An improved corrective smoothed particle method approximation for second order derivatives

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An improved corrective smoothed particle method approximation for second-order derivatives

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Abstract
To solve (partial) differential equations it is necessary to have good numerical approximations. In SPH, most approximations suffer from the presence of boundaries. In this work a new approximation for the second-order derivative is derived and numerically compared with two other approximation methods for a simple test case. The new method is slightly more expensive, but leads to a significantly improved accuracy.

I INTRODUCTION
Smoothed Particle Hydrodynamics (SPH) is a numerical method for solving partial differential equations. It is a mesh-free, Lagrangian method in which the state of the system is represented by a finite set of particles. Although SPH was originally developed to solve astrophysical problems [5, 7] in which boundaries are not present, the method has attracted attention in other areas like fluid and solid mechanics. This has led to significant extensions and improvements to the original method [1].

However, in many areas the presence of boundaries is still leading to inaccurate approximations. This also holds for the second-order derivative. The original SPH approximation for the second-order derivative includes the second-order derivative of the kernel function, which is very sensitive to particle disorder [2, 10]. Therefore alternatives based on the first-order derivative [2] of the kernel function and the kernel function itself [4] have been proposed. Also it is suggested to include boundary terms in the approximation [8].

In this work we will consider the methods described in [4] and [8], as well as an improved version of the one in [4]. A one-dimensional setting will be assumed throughout this work. We will start by stating the kernel function we use, whereafter all three methods are briefly explained. The numerical comparison of the methods focuses on both uniformly and non-uniformly distributed particles.

II WENDLAND KERNEL
There are several options for the kernel function. Originally a Gaussian function was used [5]. A disadvantage of this function is that it does not have compact support, which is computationally more expensive. Other examples are a truncated Gaussian or B-spline functions. A short overview is given in [6]. Throughout this work we will use the Wendland kernel of fifth degree [9, 13], given by:

\[ W_h(x - y) = \alpha_d \cdot \begin{cases} (2 - |q|)^5 (2|q|^2 + \frac{5}{4}|q| + 1) & \text{for } |q| < 2, \\ 0 & \text{for } |q| \geq 2, \end{cases} \]

where \( h \) is the smoothing length, \( \alpha_d = 3/(128h) \) is a normalizing and spatial-dimension-dependent factor and \( q = (x - y)/h \). The first-order derivative with respect to \( y \) of this function is given by:

\[ W'_h(x - y) = \frac{7\alpha_d}{h} \cdot \begin{cases} q(2 - |q|)^4 (2|q| + 1) & \text{for } |q| < 2, \\ 0 & \text{for } |q| \geq 2. \end{cases} \]

Since \( \alpha_d = O(h^{-1}) \) and \( q = O(h) \) as \( h \to 0 \), it follows that for this kernel we have:

\[ W_h(x - y) = O(h^{-1}) \quad \text{as } h \to 0, \quad (1) \]
\[ W'_h(x - y) = O(h^{-2}) \quad \text{as } h \to 0. \quad (2) \]

These orders play an important role in the accuracy of the kernel approximations. In the following sections we will consider several SPH approximations for the second-order derivative. In the accuracy analysis of these approximations we will implicitly use equations (1) and (2).

III APPROXIMATING A FIRST-ORDER DERIVATIVE
Before considering second-order derivatives, let us first have a look at the first-order derivative approximation. We will need this approximation later. In SPH, most approximations can be derived from the well-known Taylor series expansion of a function \( f \) around a point \( x \):

\[ f(y) = f(x) + (y - x)f'(x) + \frac{(y - x)^2}{2}f''(x) + \ldots \quad (3) \]

To find the value of the derivative at \( x \), we could start by subtracting \( f(x) \) from both sides of the equation. Multiplying the
entire equation with the odd function $W'_h$ and integrating over the computational domain $\Omega := [x_l, x_r]$ then gives:

$$\int_{\Omega} (f(y) - f(x)) W'_h(x - y) \, dy = \frac{f'(x)}{2} \int_{\Omega} (y - x) W_h(x - y) \, dy + \mathcal{O}(h).$$

For $x$ satisfying $|x - 2h, x + 2h| \subset \Omega$ this leads to a second-order accurate approximation, since in this case the first-order error term vanishes and the integral on the right-hand side equals 1. If $x$ is too close to a boundary this integral is unequal to 1, which causes a zero-order error. To obtain a first-order accurate approximation for these positions one could use the following approximation:

$$\langle f'(x) \rangle_{\text{CSPM}} := \frac{1}{\gamma(x)} \int_{\Omega} (f(y) - f(x)) W'_h(x - y) \, dy,$$  

where

$$\gamma(x) := \int_{\Omega} (y - x) W'_h(x - y) \, dy.$$  

Since $\gamma(x) = 1$ for $x$ in the interior of $\Omega$, dividing by it only affects the approximation close to the boundaries. This approximation is known as the Corrective Smoothed Particle Method (CSPM) approximation for the first derivative and was first proposed in [3].

