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Citation for published version (APA):

Document status and date:
Published: 01/01/2015

Document Version:
Publisher’s PDF, also known as Version of Record (includes final page, issue and volume numbers)

Please check the document version of this publication:
• A submitted manuscript is the version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher’s website.
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An improved CSPM approximation for multi-dimensional second-order derivatives

by

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An improved CSPM approximation for multi-dimensional second-order derivatives

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Abstract

Many SPH approximations for second-order derivatives, or the Laplacian, suffer from the presence of boundaries and irregularities in the particle distribution. In this paper we discuss four estimates to the Laplacian: the Brookshaw approximation, CSPM, MSPH and ICSPM – the latter of which is derived in this work. We theoretically derive the convergence rate of these methods and validate the results with numerical experiments. We show that the widely used Brookshaw method suffers the most from boundaries or random particles, while MSPH and the method derived in this work (ICSPM) are able to stay accurate. ICSPM uses smaller matrices than MSPH and is therefore computationally more attractive.

I Introduction

Smoothed Particle Hydrodynamics (SPH) is a mesh-free Lagrangian method to solve differential equations. The state of the system is represented by a finite set of particles. SPH was originally developed to solve astrophysical problems [6, 8] in which boundaries are not present, but the method has gained attention from other disciplines. This has led to significant extensions and improvements to the original method [1].

In many areas, the presence of boundaries leads to inaccurate approximations. Second-order derivatives are no exception to this. It is important to have good estimates for second-order derivatives, or for the Laplacian, because they are used in viscous terms. Also, in incompressible SPH (ISPH) the Laplacian is important. Originally, second-order derivatives were calculated by using second-order derivatives of the kernel function, which are 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. Other researchers have suggested to include boundary terms in the approximation [9].
We consider the method described by Brookshaw [2], Chen et al. [3, 4, 5] and Zhang and Batra [12]. We also propose an improvement to the estimate by Chen et al. The approximations are valid for any number of dimensions (1, 2 or 3). We compare numerical results for both uniformly and non-uniformly distributed particles, but are especially interested in the latter, because it most accurately resembles particle distributions from actual simulations.

II Approximations for second-order derivatives

Many methods for estimating second-order derivatives or the Laplacian are available in literature. The originial approximation is based on second-order derivatives of the kernel function, but these showed to be too sensitive to particle disorder [10]. Therefore Brookshaw [2] proposed an approximation based on the kernel’s first derivative:

\[ \langle \nabla^2 f(x) \rangle_B = 2 \int_\Omega (f(y) - f(x)) \frac{\xi^T \nabla W}{|\xi|^2} d\gamma. \tag{2.1} \]

Here, \( \nabla W := \nabla W(x - y, h) \) and \( \xi := y - x \). This simple expression works very well in the absence of boundaries. Unfortunately, when particles are close to boundaries the approximation in (2.1) is not so good. In fact, using Taylor series it can be shown that it is of order \( O(h^{-1}) \). Moreover, it does not compute all second-order derivatives separately, which may be required in some cases. Instead, it computes the Laplacian directly.

A more accurate, but also more expensive approximation is the corrective smoothed particle method (CSPM) by Chen et al. [3, 4, 5]. This method computes all second-order derivatives separately. It is derived from:

\[ f(y) - f(x) = \xi^T \nabla f(x) + \frac{1}{2} \xi^T H_f(x) \xi, \tag{2.2} \]

where \( H_f \) denotes the Hessian matrix of \( f \). The vector with all second-order derivatives of \( f \), including mixed derivatives, will be denoted by \( h_f \). In CSPM, (2.2) is multiplied with \( h_W := h_W(x - y, h) \) and integrated over the domain. This gives:

\[ \int_\Omega (f(y) - f(x)) h_W d\gamma = \int_\Omega \xi^T \nabla f(x) h_W d\gamma + \int_\Omega \frac{1}{2} \xi^T H_f(x) \xi h_W d\gamma. \tag{2.3} \]

