot \nabla W}{|\mathbf{r} - \mathbf{r}'|^2} \mathrm{d}V' + \frac{1}{2} \frac{\partial^2 T}{\partial x^\alpha \partial x^\beta} \int (\mathbf{r} - \mathbf{r}')^\alpha (\mathbf{r} - \mathbf{r}')^\beta \frac{(\mathbf{r} - \mathbf{r}') \cdot \nabla W}{|\mathbf{r} - \mathbf{r}'|^2} \mathrm{d}V'. \tag{71}$$

The first integral vanishes for spherically symmetric kernel functions and the second integral equals to a delta function, hence the second term results in $\nabla^2 T$.
For the sake of completeness, we will also provide the approximation for a vector function $\mathbf{T}$. It is

$$\frac{\partial^2 \mathbf{T}}{\partial x^\alpha \partial x^\beta} \approx \int \left[\mathbf{T}(\mathbf{r}) - \mathbf{T}(\mathbf{r}')\right] \left[5(\mathbf{r} - \mathbf{r}')^\alpha (\mathbf{r} - \mathbf{r}')^\beta - \delta^{\alpha\beta}\right] \frac{(\mathbf{r} - \mathbf{r}') \cdot \nabla W}{|\mathbf{r} - \mathbf{r}'|^2} \mathrm{d}V', \tag{72}$$

with the SPH representation

$$\frac{\partial^2 \mathbf{T}_i}{\partial x^\alpha \partial x^\beta} = \sum_{j=1}^{N} \frac{m_j}{\varrho_j} \left[\mathbf{T}_i - \mathbf{T}_\mathbf{j}\right] \left[5\mathbf{r}_{ij}^\alpha \mathbf{r}_{ij}^\beta - \delta^{\alpha\beta}\right] \frac{\mathbf{r}_{ij} \nabla_i W_{ij}}{\mathbf{r}_{ij}^2}, \tag{73}$$

with $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$.
The (1D-)SPH equation for solving the heat equation in a homogeneous medium with constant diffusion coefficient K is then given by

$$\frac{\mathrm{d}}{\mathrm{d}t} T_i = 2K \sum_{j=1}^{N} \frac{m_j}{\varrho_j} \frac{T_i - T_j}{x_i - x_j} \frac{\partial W_{ij}}{\partial x_i}. \tag{74}$$

9.4.7 Gravitation

Gravitation is of great importance in astrophysics. External gravitational forces can be implemented straight forwardly into the SPH method. Hence, the attracting force from a central star on the rotating gas in the accretion disk around it or the additional gravitational force from a planet moving inside the disk are simply added as external forces for each particle. Much more complicated and at a very much higher computational cost, is the gravitational force between the particles themselves, the so called self gravity. For example, for the simulation of the gravitative collapse of a molecular cloud, we have to include the gravitational force of the gas on itself.

External gravitational forces. External gravitational accelerations **a**, which result from additional masses in the system and do not originate from the mass of the fluid, the SPH particles themselves, can be feasibly added to the equation of motion. If $\phi(\mathbf{r})$ is the known gravitational potential of the masses, the additional term for the calculation of the acceleration of particle i reads

$$\left.\frac{\mathrm{d}\mathbf{v}_i}{\mathrm{d}t}\right|_{\text{grav.}} = \mathbf{a}_i = -\nabla\phi(\mathbf{r}_i). \tag{75}$$

For example: A point mass M_{star} at the position $\mathbf{r}_{\text{star}}$. The gravitational acceleration of particle i by this mass (e.g., a star in the simulation domain) is then given by

$$\left.\frac{\mathrm{d}\mathbf{v}_i}{\mathrm{d}t}\right|_{\text{grav.}} = -\frac{GM_{\text{star}}}{|\mathbf{r}_i - \mathbf{r}_{\text{star}}|^3}\left(\mathbf{r}_i - \mathbf{r}_{\text{star}}\right). \tag{76}$$