### IV APPROXIMATING A SECOND-ORDER DERIVATIVE

#### IV.I CSPM approach

To find an approximation for the second-order derivative a similar path can be taken. By performing the same steps, only substituting $W'_h$ by the even function $W_h$, we find:

$$\int_{\Omega} (f(y) - f(x)) W_h(x - y) \, dy = f'(x) \int_{\Omega} (y - x) W_h(x - y) \, dy + f''(x) \int_{\Omega} \frac{(y - x)^2}{2} W_h(x - y) \, dy + \mathcal{O}(h^3).$$

Since the second integral on the right-hand side of this equation is not identically equal to one, we define it as $\gamma^*(x)$ and divide the entire equation by it. Note that for all $x$, $\gamma^*(x) = \mathcal{O}(h^2)$ as $h \to 0$ and as a consequence dividing by this factor reduces the order of all terms. For example, the remaining error term changes from $\mathcal{O}(h^3)$ to $\mathcal{O}(h)$. This gives a second-order accurate approximation for $x$ satisfying $[x - 2h, x + 2h] \subset \Omega$. This is because the first integral on the right-hand side and the first-order error term both vanish because $W_h$ is even. For $x$ close to a boundary these integrals are not zero and we end up with a very bad approximation.

To deal with this issue it is suggested in [4] to also subtract $(y-x)f'(x)$ from equation (3), before it is multiplied with $W_h$ and integrated over $\Omega$. Since $f'$ is unknown we have to approximate this value as well. Using the approximation in (4) leads to the following approximation for the second-order derivative:

$$\langle f''(x) \rangle_{\text{CSPM}} := \frac{1}{\gamma^*(x)} \int_{\Omega} (f(y) - f(x)) W_h(x - y) \, dy - \frac{1}{\gamma^*(x)} \langle f'(x) \rangle_{\text{CSPM}} \int_{\Omega} (y - x) W_h(x - y) \, dy,$$  

where

$$\gamma^*(x) := \int_{\Omega} \frac{(y - x)^2}{2} W_h(x - y) \, dy.$$  

Again, the approximation in (6) uses (4), since the exact first-order derivative of $f$ is unknown.

#### IV.II Boundary Integral approach

As we will see later, the CSPM approximation for a second-order derivative gives poor results when applied to a ‘direct’ problem. By this we mean that a second-order derivative is computed from a known function $f$. In a way this is the opposite of a boundary value problem, in which a second-order derivative and some boundary conditions are known and the original function $f$ is to be found. In this work we will consider both types of problems.

To improve the accuracy at the boundaries, in [8] a method is proposed that adds boundary integral terms to the approximation given in [2]:

$$\langle f''(x) \rangle_{\text{BIM}} := \frac{2}{\gamma(x)} \int_{\Omega} \frac{f(y) - f(x)}{y - x} W_h'(x - y) \, dy + \frac{f(x) - f(x_\ell)}{x - x_\ell} W_h(x - x_\ell) - \frac{f(x) - f(x_l)}{x - x_l} W_h(x - x_l),$$  

where $\gamma$ is the so-called Shepard normalization factor defined by:

$$\gamma(x) := \int_{\Omega} W_h(x - y) \, dy.$$  

For $x$ in the interior of $\Omega$ the boundary integral terms in (8) equal 0. For those positions the approximation is second-order accurate, just like the CSPM approximation. However, it can be shown that for $x$ close to a boundary the method is still first-order accurate, which is an improvement to the CSPM approximation. A complete derivation can be found in [8].

#### IV.III An improved CSPM approach

If one takes a closer look at (8), it is noticed that $x = x_\ell$ or $x = x_l$ leads to a 0-divided-by-0 situation. Although this may not cause a problem in the case of a boundary value problem with Dirichlet boundary conditions, it is undesirable. Therefore in this work a method is derived that avoids this situation, but still has first-order accuracy.

