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A SECOND-ORDER CORRECTED KERNEL FOR SPH METHOD TO ENHANCE CONVERGENCE AND CONSISTENCY

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Summary. The application of smoothed particle hydrodynamics (SPH) encounters challenges related to consistency, stability, and accuracy. Inconsistencies in SPH arise from non-uniform particle distribution and a lack of neighboring particles at the boundary, leading to numerical instability and inaccurate particle approximations. Various methods have been proposed to address these issues. One such framework is the corrected SPH, designed to ensure consistency of the method. In this work, performance of some correction procedures are analysed through gradient calculations of a function. The root mean square error of the gradient approximation is analysed to justify the method's convergence and accuracy.

1 INTRODUCTION

The smoothed particle hydrodynamics (SPH), which is originally proposed to simulate astrophysics problems [1, 2], become more popular for fluid dynamics [3], solid mechanics [4, 5, 6, 7], and fracture mechanics [8, 9, 10] analysis. SPH is a Lagrangian meshfree method, which represent the physical domain using a set of particles. Particle arrangement can be uniformly or arbitrary distributed. Therefore, the SPH is suitable to be implemented for complex geometry, free surface, and deformable boundary.

The SPH have been successfully to be implemented in computational mechanics. However, there are several challenges in the application of SPH, which include consistency, convergence, stability, computational time cost, and real industrial problems [11]. Lack of consistency in SPH arise from incomplete support domain due to the boundary effect and particle disorder. This inconsistency reduces the convergence rate of the method, which leads to low accuracy on the analysis.

Many treatments have been proposed to solve the inconsistency of SPH. The simplest method is the use of ghost particle to overcome the boundary effect. However, there are some limitation in the implementation of ghost particle. Arrangement of ghost particle on a complex geometry is not straightforward, and it can prohibit the surface interaction in the problem with contact. Besides, the ghost particle cannot solve the inconsistency due to particle disorder. Moreover, additional particle number will increase the computational time cost.

Other works without additional ghost particle was proposed. A corrective procedure using Taylor series expansion is implemented to improve the consistency of the SPH [12]. This method yield a good approximation of first derivative and Laplacian of a function, which have been successfully implemented for heat transfer problems. Other works [13, 14, 15] reported a corrected SPH, which the correction term is implemented to ensure the consistency of the SPH up to n-order of completeness. Generally, satisfaction of the zeroth and first order completeness yield a proper accuracy, as well as efficient computational time cost.

In this work, the convergence rate of several correction frameworks is compared using the root mean square error (RMSE) when calculating the gradient of a polynomial function. A kernel and its gradient which satisfy the zeroth, first, and second order completeness is presented. Then, the performance of convergence rate is compared to the common kernel which only satisfy the zeroth and first order consistency. The study shows that the kernel with a second order correction provides a better convergence rate. On the other hand, various form of correction which satisfy the zeroth and first order completeness leads to the same performance compared to each other.

2 SMOOTHED PARTICLE HYDRODYNAMICS

The concept of smoothed particle hydrodynamics (SPH) originates from a kernel approximation of an arbitrary function $f(\boldsymbol{x})$, expressed as

$$f(\boldsymbol{x}) = \int_{\Omega} f(\boldsymbol{x}')W(\boldsymbol{x}-\boldsymbol{x}', h)d\boldsymbol{x}' \,. \tag{1}$$

Variable $W(\boldsymbol{x}-\boldsymbol{x}', h)$ is a smoothing function usually called kernel, which is calculated with the centre at coordinate $\boldsymbol{x}$ and neighbours $\boldsymbol{x}'$ within a domain Ω bounded by the radius κh, as illustrated in Figure 1. The constant κ is a user defined parameter which depend on the type of the smoothing function, and smoothing length h is defined by $h = \eta dx$, which η is scaling factor and dx is particle spacing.

