Momentum conserving methods that reduce particle clustering in SPH

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Momentum conserving methods that reduce particle clustering in SPH

by

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Abstract

In this paper we present two remedies for particle clustering in SPH. Since particle clustering is the consequence of a diminishing kernel gradient for small inter-particle distances, the first method uses a convex kernel with a non-zero kernel gradient at the origin. The second method is based on inter-particle collisions. They are both compared with conventional SPH in several case studies. The results show a great improvement in particle distribution, where particle clustering is strongly reduced or absent, with only a small influence on the accuracy of the computations.

I Introduction

One of the unsolved problems in SPH is the pairing, or clustering, of particles. This process in some situations mimics physical processes and fragmentation, making it hard to detect as a numerical artifact [18]. Particle clustering reduces the resolution of the simulation. This not only endangers the accuracy of the results, it is also a waist of computational effort. It is thus of great importance to reduce the numerical clustering of particles as much as possible.

In the battle against particle clustering there is confusion about what is causing the particles to cluster. This confusion is caused by the presence of two types of particle clustering. On the one hand there is an instability known as the tensile instability [14, 18]. This instability can be present in
Figure 1: **Particle clustering in action.** The left picture shows the initial configuration. The right picture shows the results when the Wendland kernel as in (1.1) is used. The clustering of particles is clearly visible.

simulations that allow for a negative pressure, but it is also known to occur in problems where the pressure is always positive [14]. SPH particles being subjected to a compressive/tensile stress will repel/attract each other, just like real particles, e.g. atoms, would do. However, in the case of tensile stress this leads to an instability where particles cluster.

On the other hand, there is an instability usually known as the pairing or clumping instability. This instability has little to do with the sign of the stresses, instead it is caused by a diminishing repelling force for approaching particles. Because the gradients of the most commonly used kernels tend to zero for small inter-particle distances, the forces or accelerations calculated from the momentum equation will also tend to zero. This makes that particles cannot get away from each other. This is the type of instability we consider in this paper. To avoid any confusion regarding the tensile instability we will not use the word ‘instability’, rather we will speak about ‘particle clustering’.

In [3] it is argued that not the diminishing kernel gradient is causing the clustering, but it is in fact caused by a (partly) negative Fourier transform. Since Wendland kernels are constructed to have a positive Fourier transform, they should not suffer from particle clustering. This statement does not agree with our results, as can be seen in Figure 1. The left picture shows the initial situation of a box with periodic boundary conditions. The box is filled with air and all particles have the same mass and are randomly
distributed. From a gas we expect that over time it distributes itself more or less uniformly over the domain. However, in the second picture, for which we used the Wendland kernel:

\[
W(R) = \alpha_d \begin{cases} 
(2 - R)^3 \left( \frac{3}{2} R + 1 \right) & R \leq 2, \\
0 & R > 2,
\end{cases}
\] (1.1)

the particles are not distributed uniformly over the domain, but are even forming clusters. For more details we refer to Section V.I. Thus also with Wendland kernels particle clustering can occur, which makes us consider the diminishing kernel gradient as the reason for the clustering.

In Section II we state the governing equations. We propose two methods to tackle particle clustering in Sections III and IV. The two methods are then applied and compared to traditional results in Section V, after which we summarize the paper in Section VI.

II Governing equations

We consider the compressible Navier-Stokes equations. The derivation of the discrete equations is not unique, as they can be found by the “interpolation-method” as well as the “Lagrangian-method”, see e.g. [12, 15]. We will not give a derivation here, but only state the equations we use. The density is estimated by:

\[
\langle \rho_i \rangle = \sum_{j \in S_i} m_j W_{ij},
\] (2.2)

where \( S_i \) is the set containing all particles that are within the support domain of particle \( i \). For the momentum equation we adopt:

\[
\left\langle \frac{Dv_i}{Dt} \right\rangle = -\sum_{j \in S_i} m_j \left( \frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} + \Pi_{ij} \right) \nabla_i W_{ij}.
\] (2.3)

