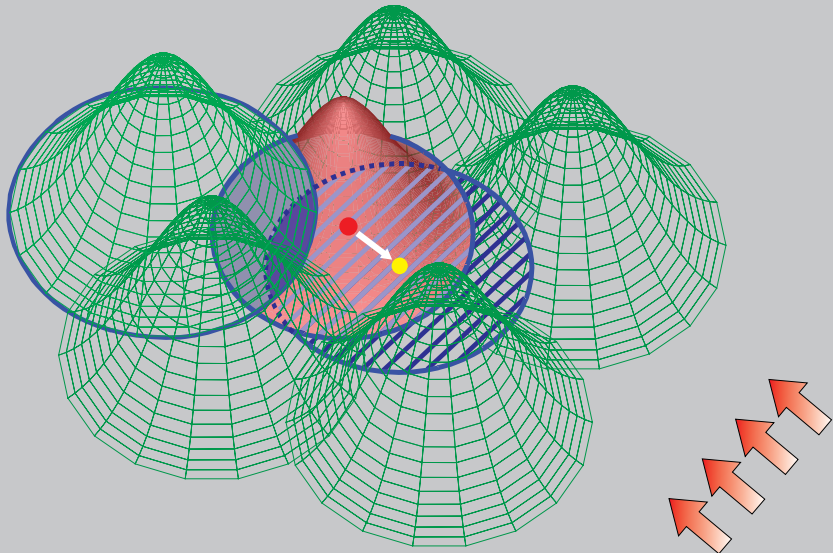


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Particle Methods for a 1D Elastic Model Problem: Error Analysis and Development of a Second-Order Accurate Formulation

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Abstract: Particle methods represent some of the most investigated meshless approaches, applied to numerical problems, ranging from solid mechanics to fluid-dynamics and thermo-dynamics. The objective of the present paper is to analyze some of the proposed particle formulations in one dimension, investigating in particular how the different approaches address second derivative approximation. With respect to this issue, a rigorous analysis of the error is conducted and a novel second-order accurate formulation is proposed. Hence, as a benchmark, three numerical experiments are carried out on the investigated formulations, dealing respectively with the approximation of the second derivative of given functions, as well as with the numerical solution of the static problem and with the approximation of the vibration frequencies for an elastic rod. In each test, the obtained numerical results are compared with exact solutions and the main criticalities of each formulation are addressed.

Keywords: Meshless Methods, Particle Methods, Reproducing Kernel Particle Methods, Second Order Finite Particle Method, Error Evaluation

1 Introduction

A variety of numerical methods has been recently proposed in the literature to address advanced mechanical problems, such as those involving rapid deformations, high intensity forces, large displacement fields. In many of these cases, in fact, classical finite element methods (FEM) suffer from mesh distortion, numerical spurious errors and, above all, mesh sensitiveness. Hence, to overcome such issues, a number of numerical methods, belonging to the family of the so-called meshless

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techniques, has been widely investigated and applied. The objective of employing these methods is to avoid the introduction of a mesh for the continuum, preferring a particle discretization, with the goal of obtaining an easier treatment of large and rapid displacements. Thus, meshless methods have been widely applied, mainly to fluid dynamics problems, where particle approaches appear to be more feasible. However, recently, a number of researchers have tried to extend meshless methods also to solid mechanics problems.

Among the several meshless numerical methods proposed, particle methods, and in particular Smoothed Particle Hydrodynamics (SPH), have been widely implemented and investigated. Historically, SPH was introduced by Lucy (1977) and Gingold and Monaghan (1977) to treat astrophysics problems, and, then, a variety of formulations has been proposed to apply its principles to different problems, such as incompressible flows (Monaghan, 1994), elasticity (Lidersky and Petschek, 1991), fracture of solids (Benz and Asphaug, 1994, 1995), heat conduction (Cleary and Monaghan, 1994), large deformations (Wong and Shie, 2008), explosions (Ma, Zhang, Lian and Zhou, 2009). Furthermore, in order to address a number of criticalities and issues, several improvements have been proposed: for instance, Swegle, Hicks and Attaway (1995) highlighted “tension instability”, fixing it through a viscosity-based procedure whereas Dyka, Randles and Ingel (1997) and Randles and Libersky (2000) addressed the same problem through a stress point procedure; Johnson and Beissel (1996) proposed a method to improve strain calculation and Liu, Jun, Li and Zhang (1995) and Liu, Jun, Li, Adee and Belytschko (1995) introduced the so-called Reproducing Kernel Particle Method (RKPM) to overcome deficiencies occurring on the boundary. Nowadays, SPH represents itself a family of methods, given the large variety of formulations available in the literature stemmed from the original SPH approach.