In this work, the cubic spline smoothing function is employed to perform the kernel approximation. By implementing the convolution identity, derivative of a function can be calculated by using

$$f'(\boldsymbol{x}) = \int_{\Omega} f(\boldsymbol{x}')W'(\boldsymbol{x}-\boldsymbol{x}', h)d\boldsymbol{x}' \,. \tag{2}$$

In order to employ a numerical calculation, the exact integral in the kernel approximation must be discretised, which leads to a discrete particle approximation of SPH. The relation can be expressed as

$$f(\boldsymbol{x}_i) \approx \sum_{j\in\mathcal{N}(x_i)} V_j f(\boldsymbol{x}_j) W_j(\boldsymbol{x}_i) \,, \tag{3a}$$

$$\nabla f(\boldsymbol{x}_i) \approx \sum_{j\in\mathcal{N}(x_i)} V_j f(\boldsymbol{x}_j) \nabla W_j(\boldsymbol{x}_i) \,. \tag{3b}$$

Note that $W_j(\boldsymbol{x}_i)$ is the kernel value at particle-i due to interaction with particle-j, and $\mathcal{N}(x_i)$ represents all particles within the support domain of particle-i. Variable V_j is the volume occupied by particle-j, in 2D problems it becomes area A_j, and particle spacing dx_j for 1D problems.. In this study, scope of the work is limited to 1D problems for prove of concept.

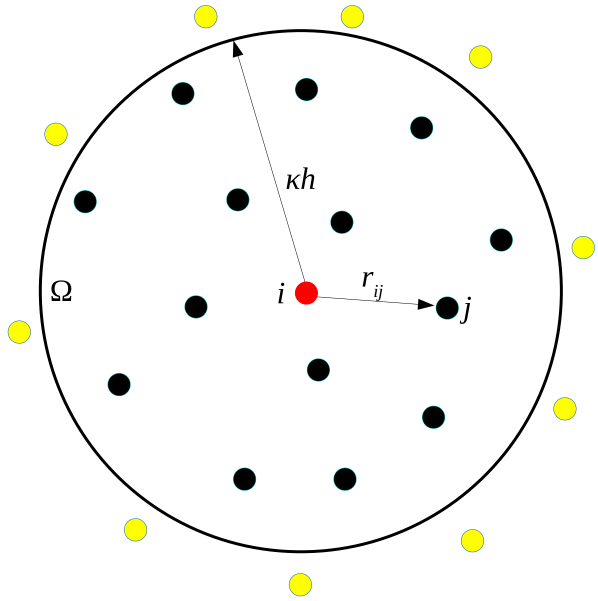

Figure 1: Support domain of particle-i

3 CORRECTED SMOOTHED PARTICLE HYDRODYNAMICS

In handling problems at the boundary or non-uniform spatial discretisation, the original SPH suffers from inconsistency which affect the convergence of the analysis. Correction framework for the kernel and its gradient is more popular to be implemented to overcome the inconsistency. It can improves the consistency due to both boundary effect and non-uniform spatial discretisation. In order to optimise the consistency and computational time efficiency, a correction term which satisfies the zeroth and first order completeness is usually implemented for SPH. In this work, various correction frameworks are analysed to justify the convergence rate given by each correction.

3.1 Corrected kernel gradient

The simplest correction method for the kernel gradient is by directly correcting the kernel gradient, as represented by

$$\widetilde{\nabla} W_j(x_i) = L_i \, \nabla W_j(x_i)\,. \tag{4}$$

Matrix L is derived from the first order completeness condition, which leads to

$$L_i = \left(\sum_{j \in \mathcal{N}(x_i)} dx_j (x_j - x_i) \otimes \nabla W_j(x_i) \right)^{-1} . \tag{5}$$

Approximation of the derivative of a function using Equation 3b and the corrected kernel gradient in Equation 4 still cannot satisfy the zeroth order completeness. Consequently, it can not reproduce gradient of a constant function. In order to solve such problem, the form of the formulation can be modified by employing the zeroth order completeness condition, which leads to

$$\nabla f(x_i) \approx \sum_{j \in \mathcal{N}(x_i)} dx_j \left(f(x_j) - f(x_i) \right) \widetilde{\nabla} W_j(x_i) \,. \tag{6}$$

Approximation of a gradient of a function using Equation 6 provides both zeroth and first order consistency, as well as maintain the simplicity and computational time efficiency of the SPH method.