Here \( \Pi_{ij} \) is an artificial viscosity term proposed by Monaghan [12], with two parameters \( \alpha_\Pi \) and \( \beta_\Pi \). In our computations we always use \( \beta_\Pi = 0 \). It is worth noting that equations (2.2) and (2.3) form a consistent pair according to the “Lagrangian derivation” [15]. A coupling between density and pressure is made by the equation of state:

\[
\langle p_i \rangle = p_0 + \frac{\rho_0 c^2}{\gamma} \left[ \left( \frac{\langle \rho_i \rangle}{\rho_0} \right)^\gamma - 1 \right],
\] (2.4)
which is usually referred to as the Tait equation, but in fact was proposed in this form by MacDonald [6]. In all case studies in Section V we will use $\gamma = 1$. Finally, we use (2.3) to compute new velocities. These velocities are then used to find the new positions of the particles.

III Convex kernel

The problem with the most commonly used kernel or smoothing functions in SPH, e.g. the cubic spline or the Gaussian, is that they are quite flat for small inter-particle distances. This is a favourable property, because as a consequence the density estimate (2.2) is not too sensitive for small changes in positions of close particles [15]. Except for the density estimate, the choice of kernel function also has an effect on the approximations of the accelerations of the particles. In contrast to the density estimate, where the kernel function itself is used, the accelerations are estimated with the gradient of the kernel function. The flat shape of the kernel function for small inter-particle distances implies that for those distances the kernel gradient is small. As a consequence the (repulsive) force between close particles is small. This makes that particles that at some point happen to be close will stay close, unless some external force separates them. This is why Monaghan introduced a repulsive force (resembling an artificial pressure) similar to the Lennard-Jones force [14]. Obviously, regridding as described in [1] also prevents particles from clustering, but it has disadvantages as well. Regridding implies interpolation, which has an effect on the accuracy and makes it computationally expensive. Moreover, it makes SPH lose one of its biggest advantages: not having a predefined mesh.

Because particle clustering is caused by a diminishing kernel gradient, an obvious treatment would be to use a kernel function that does not have such a gradient. More specific, we would like to use a convex kernel. Since a convex kernel has no inflection point, the kernel gradient will not go to zero. Instead, it will keep decreasing for lower input values. Such kernels have been introduced in the past. For example, Read et. al. [16] constructed kernel functions with derivatives that are constant between $R = 0$ and some value $R_m$. This $R_m$ is the value for $R$ where the derivative of a traditional kernel function would reach its minimum value. Despite this artificial construction that leads to an oddly shaped derivative, it was reported to reduce the clustering of particles.
Much earlier, Schüssler and Schmitt [17] introduced a kernel of the form:

$$W(R) = \alpha_d \begin{cases} \sqrt{2} - \sqrt{R} & R \leq 2, \\ 0 & R > 2. \end{cases} \quad (3.5)$$

Here, and in the rest of this paper, $R$ denotes the ratio of inter-particle distance and smoothing scale $h$ and $\alpha_d$ denotes a normalising constant dependent on the number of dimensions. The kernel derivative of Schüssler and Schmitt tends to infinity for small inter-particle distances, but in practice this never happens [17].

Another convex kernel was introduced by Johnson and Beissel [7]. Their work did not specifically focus on particle clustering, but they did experiment with a kernel function of the form:

$$W(R) = \alpha_d \begin{cases} \frac{1}{4} R^2 - R + 1 & R \leq 2, \\ 0 & R > 2. \end{cases} \quad (3.6)$$

Although both kernel functions (3.5) and (3.6) should prevent or at least reduce particle clustering, they are not widely used in literature. Monaghan argues that the kernel function of Johnson and Beissel does not have continuous second derivatives, making it more dispersive and sensitive to particle disorder than traditional kernels [14]. Obviously the kernel of Schüssler and Schmitt does not even have continuous first derivatives. It is possible however, to construct a convex kernel that has continuous first and second derivatives (with respect to $R$).