The value for \( \langle h_f(x) \rangle \) comes from the second integral on the right-hand side. Therefore the approximation in (2.3) can be made more accurate by subtracting an estimate of the first integral on the right-hand side. This requires an approximation for \( \nabla f(x) \), which is found by multiplying (2.2) by \( \nabla W \) instead of \( h_W \):

\[ \int_\Omega (f(y) - f(x)) \nabla W d\gamma = \int_\Omega \xi^T \nabla f(x) \nabla W d\gamma + \int_\Omega \frac{1}{2} \xi^T H_f(x) \xi \nabla W d\gamma. \tag{2.4} \]
The right-hand side of (2.4) can be written $\Gamma_1 \nabla f(x) + O(h)$, with $\Gamma_1 = \Gamma_1(x)$ a normalisation matrix. Hence:

$$\langle \nabla f(x) \rangle := \Gamma_1^{-1} \int_{\Omega} (f(y) - f(x)) \nabla W \, dy$$

$$= \nabla f(x) + O(h).$$

The approximation for the gradient in (2.5) is substituted for $\nabla f(x)$ in the first integral on the right-hand side of (2.3). Next, the entire integral is subtracted from both sides of the equation. Finally, the remaining integral on the right-hand side of (2.3) is written:

$$\int_{\Omega} \frac{1}{2} \xi^T H_f(x) \xi h_W \, dy =: \Gamma_2 h_f(x),$$

with $\Gamma_2 = \Gamma_2(x)$ another normalisation matrix. Multiplying both sides of the equation with $\Gamma_2^{-1}$ gives the approximation of Chen et al.:

$$\langle h_f(x) \rangle_{\text{CSPM}} := \Gamma_2^{-1} \left( \int_{\Omega} (f(y) - f(x)) h_W \, dy - \int_{\Omega} \xi^T \langle \nabla f(x) \rangle h_W \, dy \right),$$

with $\langle \nabla f(x) \rangle$ as defined in (2.5). The Laplacian is then found by adding up the relevant terms of $\langle h_f(x) \rangle$. Based on the first-order accuracy of the gradient approximation in (2.5), one could hope that

$$\langle h_f(x) \rangle_{\text{CSPM}} = h_f(x) + O(h),$$

but this is in general not true. Instead, we only have:

$$\langle h_f(x) \rangle_{\text{CSPM}} = h_f(x) + O(1).$$

The reason is that part of the solution is in the $O(h)$-term in (2.6), which depends on $H_f(x)$.

Another method was proposed by Zhang and Batra [12]. In the modified smoothed particle hydrodynamics method (MSPH) a vector $\varphi$ is computed that consists of an approximation of $f$ itself, all its first-order derivatives and all its second-order derivatives. Because all unknowns are put in one single vector, this method requires larger matrices. Hence, all the derivative estimates depend on each other, which leads to more accurate results than the previous methods. In fact, if we isolate $h_f$ from $\varphi$, we find:

$$\langle h_f(x) \rangle_{\text{MSPH}} = h_f(x) + O(h).$$

It is possible to achieve similar accuracy without using large matrices. For that we need only one extra normalisation step in CSPM. This is described in the next section.
III An improvement to CSPM

To improve the CSPM approximation, we investigate how the error of \( \langle \nabla f \rangle \) influences the error of \( \langle h f \rangle \). This approach is analogous to the improvement to the one-dimensional approximation described in [7]. Combining (2.4), (2.5) and (2.6) gives:

\[
\langle \nabla f(x) \rangle = \nabla f(x) + \Gamma_1^{-1} \int_{\Omega} \frac{1}{2} \xi^T H_f(x) \xi \nabla W \, dy + O(h^2). \tag{3.12}
\]

Substituting this equation for \( \langle \nabla f(x) \rangle \) in (2.8) leads to:

\[
\langle h f(x) \rangle_{\text{CSPM}} = \frac{1}{2} \int_{\Omega} (f(y) - f(x)) h_W \, dy
- \Gamma_2^{-1} \int_{\Omega} \xi^T \left( \nabla f(x) + \Gamma_1^{-1} \int_{\Omega} \frac{1}{2} \xi^T H_f(x) \xi \nabla W \, dy + O(h^2) \right) h_W \, dy. \tag{3.13}
\]

