



# Error estimation in smoothed particle hydrodynamics and a new scheme for second derivatives

R. Fatehi, M.T. Manzari\*

Center of Excellence in Energy Conversion, School of Mechanical Engineering, Sharif University of Technology, Tehran, Iran

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## ABSTRACT

Several schemes for discretization of first and second derivatives are available in Smoothed Particle Hydrodynamics (SPH). Here, four schemes for approximation of the first derivative and three schemes for the second derivative are examined using a theoretical analysis based on Taylor series expansion both for regular and irregular particle distributions. Estimation of terms in the truncation errors shows that only the renormalized (the first-order consistent) scheme has acceptable convergence properties to approximate the first derivative. None of the second derivative schemes has the first-order consistency. Therefore, they converge only when the particle spacing decreases much faster than the smoothing length of the kernel function.

In addition, using a modified renormalization tensor, a new SPH scheme is presented for approximating second derivatives that has the property of first-order consistency. To assess the computational performance of the proposed scheme, it is compared with the best available schemes when applied to a 2D heat equation. The numerical results show at least one order of magnitude improvement in accuracy when the new scheme is used. In addition, the new scheme has higher-order convergence rate on regular particle arrangements even for the case of only four particles in the neighborhood of each particle.

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## 1. Introduction

Smoothed Particle Hydrodynamics (SPH) was first introduced by Gingold and Monaghan [1] and Lucy [2] in 1977 and has emerged as a viable numerical scheme in the context of mesh-free methods. The method has been successfully applied to numerous scientific applications. Like most other numerical schemes, however, the SPH method experiences continual theoretical and technical developments. In particular, various numerical schemes have been devised to approximate the first and second spatial derivative terms which appear in the governing equations. A typical first derivative term is the pressure gradient which plays an important role in the flow equations. Various numerical schemes have been proposed to deal with such terms including both symmetric [3] and non-symmetric [4] forms. On the other hand, second derivatives are manifested typically in flow problems as viscous terms. At least three different types of schemes have been introduced to discretize such second derivatives [5]. The computational performance of various methods have been investigated and reported in [4,6,7,5]. Despite these valuable efforts, it seems that a sound and fairly general theoretical analysis on this issue is yet to be presented.

To have a numerical method of a desired order of accuracy, it is required that each term in the differential equation be discretized with a certain order of accuracy. In the mesh-free methods like SPH, the spatial derivatives are of particular importance. Another property of numerical methods which is related to accuracy is the rate of convergence. The convergence rate of a numerical method depends on the leading error term in its modified equation. Practically, each term in the

\* Corresponding author. Tel.: +98 21 6616 5689; fax: +98 21 6000 0021.

E-mail address: [mtmanzari@sharif.edu](mailto:mtmanzari@sharif.edu) (M.T. Manzari).

governing equation can be discretized using different methods for computation of derivatives which potentially lead to errors of different magnitudes. Therefore, the choice of appropriate approximations for various derivative terms is of crucial importance especially in the SPH method.

In the context of the SPH method, Monaghan and Lattanzio [8] showed that the error of the so-called integral interpolant of SPH is of second order in terms of smoothing length  $h$  and also demonstrated that using a higher-order kernel function can improve the accuracy to  $h^4$ . This argument is however valid only for the continuous interpolation of field functions. In the discrete summations which are used in the computation of derivatives, there are also other sources of errors. In 1987, Mas-Gallic and Raviart [9] proved that a discrete form for  $n$ th derivatives in SPH has an error of order  $h^2 + h^{-n}(\Delta/h)^2$  where  $\Delta$  is the distance between the neighboring particles in one dimension. This means that decreasing the smoothing length  $h$  does not lead to convergence unless the particle spacing  $\Delta$  decreases much faster than  $h$ . The dependency of convergence of the SPH method on both particle spacing  $\Delta$  and smoothing length  $h$  was also confirmed in the work of Ben Moussa and Vila [10]. They also showed that to obtain a convergent first derivative approximation in the SPH method, it is required to satisfy both  $h \rightarrow 0$  and  $\Delta/h^2 \rightarrow 0$  conditions.

Another property associated with the numerical schemes is the notion of consistency which is a requirement for convergence. Unlike grid-based methods, in general, evaluation of consistency is not a straightforward matter for mesh-free methods. For these types of methods, Belytschko et al. [11] have defined the order of consistency as the maximum order of a polynomial which is represented exactly by an approximation technique. Here, it is shown that the order of accuracy of a scheme is highly affected by its order of consistency.

An extra difficulty arises when one deals with moving particles. In such cases, the spacing between particles can continually change and therefore the assumption of equally spaced particle distribution is no longer valid. As a result, the error estimates based on regular arrangement of particles need to be modified. Colagrossi reported that the convergence rate of a method can be as much as one to three orders of magnitude lower than that for ordered particles [12]. Quinlan et al. [13] studied convergence of two SPH schemes for the computation of the first derivative in one dimension. They calculated the derivative of a sinusoidal function using the standard and first-order consistent SPH schemes when particle arrangement is either ordered or disordered. By investigating the numerical errors, they showed that for a uniform distribution, the error of the standard scheme decays as a function of  $h^2$  up to a certain limit which is itself a function of the fraction  $h/\Delta$ . In the case of the first-order consistent scheme on an ordered particle distribution, however, the method retains its second-order convergence. When the particles are disordered, error of the standard scheme can grow as  $h$  is reduced. This highlights the complex behavior of the SPH even for approximation of the first derivative of a fairly simple function.

Concerning the accuracy of second derivative approximations in SPH, there are even fewer works in the literature. Fatehi et al. [14] compared three forms of discretization of the second derivative for a heat-like equation in one dimension. Graham and Hughes [7] numerically studied a SPH scheme in 1D and 2D for random placement of particles and concluded that the method converges only in the case of regular particle arrangement and for special values of  $h/\Delta$ .

In the present paper, a mathematical framework is presented to compare the truncation errors and convergence properties of general SPH schemes for discretization of both first and second spatial derivatives. Four schemes for the first derivative and three schemes for the second derivative are considered. The schemes are briefly presented in the following section. Next, the truncation error associated with each scheme is found using a Taylor series expansion. In Section 4, the order of magnitude of different terms in the truncation errors are estimated both for regular and irregular particle arrangements. Finally, a new scheme for approximation of the second derivative is introduced in Section 5 and its performance is assessed by solving a 2D heat equation in Section 6.

## 2. SPH approximation of derivatives

SPH is a Lagrangian particle-based method in which each computational point is a part of a substance and is called particle. The SPH method is built on the notion of interpolation. For an arbitrary field function  $u$  the interpolated value  $\langle u \rangle$  in terms of the values at neighboring particles  $u_j$  is found from

$$\langle u(\mathbf{r}) \rangle = \sum_j \omega_j u_j W(\mathbf{r} - \mathbf{r}_j, h), \quad (1)$$

where  $\omega_j$  is the weight or the volume of neighboring particle  $j$  and  $W$  represents the smoothing or kernel function which is a smoothed version of the Dirac delta function and is positive for  $|\mathbf{r} - \mathbf{r}_j| < h$  with a compact support of radius  $h$  [1].

Several techniques have been used in SPH to discretize the first and the second spatial derivatives. In this section, a number of frequently used schemes are summarized.

### 2.1. First derivative

The first derivative of field function  $u$  can be approximated using either of the following schemes.

**Scheme F1.** Standard scheme as first introduced by Monaghan [1]:

$$\langle \nabla u \rangle_i = \sum_j \omega_j u_j \nabla_i W_{ij}, \quad (2)$$

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