As a starting point for our derivation we take an existing kernel function. Wendland kernels consist of only one non-zero expression, making them more convenient for our derivation than, for instance, the cubic or quartic spline. We choose to start with the following Wendland kernel:

$$W(R) = \alpha_d \begin{cases} (2 - R)^2 (R + 1) & R \leq 2, \\ 0 & R > 2. \end{cases} \quad (3.7)$$

As mentioned earlier, the derivative tends to zero for $R \to 0$. The kernel function itself keeps increasing though, a property we would like to have for the derivative (with opposite sign). Therefore we take the kernel function (3.7), change the sign and define it as the derivative of what will be our new kernel function $K$. What we then need to do is perform an integration and a normalisation step, so that it satisfies:

$$\int_{\Omega} K(x - y, h) \, dy = 1, \quad (3.8)$$
where $\Omega$ is the computational domain. This leads to the following convex kernel:

$$K(R) = \alpha_d \begin{cases} (2 - R^3) \left( \frac{1}{2} R + 1 \right) & R \leq 2, \\ 0 & R > 2, \end{cases}$$

where $\alpha_d = 5/(48h)$, $15/(64\pi h^2)$ or $21/(128\pi h^3)$ in a 1-, 2- or 3-dimensional domain, respectively. For the 1-dimensional case it is shown and compared to other kernels in Figure 2.

The algorithm used to find (3.9) is not restricted to (3.7) as starting kernel, but can be applied to any kernel function. The result will always be a function that is a decreasing function of $R$. Moreover, the convex kernel in (3.9) satisfies most usual requirements for an SPH kernel function, see e.g. [9]; it is radially symmetric, has compact support, is positive for all $R$, is monotonically decreasing, converges to the Dirac delta distribution for $h \to 0$ and satisfies the unity condition (3.8).

It is not twice differentiable with respect to $x$ or $y$ though. This is required by some authors (see, e.g., [3]), because it implies smooth forces. Also, as its derivative is constructed not to be zero for $R = 0$, it is impossible to reconstruct linear functions on a uniform grid, as argued by Fulk and Quinn [4]. The latter argument seems unimportant, since a uniform grid of particles in practice seldom occurs in SPH, as does the need to reconstruct a linear function.
A good argument against a convex kernel is given by Price [15]. He states that convex kernels do not have a flat central portions, so that density estimates are more sensitive for small changes in neighbour positions. Although it is true that a kernel function with a flat central portion is desirable for the density estimate, the opposite seems to be true for the momentum equation. The higher sensitivity of (3.9) in the density estimate can be reduced by choosing a larger smoothing scale. Because of the convexity of the function this increase should not lead to particle clustering.

IV Particle collisions

The suggested convex kernel leads to a repulsive force when implemented in the momentum equation. As such it influences the forces in the system. Unfortunately, a concept based on forces cannot guarantee that particle clustering does not occur. Therefore we also propose a concept based on particle collisions. The idea of collisions in SPH is not new, see e.g. [8, 11], but to our knowledge has not been applied in the way we propose. The model we use is derived from kinetic collision theory, satisfying conservation of momentum (for inelastic and elastic collisions) and energy (for elastic collisions). The concept takes the form of a typical SPH viscosity model. It directly influences the approach velocities of the particles and is therefore robust.

Let us consider two colliding particles $i$ and $j$. We define $\mathbf{u}_i$, $\mathbf{u}_j$ and $\mathbf{v}_i$, $\mathbf{v}_j$ as the velocities before and after the collision respectively. In a fully elastic collision there is conservation of momentum and energy:

\[
m_i \mathbf{u}_i + m_j \mathbf{u}_j = m_i \mathbf{v}_i + m_j \mathbf{v}_j,
\]

\[
\frac{1}{2} m_i |\mathbf{u}_i|^2 + \frac{1}{2} m_j |\mathbf{u}_j|^2 = \frac{1}{2} m_i |\mathbf{v}_i|^2 + \frac{1}{2} m_j |\mathbf{v}_j|^2.
\]

These two equations have two unknowns, $\mathbf{v}_i$ and $\mathbf{v}_j$. Rewriting the first equation as an expression for $\mathbf{v}_j$ and substituting it into the second equation gives an expression for the velocity of particle $i$ after the collision:

\[
\mathbf{v}_i = \frac{(m_i - m_j) \mathbf{u}_i + 2 m_j \mathbf{u}_j}{m_i + m_j}.
\]

In a fully inelastic collision the particle velocities are equal after the collision. Since energy is dissipated, there is only conservation of momentum. This gives:

\[
m_i \mathbf{u}_i + m_j \mathbf{u}_j = (m_i + m_j) \mathbf{v}_i,
\]

\[
(4.13)
\]
which can be rewritten as:

\[ \mathbf{v}_i = \frac{m_i \mathbf{u}_i + m_j \mathbf{u}_j}{m_i + m_j}. \]  