3.2 Corrected gradient of corrected kernel

The next method to obtain a corrected kernel gradient is by implementing the corrected gradient of corrected kernel [13]. First, the kernel itself is corrected to satisfy the zeroth order completeness, as follows

$$\widetilde{W}_j^0(x_i) = \frac{W_j(x_i)}{\sum_{j \in \mathcal{N}(x_i)} dx_j W_j(x_i)} \,. \tag{7}$$

Then, the gradient of zeroth order corrected kernel is calculated using the derivative rule, which leads to

$$\nabla \widetilde{W}_j^0(x_i) = \frac{\nabla W_j(x_i) - W_j(x_i)\gamma(x_i)}{\sum_{j \in \mathcal{N}(x_i)} dx_j W_j(x_i)} \,, \tag{8}$$

where

$$\gamma(x_i) = \frac{\sum_{j \in \mathcal{N}(x_i)} dx_j \nabla W_j(x_i)}{\sum_{j \in \mathcal{N}(x_i)} dx_j W_j(x_i)} \,. \tag{9}$$

Finally, a correction procedure is applied to the gradient of zeroth order order corrected kernel to obtain a first order completeness condition. Therefore, the corrected gradient of corrected kernel is represented by

$$\widetilde{\nabla} \widetilde{W}_j^0(x_i) = L_i \, \nabla \widetilde{W}_j^0(x_i) \,, \tag{10}$$

where the correction matrix L is calculated using the gradient of zeroth order corrected kernel as follows

$$L_i = \left(\sum_{j \in \mathcal{N}(x_i)} dx_j (x_j - x_i) \otimes \nabla \widetilde{W}_j^0(x_i) \right)^{-1} \,. \tag{11}$$

This correction procedure leads to zeroth and first order completeness, which leads to the gradient reconstruction of a constant and linear function give an exact value up to machine precision. The particle approximation of the SPH method using this correction procedure is given by

$$\nabla f(x_i) \approx \sum_{j \in \mathcal{N}(x_i)} dx_j f(x_j) \widetilde{\nabla} \widetilde{W}_j^0(x_i) \,. \tag{12}$$

Note that using this correction, the form of the formulation is not modified as in Equation 6.

3.3 Gradient of first order corrected kernel

The last correction method to achieve the zeroth and first order completeness is by calculating the gradient of zeroth and first order corrected kernel [3]. First, the kernel is corrected using the term α and β which are derived from the zeroth and first order completeness condition as follows

$$\widetilde{W}_j^1(x_i) = \alpha_i \left(1 + \beta_i \cdot (x_i - x_j)\right) W_j(x_i)\,. \tag{13}$$

where

$$\beta_i = \left(\sum_{j \in \mathcal{N}(x_i)} dx_j (x_i - x_j) \otimes (x_i - x_j) W_j(x_i) \right)^{-1} \sum_{j \in \mathcal{N}(x_i)} dx_j (x_j - x_i) W_j(x_i)\,, \tag{14a}$$

$$\alpha_i = \frac{1}{\sum_{j \in \mathcal{N}(x_i)} dx_j W_j(x_i) \left(1 + \beta_i \cdot (x_i - x_j)\right)}\,. \tag{14b}$$