To avoid divergence for particles very close to the point mass, the potential term is smoothed as follows

$$-\frac{1}{|\mathbf{r}_i - \mathbf{r}_{\text{star}}|} \rightarrow -\frac{1}{\sqrt{|\mathbf{r}_i - \mathbf{r}_{\text{star}}|^2 + \varepsilon^2}}. \tag{77}$$

Self gravity. The calculation of the gravity of the fluid onto itself, which means the gravitational force of each particle i on every other particle is unevenly more expensive than the handling of external gravitational forces and yields a N^2 scheme for N particles. Therefore, additional methods have been developed to calculate the self gravity. One possibility is the calculation of the potential by solving the Poisson equation

$$\nabla^2\phi(\mathbf{r}) = 4\pi G\varrho(\mathbf{r}). \tag{78}$$

In this case, a helping grid is used and the densities at the grid points are calculated from the SPH particle distribution. By solving the Poisson equation one gets the gravitational potential and consequently (see equation 75) the force acting on each particle. A more elegant and more suitable to the particle character of the SPH method option is the usage of a Barnes-Hut tree. The construction of a BH tree and the search of the interactions using this data structure has been already explained in detail in section 9.4.3. We now want to describe how the BH tree can be used to calculate also the self gravity. In the tree method the contribution of the gravitational potential, which originates from a distant group of point masses, is approximated by multipole expansion. Therefore, the whole group of the distanced mass particles are regarded as one single object at the centre of this mass distribution. During the construction of the BH tree, simultaneously for all nodes, all centre of masses, as well as the masses and the multipole moments (in most cases up to the quadrupole moments) are calculated and saved. The gravitational potential $\phi(\mathbf{r})$ of a mass distribution $\varrho(\mathbf{r})$

$$\phi(\mathbf{r}) = -\int \frac{G\varrho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}\mathrm{d}V' \tag{79}$$

can be expanded using multipoles. In cartesian coordinates, we consider the Taylor expansion of $\frac{1}{|\mathbf{r}-\mathbf{r}'|}$

$$\frac{1}{|\mathbf{r} - \mathbf{r}'|} = \sum_{n=0}^{\infty} \frac{1}{n!}\left(-\mathbf{r}' \cdot \nabla\right)^n \frac{1}{r} \tag{80}$$

and expand the gravitational potential in multipoles (for a detailed derivation see, e.g., Jackson, Elektrodynamik)

$$\phi(\mathbf{r}) = -G\frac{M}{r} - G\frac{\mathbf{p}\cdot\mathbf{r}}{r^3} - \frac{1}{2}GQ^{\alpha\beta}\frac{x^\alpha x^\beta}{r^5} - \ldots, \tag{81}$$

with the total mass

$$M = \int \varrho(\mathbf{r}')\mathrm{d}V', \tag{82}$$

the dipole moment

$$\mathbf{p} = \int \mathbf{r}'\varrho(\mathbf{r}')\mathrm{d}V', \tag{83}$$

the quadrupole moment

$$Q^{\alpha\beta} = \int \left[3x'^{\alpha}x'^{\beta} - r'^{2}\delta^{\alpha\beta}\right]\varrho(\mathbf{r}')\mathrm{d}V' \tag{84}$$

and the mass distribution $\varrho(\mathbf{r})$. The centre of mass $\mathbf{r}_{\mathrm{CM}}$ of the mass distribution is calculated as follows

$$\mathbf{r}_{\mathrm{CM}} = \frac{1}{M}\int \mathbf{r}'\varrho(\mathbf{r}')\mathrm{d}V'. \tag{85}$$

For the special choice of coordinates in the centre of mass system of the fluid, the dipole moment vanishes

$$\mathbf{p} = \int \mathbf{r}'\varrho(\mathbf{r}' + \mathbf{r}_{\mathrm{CM}})\mathrm{d}V' = \int (\mathbf{r}' - \mathbf{r}_{\mathrm{CM}})\varrho(\mathbf{r}')\mathrm{d}V' = \int \mathbf{r}'\varrho(\mathbf{r}')\mathrm{d}V' - \mathbf{r}_{\mathrm{CM}}M = 0. \tag{86}$$

