This paper seeks to reformulate moving particle semi-implicit method (MPS) in order to provide a mathematical interpretation of the method. It is shown that gradient and Laplace operators are evaluated by using volume integral of the Taylor series expansion of a target function and that the form of the volume integral evaluation of the differential operators is similar to MPS, suggesting that the volume integral evaluation is a mathematical interpretation of MPS. Numerical experiments using one-dimensional setting indicate a possibility of improving the accuracy of computing the differential operators when the reformulated MPS is used. Remarks on directions towards improving the accuracy of MPS are made.

**Key Words:** moving particle semi-implicit method, free boundary problem, particle method, volume integration identity, accuracy improvement

### 1. INTRODUCTION

A free boundary problem remains a challenging problem of computational mechanics, since a robust methodology is not established to determine the configuration of the free boundary; see articles relevant to civil engineering\(^1\),\(^2\),\(^3\). For instance, it is almost impossible for finite element method to generate meshes unless the configuration of the boundary is known in advance. While many techniques have been proposed, a numerical method that decomposes a target domain has inherent disadvantage in solving the free boundary problem.

A particle or meshless method has been recognized as a suitable numerical analysis method for solving the free boundary problem, since it does not require grid generation. There are numerous methods that are applied to the free boundary problem. Representative are Smoothed Particle Hydrodynamics (SPH)\(^4\) and Moving Particle Semi-Implicit Method (MPS) proposed by Koshizuka and Oka\(^5\). Although the formulation of SPH and MPS appears similar to each other, it is taken for granted that SPH is a mathematical method, while MPS proposes a new physical modeling, according to the Handbook of Computational Mechanics\(^6\).

In the authors’ eyes, it seems that MPS has higher accuracy, compared with SPH, mainly because of the characteristics of MPS as a new physical modeling. However, the characteristics might not be good enough to be used in solving a free boundary problem that is mathematically well-posed and needs no additional physical modeling. MPS has less popularity than SPH, which is readily applicable to many free boundary problems; moreover, the popularity of SPH owes its simple but clear characteristics as a tool for solving the free boundary problems.

In this paper, we seek to interpret MPS in a mathematical manner, despite the current understanding that MPS is a physical modeling, so that higher accuracy and popularity is achieved for MPS. As explained later, we regard MPS as a *rigorous* method for evaluating differential operators using volume integral. This interpretation sounds surely tricky, but we seek to prove the rigorousness that is embedded in MPS. We also seek to improve the accuracy of MPS as a method for solving free boundary problems, taking advantage of this interpretation.
The contents of the present paper are organized as follows. First, in Section 2, we summarize the present formulation of MPS. In Section 3, we seek to reformulate MPS using Taylor series expansion. Numerical experiments, which are often made in one-dimensional setting, are carried out in Section 4, to examine the effectiveness of the reformulation. Some attempts are made to improve the accuracy of computing the differential operators in Section 5. In the numerical experiments, it is shown that the differential operators can be computed accurately by applying the reformulated MPS. A few remarks on future studies towards improving the accuracy of MPS are made in Section 6.

2. OVERVIEW OF MPS

MPS\textsuperscript{5,7,8,9,10} assumes that a continuum is replaced with a set of particles, each of which is assigned a value of a target function. It is further assumed that there are interactions among the particles that are expressed in terms of two differential operators, gradient and Laplacian. Fig. 1 shows particles in the two-dimensional setting. A set of particles are distributed in a domain, which is a part of the continuum, and a green particle interacts with surrounding blue parties, which are located within a circular of radius \( R \).

When the location and value of the \( \alpha \)-th particle are denoted by \( x^\alpha \) and \( f^\alpha \), the value of the gradient operator of the \( \alpha \)-th particle is determined in a similar manner, i.e.,

\[
\nabla f^\alpha = \sum_{|x^\beta-x^\alpha|<R} d \left( f^\beta - f^\alpha \right) \frac{x^\beta - x^\alpha}{|x^\beta - x^\alpha|^2} \frac{\psi(|x^\beta - x^\alpha|)}{\sum_{j} \psi(|x^\gamma - x^\alpha|)},
\]

(1)

where \( d \) is a dimension number, and \( \psi \) is a kernel function, which plays a role of putting a weight to a summed term.