(4.14)

Defining \( C_R \) as the coefficient of restitution, we can make any linear combination between an elastic and an inelastic collision. Combining equations (4.12) and (4.14) gives:

\[ \mathbf{v}_i = \frac{(m_i - C_R m_j) \mathbf{u}_i + (1 + C_R) m_j \mathbf{u}_j}{m_i + m_j}. \]  

(4.15)

It is easy to check that choosing \( C_R = 0 \) indeed corresponds to the post collision velocity of an inelastic collision (4.14) and \( C_R = 1 \) corresponds to the velocity after a fully elastic collision (4.12). The difference between the velocity before and after the collision can now be found by subtracting the original velocity from (4.15), giving:

\[ \mathbf{v}_i - \mathbf{u}_i = \frac{-m_j}{m_i + m_j} (1 + C_R) (\mathbf{u}_i - \mathbf{u}_j). \]  

(4.16)

Since we would only like to change the velocity in the so-called inter-particle direction, we need to find the component of the velocity difference in this direction. A unit vector in this direction is given by:

\[ \mathbf{e}_{ij} = \frac{\mathbf{r}_{ij}}{|\mathbf{r}_{ij}|} = \frac{\mathbf{r}_{ij}}{d_{ij}}, \]  

(4.17)

where \( \mathbf{r}_{ij} := \mathbf{r}_i - \mathbf{r}_j \) is the difference of the position vectors of particle \( i \) and \( j \) and \( d_{ij} \) is the distance between the particles. Now we find the approach velocity \( \mathbf{u}_{ij} := \mathbf{u}_i - \mathbf{u}_j \) to be:

\[ \mathbf{u}_{ij} = (\mathbf{u}_{ij} \cdot \mathbf{e}_{ij}) \mathbf{e}_{ij} = \frac{(\mathbf{u}_{ij} \cdot \mathbf{r}_{ij}) \mathbf{r}_{ij}}{d_{ij}^2}. \]  

(4.18)

Combining equations (4.16) and (4.18) gives the velocity of particle \( i \) after the collision with particle \( j \):

\[ \mathbf{v}_i = \mathbf{u}_i - \frac{m_j}{m_i + m_j} (1 + C_R) \frac{(\mathbf{u}_{ij} \cdot \mathbf{r}_{ij}) \mathbf{r}_{ij}}{d_{ij}^2}. \]  

(4.19)

Finally, we have to do this for all particles with which particle \( i \) is colliding. For that purpose we define \( \delta_c d_{ref} \) as the collision distance, where \( \delta_c \) is the collision distance parameter and \( d_{ref} \) is the reference particle spacing distance. All particles that are closer than \( \delta_c d_{ref} \) to each other are considered
to be colliding. If we define \( C_i \) as the set of particles colliding with particle \( i \), we find the velocity of particle \( i \), taking into account all its collisions, to be:

\[
v_i = u_i - \sum_{j \in C_i} \frac{m_j}{m_i + m_j} \left(1 + C_R \right) \frac{(u_{ij} \cdot r_{ij}) r_{ij}}{d_{ij}^2}.
\]

(4.20)

The particle collision concept is based on velocities. To make the step to forces we assume for the contact time between two particles:

\[
\Delta t_{col}^{ij} = N_{col}^{ij} \frac{d_{ij}}{|u_{ij}|},
\]

(4.21)

where \( N_{col}^{ij} \) is introduced as a collision number. Note that \( \Delta t_{col}^{ij} \) may be much smaller than the time step in the SPH simulation. Combining this with (4.20) gives:

\[
\frac{v_i - u_i}{\Delta t_{col}^{ij}} = - \sum_{j \in C_i} m_j \left[ \frac{|u_{ij}| \left(1 + C_R \right)}{N_{col}^{ij} (m_i + m_j)} \right] \frac{(u_{ij} \cdot r_{ij}) r_{ij}}{d_{ij}^3},
\]

(4.22)

which is basically an expression for the acceleration. This means that the formulation of the force due to a collision is very similar to that of a viscous force. In that sense the concept may be considered as a time dependent SPH viscosity model. However, the essential difference is that the force may become extremely high, since the collision takes place in a very short time frame. Small contact times are associated with high particle accelerations, which cannot be described by traditional viscosity models.

