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A New Corrective Scheme for SPH

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A new corrective scheme for Smoothed Particle Hydrodynamics (SPH) is introduced which greatly improves its accuracy, particularly in regions of particle deficiency or when particles are irregularly distributed. The scheme is based on the Taylor expansion of the SPH kernel estimates. The corrective equations are derived up to the second derivative in an arbitrary number of dimensions. Test applications for the new scheme include the interpolation of functions and the numerical solution of the heat equation in one and two dimensions.

Keywords: SPH, particle deficiency, particle inconsistency, corrective scheme

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I. INTRODUCTION

Smoothed Particle Hydrodynamics (SPH) is a technique used for the solution of partial differential equations (PDEs) first formulated by Lucy [1] and Gingold and Monaghan [2]. Although its early application was in the fields of astrophysics and cosmology (see [3, 4] for a review of the early development of SPH), it is now extensively used in a wide range of applications. For example, several non-hydrodynamic PDEs are investigated within the technique of Smoothed Particle Interpolation (SPI) in [5], while the Maxwell curl equations are solved using the technique of Smoothed Particle ElectroMagnetics (SPEM) in [6]. A number of other applications, primarily in the engineering field, are discussed in [7].

SPH is a mesh-free particle method particularly effective at solving problems involving large deformation, where traditional grid-based techniques run into issues. As a particle method, SPH does not solve differential equations by discretising spacetime on a grid, as done in finite difference methods. Instead, the space is discretised into particles which are free to move. The particles are given volume and assigned values of the observable properties of the problem domain. The value of a property at an arbitrary point in the domain is calculated as a weighted average over the neighbouring particles within a certain radius of that point.

One advantage of SPH over traditional grid-based techniques is that the computation can be efficiently distributed over the problem domain. The equivalent of a finer mesh can be created in areas of greater change by placing more particles there. For fluids, the movement property is especially valuable in that it avoids entangled meshes and the computational cost of remeshing found in finite difference methods. Irregularly shaped regions are also handled far more easily.

SPH is, however, not without its issues [8]. The imposition of non-trivial boundary conditions is a challenge and the problem of particle deficiency near the boundary of the problem domain needs to be overcome. The particle approximation of SPH may also lead to inconsistency, particularly when the particles are irregularly distributed.

Several algorithms have been proposed in the literature to diminish the effect of these issues: including ghost particles [8, 9] and scalar corrective factors [8, 10–12], the inclusion of boundary terms in expressions for derivatives [13], the construction of reproducing kernel functions [7, 14, 15] and by correcting SPH discretisations using higher-order Taylor series approximations [16–20]. Several authors have investigated the second derivative. Most notably, Brookshaw [21] introduced a form of the Laplacian based on gradients, while Schwaiger [22] introduced a correction term to this result based on the Corrective Smoothed Particle Method (CSPM) [16].

In this paper we investigate in some detail the issues of particle deficiency, boundary effects, and inconsistency arising from irregular particle spacing. We follow most closely the approach of [16] leading to a new corrective scheme that outperforms that of [16] in the case of first and higher order derivatives. In contrast to the approach taken in [18–20] and in the Modified Smoothed Particle Hydrodynamics (MSPH) technique [17], our scheme sequentially solves for the corrections to higher derivatives, which is less computationally expensive.

The paper is organised as follows. The standard formulation of SPH is discussed in Section II. In Section III we introduce the problems of particle deficiency and inconsistency arising from irregular particle spacing by applying SPH to function interpolation. The new corrective scheme is then introduced for one spatial dimension in Section IV and test cases in 1D are described in Section V. Corrections in higher dimensions are derived in Section VI and test cases in 2D are discussed in Section VII. The article closes with discussion and conclusions in Section VIII.

II. STANDARD FORMALISM OF SPH

As implied by the name, the idea behind SPH is first to smooth over a region (the smoothing approximation) and then to discretise the region into particles (the particle approximation). In this section, we will introduce the one-dimensional case in detail. The results are easily generalized to higher dimensions.

A. Smoothing Approximation

Given a function $f(x)$, we can write it as the integral over a delta function:

$$f(x) = \int_{-\infty}^{+\infty} \mathrm{d}x' \, f(x')\delta(x - x'). \tag{1}$$

Replacing the delta function by a "kernel" function $\frac{1}{h} w\left(\frac{x-x'}{h}\right)$, we obtain the "smoothing approximation" to $f(x)$ given by

$$\langle f(x) \rangle = \int_{-\infty}^{+\infty} \mathrm{d}x' \, f(x') \left[\frac{1}{h} w\left(\frac{x - x'}{h}\right)\right]. \tag{2}$$

The parameter h is called the smoothing length because it is a measure of the size of the smoothing region. In Equation (2), the limits of integration extend to infinity. However, it is often the case that the problem domain over which $f(x)$ is defined is a finite region. In this case, the limits of integration have to be replaced by the limits of the problem domain. We require the kernel function to be smooth so that it can be Taylor expanded.

The smoothing approximation introduces an error $\langle \epsilon \rangle$ such that

$$\langle f(x) \rangle = f(x) + \langle \epsilon \rangle \,. \tag{3}$$

We will now calculate this error. Using the substitution $u = x - x'$ in Equation (2) and replacing $f(x')$ by its Taylor series gives:

$$\begin{aligned} \langle f(x) \rangle &= \int_{-\infty}^{+\infty} \mathrm{d}u \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} f^{(n)}(x) \; u^n \left[\frac{1}{h} w\left(\frac{u}{h}\right)\right] \\ &= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} f^{(n)}(x) \int_{-\infty}^{+\infty} \mathrm{d}u \, u^n \left[\frac{1}{h} w\left(\frac{u}{h}\right)\right]. \end{aligned} \tag{4}$$

Now use the substitution $v = u/h$ in the integral to obtain

$$\langle f(x) \rangle = M_0 f(x) - hM_1 f'(x) + h^2 \frac{M_2}{2} f''(x) - \cdots \,, \tag{5}$$

where we have defined the moments of the kernel M_n to be

$$M_n \equiv \int_{-\infty}^{+\infty} \mathrm{d}v \, v^n \; w(v). \tag{6}$$

These moments are constants of the kernel and are independent of h. Since we require $\langle f(x) \rangle$ to approach $f(x)$ as $h \to 0$, we must have $M_0 = 1$. This amounts to a normalization condition on the kernel. To get an $O(h^2)$ approximation, we require $M_1 = 0$. This is satisfied by kernels that are even functions. It is impossible to find a non-negative kernel that also has $M_2 = 0$. The best we can do is to choose a kernel with a small second moment.

Now consider the smoothing approximation for derivatives:

$$\begin{aligned} \langle f'(x) \rangle &= \int_{-\infty}^{+\infty} \mathrm{d}x' \, f'(x') \left[\frac{1}{h} w\left(\frac{x - x'}{h}\right)\right] \\ &= f(x') \left[\frac{1}{h} w\left(\frac{x - x'}{h}\right)\right]\Bigg|_{\mathrm{d}\Omega} - \int_{-\infty}^{+\infty} \mathrm{d}x' \, f(x') \frac{d}{dx'} \left[\frac{1}{h} w\left(\frac{x - x'}{h}\right)\right] \\ &= f(x') \left[\frac{1}{h} w\left(\frac{x - x'}{h}\right)\right]\Bigg|_{\mathrm{d}\Omega} + \int_{-\infty}^{+\infty} \mathrm{d}x' \, f(x') \left[\frac{1}{h^2} w'\left(\frac{x - x'}{h}\right)\right], \end{aligned} \tag{7}$$

where the derivative of the kernel function is with respect to its argument and $\mathrm{d}\Omega$ represents the boundary of the problem domain. If the problem domain is infinite, then the boundary term vanishes because the kernel goes to zero at infinity. If the problem domain is finite, then the boundary term need not vanish. Nevertheless, in the simplest formulation of SPH (which we will refer to as standard SPH), the boundary term is always discarded. We will return to this point in Section III.

The result for the derivative is quite remarkable: the derivative acts only on the kernel, so it is not necessary to know anything about the derivative of the function in order to approximate it. We can expand $\langle f'(x)\rangle$ as a power series in h using a similar procedure as for $\langle f(x)\rangle$:

$$\langle f'(x)\rangle = \frac{1}{h}M_0' f(x) - M_1' f'(x) + h\frac{M_2'}{2} f''(x) - \cdots \,, \tag{8}$$

where

$$M_n' \equiv \int_{-\infty}^{+\infty} \mathrm{d}v \, v^n \; w'(v). \tag{9}$$

The conditions $M_0 = 1$ and $M_1 = 0$ automatically ensure that $M_0' = 0$, $M_1' = -1$ and $M_2' = 0$, so that the smoothing approximation of $f'(x)$ is again of second order.

The smoothing approximation for any order of derivative can be calculated in this way, provided the kernel has continuous derivatives of that order. Therefore we define:

$$\left\langle f^{(n)}(x)\right\rangle \equiv \int_{-\infty}^{+\infty} \mathrm{d}x \, f(x') \left[\frac{1}{h^{n+1}} w^{(n)}\left(\frac{x-x'}{h}\right)\right], \tag{10}$$

which leads to the power series expansion:

$$h^n \left\langle f^{(n)}(x)\right\rangle = M_0^{(n)} \; f(x) - hM_1^{(n)} \; f'(x) + h^2 \frac{M_2^{(n)}}{2} f''(x) - \cdots \,, \tag{11}$$

where

$$M_k^{(n)} \equiv \int_{-\infty}^{+\infty} \mathrm{d}v \, v^k w^{(n)}(v). \tag{12}$$

Note that the boundary terms have been implicitly discarded in this definition of the smoothing approximation.