The value of Laplace operator of the \( \alpha \)-th particle is determined in a similar manner, i.e.,

\[
\nabla^2 f^\alpha = \sum_{|x^\beta-x^\alpha|<R} 2d \left( f^\beta - f^\alpha \right) \frac{1}{|x^\beta - x^\alpha|^2} \frac{\psi(|x^\beta - x^\alpha|)}{\sum_{j} \psi(|x^\gamma - x^\alpha|)}
\]

(2)

Another Laplacian operator is recommended by Koshizuka and Oka\textsuperscript{5}. That is,

\[
\nabla^2 f^\alpha = \sum_{|x^\beta-x^\alpha|<R} 2d \left( f^\beta - f^\alpha \right) \frac{\psi(|x^\beta - x^\alpha|)}{\sum_{j} \psi(|x^\gamma - x^\alpha|)|x^\gamma - x^\alpha|^2};
\]

this operator is developed in view of solving a diffusion equation.

In the literature review, we find that these differential operators are formulated based on the physical consideration. More specifically, the operators are formulated by defining the interaction between two particles, which is averaged by using a kernel function, \( \psi \). The terms that define the interaction are

\[
\left( f^\beta - f^\alpha \right) \frac{x^\beta - x^\alpha}{|x^\beta - x^\alpha|^2} \quad \text{and} \quad \left( f^\beta - f^\alpha \right) \frac{1}{|x^\beta - x^\alpha|^2},
\]

for the gradient and Laplace operators, respectively; see Eqs. (1) and (2). While these two terms appear natural in expressing the first- and second-order derivatives, it is not clear how suitably they express the interaction; see references related to improvement of MPS\textsuperscript{6,17,18,19,20,21}.

Furthermore, there are three enigmatic terms involved in computing the differential operators. Fig. 2 points out these terms for the gradient operator; see Eq. (1). The first term is the appearance of the dimension number, \( d \), in the Laplace operator, it is replaced by \( 2d \). The second term is indeed the term that expresses the interaction effect. As mentioned, the form of the second term seems natural. However, questions arise such as “why is this form suitable to account for the interaction?” or “is there any better form to account for the particle location?” and so on. The last term is the appearance of the kernel function. Just like the second term, it raises a question of “why is this function or this form suitable?” even though the form appears natural as a kind of weighting factor.
3. REFORMULATION OF MPS

We start the reformulation of MPS by considering the Taylor series expansion of a function in which a series of differential operators appear; see articles on an approach similar to the present paper that is applied to SPH\textsuperscript{11,12,13,14,15}. We consider a general $d$-dimensional setting. If a target function $f(x)$ is smooth in the neighborhood of, say, $0$, it admits the following expansion:

$$f(x) = f(0) + \nabla f(0) \cdot x + \frac{1}{2} \nabla \nabla f(0) : x \otimes x + \cdots,$$
(3)

where $\cdot$ and $\otimes$ are first-, second-order contraction and tensor product, and $\nabla f$ and $\nabla \nabla f$ are the first- and second-order derivatives of $f$, respectively; in a Cartesian coordinate system, $(x_i)$, the components of $\nabla f$ and $\nabla \nabla f$ are

$$(\nabla f)_i = \frac{\partial f}{\partial x_i} \quad \text{and} \quad (\nabla \nabla f)_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j},$$

for $i, j = 1, \ldots, d$. The neighborhood of $0$ could be given as a $d$-dimensional sphere of radius $R$, i.e., $|x| < R$ with $|x|^2 = \sum x_i^2$. This sphere is denoted by $V$.

Multiplying the both sides with $\frac{1}{|x|^2}$ and computing the volume integral over $V$, we derive the following equation from Eq. (3):

$$\int_V \left( \frac{f(x) - f(0)}{|x|^2} \right) dv = \nabla f(0) \cdot \int_V \frac{x}{|x|^2} dv$$
$$+ \frac{1}{2} \nabla \nabla f(0) : \int_V \frac{x \otimes x}{|x|^2} dv + \cdots.$$  
(4)

Note that $\nabla f(0)$ or $\nabla \nabla f(0)$ is regarded as a constant vector or tensor, and that it is not included in the volume integral.

