Research Article

New Kernel Function for the Approximation of Third Order Derivatives

Yaiche Ilham[a], Zaoui EL Miloud[a]

[a]Mohammadia School of Engineering, Mohamed V University, Rabat, Morocco.
E-mail: ilhamyaiche2@gmail.com
[b]Department of industrial Engineering, E.N.S.M.R, Rabat, Morocco. E-mail: zaoui.elmiloud@enim.ac.ma

Article History: Received: 11 January 2021; Accepted: 27 February 2021; Published online: 5 April 2021

Abstract: A new kernel function is developed to approximate the third order derivative by mean of the Smoothed Particle Hydrodynamics (SPH) method. It has the advantage to be efficiently used with gridded data and random distributions. Due to the discrepancy of the particles in the former distribution, we extended the use of the CSPM method for the approximation of third order derivatives. Our new kernel function provides three accurate numerical schemes, in conjunction with the trapezoidal rule, Simpson's rule and the CSPM method respectively.

Keywords: SPH Method, Third Order Derivative, Kernel Function.

1. Introduction

The Smoothed particle hydrodynamics is a Lagrangian meshless method that approximates the field function and its derivatives using a weighting function, usually called a *smoothing kernel*. It was invented by (Lucy, 1977) and (Gingold & Monaghan, 1977), separately.

The advantage of this method over gridded based methods like FEM is that it is inherently suitable for problems with large deformations, complex geometries, and moving interfaces. This is due to the representation of the simulation domain using free particles without any connectivity, and also the possibility of adding effortlessly more particles in areas of interest for more accuracy.

Since its invention, the SPH method has been used in the simulation of many scientific and engineering problems. However, it was mainly used to solve no higher than second order partial differential equations. In fact, the accuracy of the approximation of the field function and its derivatives depend on the smoothing kernel and its derivatives. Therefore, numerical inconsistencies can be generated since the smoothing kernel bear multiple differentiations.

Since many interesting phenomena reduce to third order differential equations such as the KdV equation (Korteweg and de Vries, 1895), and the regulation and control of actions' type of problems, we're interested in constructing a new kernel function that is specifically customized for the approximation of the third order derivative, that can be used well for both random and gridded data due to its simplicity.

2. New Kernel Function

Before we start developing our new kernel, we will recall briefly the layout of the SPH method and give examples on well-known smoothing kernels and recent discontinuous kernels (Belly, 2009).

2.1 SPH Method Formalism

The SPH method approximates a function f using the smoothing kernel W that is compactly supported, the integral over its support domain, delimited using a parameter h called the *smoothing length* is equal unity.

$$f(x) = \int f(x')W(x - x')dx' \qquad (1)$$

Examples of smoothing kernels

- B-cubic Spline.

$$W(R,h)=\alpha_d\begin{cases}\frac{2}{3}-R^2+\frac{1}{2}R^3 & 0\ \leq R<1\\ \frac{1}{6}(2-R)^3 & 1\ \leq R<2\\ 0 & R\ \leq 2,\end{cases}$$

- Gaussian kernel.

$$W(R,h)=\alpha_d\begin{cases}e^{-R^2} & R\leq 2\\ 0 & otherwise\end{cases}$$

Examples of discontinuous kernel functions

- δ function

$$\delta_{[-h,h\ ]}(x)=\begin{cases}\frac{1}{2h} & -h\leq x\leq h\\ 0 & otherwise,\end{cases}$$

- δ' function

$$\delta'_{[-h,h]}(x)=\begin{cases}\frac{1}{h^2} & -h\leq x\leq 0\\ -\frac{1}{h^2} & 0\ <x\leq h\\ 0 & otherwise,\end{cases}$$

- δ'' function

$$\delta''_{[-h,h]}(x)=\begin{cases}\frac{4}{h^3} & h/2<|x|<h\\ -\frac{4}{h^3} & 0\ \leq|x|<h/2\\ 0 & otherwise,\end{cases}$$

The particle approximation of the field function f at the particle x_i is then achieved, by replacing the integral with the sum over all its neighbouring particles inside the support domain of the smoothing kernel W.

Then, the formula (1) becomes

$$f(x_i)=\sum_{i=1}^{N}f(x_j)W(x_i-x_j)\Delta x_j \qquad (2)$$

2.2 New Kernel Function Construction

2.2.1 Theoretical Definition

Let’s call the new function. Using the formalism of the SPH method we write the approximation of $f^{(3)}$ at a point x as

$$<f^{(3)}(x)>=\int f(x')\psi(x-x')dx' \qquad (3)$$

The integral is over the support domain of ψ centred on x which is [x- h, x+ h].