Using (2.3) and the definition of \( \Gamma_2 \) in (2.7) we know that:

\[
\Gamma_2^{-1} \int_{\Omega} (f(y) - f(x)) h_W \, dy - \Gamma_2^{-1} \int_{\Omega} \xi^T \nabla f(x) h_W \, dy = h_f(x) + O(h), \tag{3.14}
\]

which, combined with (3.13), gives:

\[
\langle h f(x) \rangle_{\text{CSPM}} = \frac{1}{2} \int_{\Omega} \xi^T \left( \Gamma_1^{-1} \int_{\Omega} \frac{1}{2} \xi^T H_f(x) \xi \nabla W \, dy + O(h^2) \right) h_W \, dy
+ h_f(x) + O(h). \tag{3.15}
\]

We can write the first term on the right-hand side of (3.15) as:

\[
- \Gamma_2^{-1} \int_{\Omega} \xi^T \left( \Gamma_1^{-1} \int_{\Omega} \frac{1}{2} \xi^T H_f(x) \xi \nabla W \, dy + O(h^2) \right) h_W \, dy
= \tilde{K} h_f(x) + O(h), \tag{3.16}
\]

for some matrix \( \tilde{K} = \tilde{K}(x) \). Combining this with (3.15) shows that, instead of (2.9), we have:

\[
\langle h f(x) \rangle_{\text{CSPM}} = \tilde{K} h_f(x) + O(h), \tag{3.17}
\]

where \( K = K(x) \), defined as \( K := I + \tilde{K} \), is a normalisation matrix. Hence, we can improve the approximation by multiplying with the inverse of \( K \):

\[
\langle h f(x) \rangle_{\text{ICSPM}} := K^{-1} \langle h f(x) \rangle_{\text{CSPM}} \tag{3.18}
\]

and we have:

\[
\langle h f(x) \rangle_{\text{ICSPM}} = h_f(x) + O(h), \tag{3.19}
\]
as desired. We validate this analysis in the next section, where we perform numerical experiments and compare various methods.
IV Numerical experiments

Although the approximations described in the previous section are valid in any number of dimensions, we will restrict ourselves to two-dimensional problems. We consider three test cases, of which the first two were also discussed in [11], namely:

\[ f(x, y) = x^5 + y^5, \]  
\[ f(x, y) = (xy)^5, \]

in the unit square \( \Omega := [0, 1] \times [0, 1] \). The four methods in the previous section will be used to compute the Laplacian of these functions, which are shown in Figure 1.

We consider both uniformly and randomly distributed particles. The random grid is obtained by distorting the uniform grid. Corner particles are not distorted and other boundary particles are distorted in only one dimension, such that they stay on the boundary. The areas covered by the particles are obtained from a Voronoi tessellation, as shown in Figure 2. This means that the particles cover the entire domain \( \Omega \).

We use a smoothing length \( h = 1.2 \delta \) in our computations, with \( \delta \) a reference particle spacing. We choose \( \delta \) to be the distance between particles in case of a uniform particle distribution.

Plotting the full numerical Laplacian would require a surface plot. Unfortunately, a figure with all numerical solutions would be unclear and not much could be concluded from it. Therefore we look at subsets of particles, e.g., one particle or a line of particles. Figures 3 and 4 show the relative errors of all methods on the line \( x = y \) on a logarithmic scale. These results were found with \( N = 1089 \) randomly distributed particles and are shown only for \( (x, y) > (0.75, 0.75) \). The results suggest that, as we expected, CSPM is more accurate than the Brookshaw approximation and both ICSPM and MSPH are more accurate than CSPM. Based on other experiments, this seems to be true in general. Figures 3 and 4 also show that this conclusion is not true for every single particle. However, it should be noted that the results shown in these figures are just examples of how the methods be-
have in case of randomly distributed particles. The actual behaviour is in fact quite strongly dependent on the particle distribution.