Then, the kernel gradient $\nabla \widetilde{W}_j^1(x_i)$ is evaluated through multiple chain rule of derivation. This correction procedure leads to a complex formulation, which may affect the computational time cost when implemented for the updated Lagrangian version of SPH. The form of formulation for the particle approximation can be represented as follows

$$\nabla f(x_i) \approx \sum_{j \in \mathcal{N}(x_i)} dx_j f(x_j) \nabla \widetilde{W}_j^1(x_i)\,. \tag{15}$$

3.4 Gradient of second order corrected kernel

In order to achieve a higher convergence rate, kernel with higher order consistency is required. In this work, a second order corrected kernel is derived to achieve the zeroth, first, and second order completeness. To simplify the form of the equation, term M_n is defined up to n-order consistency, which leads to

$$M_{0,i} = \sum_{j \in \mathcal{N}(x_i)} dx_j W_j(x_i)\,, \tag{16a}$$

$$M_{1,i} = \sum_{j \in \mathcal{N}(x_i)} dx_j (x_i - x_j) W_j(x_i)\,, \tag{16b}$$

$$M_{2,i} = \sum_{j \in \mathcal{N}(x_i)} dx_j (x_i - x_j)^2 W_j(x_i)\,, \tag{16c}$$

$$M_{3,i} = \sum_{j \in \mathcal{N}(x_i)} dx_j (x_i - x_j)^3 W_j(x_i)\,. \tag{16d}$$

Then, correction terms which are derived to conduct a correction for the kernel, as follows

$$\gamma_i' = \frac{\left(M_{2,i} - \frac{M_{1,i} M_{3,i}}{M_{2,i}} \right)}{\left(\frac{M_{3,i}^2}{M_{2,i}} - M_{4,i} \right)}\,, \tag{17a}$$

$$\beta_i' = -\frac{M_{1,i} + \gamma_i' M_{3,i}}{M_{2,i}}\,, \tag{17b}$$

$$\alpha_i' = \frac{1}{M_{0,i} + \beta_i M_{1,i} + \gamma_i' M_{2,i}}\,. \tag{17c}$$

Similar with the previous correction method, the second order corrected kernel is calculated through

$$\widetilde{W}_j^2(x_i) = \alpha_i' \left(1 + \beta_i' \cdot (x_i - x_j) + \gamma_i' \cdot (x_i - x_j)^2\right) W_j(x_i)\,. \tag{18}$$

Finally, the gradient of the second order corrected kernel $\nabla\widetilde{W}_j^2(x_i)$ is derived through multiple chain rule. The particle approximation to

$$\nabla f(x_i) \approx \sum_{j\in\mathcal{N}(x_i)} dx_j f(x_j)\nabla\widetilde{W}_j^2(x_i)\,. \tag{19}$$

4 EXAMPLES

In the first assessment, the performance of four types of correction frameworks are compared to calculate the gradient of a polynomial function

$$f(x) = (x-1)^2\ . \tag{20}$$

The support radius is varied with the value of $\kappa = 2.0$ and $\eta = \{0.5,\ 1.0,\ 2.0,\ 3.0\}$ to understand the effect of particle number within the support domain on the convergence of the method. Then, the root mean square error between the SPH approximations and the analytical results are compared, which are presented in Figure 2. Each correction types which satisfy the zeroth and first order completeness give the same performance, which the slope and the value of the RMSE are almost identical for each support radius. On the other hand, the second order corrected kernel which satisfy the zeroth, first, and second order completeness yields exact result up to machine precision. However, the second order correction is not converge when the scaling factor $\eta = 0.5$ is employed. Therefore, the second order correction require a higher particle number to conduct the approximation.