B. Particle Approximation

Having described the smoothing approximation in the previous subsection we turn our attention now to the particle approximation. A function $f(x)$ consists of an infinite number of points. Since we cannot store all of these points on a computer, we have to make do with a finite subset of them. We label these points from 1 to M and let x_i and $f_i = f(x_i)$ be respectively the coordinate and function value of point i. Since, in general, we will allow x_i to change over time, we refer to these M points as particles.

We define the particle approximation of the function $f(x)$ to be

$$[\![f(x)]\!] \equiv \frac{1}{n(x)} \sum_{i=1}^{M} f_i \left[\frac{1}{h} w\left(\frac{x-x_i}{h}\right)\right], \tag{13}$$

where $n(x)$ is the number density of particles around x. This is simply the integral in Equation (2) evaluated numerically using the midpoint rule at each particle.

Usually M is a large number so this sum is expensive to compute. Luckily, it is possible to choose kernels that decay rapidly for $|x - x'| > h$. When this is the case, particles that are far away from x have a negligible contribution to the sum and can be ignored. Thus, the number of particles included in the sum is reduced from M to a much smaller number N which is faster to compute. We will refer to the volume around x outside of which particles can be ignored as the "effective" compact support domain. It is important that we choose this volume large enough that the particles outside are really negligible compared to the approximation errors of the scheme. The density $n(x)$ is calculated as the number of particles contained in the effective compact support volume centred at x divided by the volume.

The particle approximations for the derivatives are similarly defined by

$$[\![f'(x)]\!] \equiv \frac{1}{n(x)} \sum_{i=1}^{M} f_i \left[\frac{1}{h^2} w' \left(\frac{x - x_i}{h} \right) \right], \tag{14}$$

and

$$[\![f''(x)]\!] \equiv \frac{1}{n(x)} \sum_{i=1}^{M} f_i \left[\frac{1}{h^3} w'' \left(\frac{x - x_i}{h} \right) \right]. \tag{15}$$

For the special case of uniformly distributed particles, the density is $n = 1/\Delta x$ (where Δx is the constant particle spacing) and the particle approximation for $f(x)$ becomes

$$[\![f(x)]\!] = \Delta x \sum_{i=1}^{N} f_i \left[\frac{1}{h} w \left(\frac{x - x_i}{h} \right) \right]. \tag{16}$$

In general, the error in the particle approximation has a complicated dependence on both h and Δx [23]. For uniformly spaced particles and the Gaussian kernel (discussed in the next subsection), it can be shown that [5],

$$[\![f(x)]\!] = \langle f(x) \rangle + O\left(\left(\frac{\Delta x}{h} \right)^2 \right). \tag{17}$$

C. Gaussian Kernel Function

There are many suitable kernels for SPH. The simplest (and the one that we will use throughout this article) is the Gaussian kernel:

$$w(v) = \alpha e^{-v^2}, \tag{18}$$

where α is a normalization factor. The Gaussian is an analytic function and can therefore be used for smoothing approximations at any derivative order. It is also easy to calculate its moments $M_k^{(n)}$. The normalization condition $M_0 = 1$ in one dimension leads to $\alpha = 1/\sqrt{\pi}$, while the even nature of the Gaussian ensures that $M_1 = 0$ so that the smoothing approximation is second order accurate. By evaluating M_2, we find that

$$\langle f(x) \rangle = f(x) + \frac{h^2}{4} f''(x) + \cdots. \tag{19}$$

The Gaussian also satisfies our requirement that the kernel decays rapidly for $|x - x'| > h$. We choose the effective compact support volume to be $|v| \leq 5$ so that particles with $v_i > 5$ are neglected.

III. SPH FUNCTION INTERPOLATION AND PARTICLE INCONSISTENCY

The simplest application of SPH is that of function interpolation: Given a continuous function evaluated at a discrete number of points, the interpolation problem is to determine the value of the function at an arbitrary point. This is exactly the problem solved by the smoothing and particle approximations of SPH. In fact, the derivative formula of Equation (10) allows SPH to solve the more general problem of finding the n-th derivative of the function at any point. Note that the SPH interpolation is not exact at the interpolation points because in general $[\![f(x_i)]\!] \neq f(x_i)$.

In this study we will test SPH as an interpolation scheme for the function $f(x) = e^{-x^2}$. We also looked at other functions such as polynomials and trigonometric functions and found similar results. The tests were carried out using a Gaussian kernel with smoothing length $h = 0.1$. We worked on the finite domain interval $[-1, 1]$.

We investigated two ways of positioning the particles: uniformly spaced and randomly distributed. In the case of uniform spacing, we found that at least 20 particles are needed inside the effective compact support volume to get good approximations of the function and derivatives. Therefore, we chose $\Delta x = h/2 = 0.05$. For the random case,

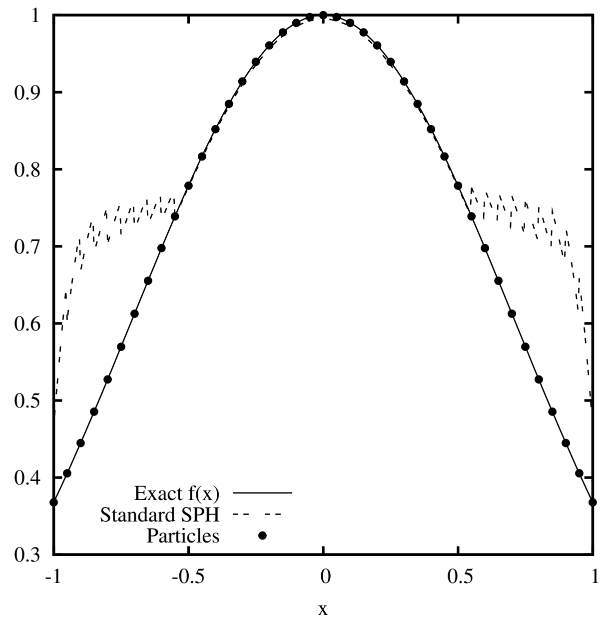

FIG. 1. The results of the standard SPH interpolation $[\![f(x)]\!]$ for $f(x) = e^{-x^2}$ with uniformly spaced particles. The particles are represented by dots in the plot. The particle spacing is $\Delta x = 0.05$ and the smoothing length is $h = 0.1$. Notice that the standard interpolation fails when the effective compact support region overlaps with the boundary.

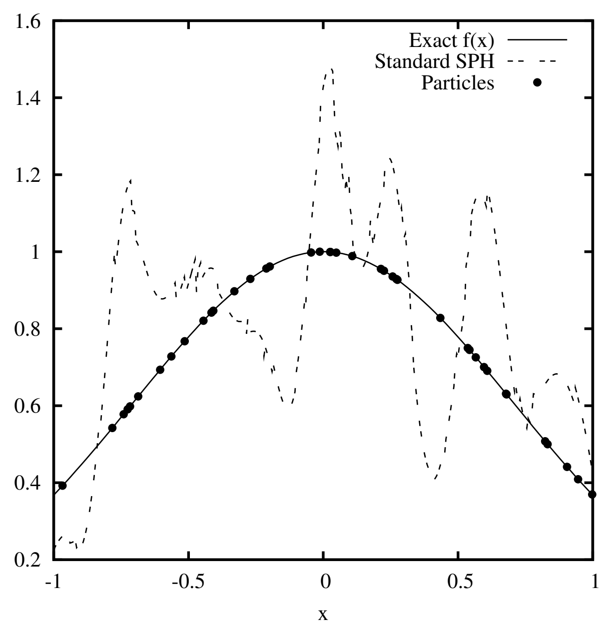

FIG. 2. The results of the standard SPH interpolation $[\![f(x)]\!]$ for $f(x) = e^{-x^2}$ with randomly distributed particles. The particles are represented by dots in the plot. There are $N = 2/\Delta x = 40$ particles and the smoothing length is $h = 0.1$. Notice that the standard interpolation is highly inaccurate everywhere.

the number of particles was set to $N = 2/\Delta x = 40$ and they were distributed randomly in the domain.

Figure 1 shows the interpolation for uniformly spaced particles. The function is well-approximated in the central portion of the interval but the interpolation fails near the boundary. The reason for this failure is that the smoothing approximations introduced in Section II were derived assuming that the problem domain extends to infinity where the kernel is zero. When the domain is finite and we are near the boundary, the effective compact support region extends past the boundary. Since there are no particles beyond the boundary, the limits of the kernel moment integrals are effectively truncated. This means that the $M_0 = 1$ and $M_1 = 0$ conditions are violated and as such the smoothing approximation is no longer $O(h^2)$ accurate. The problem of having an insufficient number of particles in the effective compact support region is called particle deficiency [8].

Figure 2 shows the interpolation for randomly distributed particles. In this case the approximation is inaccurate everywhere. The reason is that if we compute the kernel moments using the particle approximation, the $M_0 = 1$ and $M_1 = 0$ conditions will always be somewhat violated due to the randomness. This again causes the approximation to be worse than $O(h^2)$.

We have only shown the interpolation of $f(x)$ in Figure 1 and Figure 2 but the derivative interpolations have the same characteristics. This problem has been investigated by several authors and has led to a number of proposed correction methods [8, 9, 13, 14, 16–20]. In the next section we present a new corrective scheme, similar to the ones developed in [16–20] but with some important differences.