The volume integral in the right side of Eq. (4) is analytically computable for the spherical domain. Indeed, we have

$$\int_V \frac{x \otimes x}{|x|^2} dv = \frac{V}{d} \delta$$
(5)

where $\delta$ is the second-order identity tensor, and $V$ stands for the volume of the $d$-dimensional sphere. We also have another identity,

$$\int_V \frac{x \otimes x \otimes x}{|x|^2} dv = 0;$$

see Appendix A for the derivation of Eq. (5) and this identity. Therefore, we can evaluate $\nabla f(0)$ as

$$\nabla f(0) = \frac{d}{V} \int_V \frac{(f(x) - f(0))}{|x|^2} x dv,$$
(6)

ignoring higher-order terms in Eq. (4).

The right side of Eq. (6) is similar in form to the original gradient operator of MPS; the first and second enigmatic terms, $d$ and $x/|x|^2$, appear. The third enigmatic term is interpreted as the evaluation of the volume integral, if a collocation method is used for the volume integral of the right side and particles are regarded as points of the collocation method.

Multiplying the both sides with $\frac{1}{|x|^2}$ and computing the volume integral over $V$, we derive the following equation from Eq. (3):

$$\int_V \left( \frac{f(x) - f(0)}{|x|^2} \right) dv = \nabla f(0) \cdot \int_V \frac{x}{|x|^2} dv$$
$$+ \frac{1}{2} \nabla \nabla f(0) : \int_V \frac{x \otimes x}{|x|^2} dv + \cdots.$$  
(7)

In view of an identity of

$$\int_V \frac{x}{|x|^2} dv = 0,$$

we can evaluate $\nabla^2 f(0)$ as

$$\nabla^2 f(0) = \frac{2d}{V} \int_V \frac{(f(x) - f(0))}{|x|^2} x dv,$$
(8)

ignoring higher-order terms. Just like Eq. (6) for the gradient operator, Eq. (8) provides an expression of the Laplace operator that is similar to MPS, as it includes the first and second enigmatic terms and the third term is interpreted as the evaluation of the volume integral.

The procedures of deriving Eqs. (6) and (8) from Eq. (3) are essentially the same. Approximating the volume integral by the collocation method without introducing weight terms given by $\psi$, we can reformulate the gradient and Laplace operators, as

$$\nabla f^\alpha = \sum_{|x^\beta - x^\alpha| < R} \frac{d}{N} \left( f^\beta - f^\alpha \right) \frac{x^\beta - x^\alpha}{|x^\beta - x^\alpha|^2},$$
(9)

and

$$\nabla^2 f^\alpha = \sum_{|x^\beta - x^\alpha| < R} \frac{2d}{N} \left( f^\beta - f^\alpha \right) \frac{1}{|x^\beta - x^\alpha|^2}. $$
(10)

Note that the same volume is assigned to each term in the summation, and hence $1/N$ appears in the summation.

As mentioned, essentially the same approach as explained in the above has been studied for SPH\textsuperscript{11,12,13,14,15}. The originality of this paper, however, is mathematical derivation of the integration evaluation of differential operators, which does not include physical interpretation. Hence, as shown in the next sections, we can concentrate on the improvement of the accuracy in evaluating the differential operators by considering a more suitable method of computing integral. While the gradient and Laplace operators are studied in this paper, the present method of the internal evaluation can be applied to any other differential operators.

4. NUMERICAL EXPERIMENTS OF REFORMULATED MPS

It is shown that the volume integral evaluation of the gradient and Laplace operators, Eqs. (6) and (8), is
similar in form to the original MPS and that these operators are reformulated as Eqs. (9) and (10), based on the volume integral evaluation. In order to examine the effectiveness of this reformulation in computing the differential operators, we carry out simple numerical experiments. The experiments use \(N\) particles, the center of which is \(x^\alpha\) with \(\alpha = 1, \ldots, N\), are randomly distributed in \(V\), and assign an exact value of a target function \(f\) to each particle, \(f^\alpha = f(x^\alpha)\).