V Case studies

In this section we compare traditional results with the ones of our convex kernel and with the addition of particle collisions. We consider four cases.

V.I Gas-filled box

Our first case study will just act as a proof of concept. We consider a box of \( 1 \times 1 \) m with with periodic boundaries, filled with air; \( \rho = 1 \) kg/m\(^2\). Initially the particles are distributed randomly, so as to mimic a simulation that has gone wrong in the sense that particles have gotten too close. They all start with a zero velocity. The density estimate (2.2) will detect density differences, which will ultimately make the particles move.

We already saw in Figure 1 that with the Wendland kernel (1.1) the particles did not move away from each other. There we used a smoothing
scale of \( h = 2d_{ref} \), where \( d_{ref} = 1/20 \) m is a reference particle distance corresponding to a uniform hexagonal distribution. Furthermore we used \( \alpha_{II} = 0.1 \) in Monaghan’s artificial viscosity term, \( c = 10 \) m/s, \( \Delta t = 10^{-4} \) s and \( t_{\text{end}} = 2.0 \) s.

With our convex kernel (3.9), or with the inclusion of particle collisions (4.20), the particle distribution is much better. This is shown in Figure 3. Clearly the particles have been pushed away from each other, which has resulted in an almost hexagonal distribution. For the particle collisions we assumed \( C_R = 0.01 \) and \( \delta_c = 0.85 \), which means that every particle pair that gets closer than 0.85 times the reference distance \( d_{ref} \) is considered to be colliding, with the collision being almost fully inelastic.

V.II Hydrostatic pressure-tank

In our next case study we investigate the accuracy of the pressure of a column of fluid. We assume the fluid to be water, so that \( \rho = 1000 \) kg/m\(^2\). The height of the column is 1.0 m, with periodic boundary conditions in the horizontal direction. Below the bottom of the column are several layers of ghost particles, to keep the fluid particles from leaving the domain. Initially all particles are at rest and have an analytically correct pressure of \( \rho g (1 - H_i) \), with \( H_i \) the height of particle \( i \). They form a uniform hexagonal grid with \( d_{ref} = 1/100 \) m. Other parameters are chosen as \( c = 30 \) m/s and \( \alpha_{II} = 1.0 \).
Figure 4: **Hydrostatic pressure-tank.** The initial configuration of a column of water. The pressure unit is Pa. Particles with a negative height are ghost particles.

Finally, the time step is $\Delta t = 10^{-5}$ s and $t_{\text{end}} = 1.0$ s. The setup is shown in Figure 4.

Because of the free surface at the top of the column, the density estimate in (2.2) will not give good results. An equation that can deal with the free surface in a better way is:

$$\left\langle \frac{D\rho_i}{Dt} \right\rangle = \rho_i \sum_{j \in S_i} m_j \frac{\rho_j}{\rho_i} v_{ij} \cdot \nabla W_{ij},$$

(5.23)

where $v_{ij} := v_i - v_j$ is the relative velocity. Because we would like to use a consistent set of equations with respect to the “Lagrangian derivation” mentioned earlier, we adopt the following equation for the momentum equation:

$$\left\langle \frac{Dv_i}{Dt} \right\rangle = - \sum_{j \in S_i} m_j \left( \frac{p_i + p_j}{\rho_i \rho_j} + \Pi_{ij} \right) \nabla_i W_{ij}.$$  

(5.24)

These equations are completed with the same equation of state (2.4) and are used for this problem only.

Before computing the numerical pressure gradient, we remove 10% of the fluid particles both at the top and the bottom of the domain, to decrease the influence of the free surface and the ghost particles. The pressures of the particles can then be used to find the pressure gradient. Since we know that the pressure gradient should equal $-\rho g$, we can calculate the error we make.

During the simulation, the pressures fluctuate around the correct analytical values. This is due to the compressibility of the fluid. The fluctuations become smaller over time and the system converges to an equilibrium state, which differs from the correct one. This is shown in Figure 5.