Further assessment of the correction frameworks is conducted by employing a higher order polynomial function. Since each type of first order correction yield a similar result, in this test, only the second order correction $\nabla\widetilde{W}^2$ and one type of first order correction $\nabla\widetilde{W}^1$ are compared. The scaling factor is varied with $\eta = \{1.0,\ 2.0,\ 3.0,\ 4.0,\ 5.0\}$ for $\nabla\widetilde{W}^2$, and $\eta = \{1.0,\ 2.0,\ 3.0\}$ for $\nabla\widetilde{W}^1$. The gradient of a cubic polynomial is approximated with

$$f(x) = (x-1)^3\ . \tag{21}$$

Then, the convergence and accuracy of the method is evaluated, which are presented in Figure 3. The convergence rate of the second order corrected kernel is higher than the first order corrected kernel, which indicated by a higher slope of root mean square error. The optimum choice of the scaling factor for the second order corrected kernel is $\eta = 3$, which provides a higher slope and accuracy compared to others. On the other hand, the support radius will be larger, which increase the computational time cost. Optimum support radius must be justified by balancing the accuracy and computational time.

5 CONCLUSIONS

In this work, performance of four types correction frameworks for SPH method is evaluated. The second order corrected kernel is presented, which yield a higher convergence rate compared to the common used kernel with a zeroth and first order completeness. On the other hand, the