The CSPM approximation in (6) uses the approximation for the first-order derivative in (4). As mentioned earlier, the approximation for the first-order derivative is second-order accurate in the interior of $\Omega$ and first-order accurate for $x$ close to a boundary. Therefore this may seem like a good approach, but let us have a more detailed look at this first-order error. If we keep track of one
more term in the derivation of the first-order derivative approximation we find that:

$$\langle f'(x) \rangle_{\text{CSPM}} = f'(x) + \frac{f''(x)}{\gamma(x)} \int_{\Omega} \frac{(y-x)^2}{2} W_h(x-y) \, dy + \mathcal{O}(h^2).$$

(10)

Notice that the first error term in this equation depends on $f''$, which could play a role in the approximation for the second-order derivative. We substitute the right-hand side of (10) into (6) to investigate the accuracy of this approximation. After some arithmetic operations this gives us:

$$\langle f''(x) \rangle_{\text{CSPM}} = f''(x) + \frac{f''(x)}{\gamma(x)} \int_{\Omega} \frac{(y-x)^2}{2} W_h(x-y) \, dy \times \int_{\Omega} (y-x) W_h(x-y) \, dy + \mathcal{O}(h).$$

(11)

We thus see that the CSPM approximation for the second-order derivative has a zeroth-order error. This can easily be solved by dividing by a normalization factor. This results in the following approximation:

$$\langle f''(x) \rangle_{\text{CSPM}} := \frac{1}{\kappa(x)} \langle f''(x) \rangle_{\text{CSPM}},$$

(12)

where

$$\kappa(x) := 1 + \frac{1}{\gamma(x)} \int_{\Omega} \frac{(y-x)^2}{2} W_h(x-y) \, dy \times \int_{\Omega} (y-x) W_h(x-y) \, dy.$$

(13)

Like the previous two methods, this approximation is second-order accurate in the interior of $\Omega$. Compared to the CSPM approximation this new method (ICSPM) is an improvement though, since it is first-order accurate near boundaries. To have a more complete comparison between the approximations in (6), (8) and (12) we perform numerical experiments.

V NUMERICAL RESULTS

In order to perform numerical experiments we need to discretize the continuous approximations described in the previous section. This is done by distributing $N$ particles over $\Omega$. Each particle $i$ has its own position $x_i$ and volume of size $|\Omega_i|$. Approximations are only computed at positions where particles are located. The integral over the support domain of a particular particle is then approximated by a sum over the particles inside this support domain. Approximations (6), (8) and (12) then become:

$$\langle f'_i \rangle_{\text{CSPM}} = \frac{1}{\gamma_i} \sum_{j \in N_i} (f_j - f_i) W_{ij} |\Omega_j| - \frac{1}{\gamma_i} \langle f'_i \rangle_{\text{CSPM}} \sum_{j \in N_i} (x_j - x_i) W_{ij} |\Omega_j|,$$

(14)

$$\langle f''_i \rangle_{\text{BIM}} = \frac{2}{\gamma_i} \sum_{j \in N_i} (f_j - f_i) W_{ij} |\Omega_j| + \frac{f_j - f_i}{x_j - x_i} W_{ij} - \frac{f_i - f_j}{x_i - x_j} W_{ij},$$

(15)

$$\langle f''_i \rangle_{\text{ICSPM}} = \frac{1}{\kappa_i} \langle f''_i \rangle_{\text{CSPM}},$$

(16)

with

$$\langle f'_i \rangle_{\text{CSPM}} = \frac{1}{\gamma_i} \sum_{j \in N_i} (f_j - f_i) W_{ij} |\Omega_j|,$$

$$\gamma_i = \sum_{j \in N_i} (x_j - x_i) W_{ij} |\Omega_i|,$$

$$\gamma_i^* = \sum_{j \in N_i} \frac{(x_j - x_i)^2}{2} W_{ij} |\Omega_j|,$$

$$\kappa_i = 1 + \frac{1}{\gamma_i} \sum_{j \in N_i} \frac{(x_j - x_i)^2}{2} W_{ij} |\Omega_j| \times \sum_{j \in N_i} (x_j - x_i) W_{ij} |\Omega_j|,$$

and where $f_i := f(x_i)$, $W_{ij} := W_h(x_i - x_j)$ and $N_i$ is the set of particles within the support domain of particle $i$. Similar abbreviations as for $f_i$ hold for $\gamma_i, \gamma_i^*, \kappa_i$.

We will consider the function $f(x) = x^2 + \cos(\pi x)$ on the domain $\Omega = [0, 1]$, i.e. $x_0 = 0$ and $x_{N} = 1$. This function is a solution to the following boundary value problem:

$$\begin{cases}
  f''(x) = 2 - \pi^2 \cos(\pi x), & \text{for } x \in (0, 1), \\
  f(0) = 1, \\
  f(1) = 0.
\end{cases}$$

(17)

As mentioned before we will test the approximations in (14), (15) and (16) in a direct way, by assuming that $f$ is known and approximating its second-order derivative, and by solving the boundary value problem (17).