IV. NEW SPH CORRECTIONS IN 1D

Consider the power series expansion of Equation (5). We have chosen the kernel such that $M_0 = 1$ and $M_1 = 0$ when the limits of integration extend to infinity. However, as demonstrated in the previous section, we may effectively have $M_0 \neq 1$ and $M_1 \neq 0$ for various reasons including particle deficiency and irregularly distributed particles. Nevertheless we can still determine $f(x)$ by rearranging Equation (5):

$$\frac{\langle f(x)\rangle}{M_0} = f(x) - h\frac{M_1}{M_0}f'(x) + h^2\frac{M_2}{2M_0}f''(x) - \cdots. \tag{20}$$

Since $M_1 \neq 0$ near the boundary, this gives us an $O(h)$ approximation for $f(x)$. This is not as good as the $O(h^2)$ approximation we get away from the boundary, but it is certainly better than no correction at all. We will denote the corrected approximation by,

$$\langle f(x)\rangle_C \equiv \frac{\langle f(x)\rangle}{M_0} = f(x) - h\frac{M_1}{M_0}f'(x) + h^2\frac{M_2}{2M_0}f''(x) + O(h^3). \tag{21}$$

We next proceed to a corrected expression for $f'(x)$ starting from the power series expansion of $f'(x)$ in Equation (8). This expansion involves $f(x)$, which we do not know except at the particle positions. However, we can use $\langle f(x)\rangle_C$ to determine $f(x)$:

$$\begin{aligned}\langle f'(x)\rangle &= \frac{1}{h}M_0'\left[\langle f(x)\rangle_C + h\frac{M_1}{M_0}f'(x) - \frac{h^2}{2}\frac{M_2}{M_0}f''(x) + O(h^3)\right] - M_1'f'(x) + h\frac{M_2'}{2}f''(x) + O(h^2)\\ &= \frac{1}{h}M_0'\langle f(x)\rangle_C + f'(x)\left[\frac{M_0'M_1}{M_0} - M_1'\right] + \frac{h}{2}f''(x)\left[M_2' - \frac{M_0'M_2}{M_0}\right] + O(h^2).\end{aligned} \tag{22}$$

Solving for $f'(x)$ gives,

$$\langle f'(x)\rangle_C \equiv \frac{\langle f'(x)\rangle M_0 - \frac{1}{h}M_0M_0'\langle f(x)\rangle_C}{M_0'M_1 - M_0M_1'} \tag{23}$$

$$= f'(x) + \frac{h}{2}f''(x)\frac{M_0M_2' - M_0'M_2}{M_0'M_1 - M_0M_1'} + O(h^2), \tag{24}$$

which is once again an $O(h)$ approximation. Note that this works only when $M_0'M_1 - M_0M_1'$ is non-zero. Otherwise, there is no choice but to use the original approximation.

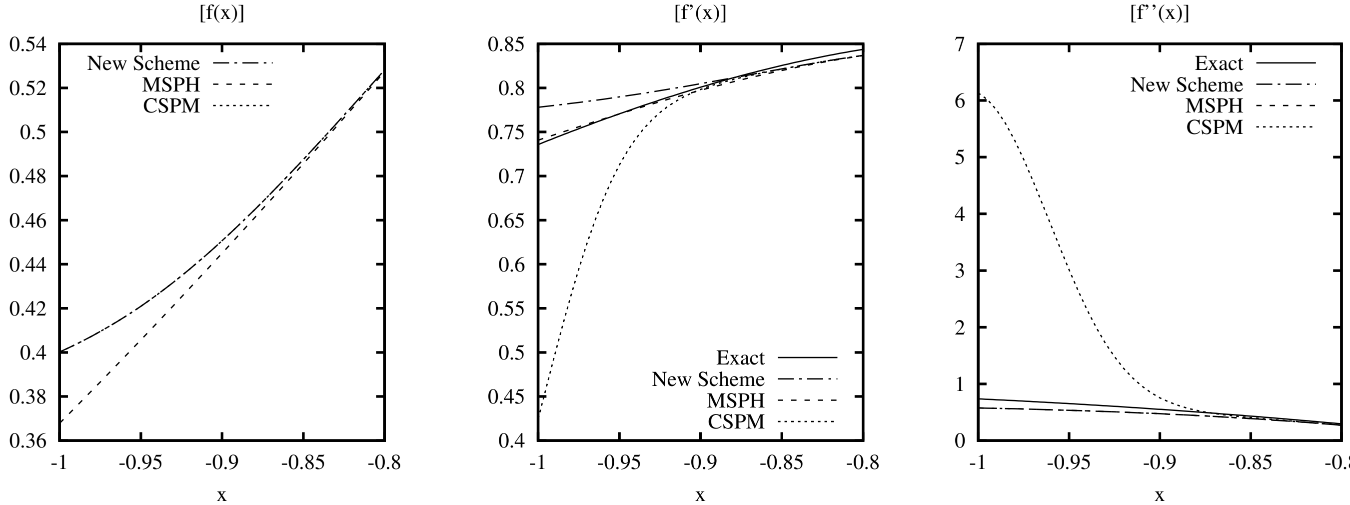

FIG. 3. Uniformly spaced particle interpolations of $f(x) = e^{-x^2}$ and its derivatives produced by the new corrective scheme compared to the exact value, CSPM and MSPH. The exact function was not plotted for $f(x)$ because it almost coincides with the MSPH result. The new scheme and CSPM results coincide for $f(x)$. The new scheme and MSPH results coincide for $f''(x)$. The particles are uniformly spaced with separation $\Delta x = 0.05$ and the smoothing length is $h = 0.1$.

A similar procedure can be followed to find the corrected approximations for higher order derivatives. For example, the correction for the second derivative is,

$$\begin{aligned}\langle f''(x)\rangle_C &= \frac{2\left[h^2 M_0 \langle f''(x)\rangle - M_0 M_0'' \langle f(x)\rangle_C - h\left(M_1 M_0'' - M_0 M_1''\right)\langle f'(x)\rangle_C\right]}{h^2\left[M_0 M_2'' - M_2 M_0'' - \left(M_1 M_0'' - M_1'' M_0\right)\left(M_2' M_0 - M_0' M_2\right)\left(M_0' M_1 - M_1' M_0\right)^{-1}\right]} \qquad (25)\\ &= f''(x) + O(h). \qquad (26)\end{aligned}$$

V. TEST STUDIES IN 1D

A. Interpolation

To illustrate the corrections introduced in the previous section, we return to the interpolation problem discussed in Section III. In Figure 3 we compare $f(x)$ and its derivatives to their uniformly spaced particle interpolations in the CSPM and MSPH schemes [16, 17], and the newly developed scheme of Section IV. The interpolation is greatly improved near the boundaries compared to standard SPH for all these schemes. The new scheme is equivalent to CSPM for $f(x)$ but is more accurate for $f'(x)$ and $f''(x)$. The MSPH scheme is more accurate than the new scheme for $f(x)$ and $f'(x)$ but is equivalent for $f''(x)$. The corrections also vastly improve interpolation for randomly spaced particles, as shown in Figure 4.

Figure 5 shows how the interpolation error depends on the smoothing length h. We quantify the interpolation error using a maximum error metric defined by

$$L_\infty = \max_i \left|[\![f(x_i)]\!] - f_{\text{exact}}(x_i)\right|, \qquad (27)$$

where the index runs over a set of sampling points. The sampling points were uniformly separated with spacing $\Delta x/10$. The results confirm the $O(h)$ error term in our new scheme. The MSPH error is seen to be $O(h^3)$ for $f(x)$, $O(h^2)$ for $f'(x)$ and $O(h)$ for $f''(x)$. The CSPM error is $O(h)$ for $f(x)$ and $O(1)$ for the derivatives. The standard SPH error is always $O(1)$.

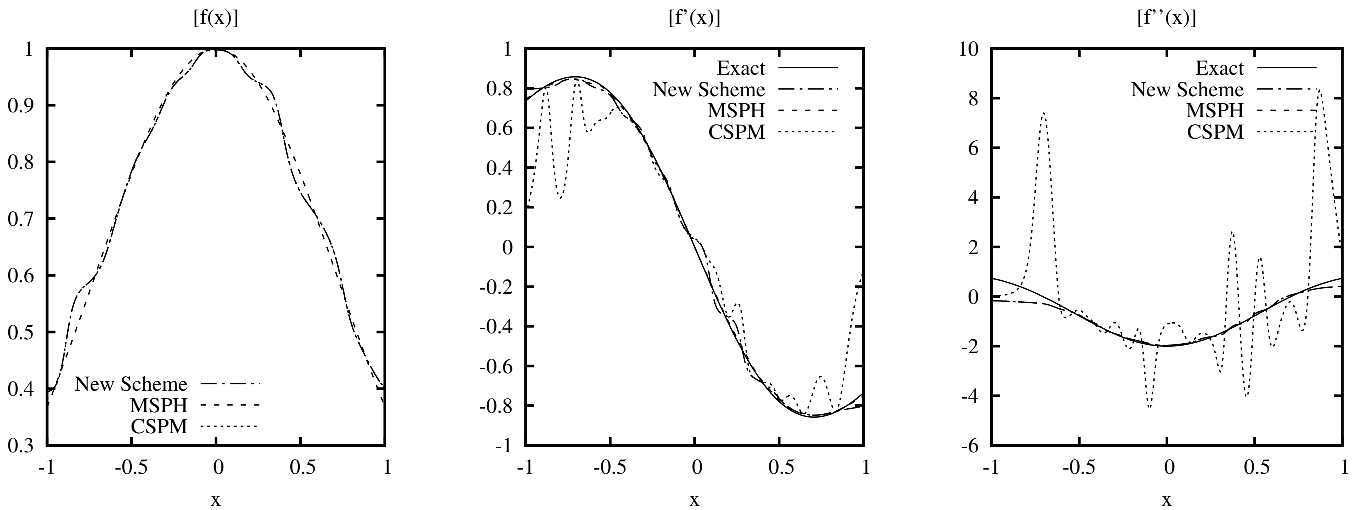

FIG. 4. Randomly distributed particle interpolations of $f(x) = e^{-x^2}$ and its derivatives produced by the new corrective scheme compared to the exact value, CSPM and MSPH. The exact function was not plotted for $f(x)$ because it almost coincides with the MSPH result. The new scheme and CSPM results coincide for $f(x)$. The new scheme and MSPH results coincide for $f''(x)$. There are $N = 2/\Delta x = 40$ randomly distributed particles and the smoothing length is $h = 0.1$.