Therefore, we need only the centre of mass and the total mass of each tree node, the dipole moments vanish. The centre of mass of a node n with N_{node} SPH particles is given by

$$\mathbf{r}_{\mathrm{CM_n}} = \frac{1}{M_n}\sum_{j=1}^{N_{\mathrm{node}}} m_j\mathbf{r}_j, \tag{87}$$

with the total mass of the node

$$M_n = \sum_{j=1}^{N_{\mathrm{node}}} m_j. \tag{88}$$

The calculation of the centre of mass and the total mass of each node is done recursively starting with the leaves. The parents always incorporate the mass of their children. Additionally, we need an indicator to decide if, when calculating the gravitational force of a distanced mass distribution onto a particle i, it is sufficient to calculate it using the centre of mass and the total mass or if the mass distribution needs to be better resolved spatially, which means the children have to be taken into account. For this, a predetermined tolerance parameter ϑ is used. It is defined by the opening angle, the ratio of the dimensions of the mass distribution d with the distance of particle i to the mass distribution r (see Figure 7).

$$\vartheta = \frac{d}{r}. \tag{89}$$

In practice the value $\vartheta = 0.5$ for methods, which only take the monopole moment into account, and $\vartheta = 0.8$ for methods, which also calculate the quadrupole moments, are used.

9.5 Appendix

9.5.1 Conservation of momentum

The Euler equation in all mentioned presentations has the following basical type

$$\frac{\mathrm{d}\mathbf{v}_i}{\mathrm{d}t} = -\sum_{j=1}^{N_p} m_j f(\varrho_i, \varrho_j; p_i, p_j)\nabla_i W_{ij}(h), \tag{90}$$

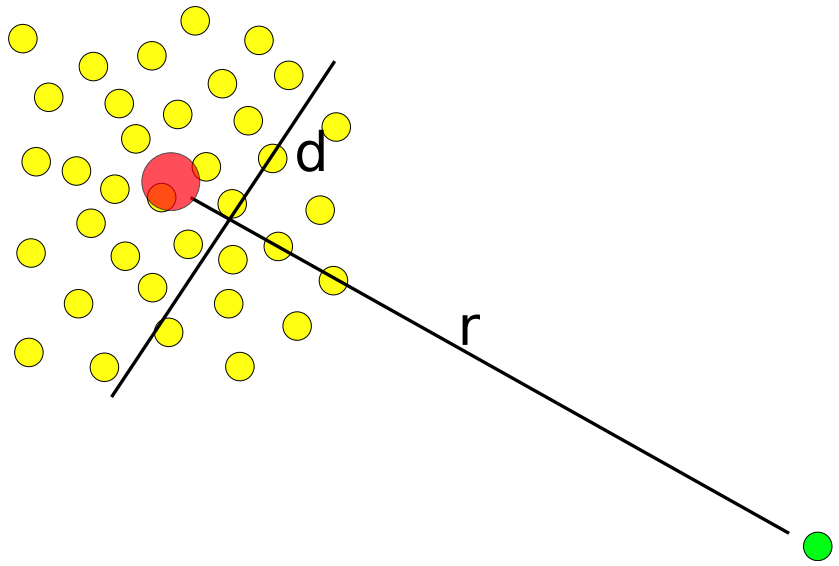

Figure 7: Illustration of the ϑ criterion for the Barnes-Hut method. The opening angle $\vartheta = d/r$ is the crucial factor if, for the calculation of the gravitational force of the yellow particles onto the green particles, the centre of mass and the total mass of the yellow particles (illustrated by the red particle) can be used or if the mass distribution has the be better resolved spatially.