The main objective of the present paper is to analyze some of the proposed particle formulations in a one dimensional setting, where a rigorous error analysis can be conducted. In particular, beside the original SPH approach, we focus on the following methods:

- Chen Beraun’s SPH formulation (Chen and Beraun, 2000);
- Finite Particle Method (FPM) (Batra and Zhang, 2004; Liu, Xie and Liu, 2005);
- first and second-order RKPM methods (Liu, Jun, Li and Zhang, 1995; Liu, Jun, Li, Adee and Belytschko, 1995; Jun, Liu and Belytschko, 1998).

Finally, we also propose a novel enhanced SPH-like procedure, based on FPM and able to guarantee second-order accurate approximations, called in the following

“second-order FPM”. Accordingly, the present paper starts with a brief introduction to classical SPH methods, followed by a review of the methods listed above and by a presentation of the main proposed methodology. Then all numerical schemes are tested against three different 1D benchmarks, all dealing with second derivative approximation, i.e.:

- Derivative test: approximation of second derivatives of given functions and evaluation of the convergence order.
- Elastic static test: approximation of the displacements of an elastic rod and evaluation of the convergence order.
- Elastic vibration test: evaluation of the eigenvalues of an elastic rod.

Finally, conclusions arising from the conducted investigations are presented and discussed.

2 Classical SPH Approach

The classical SPH approximation procedure (Lucy , 1977; Gingold and Monaghan , 1977) takes its origin from the fact that, for a generic function $B(x)$ defined in a continuous domain Ω , the value of the function in a generic point x_i can be expressed using the following relationship

$$B(x_i) = \int_{\Omega} B(x) \delta_i(x) d\Omega, \quad (1)$$

where $\delta_i(x)$ is the Dirac’s function centered in x_i . A first approximation of the above relation can be introduced replacing the Dirac’s delta with a smooth “kernel” function $W_i(x)$,

$$B(x_i) \cong \int_{\Omega} B(x) W_i(x) d\Omega. \quad (2)$$

The approximation clearly depends on how the kernel function approximates the Dirac’s delta and, so, in the original works (Lucy , 1977; Gingold and Monaghan , 1977), W_i was required to satisfy at least the following conditions:

- (1) $W_i(x) \geq 0, \forall x \in \Omega$;
- (2) $\int_{\Omega} W_i(x) d\Omega = 1$;
- (3) $W_i(x)$ regular enough, i.e., derivable many times with continuous derivatives;
- (4) $W_i(x)$ defined on a compact support.

Kernel functions may assume different expressions, but typically Gaussian or spline functions are used. Gaussian functions are often preferred, even if they do not respect the last of the listed properties. However, for practical purposes they are considered negligible outside a compact region that, with abuse of notation, is referred to as support. The diameter measure of such a support is called *smoothing length*, and is denoted by the parameter h . As h approaches zero, the kernel approaches a Dirac's delta.

A second approximation may now be introduced performing a discretization of the domain Ω , introducing a partition of Ω into a finite number N of subdomains $\Delta\Omega_j$, such that

$$\bigcup_{j=1}^N \Delta\Omega_j = \Omega. \quad (3)$$

A centroid x_j , referred to as *particle*, may be associated to each subdomain $\Delta\Omega_j$; then, equation (2) is further approximated substituting the integration with a summation of the integrand function, computed at the centroids x_j , and weighted using $\Delta\Omega_j$, i.e.

$$B(x_i) \cong \sum_{j=1}^N B(x_j) W_i(x_j) \Delta\Omega_j. \quad (4)$$

Observe that, with some abuse of notation, we denote with $\Delta\Omega_j$ both the subdomain and its measure. This approximation step can be interpreted as a numerical quadrature of equation (2).

3 Approximation of Derivatives

To obtain an expression for the approximation of derivatives via the SPH approach, several procedures may be proposed. The following paragraphs examine and compare some of the most significant methods available in the literature, investigating in particular the corresponding error orders. For the sake of simplicity, only the 1D case is discussed.