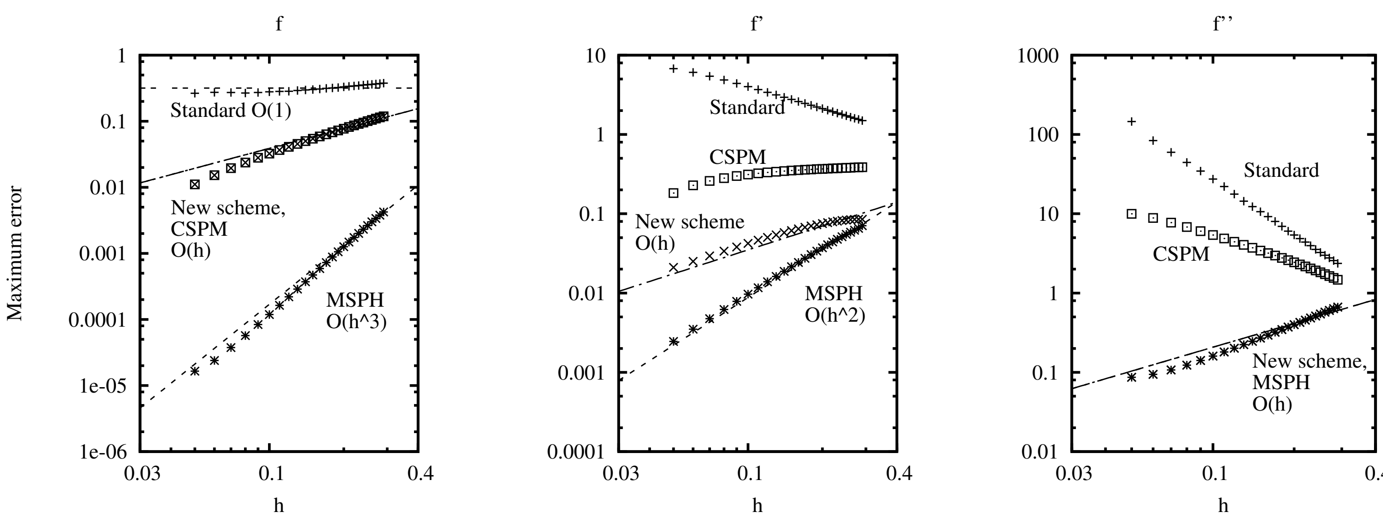

FIG. 5. The L_∞ maximum error of the various interpolation schemes as a function of the smoothing length h. The plots show the interpolation errors for $f(x)$, $f'(x)$ and $f''(x)$ respectively. Fitted $O(1)$, $O(h)$, $O(h^2)$ and $O(h^3)$ curves are indicated. The particles were uniformly spaced with separation $\Delta x = 0.05$ and the test function $f(x) = e^{-x^2}$ was used.

B. Solution of the 1D Heat Equation

As a simple application of the new scheme, we set out in this section to solve the heat equation in one spatial dimension:

$$\frac{\partial u(x,t)}{\partial t} = \kappa \frac{\partial^2 u(x,t)}{\partial x^2}, \tag{28}$$

where κ is a constant. Physically this represents the evolution of the temperature u along a uniform bar with thermal diffusivity κ. We assume the bar has a finite length ($-1 \leq x \leq 1$), thermal diffusivity $\kappa = 0.01$, a sinusoidal initial condition $u(x,0) = \sin(3\pi x)$, and Dirichlet boundary conditions $u(-1,t) = u(1,t) = 0$. In this case, an analytic solution is known:

$$u_{\text{exact}}(x,t) = \sin(3\pi x)\, e^{-9\pi^2 \kappa t}.$$

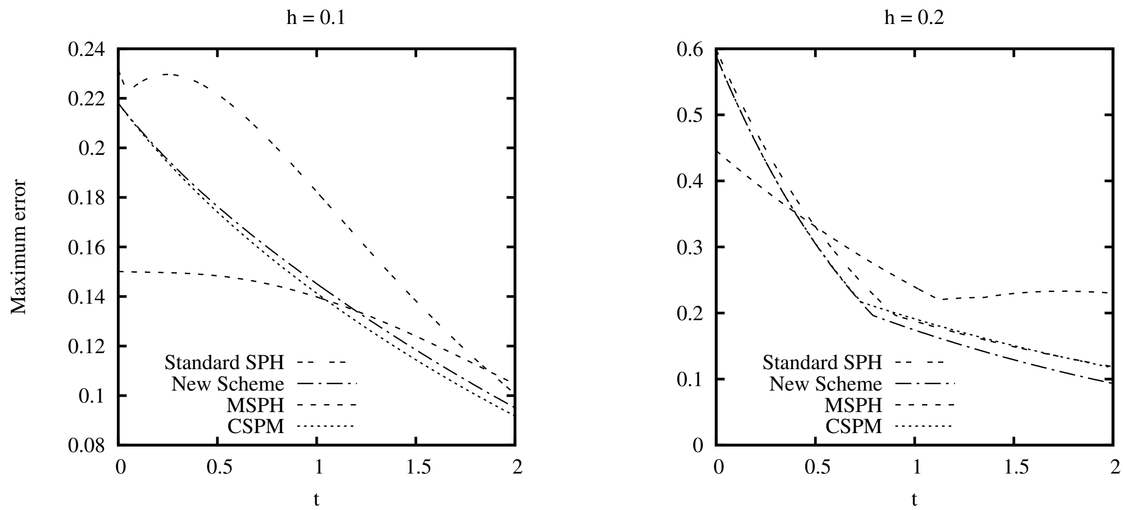

FIG. 6. The L_∞ maximum error as a function of t for the heat equation problem described in Section V B. Results are shown for standard SPH, CSPM, MSPH, and the new corrective scheme. Smoothing length $h = 0.1$ was used for the left plot and $h = 0.2$ was used for the right plot. The set of particle positions were used as the sampling points to compute L_∞.

SPH allows us to express spatial derivatives in terms of particles, but there is no such result for temporal derivatives. In this study, we use a forward difference approximation for the time derivative and the particle approximation for the second spatial derivative:

$$u(x_i, t + \Delta t) = u(x_i, t) + \kappa \Delta t \, [\![u''(x_i, t)]\!] + O((\Delta t)^2) + O(h^2). \tag{29}$$

Equation (29) represents an explicit scheme. Given $u(x, 0)$, it can be applied n times to obtain $u(x, n\Delta t)$. We used $\Delta t = 0.01$ and uniformly spaced, static particles with spacing $\Delta x = 0.05$. We tested two choices for the smoothing length: $h = 0.1$ and $h = 0.2$.

The Dirichlet boundary conditions are imposed by adding ghost particles outside the boundary on either side. These ghost particles are used only as a means to impose the boundary conditions, not as a way to avoid particle deficiency. Since the boundary conditions only involve $u(x, t)$, the ghost particles are ignored when computing derivatives.

Figure 6 shows the L_∞ error obtained for the different SPH schemes. For $h = 0.1$, the error is improved for all corrective schemes compared to standard SPH. The error for the new scheme and CSPM are comparable. MSPH has a lower error due to its more accurate interpolation of $[\![u(x_i, t)]\!]$ when computing L_∞. The actual particle values are equal for MSPH and the new scheme because the second derivative interpolations are equal. For $h = 0.2$, standard SPH, the new scheme and CSPM perform similarly. MSPH is more accurate than the other schemes at early times but becomes less accurate later.

VI. GENERALIZATION OF CORRECTIONS TO HIGHER DIMENSIONS

In this section we generalize our corrections to multiple dimensions. In D dimensions, the smoothed approximations of the function and its derivatives are defined by

$$\langle f(\mathbf{x}) \rangle = \int \mathrm{d}^D x' \, f(\mathbf{x}') \left[\frac{1}{h^D} w \left(\frac{\mathbf{x} - \mathbf{x}'}{h} \right) \right], \tag{30}$$

$$\langle \partial_i f(\mathbf{x}) \rangle = \int \mathrm{d}^D x' \, f(\mathbf{x}') \left[\frac{1}{h^{D+1}} (\partial_i w) \left(\frac{\mathbf{x} - \mathbf{x}'}{h} \right) \right], \tag{31}$$

$$\langle \partial_i \partial_j f(\mathbf{x}) \rangle = \int \mathrm{d}^D x' \, f(\mathbf{x}') \left[\frac{1}{h^{D+2}} (\partial_i \partial_j w) \left(\frac{\mathbf{x} - \mathbf{x}'}{h} \right) \right], \tag{32}$$

where $w(\mathbf{v})$ is the dimensionless kernel function in D dimensions and boldface variables denote vectors (e.g. $\mathbf{x}$ is a column vector with components x^i). We will use the Einstein summation convention for repeated indices.