where f is symmetric regarding the particle indices i and j, so the condition

$$f(\varrho_i, \varrho_j; p_i, p_j) = f(\varrho_j, \varrho_i; p_j, p_i)$$

is fulfilled. The conservation of momentum follows immediately since forces occur pairwise. The force $\mathbf{F}_{ij}$ from particle j onto particle i is obviously

$$\mathbf{F}_{ij} = \left[m_i \frac{\mathrm{d}\mathbf{v}_i}{\mathrm{d}t} \right]_j = -m_i m_j f(\varrho_i, \varrho_j; p_i, p_j) \nabla_i W_{ij}(h). \tag{91}$$

Because of the symmetry of function f and the anti-symmetry of $\nabla_i W_{ij}(h)$ regarding the indices i and j, Newton's third law, that the force of particle j onto i is the negative of the force of particle i onto j ($\mathbf{F}_{ij} = -\mathbf{F}_{ji}$), follows directly. The conservation of momentum is always guaranteed since the time derivative of the total momentum automatically vanishes

$$0 \stackrel{!}{=} \sum_{i=1}^{N_p} m_i \frac{\mathrm{d}\mathbf{v}_i}{\mathrm{d}t} = \sum_{i=0}^{N_p} \sum_{j=1}^{N_p} \mathbf{F}_{ij} = \frac{1}{2} \sum_{i,j}^{N_p} \left(\mathbf{F}_{ij} + \mathbf{F}_{ji} \right) = 0. \tag{92}$$

9.5.2 Conservation of angular momentum

The conservation of angular momentum is also automatically fulfilled because of the anti-symmetry of the particle forces $\mathbf{F}_{ij}$. The torque onto a particle reads

$$\mathbf{M}_i = \mathbf{r}_i \times m_i \frac{\mathrm{d}\mathbf{v}_i}{\mathrm{d}t} = \mathbf{r}_i \times \sum_{j=1}^{N_p} \mathbf{F}_{ij}. \tag{93}$$

The total torque onto the whole system vanishes

$$\sum_{i=1}^{N_p} \mathbf{M}_i = \sum_{i,j}^{N_p} \mathbf{r}_i \times \mathbf{F}_{ij} = \frac{1}{2} \sum_{i,j}^{N_p} \left(\mathbf{r}_i \times \mathbf{F}_{ij} + \mathbf{r}_j \times \mathbf{F}_{ji} \right) = 0, \tag{94}$$

so the angular momentum of the whole system is conserved. For the last step following relation was used

$$\mathbf{F}_{ij} \propto \nabla_i W_{ij}(h) \propto (\mathbf{r}_i - \mathbf{r_j}). \tag{95}$$

9.5.3 Conservation of energy

As already mentioned, there exists also a variety of different SPH presentations for the energy equation. To ensure an exact energy equation, the SPH representation of the Euler equation and the energy equation should not be chosen independently. The relation between the Euler and the energy equation comes from the SPH representation of the total energy E_{tot} and is

$$\frac{\mathrm{d}E_{\text{tot}}}{\mathrm{d}t} = \sum_{i=1}^{N_p} \left(m_i \frac{\mathrm{d}\epsilon_i}{\mathrm{d}t} + m_i \left(\mathbf{v}_i \cdot \frac{\mathrm{d}\mathbf{v}_i}{\mathrm{d}t} \right) \right) \stackrel{!}{=} 0. \tag{96}$$

If this condition for the SPH presentations of $\mathrm{d}\epsilon_i/\mathrm{d}t$ and $\mathrm{d}\mathbf{v}_i/\mathrm{d}t$ is not fulfilled then the total energy is only conserved in the order $O(h^2)$. To show this, one has to simply put the Euler and the energy equation with the same representation into equation (96). For the representation with the Euler equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{v}_i = -\sum_{j=1}^{N} m_j \left[\frac{p_i}{\varrho_i^2} + \frac{p_j}{\varrho_j^2} \right] \nabla_i W_{ij}(h). \tag{97}$$

and the energy equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\varepsilon_i = \frac{1}{2} \sum_{j=1}^{N} m_j \left[\frac{p_i}{\varrho_i^2} + \frac{p_j}{\varrho_j^2} \right] (\mathbf{v}_i - \mathbf{v}_j) \cdot \nabla_i W_{ij}(h). \tag{98}$$