2.2.2 Accuracy and Efficiency Requirements

In order to obtain the shape and a good accuracy for , we will approximate the function f in the integrand using use a fifth degree Taylor polynomial and derive the appropriate conditions.

First, we write

$$f(x')=\sum_{i=0}^{5}f^{(j)}(x)\frac{(x'-x)^{(j)}}{j!} \qquad (4)$$

Thus,

$$< f^{(3)}(x) >= f(x)\mathrm{M}_0 + f'(x)\mathrm{M}_1 + \frac{1}{2}f''(x)M_2 + \frac{1}{6}f^{(3)}(x)\mathrm{M}_3 + \frac{1}{24}f^{(4)}(x)\mathrm{M}_4 + \frac{1}{120}\, f^{(5)}(x)M_5 \quad (5)$$

Provided that

$$M_i = \int_{x-h}^{x+h} (x'-x)^{(i)}\psi(x-x')dx'$$
$$= -\int_{-h}^{h} r^{(i)}\psi(r)dr \qquad (6)$$

Where the index (i) varies from 0 to 5.

Therefore, in order to approximate the third order derivative accurately, the M_i elements for i=0 to 2 must be null, M_3 must equal - 6 and $\mathrm{M}_4 = 0$.

For efficiency purposes, we add another requirement for ψ to be a constant wise kernel.

2.2.3 Kernel Function Development

In order to fulfil the conditions where the integrals M_i must be null for the indexes 0, 2 and 4, we designed the kernel function ψ as a step function that it is symmetric around the origin as follows

$$\psi(x) = \begin{cases} c_1 \; -h \le x \le -a \\ c_2 \; -a < x \le 0 \\ -c_1 \; 0 < x \le a \\ -c_2 \; a < x \le h \\ 0 \; elsewhere, \end{cases}$$

We calculate then, the integrals $M_1$and M_3 using this form of ψ and get the following resulting conditions.

$$c_1(a^2 - h^2) - c_2 a^2 = 0 \qquad (7)$$
$$c_1(a^4 - h^4) - c_2 a^4 = -12 \qquad (8)$$

Multiplying (6) by $(a^2 + h^2)$ and then subtracting (7), give us a relation between a and c_2 such that

$$c_2 a^2 h^2 = -12 \qquad (9)$$

We choose a=h/2, which results to $c_2 = -48/h^4$. Replacing the value of c_2 in equation (7) leads to $c_1 = 16/h^4$. Therefore, we define the kernel function ψ as

$$\psi(x) = \begin{cases} \frac{16}{h^4} \; -h \le x \le -h/2 \\ -\frac{48}{h^4} \; -h/2 < x \le 0 \\ \frac{48}{h^4} \; 0 < x \le h/2 \\ \frac{16}{h^4} \; h/2 < x \le h \end{cases}$$

2.3 Numerical Schemes

Using the definition of ψ, we write the approximation of f^3 at a point x as

$$f^3(x) = \int_{x-h}^{x+h} f(x')\,\psi(x-x')dx' + O(h^2) \qquad (10)$$

We divide the [x-h, x +h] on 4 subdomains and we substitute the value of ψ in each subdomain and get

$$f^3(x) \approx \frac{16\,A_\psi - 48\,B_\psi + 48\,C_\psi - 16\,D_\psi}{h^4} \qquad (11)$$

Provided that,

$$A_{\psi} = \int_{x+\frac{h}{2}}^{x+h} f(x')dx' \;\; B_{\psi} = \int_{x}^{x+\frac{h}{2}} f(x')dx'$$
$$C_{\psi} = \int_{x-h/2}^{x} f(x')dx' \;\; D_{\psi} = \int_{x-h}^{x-h/2} f(x')dx'$$

2.3.1 Numerical Scheme with Trapezoidal Rule

Using the trapezoidal rule in the evaluation of the integrals in (11) gives

$$A_{\psi_i} = \frac{h}{4}\,(f(x_i + h) - f(x_i + \frac{h}{2}))$$
$$B_{\psi_i} = \frac{h}{4}(f(x_i + \frac{h}{2}) - f(x_i))$$
$$C_{\psi_i} = \frac{h}{4}(f(x_i) - f(x_i - \frac{h}{2}))$$
$$D_{\psi_i} = \frac{h}{4}(f\left(x_i - \frac{h}{2}\right) - f(x_i - h))$$

Therefore, the numerical approximation of the third order derivative f^3 at a particle x_i is given by

$$f^3(x_i) = \frac{4}{h^3}\left[f(x_i + h) - 2f\left(x_i + \frac{h}{2}\right) + 2\,f\left(x_i - \frac{h}{2}\right) - f(x_i - h)\right] \quad (12)$$

2.3.2 Numerical Scheme Using Simpson's rule

In this subsection we used the Simpson's rule to evaluate each integral of (11) and got a new formula

$$f^3(x_i) = \frac{4}{3h^3}\left[f(x_i + h) + 4f\left(x_i + \frac{3h}{4}\right) - 4\,f\left(x_i - \frac{3h}{4}\right) + 2\,f\left(x_i - \frac{h}{2}\right) - 2\,f\left(x_i + \frac{h}{2}\right) + 12\,f\left(x_i - \frac{h}{4}\right) - 12\,f\left(x_i + \frac{h}{4}\right) - f(x_i - h)\right] \quad (13)$$

This scheme is slightly equivalent to the former one, but requires more data points.