Correction terms in higher dimensions are derived in exactly the same way as in the 1D case, starting from the multi-dimensional Taylor expansion:

$$\langle f(\mathbf{x})\rangle = f(\mathbf{x})M_0 - h\partial_i f(\mathbf{x})M_1^i + \frac{1}{2}h^2\partial_i\partial_j f(\mathbf{x})M_2^{ij} + O(h^3), \tag{33}$$

where the M quantities are multi-dimensional moments of the kernel defined by

$$M_n^{i_1 i_2 \cdots i_n} \equiv \int \mathrm{d}^D v\, v^{i_1} v^{i_2} \cdots v^{i_n} w(\mathbf{v}). \tag{34}$$

Just as in the 1D case, these moments are constants of the kernel and independent of h. Clearly a good approximation of the function follows if $M_0 = 1$ and $M_1^i = 0$. The first requirement is just a normalization condition, while the second condition is met by choosing a radially symmetric kernel with $w(\mathbf{v}) = w(|\mathbf{v}|)$. If the kernel is chosen as described, then we have $\langle f(\mathbf{x})\rangle = f(\mathbf{x}) + O(h^2)$. It is impossible to have $M_2^{ij} = 0$ if the kernel is nonnegative.

The Taylor expansions for the derivatives are similar:

$$h\,\langle \partial_a f(\mathbf{x})\rangle = f(\mathbf{x})M_{0,a} - h\partial_i f(\mathbf{x})M_{1,a}^i + \frac{1}{2}h^2\partial_i\partial_j f(\mathbf{x})M_{2,a}^{ij} + O(h^3), \tag{35}$$

where,

$$M_{n,a}^{i_1 i_2 \cdots i_n} \equiv \int \mathrm{d}^D v\, v^{i_1} v^{i_2} \cdots v^{i_n} (\partial_a w)(\mathbf{v}), \tag{36}$$

and,

$$h^2\,\langle \partial_a\partial_b f(\mathbf{x})\rangle = f(\mathbf{x})M_{0,ab} - h\partial_i f(\mathbf{x})M_{1,ab}^i + \frac{1}{2}h^2\partial_i\partial_j f(\mathbf{x})M_{2,ab}^{ij} + O(h^3), \tag{37}$$

where,

$$M_{n,ab}^{i_1 i_2 \cdots i_n} \equiv \int \mathrm{d}^D v\, v^{i_1} v^{i_2} \cdots v^{i_n} (\partial_a\partial_b w)(\mathbf{v}). \tag{38}$$

If the kernel is chosen so that $M_0 = 1$ and $M_1^i = 0$, it follows that $M_{0,a} = 0$, $M_{1,a}^i = -\delta_a^i$ and $M_{2,a}^{ij} = 0$. The Taylor expansion then gives $\langle \partial_a f(\mathbf{x})\rangle = \partial_a f(\mathbf{x}) + O(h^2)$. There are similar relations for the second and higher order derivatives.

As we saw in the 1D case, even if we choose a kernel such that $M_0 = 1$ and $M_1^i = 0$ over an infinite domain, these conditions can be effectively violated near the boundary or when the particles are irregularly distributed. We will now derive a set of corrective approximations.

Rearranging the expansion of Equation (33), we arrive at:

$$f(\mathbf{x}) = \frac{\langle f(\mathbf{x})\rangle}{M_0} + h\partial_i f(\mathbf{x})\frac{M_1^i}{M_0} - \frac{1}{2}h^2\partial_i\partial_j f(\mathbf{x})\frac{M_2^{ij}}{M_0} + O(h^3). \tag{39}$$

Thus, we define the corrected approximation as

$$\langle f(\mathbf{x})\rangle_C = \frac{\langle f(\mathbf{x})\rangle}{M_0}, \tag{40}$$

which is $O(h)$ accurate.

We can obtain a similar correction for $\partial_a f(\mathbf{x})$ by inserting Equation (39) into Equation (35) and rearranging:

$$\left[h\,\langle \partial_a f(\mathbf{x})\rangle - \langle f(\mathbf{x})\rangle_C M_{0,a}\right] = h\partial_i f(\mathbf{x})\left[\frac{M_{0,a}M_1^i}{M_0} - M_{1,a}^i\right] + \frac{1}{2}h^2\partial_i\partial_j f(\mathbf{x})\left[M_{2,a}^{ij} - \frac{M_{0,a}M_2^{ij}}{M_0}\right] + O(h^3). \tag{41}$$

To make this equation easier to handle, introduce three quantities A, B and C defined by

$$\begin{aligned} A_a &= h\left\langle \partial_a f(\mathbf{x})\right\rangle - \left\langle f(\mathbf{x})\right\rangle_C M_{0,a}, \\ B_a^i &= \frac{M_{0,a}M_1^i}{M_0} - M_{1,a}^i, \\ C_a^{ij} &= M_{2,a}^{ij} - \frac{M_{0,a}M_2^{ij}}{M_0}. \end{aligned} \tag{42}$$

These three quantities can be easily computed using the particle approximation. Equation (41) rewritten in terms of A, B and C is

$$A_a = h\partial_i f(\mathbf{x})B_a^i + \frac{1}{2}h^2\partial_i\partial_j f(\mathbf{x})C_a^{ij} + O(h^3). \tag{43}$$

Assuming that the matrix B_a^i has an inverse $(B^{-1})_k^a$ such that $B_a^i(B^{-1})_k^a = \delta_k^i$, contract both sides with $(B^{-1})_k^a$ and rearrange to get:

$$\partial_k f(\mathbf{x}) = \frac{1}{h}A_a(B^{-1})_k^a - \frac{1}{2}h\partial_i\partial_j f(\mathbf{x})C_a^{ij}(B^{-1})_k^a + O(h^2). \tag{44}$$

Here we identify the corrected derivative

$$\left\langle \partial_k f(\mathbf{x})\right\rangle_C = \frac{1}{h}A_a(B^{-1})_k^a, \tag{45}$$

which is again an $O(h)$ approximation of $\partial_k f(\mathbf{x})$.

This procedure can be repeated once again to obtain an equation involving the second derivatives:

$$E_{ab} = \frac{1}{2}h^2\partial_i\partial_j f(\mathbf{x})F_{ab}^{ij} + O(h^3), \tag{46}$$

where,

$$\begin{aligned} E_{ab} &= h^2\left\langle \partial_a\partial_b f(\mathbf{x})\right\rangle - \left\langle f(\mathbf{x})\right\rangle_C M_{0,ab} - hD_{ab}^k\left\langle \partial_k f(\mathbf{x})\right\rangle_C, \\ F_{ab}^{ij} &= M_{2,ab}^{ij} - \frac{M_2^{ij}M_{0,ab}}{M_0} - C_l^{ij}(B^{-1})_k^l D_{ab}^k, \\ D_{ab}^k &= \frac{M_1^k M_{0,ab}}{M_0} - M_{1,ab}^k. \end{aligned} \tag{47}$$

The D, E and F quantities can be computed using the particle approximation. Unlike before, we cannot solve Equation (46) simply by contracting it with $(F^{-1})_{lm}^{ab}$ (using $(F^{-1})_{lm}^{ab}F_{ab}^{ij} = \delta_l^i\delta_m^j$) because no such inverse exists. To see why, assume $f(\mathbf{x})$ has continuous second partial derivatives so that $\partial_i\partial_j f(\mathbf{x}) = \partial_j\partial_i f(\mathbf{x})$. As a result, D, E and F are symmetric in their lower indices: $D_{ab}^i = D_{ba}^i$, $E_{ab} = E_{ba}$ and $F_{ab}^{ij} = F_{ba}^{ij}$. Since the moments are symmetric in their upper indices, it follows also that $F_{ab}^{ij} = F_{ab}^{ji}$. These symmetries introduce redundancy which makes the linear system of Equation (46) indeterminate. However, one can remove the redundancy by limiting the range of the indices to

$$\begin{aligned} a &= 1, ..., D \\ b &= 1, ..., a \\ i &= 1, ..., D \\ j &= 1, ..., i, \end{aligned} \tag{48}$$

and doubling the $i \neq j$ elements of F_{ab}^{ij}. The linear system of Equation (46) can then be solved using these index limits to get,

$$\left\langle \partial_i\partial_j f(\mathbf{x})\right\rangle_C = \partial_i\partial_j f(\mathbf{x}) + O(h). \tag{49}$$

In order for these correction formulae to be well-defined, the matrices B_a^i and F_{ab}^{ij} (with limited indices) must be invertible. We have found experimentally that B_a^i is invertible as long as there are at least 2, 3 and 4 particles in the effective compact support volume in 1, 2 and 3 dimensions respectively. Similarly, we found that F_{ab}^{ij} is invertible as long as there are at least 3, 6 and 12 particles in 1, 2 and 3 dimensions respectively.

As a consistency check, it is possible to calculate the determinants of the B_a^i and F_{ab}^{ij} matrices analytically in the smoothing approximation assuming an infinite domain. The result is that the matrices are always invertible if the kernel is symmetric, non-zero and tends to zero at infinity.

VII. TEST STUDIES IN 2D

In this section we apply the generalized formulae derived in the previous section to the case of $D = 2$ dimensions to demonstrate their validity. Results are compared to standard SPH, CSPM and MSPH.