In a one-dimensional setting \((d = 1)\), we first compare terms that are summed in the original and reformulated MPSs. Points are randomly generated around \(x = 1\) with \(N = 20\) and \(R = 0.1\). **Fig. 3** shows a typical example of the distribution of the summed terms for the case of \(f(x) = x^2\) at \((x_1) = (1)\). As is seen, the reformulated MPS (designated as “reformulated”) has a smoother distribution of the integrand, compared with the original MPS (designated as “original”), but they have a much wilder distribution for the Laplacian. This is well understood if we see Eqs. (6) and (8) or the integral evaluation of MPS; the integrand is singular at the origin.

Generating 80, 160, 320, 640, 1,280 sets of the particles, we compare the convergence of the mean and the standard deviation of \(\nabla f\) and \(\nabla^2 f\) in **Fig. 4**: the horizontal axis is the number of the sets in logarithmic scale and the vertical axis is the relative error of the mean or the standard deviation divided by the exact value, respectively. As for the gradient, the original and reformulated MPSs do not have a significant difference; the standard deviation of the reformulated MPS is slightly larger than that of the original MPS.
Fig. 5 Comparison of standard deviation of original and reformulated MPS by changing particle number ($N$) for $d = 1$.

Fig. 6 Comparison of standard deviation of original and reformulated MPS by changing domain radius ($R$) for $d = 1$; the graphs of $N = 10$ are omitted in c) and d) because they are out of the range.

As for the Laplacian, the reformulated MPS shows faster convergence; the relative error of the mean and the standard deviation are significantly reduced, compared with the original MPS.

We examine the effects of the particle number and the domain radius, $N$ and $R$, on the accuracy of computing the differential operators. The results are presented in Fig. 5 and Fig. 6, respectively, for $N$ and $R$; the target function is $f = x^2$ and 160 sets of randomly generated particles are used. In view of Fig. 4, we use the standard deviation divided by the exact value of the Laplacian as a measure of the accuracy.
in these figures. As for the gradient, the original MPS has slightly smaller standard deviation than the reformulated MPS; the difference is in the order of 1% of the exact value of the gradient. As for the Laplacian, the reformulated MPS has much smaller standard deviations for all the cases of varying $N$ and $R$ (the cases of $N = 10$ are omitted in the figure as the graphs are out of the range). This suggests the usefulness of the reformulated MPS.

We have to point out that as for the reformulated MPS, the standard deviation of the gradient increases as $N$ increase or $R$ decreases in Fig. 5 or Fig. 6, respectively. This is odd, because using a larger number of particles contributes to the increase in the accuracy or because higher-order terms of Taylor series expansion vanishes faster in a smaller domain. This is probably due to the limitation of the collocation method that is used in the volume integral.

The convergence of the mean and the standard deviation is compared for the case of $d = 2$; a target function is $f(x) = (x_1 + x_2)^2$, and the point $(x_1, x_2) = (1, 1)$ is used. The results are presented in Fig. 7: “original 1, 2” or “reformulated 1, 2” stands for the $x_1, x_2$-component of $\nabla f$ computed by the original or reformulated MPS, respectively. As for the gradient, the reformulated MPS has a slightly smaller error for the mean and a smaller standard deviation. The improvement is more significant for the Laplacian. The relative error of the mean and the standard deviation of the reformulated MPS are almost 10% of the original MPS. However, we have to point out that the standard deviation of the Laplacian remains 10 times larger than the exact value, even when more than 1,000 particles are used. This is a significant loss of the accuracy in computing the Laplacian.

5. IMPROVEMENT OF ACCURACY OF REFORMULATED MPS

In order to improve the accuracy of reformulated MPS, we focus on the simplest case of $d = 1$ and seek to find a better way of computing the volume integral. We should emphasize that unlike the original MPS that is interpreted as a new physical model, the reformulated MPS does not involve any physical assumption nor modeling. The improvement of the accuracy is thus made by considering a better mathematical treatment only.

1. Use of other volume integral identities

It is easily understood that multiplying the both sides of Eq. (3) with $x|x|^m$ of a suitable $m$, we can derive another evaluation of the gradient operator,

\[
\left( \int_V x \otimes x|x|^m \, dv \right) \cdot \nabla f(0) = \int_V (f(x) - f(0)) \cdot x|x|^m \, dv,
\]

(11)

ignoring higher order terms. Note that the term that includes $\nabla \nabla f(0)$ vanishes since the corresponding integrand becomes an odd function with respect to each
Fig. 8 Comparison of convergence of mean and standard deviation of gradient and Laplacian of original MPS and reformulated MPS using $|x|^m$ of $m = 1$ as increasing sets of randomly generated particles.