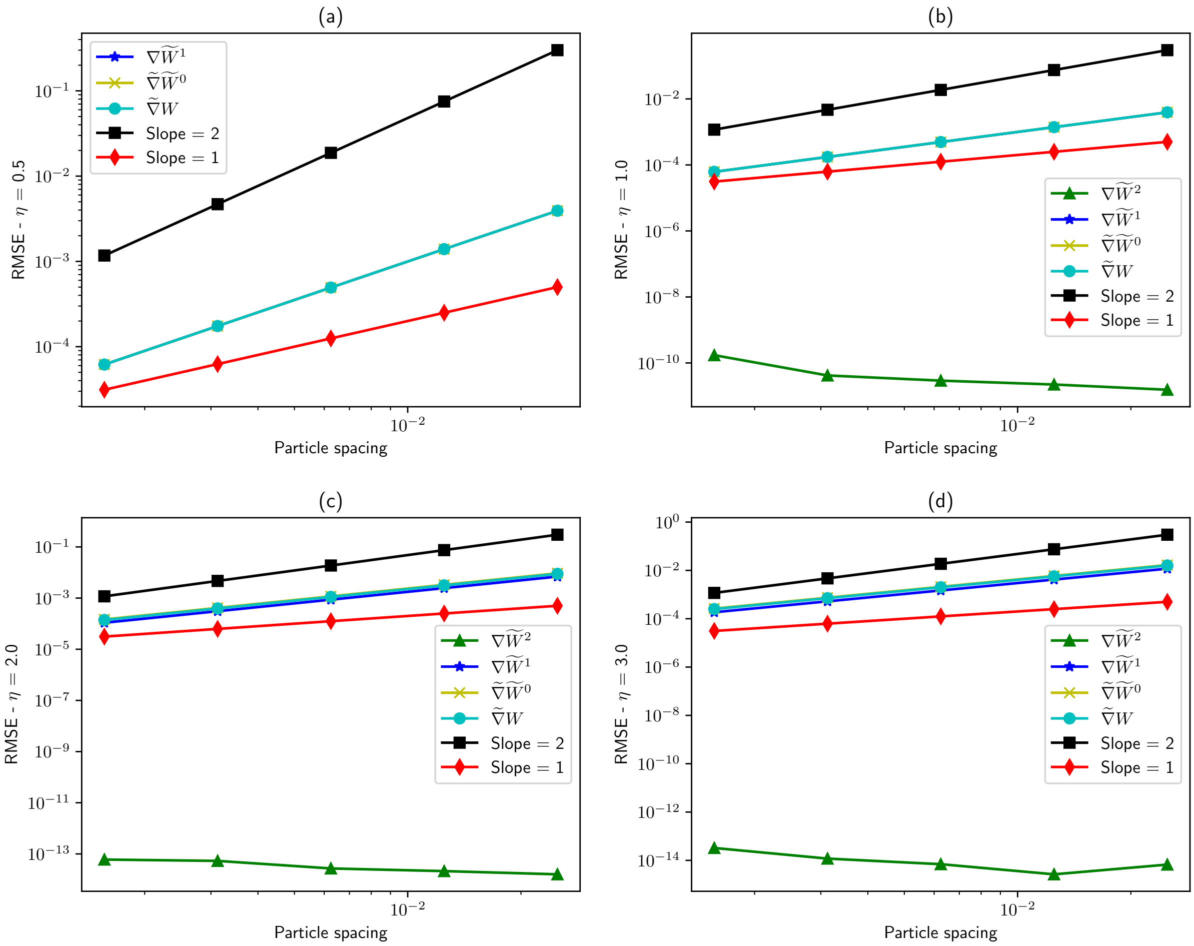

Figure 2: RMSE of various correction frameworks when calculating the gradient of a quadratic polynomial

use of second order corrected kernel require a larger support radius, which can affect the cost efficiency of the method. Therefore, justification to use the first order or second order corrected kernel is based on the balance of accuracy and computational time cost.

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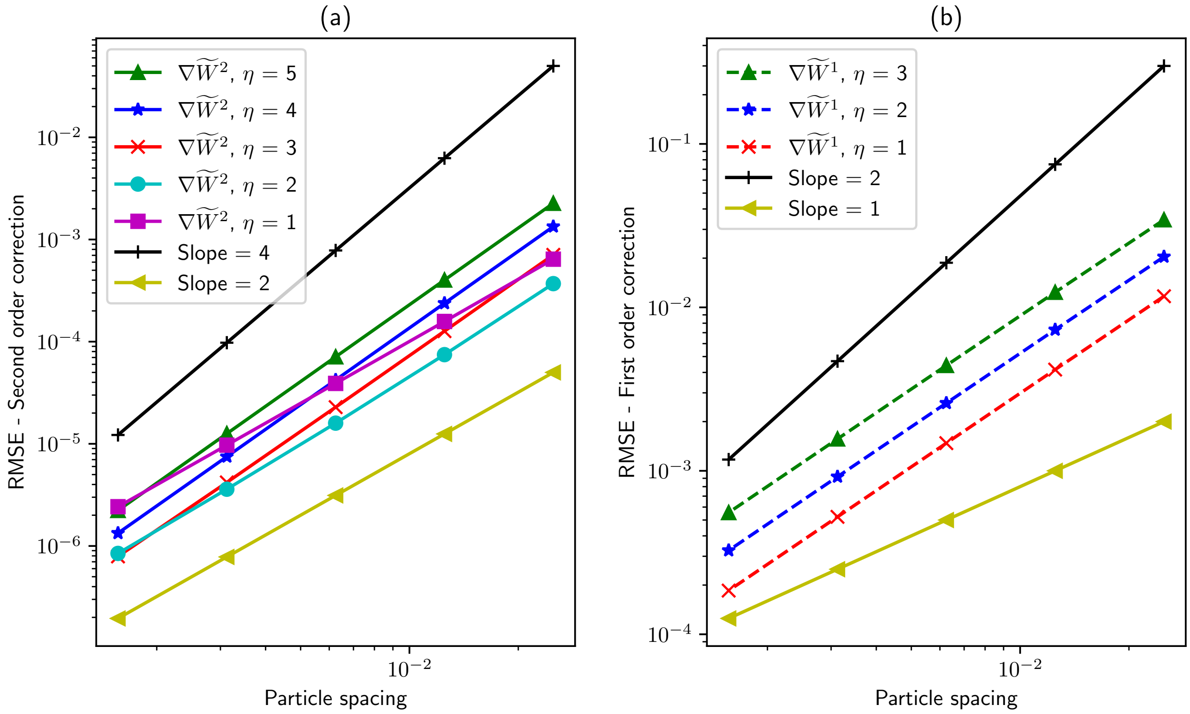

Figure 3: RMSE of the gradient of a cubic polynomial: (a) second order correction, (b) first order correction

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