A. Interpolation

For the first 2D interpolation test, we consider the xy-derivative of the function $g(x, y) = e^{-(x^2+y^2)}$. The Gaussian kernel was used for the interpolation with smoothing length $h = 0.5$. We used randomly distributed particles with average spacing $\Delta x = 0.25$ on the domain $[-5, 5]^2$. Comparing the plots of Figure 7 we find that standard SPH performs badly under these conditions, while the new scheme fares comparatively well. The results for the new corrective scheme and MSPH are similar and better than CSPM.

For the second test, we consider the polynomial $p(x, y) = x^3 + 3x^2 + 6x + 2y^2 + x^2y^2 + 5$ on the domain $[-5, 5]^2$. This time the particles were uniformly spaced over the domain with spacing $\Delta x = 0.25$. The xy-derivative interpolation of the polynomial in the $[4, 5]^2$ corner is shown in Figure 8. The standard SPH interpolation has an error of order 10^3, while the new corrective scheme fares much better with an error of order 10. The MSPH and new corrective scheme interpolations are again similar and much better than CSPM. The L_∞ error is plotted as a function of h in Figure 9 for p, $\partial p/\partial x$ and $\partial^2 p/\partial x \partial y$.

B. 2D Diffusion Equation

In this test, we solve the 2D diffusion equation,

$$\frac{\partial u(x, y, t)}{\partial t} = \kappa \nabla^2 u(x, y, t), \tag{50}$$

on the domain $[-1, 1]^2$, with Dirichlet boundary conditions

$$u(x, y, t)|_{\text{boundary}} = x + y, \tag{51}$$

and initial condition

$$u(x, y, 0) = \sin(3\pi x) \sin(2\pi y) + x + y. \tag{52}$$

The analytical solution is

$$u_{\text{exact}}(x, y, t) = \sin(3\pi x) \sin(2\pi y) \exp(-13\pi^2 \kappa t) + x + y. \tag{53}$$

We used the explicit method:

$$u(x_i, y_j, t + \Delta t) = u(x_i, y_j, t) + \kappa \Delta t [\![\nabla^2 u(x_i, y_j, t)]\!], \tag{54}$$

with parameters $\kappa = 0.01$ and $\Delta t = 0.1$. The particles were uniformly spaced with spacing $\Delta x = 0.05$. We used two choices for the smoothing length: $h = 0.1$ and $h = 0.2$. In order to impose the boundary conditions, ghost particles were placed outside the domain and set to the value of the boundary condition at the closest boundary point. Since we

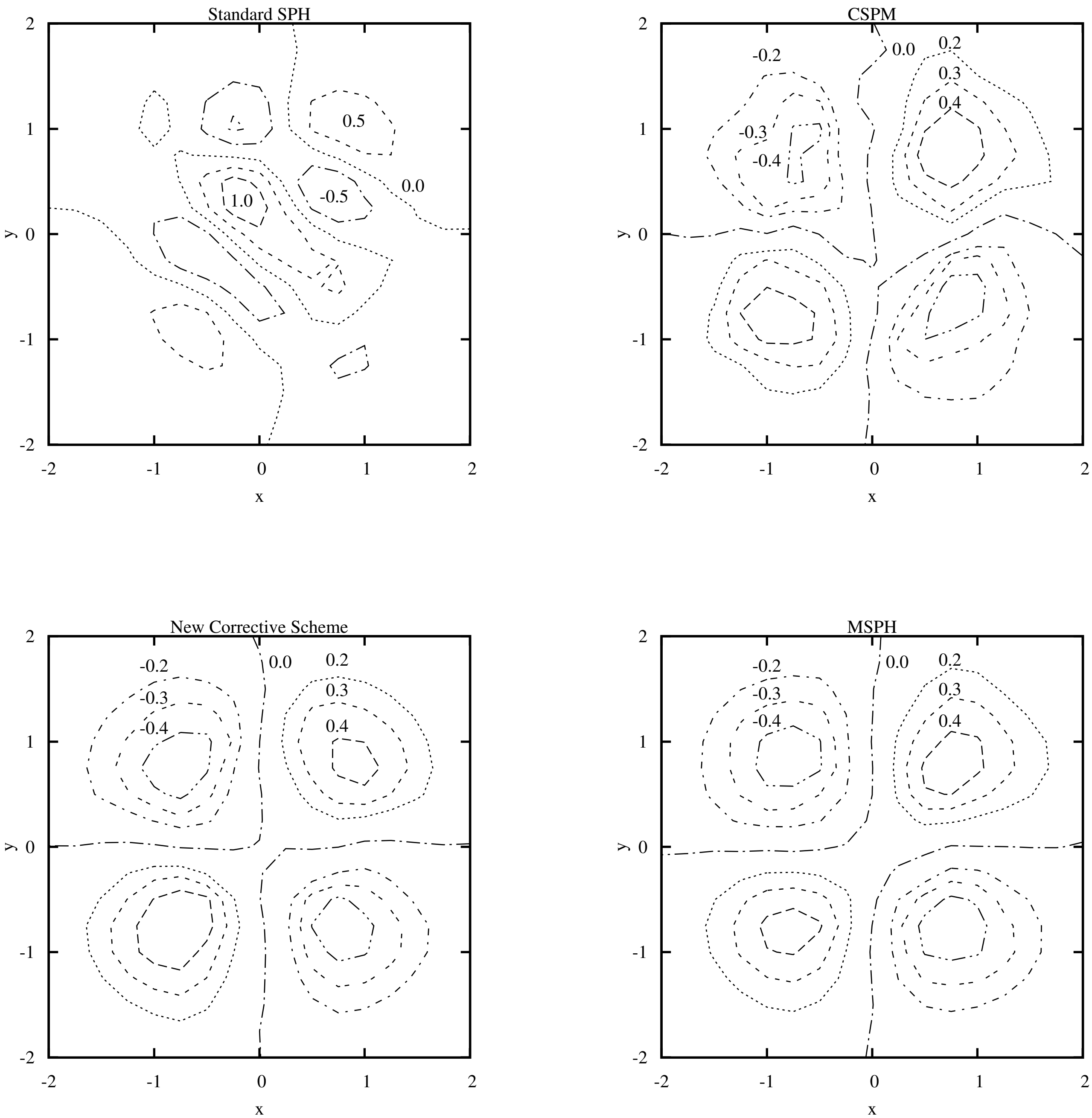

FIG. 7. SPH interpolation of the xy-derivative of $g(x, y) = e^{-(x^2+y^2)}$ using randomly distributed particles with an average particle spacing $\Delta x = 0.25$ and smoothing length $h = 0.5$. The panels show the interpolations from standard SPH, CSPM, the new corrective scheme and MSPH.

are using Dirichlet boundary conditions, the ghost particles were considered when computing $[\![u]\!]$ but ignored for $[\![\nabla^2 u]\!]$.

The L_∞ errors obtained using standard SPH, MSPH, CSPM and the new scheme are shown in Figure 10. All the corrective schemes fare much better than standard SPH. As seen in the 1D heat equation test, MSPH is more accurate than the other schemes at early times but becomes less accurate later.

VIII. DISCUSSION AND CONCLUSIONS

Our corrective scheme is based on Taylor expansion of the SPH smoothing approximation. CSPM [16], MSPH [17], and the methods derived in [18–20] are also based on similar Taylor expansions. However, our method has some different properties which we will discuss in this section. Appendix A describes CSPM and MSPH using the notation of Section II.

The CSPM correction to $f(x)$ is equivalent to our correction. However, for first and higher derivatives, the CSPM scheme is only $O(h)$ accurate when $f(x)$ and $f'(x)$ are known exactly. When interpolating to a point where these values are not known, the scheme has an $O(1)$ error. In contrast, our method is always $O(h)$ accurate at any point. Therefore, our scheme outperforms CSPM for interpolation of first and higher derivatives, as demonstrated in our tests.

MSPH and the method from [19] expand $f(x)$, $f'(x)$ and $f''(x)$ up to the first three terms in the Taylor expansion and invert these coupled equations to solve for the corrective values. This method obtains $\langle f(x)\rangle_{\mathrm{MSPH}}$, $\langle f'(x)\rangle_{\mathrm{MSPH}}$ and $\langle f''(x)\rangle_{\mathrm{MSPH}}$ with $O(h^3)$, $O(h^2)$ and $O(h)$ accuracy respectively. Our method calculates $\langle f(x)\rangle_C$, $\langle f'(x)\rangle_C$ and $\langle f''(x)\rangle_C$ sequentially and always with $O(h)$ accuracy. Indeed, the tests show that our interpolation matches MSPH for f'' but that MSPH is more accurate for f and f'. However, our scheme requires less computation than MSPH. For example, for $D = 1$, MSPH requires a 3×3 matrix inversion while our method doesn't require any matrix inversions. For $D = 2$, MSPH requires a 6×6 matrix inversion while our method requires a 2×2 and a 3×3 matrix inversion, which is less expensive. The saving becomes even greater when more dimensions and higher order derivatives are needed.

The method from [20] is similar to ours except that it assumes $f(x)$ is known exactly. When this is the case, the equations are simplified and only a single matrix inversion is needed. Another difference is that this method allows a set of independent projection or basis functions to be used instead of using a single kernel function and its derivatives. The method from [19] also allows for this (and it differs from MSPH in this respect).

In conclusion, we have developed corrections to SPH that vastly improve interpolation accuracy in areas of particle deficiency such as near boundaries and when particles are irregularly distributed. This was demonstrated by test applications in function interpolation and in solving PDEs. We have shown how the method generalizes to any number of dimensions.

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[1] L. B. Lucy, A numerical approach to the testing of the fission hypothesis, Astron. J. 82 (1977) 1013–1024. http://dx.doi.org/10.1086/112164 doi:10.1086/112164.