Fig. 9 Comparison of convergence of mean and standard deviation of gradient and Laplacian of reformulated MPS using $|x|^m$ of $m = 1$, 2 and 3 as increasing sets of randomly generated particles.

component of $x$. The volume integral on the left side is analytically computed as

$$\int_V x \otimes x |x|^m \, dv = \begin{cases} \frac{d^m}{S \log R} & m \neq -d - 2, \\ \log R \delta & m = -d - 2, \end{cases}$$

where $S$ stands for the $d$-dimensional surface area of $V$. Choosing a suitable $m$, we may be able to increase the accuracy of computing the gradient operator, since the integrand becomes less wild at $0$. It should be noted that the value of $\nabla f(0)$ should not depend on the choice of $m$, but the accuracy of computing $\nabla f(0)$ depends on $m$. We thus study the effect of $m$ on $\nabla f(0)$, varying the value of $m$. 

Fig. 10 Comparison of distribution of mean and standard deviation of gradient and Laplacian of original MPS, reformulated MPS, and reformulated MPS using $|x|^m$.

We continue the numerical experiments made in the preceding section. The volume integral is computed by the collocation method, and the gradient and Laplace operators are evaluated as

$$\nabla f(0) = \frac{(m + 3) N}{R^{m+3} S} \sum_{\alpha=1}^N (f^{(\alpha)} - f^0) \frac{x^\alpha}{|x^\alpha|^{1+m}} \quad (13)$$

and

$$\nabla^2 f(0) = \frac{(m + 3) 2 N}{R^{m+3} S} \sum_{\alpha=1}^N (f^{(\alpha)} - f^0) \frac{1}{|x^\alpha|^{1+m}} \quad (14)$$

see Eqs. (9) and (10) as the case of $m = 0$.

First, we examine the convergence of the mean and the standard deviation of the gradient and Laplacian for $f = x_1^2$, generating 80, 160, 320, 640, 1,280 sets of the particles for $N = 20$ and $R = 0.1$, just like Fig. 4. The results are shown in Fig. 8 for $m = 1$; the relative error of the mean and the standard deviation divided by the exact value are plotted. As is seen, faster convergence is observed for the reformulated MPS using $|x|^m$ which is designated by “improved.”

Fig. 9 shows the convergence of the mean and the standard deviation with respect to the increasing number of $N$, varying the values of $m$; $m = 1, 2,$ and 3 are used. There are no significant differences for the three cases of $m$. The standard deviation divided by the exact value is around 0.2 or 10 for the gradient and the Laplacian, respectively. This poor accuracy is partially due to the use of only 20 particles for each set in computing the differential operators. Still, some improvement is necessary.

For the case of 320 sets of generated particles, Fig. 10 presents the distribution of the mean and the standard deviation computed by the original MPS (“original”), the reformulated MPS (“reformulated”), and the reformulated MPS using $|x|^m$ (“improved”); and the horizontal axis is the value divided by the exact value. As for the gradient, the distribution is slightly different for the three methods; the reformulated MPS has the sharpest distribution around the exact value, and others are distributed ±20%. The Laplacian has a much wider distribution compared with the gradient, and hence the standard deviation of the Laplacian converges much more slowly than the gradient. Moreover, the value of the standard deviation divided by the exact value of the Laplacian is around 10. This does not indicate that sufficiently high accuracy is achieved in computing the volume integral.

(2) Use of midpoint rule for volume integral

A simple improvement of the accuracy of computing the volume integral is the use of the midpoint rule, i.e.,

$$\int_V (f(x) - f(0)) x|x|^m \, dv = \sum_{\alpha=1}^N (f^{(\alpha)} - f^0) \frac{x^\alpha}{|x^\alpha|^{1+m}} \nu^\alpha, \quad (15)$$

where $\nu^\alpha$ is the volume of the domain that the particle at $x^\alpha$ occupies within $V$. In the case of $d = 1$, this $\nu^\alpha$ is easily determined; see Fig. 11, in which $\nu^\alpha$ is the segment between $\frac{x^\alpha + x^{\alpha+1}}{2}$ and $\frac{x^\alpha - x^{\alpha+1}}{2}$ when the particle order is rearranged in an ascending order and $x^\alpha$ is placed at the $\alpha$-th position. This is the use of simple
midpoint rule for the one-dimensional integration; $x'$ is regarded as the midpoint of $\frac{x_1+x_2}{2}$ and $\frac{x_1+x_2+1}{2}$.