Clearly, with equal smoothing scales, the regular Wendland kernel behaves better than our convex kernel. Not only is the average error smaller,
Figure 5: Error fluctuations of the numerical pressure gradient. The percentage errors of the numerical pressure gradient with respect to the analytical value of $-\rho g$. The blue line corresponds to the Wendland kernel (1.1), either with or without particle collisions. The red line shows the error for our convex kernel (3.9) when $h = 1.5d_{\text{ref}}$, while for the cyan line $h = 2.0d_{\text{ref}}$.

![Graph showing error fluctuations of the numerical pressure gradient.](image)

Table 1: Average numerical errors of the pressure gradient. Average errors of the pressure gradient for the case study in Section V.II.

<table>
<thead>
<tr>
<th>Method</th>
<th>$h = 1.5d_{\text{ref}}$</th>
<th>$h = 2d_{\text{ref}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wendland kernel</td>
<td>1.32 %</td>
<td>-</td>
</tr>
<tr>
<td>Particle collisions</td>
<td>1.32 %</td>
<td>-</td>
</tr>
<tr>
<td>Convex kernel</td>
<td>2.76 %</td>
<td>1.20 %</td>
</tr>
</tbody>
</table>

also the fluctuations around this value are significantly smaller. The computations also show that adding the concept of particle collisions has no influence on the pressures, which is a very interesting result.

The numerical error of the convex kernel gets smaller when we increase the smoothing scale. This is because with more particles in the support domain of the kernel, the discrete unity condition is satisfied more closely. Since our kernel is convex, this does not lead to particle clustering. The average numerical errors are shown in Table 1.

Although the errors with the convex kernel are bigger, they are still acceptable. This is especially true if not using it would lead to particle clustering. Also, when we slightly increase the smoothing scale, the accuracy of the convex kernel is similar to the accuracy of the regular Wendland kernel.
Now that we have seen a proof of concept and investigated the accuracy of our methods, we would like to see how they behave in more extreme circumstances. Therefore we consider a flow around a rotating shaft. The radius of the shaft is 0.04 m. Around the shaft is a circular wall of radius 0.1 m. The area between the shaft and the outer wall is filled with air; $\rho = 1 \text{ kg/m}^2$. The shaft will be rotating with 1000 rpm, thereby driving the airflow. Ghost particles with a prescribed velocity inside the shaft will model the rotating shaft. Behind the outer wall are also ghost particles, to keep the fluid particles from penetrating the outer domain boundary.

Initially the particles have zero velocities. They are distributed according to a hexagonal grid with $d_{\text{ref}} = 1/200$ m. To avoid an immediate movement of the particles in the vertical direction we neglect gravity. This is a reasonable assumption, since the high shaft velocity makes the effect of gravity negligible.

We choose $\alpha = 0.1$, $c = 10 \text{ m/s}$ and a smoothing scale of $1.5d_{\text{ref}}$. Finally, we use a time step of $\Delta t = 10^{-6}$ and $t_{\text{end}} = 0.5 \text{ s}$. For $t_{\text{end}}$ the particle distributions are shown in Figure 6.

From the left picture it is clear that some kind of treatment is required. Many particles are clustering, leaving large voids, while others have even left the domain. In that respect applying the concept of particle collisions is a huge improvement. This is shown in the right picture. No particles have left the domain and the distribution is much better. Since particle collisions can be considered as a time dependent viscosity model, see Section IV, they may cause our flow to be less realistic. Because we have no analytical or experimental data available, we cannot say anything about this.

Using the convex kernel also drastically increases the quality of the particle distribution, as shown in the middle picture of Figure 6. All particles are kept inside the domain and there is far less clustering of particles. There is less regularity in distribution compared to the right picture though, especially close to the shaft. However, this makes sense because there the velocities are very high and the method is only changing forces, while the particle collisions directly influence the velocities of particles.

A dam break flow is a well-known benchmark case in SPH. See, e.g., [2, 9, 13]. Often a dam break is simulated as a single phase flow. In this paper, however, we also include the surrounding air to investigate if our methods...
are applicable to multiphase flows.