[2] R. A. Gingold, J. J. Monaghan, Smoothed particle hydrodynamics: theory and application to non-spherical stars, Mon. Not. R. Astr. Soc. 181 (1977) 375–389.

[3] W. Benz, Smooth particle hydrodynamics: a review, in: J. R. Buchler (Ed.), The Numerical modelling of nonlinear stellar pulsations: problems and prospects, Kluwer Academic Publishers, 1990.

[4] J. J. Monaghan, Why particle methods work (hydrodynamics), SIAM Journal on Scientific and Statistical Computing 3 (4) (1982) 422–433.

[5] P. Laguna, Smoothed particle interpolation, Astrophys. J. 439 (1995) 814–821. http://arxiv.org/abs/astro-ph/9402062 arXiv:astro-ph/9402062, http://dx.doi.org/10.1086/175219 doi:10.1086/175219.

[6] G. Ala, E. Francomano, A. Tortorici, E. Toscano, F. Viola, Smoothed Particle ElectroMagnetics: A mesh-free solver for transients, Journal of Computational and Applied Mathematics 191 (2006) 194–205.

[7] G. Liu, M. Liu, Smoothed Particle Hydrodynamics—a Mesh-free Particle Method, World Scientific, Singapore, 2003.

[8] P. W. Randles, L. D. Libersky, Smoothed-particle-hydrodynamics: Some recent improvements and applications, Computer Methods in Applied Mechanics and Engineering 139 (1-4) (1996) 375–408. http://dx.doi.org/10.1016/S0045-7825(96)01090-

0 doi:10.1016/S0045-7825(96)01090-0.
URL http://www.sciencedirect.com/science/article/B6V29-41FDG4T-F/2/8220aeb1a97726e157007f98e4215d5a

[9] L. D. Libersky, A. G. Petschek, Smooth particle hydrodynamics with strength of materials, in: H. E. Trease, M. F. Fritts, & W. P. Crowley (Ed.), Advances in the Free-Lagrange Method Including Contributions on Adaptive Gridding and the Smooth Particle Hydrodynamics Method, Vol. 395 of Lecture Notes in Physics, Berlin Springer Verlag, 1991, pp. 248–257. http://dx.doi.org/10.1007/3-540-54960-9˙58 doi:10.1007/3-540-54960-9_58.

[10] G. R. Johnson, R. A. Stryk, S. R. Beissel, Sph-for-high-velocity-impact-computations, Computer Methods in Applied Mechanics and Engineering 139 (1-4) (1996) 347–373. http://dx.doi.org/10.1016/S0045-7825(96)01089-4 doi:10.1016/S0045-7825(96)01089-4.
URL http://www.sciencedirect.com/science/article/B6V29-41FDG4T-D/2/79d04e49f246dbdb57e413ca98bd4cc6

[11] R. Vignjevic, J. Campbell, L. Libersky, A-treatment-of-zero-energy-modes-in-the-smoothed -particle-hydrodynamics-method, Computer Methods in Applied Mechanics and Engineering 184 (1) (2000) 67–85. http://dx.doi.org/10.1016/S0045-7825(99)00441-7 doi:10.1016/S0045-7825(99)00441-7.
URL http://www.sciencedirect.com/science/article/B6V29-3YS33Y6-K/2/91981e3d2d8480c7b6480df7927a7ad4

[12] J. Bonet, S. Kulasegaram, A-simplified-approach-to-enhance-the-performance-of -smooth-particle-hydrodynamics-methods, Applied Mathematics and Computation 126 (2-3) (2002) 133–155. http://dx.doi.org/10.1016/S0096-3003(00)00143-0 doi:10.1016/S0096-3003(00)00143-0.
URL http://www.sciencedirect.com/science/article/B6TY8-44VW0B6-1/2/9c52d6eb10669bce6e31b86025f8058a

[13] P. Campbell, DNA report DNA-TR-88-286, Tech. rep. (1989).

[14] W. K. Liu, S. Jun, S. Li, J. Adee, T. Belytschko, Reproducing kernel particle methods for structural dynamics, International Journal for Numerical Methods in Engineering 38 (10) (1995) 1655–1679. http://dx.doi.org/10.1002/nme.1620381005 doi:10.1002/nme.1620381005.

[15] M. B. Liu, G. R. Liu, K. Y. Lam, Constructing-smoothing-functions-in-smoothed -particle-hydrodynamics-with-applications, Journal of Computational and Applied Mathematics 155 (2) (2003) 263–284. http://dx.doi.org/10.1016/S0377-0427(02)00869-5 doi:10.1016/S0377-0427(02)00869-5.
URL http://www.sciencedirect.com/science/article/B6TYH-48MX4V4-3/2/50fab430c45b54747e1a92ea4bbdd00b

[16] J. K. Chen, J. E. Beraun, T. C. Carney, A corrective smoothed particle method for boundary value problems in heat conduction, International Journal for Numerical Methods in Engineering 46 (2) (1999) 231–252. -http://dx.doi.org/10.1002/(SICI)1097-0207(19990920)46:2¡231::AID-NME672¿3.0.CO;2-K doi:10.1002/(SICI)1097-0207(19990920)46:2<231::AID-NME672>3.0.CO;2-K.

[17] G. M. Zhang, R. C. Batra, Modified smoothed particle hydrodynamics method and its application to transient problems, Computational Mechanics 34 (2004) 137–146. http://dx.doi.org/10.1007/s00466-004-0561-5 doi:10.1007/s00466-004-0561-5.

[18] M. Liu, G. Liu, Restoring-particle-consistency-in-smoothed-particle -hydrodynamics, Applied Numerical Mathematics 56 (1) (2006) 19–36. http://dx.doi.org/10.1016/j.apnum.2005.02.012 doi:10.1016/j.apnum.2005.02.012.
URL http://www.sciencedirect.com/science/article/B6TYD-4FSCV3D-1/2/18b9baca41c65f1c16faa47a4bbf78a9

[19] M. Liu, W. Xie, G. Liu, Modeling-incompressible-flows-using-a-finite -particle-method, Applied Mathematical Modelling 29 (12) (2005) 1252–1270. http://dx.doi.org/DOI:-10.1016/j.apm.2005.05.003 doi:DOI:10.1016/j.apm.2005.05.003.
URL http://www.sciencedirect.com/science/article/B6TYC-4GM46BG-1/2/ba82663b15bfff65598b1266c8e0e11a

[20] D. Asprone, F. Auricchio, A. Reali, Novel-finite-particle-formulations -based-on-projection-methodologies, International Journal for Numerical Methods in Fluidshttp://dx.doi.org/10.1002/fld.2327 doi:10.1002/fld.2327.
URL http://dx.doi.org/10.1002/fld.2327

[21] L. Brookshaw, A method of calculating radiative heat diffusion in particle simulations, Proceedings of the Astronomical Society of Australia 6 (1985) 207–210.

[22] H. F. Schwaiger, An implicit corrected sph formulation for thermal diffusion with linear free surface boundary conditions, International Journal for Numerical Methods in Engineering 75 (6) (2008) 647–671. http://dx.doi.org/10.1002/nme.2266 doi:10.1002/nme.2266.

[23] N. J. Quinlan, M. Basa, M. Lastiwka, Truncation error in mesh-free particle methods, International Journal for Numerical Methods in Engineering 66 (13) (2006) 2064–2085. http://dx.doi.org/10.1002/nme.1617 doi:10.1002/nme.1617.

Appendix A: CSPM and MSPH in our notation

In order to compare our scheme to CSPM and MSPH, it is useful to rewrite the equations from [16] and [17] using our notation.

The CSPM result corresponding to our Equation (21) is:

$$\langle f(x)\rangle_{\mathrm{CSPM}} = \frac{\langle f(x)\rangle}{M_0} = f(x) + O(h). \tag{A1}$$

This is exactly equivalent to our result.

The first CSPM derivative is given by

$$\langle f'(x)\rangle_{\text{CSPM}} = \frac{M_0' f(x) - h\,\langle f'(x)\rangle}{hM_1'} + O(h). \tag{A2}$$

This result differs from our result in Equation (24). If $f(x)$ is known exactly at the interpolation point, then this expression works well. Otherwise, in the case of true interpolation, one is forced to replace $f(x)$ in Equation (A2) by $\langle f(x)\rangle_{\text{CSPM}}$. The resulting expression has an $O(1)$ term which makes it a bad approximation.

The second CSPM derivative is given by

$$\langle f''(x)\rangle_{CSPM} = \frac{h^2\,\langle f''(x)\rangle - M_0'' f(x) + hM_1'' f'(x)}{\frac{1}{2}h^2 M_2''} + O(h). \tag{A3}$$

This result differs from our second derivative correction in Equation (26). Again, if $f(x)$ and $f'(x)$ are not known exactly, then their CSPM values must be used and this leads to an $O(1)$ error term.