3.1 Original formulation

Following the original formulation proposed by Gingold and Monaghan (1977) and applying the “first approximation step” to the derivative of a generic function $B(x)$ (we remark that the differential operator is here indicated as “D”), the following relationship is obtained

$$DB(x_i) \cong \int_{\Omega} DB(x) W_i(x) d\Omega. \quad (5)$$

Employing Green's formula yields

$$DB(x_i) \cong \int_{\partial\Omega} B(x)W_i(x)ndS - \int_{\Omega} B(x)DW_i(x)d\Omega, \quad (6)$$

where $\partial\Omega$ is the boundary of Ω and n is the outward normal. If W_i is compactly supported in Ω , the first term of the right-hand-side of equation (6) is null, leading to

$$DB(x_i) \cong - \int_{\Omega} B(x)DW_i(x)d\Omega. \quad (7)$$

After discretization, by means of numerical quadrature we then obtain

$$DB(x_i) \cong - \sum_{j=1}^N B(x_j)DW_i(x_j)\Delta\Omega_j. \quad (8)$$

Accordingly, given the values $B(x_j)$, we can compute the quantities $DB(x_i)$ in a typical SPH fashion. Expression (7) is a "reasonable" approximation in the interior of Ω ; indeed, it is exact at least on constant functions when W_i is null (or negligible) on $\partial\Omega$, which implies

$$\int_{\Omega} DW_i = 0. \quad (9)$$

However, close to the boundary, that is, when W_i is not negligible on $\partial\Omega$, typically such an assumption fails, and approximations (7) and (8) deteriorate. To overcome this difficulty, many authors suggest to replace (7) by

$$DB(x_i) \cong \int_{\Omega} [B(x_i) - B(x)] DW_i(x)d\Omega. \quad (10)$$

Observe that (7) and (10) are equivalent when (9) holds, but (10) is always exact on constants. Discretizing (10), we obtain

$$DB(x_i) \cong \sum_{j=1}^N [B(x_i) - B(x_j)] DW_i(x_j)\Delta\Omega_j. \quad (11)$$

To obtain also the second derivative, this procedure can be reiterated, giving rise to the following expression

$$D^2B(x_i) \cong \sum_{j=1}^N [DB(x_i) - DB(x_j)] DW_i(x_j)\Delta\Omega_j. \quad (12)$$

It is important to remark that, though being an improvement with respect to (8), expression (11) is still not fully satisfactory, since it could be proven that it does not converge when evaluated close to the boundary (as proven in the next subsection). This motivates the development of other approaches.

3.2 Chen and Beraun's formulation

Chen and Beraun (2000) proposed a generalized SPH formulation, directly derived by Taylor's expansion of $B(x)$ up to the first derivative term, i.e.

$$B(x) = B(x_i) + (x - x_i)DB(x_i) + O(|x - x_i|^2). \quad (13)$$

In fact, multiplying both sides of equation (13) by $DW_i(x)$ and integrating over Ω yields

$$\int_{\Omega} B(x) DW_i(x) d\Omega = \int_{\Omega} B(x_i) DW_i(x) d\Omega + \int_{\Omega} (x - x_i) DB(x_i) DW_i(x) d\Omega + e, \quad (14)$$

where $e = \|DW_i\|_{L^1} \cdot O(h^2)$ is the approximation error (second-order, in this case) and $\|\cdot\|_{L^1} = \int_{\Omega} |\cdot| d\Omega$ is the L^1 -norm. From (14), we then readily get

$$DB(x_i) = \frac{\int_{\Omega} [B(x) - B(x_i)] DW_i(x) d\Omega}{\int_{\Omega} (x - x_i) DW_i(x) d\Omega} + \frac{e}{\int_{\Omega} (x - x_i) DW_i(x) d\Omega}. \quad (15)$$

Since $\int_{\Omega} (x - x_i) DW_i(x) d\Omega \cong \|DW_i\|_{L^1} \cdot h$, neglecting the second term in the right-hand-side of the previous equation results in an error of order $O(h)$. Notice that, if the second-order momentum of DW_i , $\int_{\Omega} (x - x_i)^2 DW_i d\Omega$, is null or negligible, as it typically happens far from the boundary, then $e = \|DW_i\|_{L^1} \cdot O(h^3)$ and (15) turns out to be second-order accurate when e is neglected. This is not the case, however, in a neighborhood of the boundary $\partial\Omega$. Then, discretizing by numerical quadrature, the following relationship holds

$$DB(x_i) \cong \frac{\sum_{j=1}^N [B(x_j) - B(x_i)] DW_i(x_j) \Delta\Omega_j}{\sum_{j=1}^N (x_j - x_i) DW_i(x_j) \Delta\Omega_j}. \quad (16)$$