We find with some algebra

$$\begin{aligned}
\frac{\mathrm{d}E_{\text{tot}}}{\mathrm{d}t} &= \sum_{i,j}^{N_p} m_i m_j \left(\frac{1}{2} \left[\frac{p_i}{\varrho_i^2} + \frac{p_j}{\varrho_j^2} \right] (\mathbf{v}_i - \mathbf{v}_j) \cdot \nabla_i W_{ij} - \left[\frac{p_i}{\varrho_i^2} + \frac{p_j}{\varrho_j^2} \right] \mathbf{v}_i \cdot \nabla_i W_{ij}(h) \right) && (99) \\
&= \sum_{i,j}^{N_p} m_i m_j \left(\frac{1}{2} \left[\frac{p_i}{\varrho_i^2} + \frac{p_j}{\varrho_j^2} \right] (\mathbf{v}_i - \mathbf{v}_j) \cdot \nabla_i W_{ij} - \frac{1}{2} \left[\frac{p_i}{\varrho_i^2} + \frac{p_j}{\varrho_j^2} \right] (\mathbf{v}_i - \mathbf{v}_j) \cdot \nabla_i W_{ij}(h) \right) && (100) \\
&= 0. && (101)
\end{aligned}$$

where in the second step we made use of

$$\begin{aligned}
\sum_{i,j}^{N_p} \mathbf{v}_i \cdot \nabla_i W_{ij}(h) &= \frac{1}{2} \sum_{i,j}^{N_p} \left(\mathbf{v}_i \cdot \nabla_i W_{ij}(h) + \mathbf{v}_j \cdot \nabla_j W_{ji}(h) \right) && (102) \\
&= \frac{1}{2} \sum_{i,j}^{N_p} \left(\mathbf{v}_i \cdot \nabla_i W_{ij}(h) - \mathbf{v}_j \cdot \nabla_i W_{ij}(h) \right) && (103) \\
&= \frac{1}{2} \sum_{i,j}^{N_p} (\mathbf{v}_i - \mathbf{v}_j) \cdot \nabla_i W_{ij}(h). && (104)
\end{aligned}$$

9.6 Literature

- Dai, Zili & Wang, Fawu & Huang, Yu & Song, Kun & Iio, Akinori. (2016). SPH-based numerical modeling for the post-failure behavior of the landslides triggered by the 2016 Kumamoto earthquake. Geoenvironmental Disasters. 3. 10.1186/s40677-016-0058-5.

- Benz, W., 1990, **Smooth Particle Hydrodynamics: A Review**, In: Proceedings of the NATO Advanced Research Workshop on The Numerical Modelling of Nonlinear Stellar Pulsations Problems and Prospects, held in Les Arcs, France, March 20-24, 1986. Editor, J. Robert Buchler; Publisher, Kluwer Academic Publishers, Dordrecht, The Netherlands, Boston, 1990. QB812 .N376. P.269, 1990.

- Landau & Lifschitz, 1991, **Lehrbuch der theoretischen Physik 6: Hydrodynamik**, Akademie Verlag Berlin, 5. Auflage 1991

- Monaghan, J.J., 1992, **Smoothed Particle Hydrodynamics**, In: Annual review of astronomy and astrophysics. Vol. 30 (A93-25826 09-90), p. 543-574.

- Speith, R., 1998, **Untersuchung von Smoothed Particle Hydrodynamics anhand astrophysikalischer Beispiele**, Dissertation, Universität Tübingen, 1998

- Price, Daniel, 2005, **Smoothed Particle Hydrodynamics** Chapter 3 of Thesis, `astro-ph/0507472`

- Rasio, Fred, 1999, **Particle Methods in Astrophysical Fluid Dynamics** Proc.Conf. on Comp.Physics. `astro-ph/9911360`