The MSPH corrections from [17] in 1D are defined by

$$\begin{pmatrix} \langle f(x)\rangle \\ \langle f'(x)\rangle \\ \langle f''(x)\rangle \end{pmatrix} = \begin{pmatrix} M_0 & -hM_1 & h^2M_2/2 \\ M_0'/h & -M_1' & hM_2'/2 \\ M_0''/h^2 & -M_1''/h & M_2''/2 \end{pmatrix} \begin{pmatrix} \langle f(x)\rangle \\ \langle f'(x)\rangle \\ \langle f''(x)\rangle \end{pmatrix}_{\text{MSPH}}, \tag{A4}$$

where the matrix must be inverted to obtain the corrected values. Comparing this system of equations to Equation (11), we see that

$$\begin{aligned} \langle f(x)\rangle_{\text{MSPH}} &= f(x) + O(h^3), \\ \langle f'(x)\rangle_{\text{MSPH}} &= f'(x) + O(h^2), \\ \langle f''(x)\rangle_{\text{MSPH}} &= f''(x) + O(h). \end{aligned} \tag{A5}$$

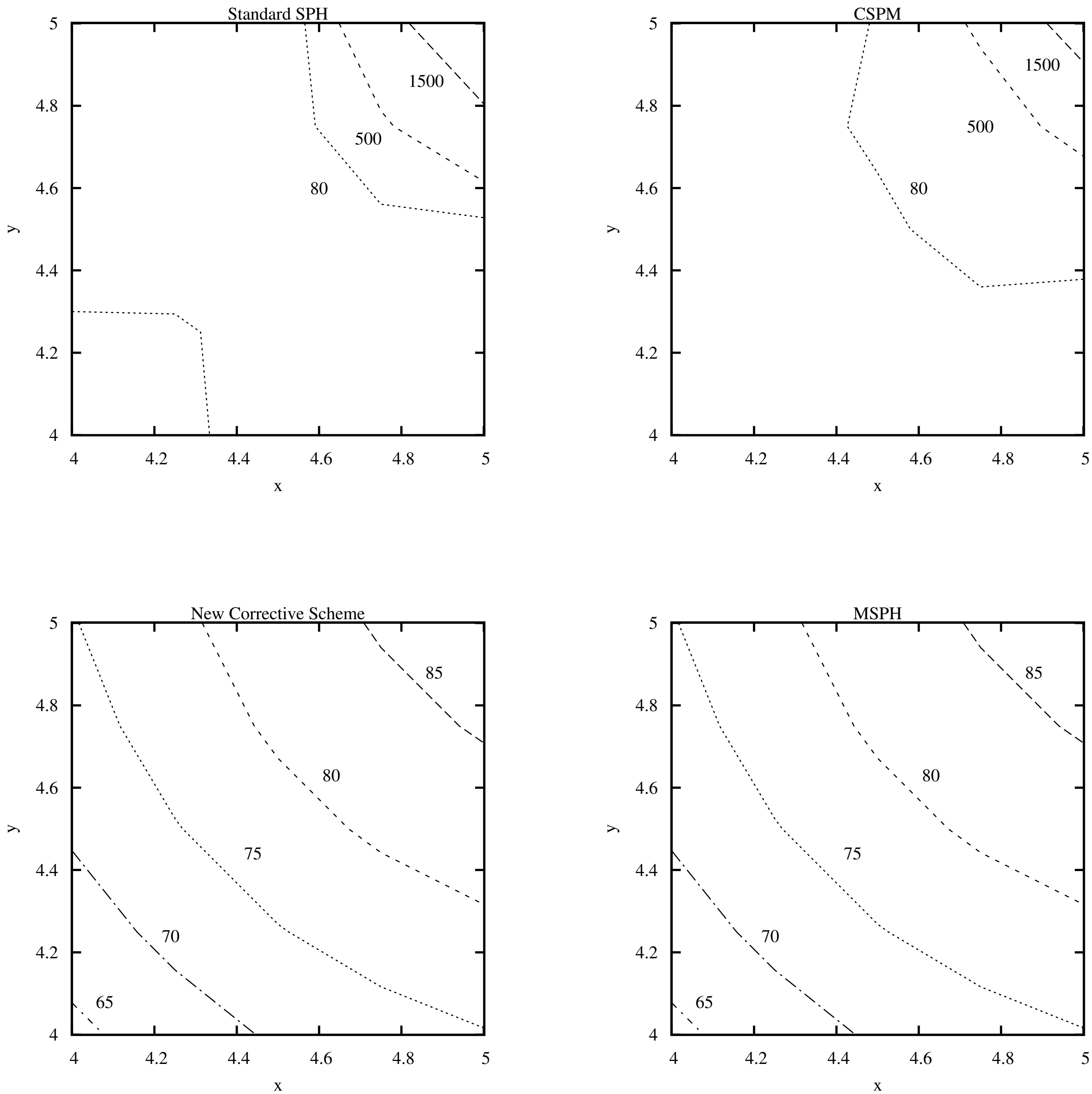

FIG. 8. SPH interpolation of the xy-derivative of $p(x,y) = x^3 + 3x^2 + 6x + 2y^2 + x^2y^2 + 5$ in one corner of the domain using uniformly-spaced particles with spacing $\Delta x = 0.25$ and smoothing length $h = 0.5$. The panels show the interpolations from standard SPH, CSPM, the new corrective scheme and MSPH.

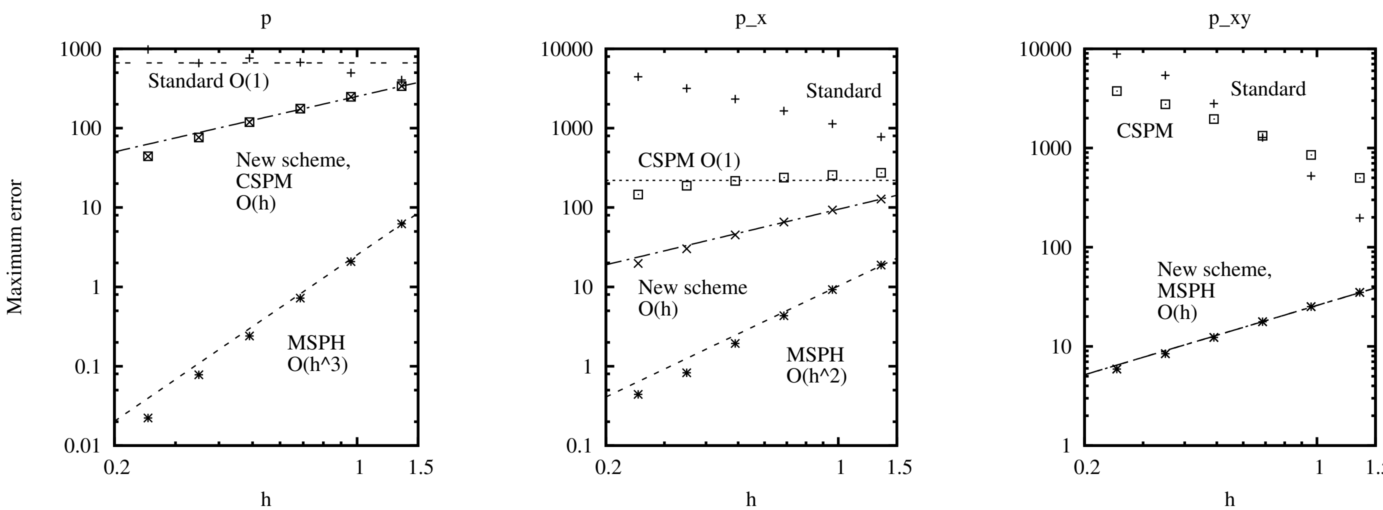

FIG. 9. The L_∞ maximum error of the various interpolation schemes as a function of the smoothing length h for the polynomial $p(x, y) = x^3 + 3x^2 + 6x + 2y^2 + x^2y^2 + 5$. Fitted $O(1)$, $O(h)$, $O(h^2)$ and $O(h^3)$ curves are indicated. The particles were uniformly spaced with separation $\Delta x = 0.25$.

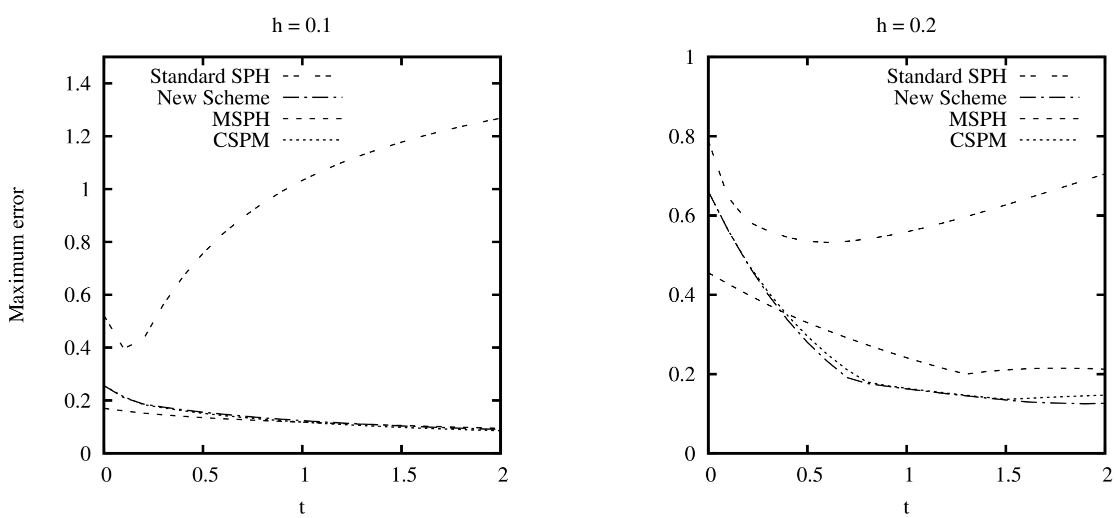

FIG. 10. The L_∞ maximum error obtained for the 2D diffusion equation test discussed in Section VII B. Smoothing length $h = 0.1$ was used for the left plot and $h = 0.2$ was used for the right plot. Results are shown for standard SPH, the new corrective scheme, CSPM and MSPH.