It can be observed that this expression is different from the original formulation (11), because it presents as denominator the static momentum of the derivative of the kernel function. Since the formulation is derived from Taylor's formula truncated at the first order, such a denominator can be considered as a correction factor, which allows to obtain a first-order approximation everywhere. Hence, if we adopt (11) instead of (16), we clearly obtain a method which is first-order where the missing denominator is close to 1 (i.e., far from the boundary) and not necessarily converging where the missing denominator is far from 1 (i.e., close to the boundary).

In order to obtain an expression for the second derivative, the procedure is reiterated starting from the Taylor's formula up to the second derivative, i.e.

$$B(x) = B(x_i) + (x - x_i)DB(x_i) + \frac{1}{2}(x - x_i)^2 D^2B(x_i) + O(|x - x_i|^3). \quad (17)$$

Multiplying both sides of (17) by $W_i(x)$ and integrating over the domain Ω yields

$$\int_{\Omega} B(x) W_i(x) d\Omega = \int_{\Omega} B(x_i) W_i(x) d\Omega + \int_{\Omega} (x - x_i) DB(x_i) W_i(x) d\Omega + \frac{1}{2} \int_{\Omega} (x - x_i)^2 D^2B(x_i) W_i(x) d\Omega + e, \quad (18)$$

where, in this case, $e = \|W_i\|_{L^1} \cdot O(h^3)$. Then, from (18), it follows

$$D^2B(x_i) = \frac{\int_{\Omega} (B(x) - B(x_i)) W_i(x) d\Omega - DB(x_i) \int_{\Omega} (x - x_i) W_i(x) d\Omega}{\frac{1}{2} \int_{\Omega} (x - x_i)^2 W_i(x) d\Omega} + \frac{e}{\frac{1}{2} \int_{\Omega} (x - x_i)^2 W_i(x) d\Omega}. \quad (19)$$

Also in this case, as in the expression for the first derivative, neglecting the error term in the right-hand-side introduces a $O(h)$ error. Far from the boundary, the term e increases again its order, becoming $\|W_i\|_{L^1} \cdot O(h^4)$, since the third order momentum of W_i vanishes; hence (19) becomes second-order accurate when e is neglected. After discretization, we finally obtain

$$D^2B(x_i) = \frac{\sum_{j=1}^N (B(x_j) - B(x_i)) W_i(x_j) \Delta\Omega_j - DB(x_i) \sum_{j=1}^N (x_j - x_i) W_i(x_j) \Delta\Omega_j}{\frac{1}{2} \sum_{j=1}^N (x_j - x_i)^2 W_i(x_j) \Delta\Omega_j}. \quad (20)$$

It should be mentioned that the proposed procedure can also be used to solve the typical SPH tension instability issue, as shown by Chen, Beraun and Jih (1999).

3.3 RKPM method

Introduced in the papers by Liu, Jun, Li and Zhang (1995), Liu, Jun, Li, Adee and Belytschko (1995), and Jun, Liu and Belytschko (1998), this method has been widely employed to correct SPH classical formulations improving their accuracy (see, e.g., Bonet and Kulasegaram (2001); Bonet and Kulasegaram (2002); and

Vidal, Bonet and Huerta (2007)). The key idea is to replace (2) by an improved representation

$$B(x_i) \cong \int_{\Omega} B(x) K_i(x) d\Omega. \quad (21)$$

where $K_i(x)$ is a particular kernel function modified for each particle as

$$K_i(x) = C_i(x) \cdot W_i(x), \quad (22)$$

where W_i is a classical Gaussian function and C_i is a polynomial, i.e.:

$$C_i(x) = a_i + b_i(x - x_i) + c_i(x - x_i)^2 + \dots \quad (23)$$

Starting from Taylor's series expansion and projecting it against K_i yields

$$\begin{aligned} \int_{\Omega} B(x) K_i(x) d\Omega &= B(x_i) \int_{\Omega} K_i(x) d\Omega + DB(x_i) \int_{\Omega} (x - x_i) K_i(x) d\Omega + \\ &\quad \frac{1}{2} D^2 B(x_i) \int_{\Omega} (x - x_i)^2 K_i(x) d\Omega + \dots \end{aligned} \quad (24)$$

Then, we impose that the zeroth-order momentum (i.e., the integral) of K_i is equal to one, and that higher-order momenta of K_i are null. Such conditions allow to define an algebraic system whose unknowns are the coefficients of the polynomial C_i in (23). Solving this system for each particle within the domain leads to determine the kernel functions K_i .