Initially all particles are distributed according to a hexagonal grid with \(d_{\text{ref}} = 1/200\). They all have zero velocities and a hydrostatic pressure distribution. The width of the water (\(\rho = 1000\ \text{kg/m}^2\)) is 0.5 m, which is half of the domain in the horizontal direction. The height of the water column is 0.2 m. The rest of the domain, up until a height of 0.5 m, is considered to be air (\(\rho = 1\ \text{kg/m}^2\)). Behind the domain boundaries are ghost particles.
to keep the fluid particles inside the domain. The initial situation is shown in Figure 7.

As an extra measure to keep particle inside the domain, we apply the particle collisions concept to all particle pairs of which exactly one particle is a ghost particle. This is done in all the simulations. Furthermore we choose $\alpha = 0.01$, $c = 10 \text{ m/s}$ and $h = 1.5d_{\text{ref}}$. Finally, we use a time step of $5 \cdot 10^{-6} \text{ s}$. Figure 8 shows the particle distributions at $t = 0.1 \text{ s}$ for the various methods.

In the top picture we clearly see difficulties arise. Especially around the interface between the water and air, large cavities appear. Due to the high pressure in the water, the rows of air particles that are close to the water start to move away from the water. In the same way, due to the low pressure in the air, the rows of water particles that are close to the air start to move towards the air. The result is that the interface between the water and air consist of several rows of closely packed particles. A similar pattern can be seen close to the domain boundaries. This is due to the zero pressures of the ghost particles.

The second picture shows the distribution when we use the convex kernel (3.9). Although the interface between the fluids looks better, there are still cavities appearing. Therefore we must conclude that the convex kernel is

Figure 7: A multiphase dam break flow. This picture shows the initial configuration of the case study in Section V.IV. Water particles are shown in black, air particles in blue, ghost particles in grey.
Figure 8: Dam break flow in an early stage. The top picture shows the particle distribution at $t = 0.1$ s when the Wendland kernel (1.1) is used. The middle picture shows the results when the convex kernel (3.9) is used. The bottom picture shows the particle distribution when the Wendland kernel (1.1) is used in combination with the concept of particle collisions.
Figure 9: Dam break flow in a later stage. The first and second picture show the particle distribution at $t = 0.7$ s when the Wendland kernel (1.1) is used, for a single phase and multiphase flow respectively. The bottom picture shows the results when the Wendland kernel (1.1) is used in combination with the concept of particle collisions.

unable to stabilize the interface between fluids with a high density ratio. The particle distribution within the fluids is much better though, which is especially noticeable at the domain boundaries.

The bottom picture in Figure 8 shows that the particle collisions lead to a great improvement in particle distribution. Despite the high density ratio, the interface between the fluids looks very good. Close to the boundaries the particle distribution remains close to uniform as well.

Finally, we look at the particle distributions at $t = 0.7$ s. These are shown in figure 9. For comparison reasons, the results for a single phase flow are shown in the first picture.
In the second picture we see that the multiphase flow is slower than the single phase flow. This is due to the interaction with the air particles. More importantly, the distribution of the particles is not good. There are many voids visible and particles are clearly clustering. In the bottom picture, where we used the particle collisions concept, the particle distribution is much better. There are hardly any voids both within the fluids and at the interface. Moreover, the flow with collisions is not slower than the flow without collisions.

VI  Summary and conclusions

In this paper we addressed the problem of particle clustering. This problem, which is not to be confused with the tensile instability, is a consequence of a diminishing kernel gradient for small inter-particle distances. We investigated the possibility of a convex kernel and the application of particle collisions.

The convex kernel greatly improves the particle distribution for single phase flows and has a small negative effect on the accuracy. The accuracy can be improved by increasing the smoothing scale, which makes it slightly more computationally expensive. We also showed that the convex kernel was not able to stabilize the interface between fluids with a high density ratio.

The second method uses particle collisions to keep particles apart. The equations are based on kinetic collision theory. Therefore this method conserves momentum (for both elastic and inelastic collisions) and energy (only for elastic collisions). The method influences the velocities of particles directly and is therefore more robust than the previous method.

Using collisions showed great improvement regarding the particle distribution. Even under extreme circumstances, like high velocities or multiphase flows with high density ratios, the method ensures that particles do not cluster. Furthermore, the concept can be applied to domain boundaries, which reduces the penetration of domain boundaries by fluid particles. However, the effect of the collision concept on the macroscopic behaviour of the flow needs more investigation.
References


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