VI Uniformly distributed particles

Although one of the biggest advantages of SPH is that it uses unconnected particles rather than a grid, we start by assuming that the particles are distributed uniformly. In particular, the first particle is put on the left boundary of the domain, $x_1 = x_0$, and the $N$'th particle is positioned on the right boundary, $x_N = x_r$. The remaining particles are positioned equidistantly between the two boundary particles. Consequently, the two boundary particles have only half the volume of the other particles. This situation is shown in Figure 1. It must be noted that this ‘finite difference like’ positioning of the particles is slightly different than the ‘finite volume like’ one used in [8], but the difference in the numerical results is negligible. We will therefore simply adopt the positioning shown in Figure 1 for all approximation methods.

![Figure 1: Uniformly distributed particles.](image-url)
We start by assuming that $f$ is known and use the three different approximation methods to compute the second-order derivative. Results for the case $N = 41$ are shown in Figure 2. Obviously the CSPM method behaves badly close to the boundaries. Notice that for the BIM method the boundary particles are neglected, because of the $0$-divided-by-$0$ situation. The BIM approximation is significantly better than the CSPM method, but the ICSPM approximation is the one that seems to suffer the least from the presence of boundaries.

Since we have an equidistant grid, we can easily investigate the order of convergence of the various approximations. This is done by performing numerical experiments with different numbers of particles, e.g., $N = 11, 21, 41, 81$ etc., thereby each time decreasing the volume of the particles by a factor 2. By defining $e_N$ as the infinity norm of the difference vector between a numerical solution with $N$ particles and the exact solution at those particles, we can approximate the order of convergence $p$ by comparing two subsequent approximations in the following way:

$$p \approx p_N := \frac{\log \left( e_{(N+1)/2} / e_N \right)}{\log 2}.$$

Furthermore, if we define $c_k$ as the ratio between smoothing length and particle ‘volume’, we have to choose between a constant $c$ and a $c$ that increases with the number of particles. In case of a constant $c$, it is recommended to choose $c \sim 1.0 - 2.0$ [12]. In this work we consider $c = 2$. Errors and convergence rates are shown in Table 1.

We clearly see that the CSPM approximation is only zeroth-order accurate. This is as expected, since in (11) we already noticed that with the original CSPM approximation we make a zeroth-order error. This is exactly what is taken into account in the ICSPM method, which is clearly second-order accurate. This is even better than de first-order accuracy we derived, but it is only due to the uniform distribution of the particles and we therefore do not expect it to hold in case of non-uniformly distributed particles.

The BIM approximation behaves quite badly, but it must be noted that we do not take into account that for this method both the particle volumes and $1/c$ must tend to zero. For instance, if we choose the smoothing length equal to $k^2$ times the particle volume, where $k = 1, 2, \ldots, 8$ is the simulation number, we get much better results. These are shown in Table 2.

![Figure 2: Second-order derivatives computed with (14), (15) and (16) in case of uniformly distributed particles. In this computation $N = 41$ and $h = 1/20$.](image)

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<th>$p_N$</th>
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Table 1: Error and convergence rates in computing the second-order derivative with uniformly distributed particles and $c = 2$.

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</table>

Table 2: Error and convergence rates in computing the second-order derivative with uniformly distributed particles and increasing $c$.
In the derivation of the kernel approximation of the BIM method, some integration steps are performed. To justify this numerically we have to choose an increasing ratio between smoothing length and particle volume, because then the sums in the particle approximations approximate the integrals in the kernel approximations better for increasing $N$. An extensive explanation is given in [11]. The increasing ratio between smoothing length and particle volume is clearly a necessity for the BIM method. The ICSPM method does not need this increasing $c$, because the error in approximating integrals is mostly taken care of by the normalization factors. In fact, an increasing $c$ in ICSPM makes the order of convergence take a lower value than 2, since a bigger $c$ implies more smoothing and therefore a less accurate kernel approximation. Moreover, every computation a bigger number of particles suffers from ‘boundary issues’. Compared to the BIM method the ICSPM method is advantageous, since the error with the same number of particles is much smaller and using a constant $c$ implies we obtain sparser matrices.

In the rest of this work we will use a constant $c$ for the CSPM and the ICSPM method and an increasing $c$ for the BIM method. The values for these $c$’s are as described previously.

We continue the comparison by solving (17) with all three methods. Since the results are too close to each other to distinguish in a simple plot, we only state the errors and convergence rates. They are listed in Table 3.