We would like to validate our statements on the convergence of the methods. To do so, we start with uniform grids. This ensures that when we increase the number of particles, positions from previous simulations are still occupied by particles. Each time we compare with the exact solution and compute the relative error. As explained before, we only look at subsets of particles. In this case we only consider the error at the $N$’th particle, located at $(x,y) = (1,1)$, since this is where the difference in performance will be most clear. The order of convergence $p$ is defined as:

$$2^p = \frac{e_M}{e_N},$$

(4.22)

where $e_k$ is the relative error with $k$ particles and $N = 2M + 1$. This means that $\delta_N = \frac{1}{2} \delta_M$ and we can estimate the order of convergence by:

$$p \approx p_N := \frac{\log(e_M / e_N)}{\log 2}.$$  

(4.23)

Results are shown in Tables 1 and 2. As we already mentioned, the Brookshaw approximation is of order $O(h^{-1})$. This is true at boundaries, but also for other particles if they are randomly distributed. For CSPM we find that, as we already stated in (2.10), it is only of order $O(1)$. ICSPM and MPSH behave similarly, with first-order convergence even at domain boundaries.

Finally, we consider a slightly more challenging problem. We will compute the Laplacian of the function:

$$f(x,y) = e^{10x \sin y}.$$  

(4.24)
Figure 3: Relative errors with randomly distributed particles for \( \langle \nabla^2 f \rangle \) on the line \( x = y \), for \( f(x, \ y) = x^5 + y^5 \).

Figure 4: Relative errors with randomly distributed particles for \( \langle \nabla^2 f \rangle \) on the line \( x = y \), for \( f(x, \ y) = (xy)^5 \).
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Table 1: Error and convergence rates when calculating the Laplacian of $f(x,y) = x^5 + y^5$ with uniformly distributed particles.

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Table 2: Error and convergence rates when calculating the Laplacian of $f(x,y) = (xy)^5$ with uniformly distributed particles.
Figure 5: Relative errors with randomly distributed particles for $\langle \nabla^2 f \rangle$ on the line $x = y$, for $f(x, y) = e^{10x}\sin y$.

The Laplacian of this function has a smooth, but steep gradient for $x$ close to unity. It is shown in Figure 6.

Looking at Figure 5, we see similar results as before, with the exception that CSPM behaves similarly to ICSPM and MSPH for particles not close to boundaries. However, we still need to keep in mind that this is just one random particle distribution. For a different particle distribution results could be different. In general, we see that CSPM is more accurate than the Brookshaw approximation and ICSPM and MSPH are more accurate than CSPM. MSPH is usually a bit more accurate than ICSPM, but it is the expectation of the authors that they can be made identical by also considering the SPH approximation to $f$, and especially the errors depending on second-order derivatives that result from that, in the derivation of ICSPM. This is implicitly also what happens in MSPH, but there everything is
Table 3: Error and convergence rates when calculating the Laplacian of $f(x, y) = e^{10x} \sin y$ with uniformly distributed particles.

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put in one large matrix. However, since this extra approximation step is not applied in ICSPM, and because smaller matrices are required, ICSPM has the potential of being computationally less expensive.

When we look at the convergence rates in case of uniformly distributed particles in Table 3, we see that all methods behave the same as before. However, for the sake of experiment, we also try to find the rate of convergence for the case of randomly distributed particles. When we increase the number of particles we do not add extra particles, but instead remove the particles and construct a fully new random distribution. However, to have a fair comparison, we use the same random distribution for specific values of $N$ for all methods. The results are shown in Table 4.

What attracts attention is the fluctuating behaviour of CSPM. Clearly, CSPM is very sensitive to irregularities in the particle distribution. ICSPM and MSPH, on the other hand, are very stable and nicely converge to first-order accuracy, with even a small advantage for ICSPM.

V Concluding remarks

In this work we compared four different approximations for the Laplacian; the widely used Brookshaw approximation, CSPM [3, 4, 5], MSPH [12] and an improvement to the CSPM approximation introduced in this paper (ICSPM). We theoretically derived and numerically validated that the Brookshaw approximation is of order $O(h^{-1})$ and CSPM of order $O(1)$ for particles close to boundaries or in case of
randomly distributed particles. In contrast, both ICSPM and MSPH are of order $O(h)$. The extra normalisation step in ICSPM compared to CSPM obviously makes it computationally more expensive, but the effect is a huge improvement in accuracy and stability, especially in case of randomly distributed particles. MSPH also has these advantages, but this method uses larger matrices, making it computationally less attractive.

References


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