2.3.3 Numerical Scheme Using Random Data

In random distributions, the contributions of the particles are not well balanced which leads to poor accuracy in the approximations.

In order to restore the consistency in the approximation of the third order derivative of a function f, we will extend the use of the CSPM method (Chen et al., 1999) to the third order derivative. However, we will need to know the values of the first derivative and the second derivative at each particle or their approximations using the smoothing kernels aforementioned.

First, we use third order Taylor polynomial in the equation (3) for f about x. Hence,

$$< f^3(x) > = \int_{x-h}^{x+h} f(x')\,\psi(x - x')dx'$$
$$= f(x)M_0 + f'(x)M_1 + \frac{1}{2}f''(x)M_2 + \frac{1}{6}f^3(x)M_3 \quad (14)$$

Therefore,

$$f^3(x) = 6\,\frac{<f^3(x)> - M_0\,f(x) - M_1 f'(x) - \frac{1}{2}M_2 f''(x)}{M_3} \quad (15)$$

We replace the integrals by summations over all the neighbouring particles of x_i inside [x_i-h, x_i +h] such that:

$$< f^3(x_i) > = \sum_{j=0}^{N} f(x_j)\psi(x_i - x_j)\Delta x_j \quad (16)$$
$$M_k = \sum_{j=1}^{N} (x_j - x_i)^k \psi(x_i - x_j)\Delta x_j \quad (17)$$

The index k takes the values from 0 to 3.

3. Numerical Examples

We approximated the third order derivatives of two functions $f(x) = \exp(x)$ and $g(x) = \sin(x)$, using 51 particles. We numbered our numerical schemes in (12), (13) and (15) as 1, 2 and 3 respectively and we measured the mean absolute error (MAE) and the root mean squared error found in the approximations.

In order to use the same distribution for both schemes 1 and 2, we took the smoothing length $h = 2\Delta x$ and $h = 4\Delta x$ respectively. Whereas for the random distribution, we used $h = 0.1$ for more neighbouring particles.

Table 1 presents the MAE and RMSE values in the approximation of third order derivative f, and Table 2 shows the value of the same metrics for the third order derivative of g.

Both schemes 1 and 2 are second order accuracy but the scheme 3 is less accurate due to particle discrepancy.

Table 1. Errors in the approximation of the third order derivative of $f(x) = exp(x)$

Numerical scheme	MAE	RMSE
1	1.72×10^{-4}	1.79×10^{-4}
2	4.59×10^{-4}	4.78×10^{-4}
3	2.41×10^{-2}	3.2×10^{-2}

Table 2. Errors in the approximation of the third order derivative of $g(x) = sin(x)$.

Numerical scheme	MAE	RMSE
1	8.4×10^{-5}	8.52×10^{-5}
2	2.24×10^{-4}	2.27×10^{-4}
3	2.96×10^{-3}	4.86×10^{-3}

4. Conclusions

In this paper, we constructed a new kernel function to approximate the third order derivative of a field function, from which we derived accurate numerical schemes adapted to gridded and random data efficiently. A generalization to multivariate functions is in perspective.

References

1. Lucy, L.B. (1977). A numerical approach to the testing of the fission hypothesis. *The astronomical journal, 82*, 1013-1024.
2. Gingold, R.A., & Monaghan, J.J. (1977). Smoothed particle hydrodynamics: theory and application to non-spherical stars. *Monthly notices of the royal astronomical society, 181*(3), 375-389.
3. Korteweg, D.J., & De Vries, G. (1895). XLI. On the change of form of long waves advancing in a rectangular canal, and on a new type of long stationary waves. *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science, 39*(240), 422-443.
4. Belley, J.M., Belley, P., Colin, F., & Egli, R. (2009). Non-smooth kernels for meshfree methods in fluid dynamics. *Computers & Mathematics with Applications, 58*(6), 1253-1272.
5. Chen, J.K., Beraun, J.E., & Carney, T.C. (1999). A corrective smoothed particle method for boundary value problems in heat conduction. *International Journal for Numerical Methods in Engineering, 46*(2), 231-252.