We continue the numerical experiments for the target function of $f(x) = x^2$ at $(x_1) = (1)$. The relative error of the mean and the standard deviation divided by the exact value are plotted in Fig. 12 and Fig. 13, respectively, for the reformulated MPS and the reformulated MPS using $|x|^m$ of $m = 2$; $N$ changes from 20 to 160 and $R$ changes from 0.025 to 0.2; and 100 sets of particles are used. As for the gradient, the accuracy is improved; there are no substantial errors in the mean, and the standard deviation is small. As for the Laplacian, however, the reformulated MPS has non-negligible errors in computing the mean and producing large standard deviations when $N$ and $R$ are small. The reformulated MPS using $|x|^m$ has much smaller errors in the mean and smaller standard deviation. In particular, the standard deviation of computing the Laplacian is drastically improved; compare Fig. 12d) with Fig. 13d).

It is of interest to see the difference between Fig. 12 and Fig. 13. The integrand of the reformulated MPS is singular at the origin, and hence it induces larger errors compared with the reformulated MPS using $|x|^m$ which eliminates the singularity. It is true that if $|x|^m$ is regarded as a kind of weight in the summation, smaller weights are put for the particles near the target particle compared with particles located far, which does not accurately produce the evaluation. In the present case, however, $|x|^m$ plays the role of eliminating the singularity of the integrand, not that of putting a weight for summed terms.

The results shown in Fig. 13 is promising to improve the accuracy of computing the gradient and the Laplacian. We have to emphasize that the error of the mean increases for smaller $R$. As mentioned in the preceding section, the less accurate evaluation of the mean for smaller $R$ is odd; in smaller $R$, the integral of polynomials of higher order vanishes faster. The source of the error for smaller $R$ might be due to the use of the midpoint rule in computing the integral. Further investigation is surely needed.

To examine the accuracy of computing the gradient and the Laplacian, we examine four functions, namely, $f(x) = x^3$, $\exp x$, $\log x$, and $\sin x$. The results of the standard deviation of the Laplacian, which is least accurately computed in the preceding numerical experiments, are presented in Fig. 14. For all the four functions, the standard deviation of computing the Laplacian tends to vanish as $N$ increases. The odd behavior of the standard deviation, i.e., a larger standard deviation of smaller $R$, is commonly observed for these four functions.

In the present numerical experiments, an exact value of a target function is assigned to all particles. The results shown in Fig. 14 suggests that even if some errors are included, they do not induce large error in computing the differential operators. When errors are randomly given to the particles, the differential operators are computed for the sum of a tar-
get function and a certain function that corresponds to these errors. The contribution of the latter to the differential operators will be small since it changes wildly and takes on small values for differential operators for lower order.

6. CONCLUDING REMARKS

In this paper, we seek the reformulation of moving particle semi-implicit method (MPS), using a Taylor series expansions and volume integral identities. Derived are similar expressions of the gradient and Laplace operators that include enigmatic terms in them. In preliminary numerical experiments, we show that the reformulated MPS generally has high accuracy in computing these operators. There are cases when the accuracy is not improved, probably because of the less accurate estimation of the volume integral; this induces opposite characteristics of the gradient and Laplace operators for the domain of integration.

Future studies are needed for a possible improvement of MPS that is based on the volume integral evaluation of the differential operators. The following would be suitable directions towards increasing the accuracy of MPS:

- The use of an ellipsoid as an integration domain; differential operators can be computed more accurately by considering many configurations of ellipsoid and components of a second-order tensor $\nabla \nabla f$ can be computed.

In Appendix B, we propose a more robust evaluation of the differential operators. We also point out that according to Eq. (3), we can evaluate the value of a function or its derivative at any points in the domain in which the Taylor series expansion is taken. This surely enlarges the application of MPS, so that boundary conditions are taken into more rigorous consideration.