We see that all methods are converging to the analytical solution. However, the BIM approximation seems to be only first-order accurate, while the CSPM and the ICSPM approximation are second-order accurate. Furthermore, the error with ICSPM is one order of magnitude smaller than with CSPM. Thus, overall the ICSPM is the best option in case of uniformly distributed particles.

### VII. Non-uniformly distributed particles

As mentioned earlier one of the most important characteristics of SPH is that particles are unconnected. A consequence of this is that when we consider a time-dependent flow and time evolves, independent of the initial configuration, the particle distribution will not remain uniform. That is why in this work also non-uniformly distributed particles are considered.

We assume that particles do not overlap. This implies that in areas with large numbers of particles, the particles have smaller ‘volumes’ than in areas with only few particles. Consequently, in general all particles have different volumes. We implement this by fixing one particle on each boundary, whereafter the remaining particles are distributed randomly over the domain. The boundaries of the sub-domains are then positioned half way between adjacent particles. An example is shown in Figure 3.

![Figure 3: Non-uniformly distributed particles.](image)

To make sure that every particle has other particles inside its support domain we choose the smoothing length dependent on the largest particle volume:

$$h = c \max_{i=1,...,N} |\Omega_i|.$$  

This time we start again with assuming a known function $f$ and compute its second-order derivative. Results with $N = 41$ are shown in Figure 4.

In both figures we clearly see that CSPM has difficulties near the boundaries, which for the biggest part are solved by ICSPM. In the top figure the BIM approximation seems to have some troubles with the non-uniformly distributed particles. However, if we increase the smoothing length this method behaves much better, as can be seen in the bottom figure. Moreover, ICSPM has some large errors close to the boundaries. From these plots we conclude that ICSPM is the better choice in case of small smoothing lengths and BIM the one for larger smoothing lengths.

With non-uniformly distributed particles, it is not trivial to compute the order of convergence. To find a reliable indication...
Figure 4: Second-order derivatives computed with (14), (15) and (16) in case of non-uniformly distributed particles. In these computations \( N = 41 \) and \( c = 2 \) (top) and \( c = 3 \) (bottom).

Figure 5: Numerical solutions when solving (17) with (14), (15) and (16) in case of non-uniformly distributed particles. In these computations \( N = 41 \) and \( c = 2 \).

Table 4: Error and convergence rates when computing the second-order derivative with non-uniformly distributed particles.

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of the convergence order we make sure that if \( N \) is increased, the first \( N \) particles have the same position as in the previous simulation. By doing this we can see to what extend the extra particles improve the previous numerical solution. The order of convergence is then approximated as described before. For the ratio between smoothing length and largest particle volume we choose \( c = 2 \) for CSPM and ICSPM and \( c = k^2 \), with \( k \) as defined before, for BIM. The results are listed in Table 4.

All methods behave more or less like one could expect. The CSPM approximation is clearly zeroth-order convergent, whereas the BIM method seems to be first-order accurate. The convergence rates for ICSPM are a bit more fluctuating, but are generally positive and bigger than 1. Also the error with ICSPM is the smallest of all three methods.

Finally, we solve (17) with non-uniformly distributed particles. Results are shown in Figure 5 and Table 5.

We see that both the BIM approximation and the ICSPM approximation behave very well. For many particles the errors with CSPM and BIM get very close, but overall the BIM method seems to behave slightly better. The ICSPM approximation is obviously the best one. The error is much smaller than with the other methods, with a difference of at least three orders of magnitude. Also the convergence rate for ICSPM, fluctuating around 2, behaves most stable of all three methods. Therefore we can conclude that also in case of non-uniformly distributed particles, the ICSPM approximation is the best one.
Table 5: Error and convergence rates when solving (17) with non-uniformly distributed particles.

VI CONCLUDING REMARKS

In this work we compared three different SPH approximations for the second-order derivative; the widely used CSPM method [4], the relatively new BIM method [8] and the ICSPM (improved CSPM) method introduced in this paper. The BIM approach gives much better results than the CSPM approach. However, the larger the total number of particles in the BIM approximation is, the larger the number of particles inside the support domain of each particle should be to get a decent accuracy. This implies that the corresponding matrices are less sparse, making the method computationally expensive. In contrast, in an ICSPM approximation the number of particles inside each support domain may remain constant and still it approximates the second-order derivative with good accuracy. The extra normalization step in ICSPM makes the method computationally slightly more expensive than CSPM, but compared to the huge accuracy improvement these extra costs are relatively small. This holds for both uniformly and non-uniformly distributed particles, but especially the latter case shows how accurate and robust the ICSPM approximation is.

References


[7] Lucy L.B. (1977); A numerical approach to the testing of the fission hypothesis. The Astronomical Journal 82 1013–1020