Appendix A  VOLUME INTEGRAL IDENTITY

We prove the volume integration identities used in Section 3. Recall that the volume integral is computed over $V$, a $d$-dimensional sphere of radius $R$ located at the origin $0$. Vanishing of integral is easily understood because the integrands, $\frac{x_k x_k}{R^d}$ and $\frac{1}{R^d}$, respectively, are an odd function with respect to each component of $x$ and the integration domain is symmetric with respect to it.

Regarding Eq. (5), we can assume isotropy for the resulting volume integral computed over $V$, which be-
Fig. 14 Standard deviation of Laplacian of reformulated MPS using $|x|^2$ of $m = 2$ and enhanced with midpoint rule; $x^3$, $\exp(x)$, $\log(x)$ and $\sin(x)$ are tested.

comes a second-order tensor\(^{22}\). That is,
\[
\int_V x \otimes x \frac{dv}{|x|^2} = A \delta,
\]
where $A$ is an unknown constant; recall that $\delta$ is an identity tensor, or a component of $\delta$ in a Cartesian coordinate system is Kronecker’s delta ($\delta_{ij} = 1$ for $i = j$ or $0$ for $i \neq j$). Taking the second-order contraction with $\delta$, we have
\[
V = dA,
\]
where $V$ stands for the volume of the $d$-dimensional sphere. Therefore, Eq. (5) is derived.

Finally, we prove Eq. (12). Denoting $|x| = r$ and writing $x = re$, we have
\[
\int_V x \otimes x |x|^m dv = \int_0^r r^{m+d+1} dr \int_S e \otimes e J ds,
\]
where $S$ is the surface of the $d$-dimensional unit sphere and $J$ is the Jacobean. It is readily seen that $\int_S e \otimes e ds$ is isotropic and given as $\frac{S}{d} \delta$ where $S$ is the area of $S$. In view of
\[
\int_0^r r^{m+d+1} dr = \left\{ \begin{array}{ll}
\frac{r^{m+d+2}}{m+d+2} & \text{for } m \neq -d-2, \\
\log r & \text{for } m = -d-2
\end{array} \right.
\]
we prove Eq. (12).

Appendix B ALTERNATIVE OF $|x|^2$

Denote by $\psi(r)$ a smooth function that is bounded at $r = 0$ and vanishes as $r$ increases. Multiplying the both sides of Eq. (1) with $x \psi(|x|)$ and integrating over $V$, we have
\[
\left( \int_V x \otimes x \psi(|x|) \frac{dv}{|x|^2} \right) \cdot \nabla f(0) = \int_V (f(x) - f(0)) x \psi(|x|) dv.
\]
Note that this equation becomes Eq. (11) if $\psi$ is replaced by $|x|^m$.

As explained in Appendix A, using $x = re$, we can calculate the volume integral on the left side as
\[
\int_V x \otimes x \psi(|x|) \frac{dv}{|x|^2} = \int_0^r r^2 \psi(r) J dr \int_S e \otimes e ds,
\]
where $J$ is the Jacobean that satisfies $dv = J dr ds$. The surface integral yields an isotropic tensor, $\frac{S}{d} \delta$. The volume integral on the right side is evaluated as
\[
\int_V (f(x) - f(0)) x \psi(|x|) dv = \sum \left( f^\alpha - f^0 \right) x^\alpha \psi(|x^\alpha|) v^\alpha,
\]
where $v^\alpha$ is a small volume element, which is approximatively computed using the collocation method ($v^\alpha = V/N$) or applying the midpoint rule ($v^\alpha = (x^{\alpha+1} - x^{\alpha-1})/2$ for $d = 1$).

We now arrive at the following evaluation of the gradient operator:
\[
\nabla f(0) = \frac{d}{S} \int_0^r r^2 \psi(r) dr \sum \left( f^\alpha - f^0 \right) x^\alpha \psi(|x^\alpha|) v^\alpha.
\]
As mentioned in Section 5, the presence of the third enigmatic term might correspond to the present $\psi$. However, we have to emphasize that $\nabla f(0)$ ought not to depend on $\psi$, just as $\nabla f(0)$ should not depend on $m$ for the use of $|\psi|^m$. We have to examine the contracting issue, i.e., the independence of $\nabla f(0)$ on $\psi$ and the choice of suitable $\psi$ that makes the estimation more accurate.

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