If only the first-order momentum of K_i is forced to be zero, the error of the Taylor's series expansion in equation (24) is second-order; hence, this approach is hereafter referred to as first-order RKPM. If, instead, both the first- and the second-order momenta of K_i are forced to be zero, the term e in equation (24) represents a third-order error and the approach is referred to as second-order RKPM.

Once "corrected" kernel functions are determined, derivatives can be expressed, adopting a classical SPH approach, through the following equations

$$DB(x_i) \cong \sum_{j=1}^N [B(x_i) - B(x_j)] DK_i(x_j) \Delta\Omega_j, \quad (25)$$

$$D^2 B(x_i) \cong \sum_{j=1}^N [DB(x_i) - DB(x_j)] DK_i(x_j) \Delta\Omega_j, \quad (26)$$

which are completely similar to (11) and (12).

It should be mentioned that the evaluation of the second derivatives through this approach is also discussed in Bonet and Kulasegaram (2000).

3.4 FPM formulation

Batra and Zhang (2004) and Liu, Xie and Liu (2005) independently proposed a different formulation to determine at the same time a function $B(x)$ and its derivatives, afterward referred to, in the literature, as Finite Particle Method (FPM). The basic idea is to project Taylor's formula on a number of independent functions. This provides a linear algebraic system for each particle x_i , whose unknowns are the approximations at x_i of the function $B(x)$ and its derivatives, up to the order of Taylor's formula. Hence, in the 1D case, considering a series expansion up to the first-order and employing as projecting function a kernel function $W_i(x)$ and its derivative $DW_i(x)$, the following relationships are obtained

$$B(x_i) \int_{\Omega} W_i(x) d\Omega + DB(x_i) \int_{\Omega} (x - x_i) W_i(x) d\Omega = \int_{\Omega} B(x) W_i(x) d\Omega + e'_1, \quad (27)$$

$$B(x_i) \int_{\Omega} DW_i(x) d\Omega + DB(x_i) \int_{\Omega} (x - x_i) DW_i(x) d\Omega = \int_{\Omega} B(x) DW_i(x) d\Omega + e'_2, \quad (28)$$

where e'_1 and e'_2 represent the errors due to series truncation. Thus, defining

$$\begin{aligned} A_{11} &= \int_{\Omega} W_i(x) d\Omega, & A_{12} &= \int_{\Omega} (x - x_i) W_i(x) d\Omega, \\ A_{21} &= \int_{\Omega} DW_i(x) d\Omega, & A_{22} &= \int_{\Omega} (x - x_i) DW_i(x) d\Omega \end{aligned} \quad (29)$$

equations (27) and (28) can be re-arranged as

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} B(x_i) \\ DB(x_i) \end{bmatrix} = \begin{bmatrix} \int_{\Omega} B(x) W_i(x) d\Omega \\ \int_{\Omega} B(x) DW_i(x) d\Omega \end{bmatrix} + \begin{bmatrix} e'_1 \\ e'_2 \end{bmatrix}. \quad (30)$$

Neglecting error terms e'_1 and e'_2 , these equations represent a linear algebraic system which can be solved with respect to $B(x_i)$ and $DB(x_i)$. To assess the corresponding error, the following considerations can be made. For particles far from the boundary, the associated kernel functions are negligible on the domain boundary; hence, given that $DW_i(x)$ is a skew-symmetric function, its second-order momentum vanishes and we have that $e'_2 = \|DW_i\|_{L^1} \cdot O(h^3)$. Being $W_i(x)$ symmetric, we also have that $e'_1 = \|W_i\|_{L^1} \cdot O(h^2)$. Moreover, considering again the symmetry of $W_i(x)$ and the skew-symmetry of $DW_i(x)$, the terms A_{12} and A_{21} vanish and the system yields

$$\begin{bmatrix} B(x_i) \\ DB(x_i) \end{bmatrix} = \begin{bmatrix} \int_{\Omega} B(x) W_i(x) d\Omega / A_{11} \\ \int_{\Omega} B(x) DW_i(x) d\Omega / A_{22} \end{bmatrix} + \begin{bmatrix} e'_1 / A_{11} \\ e'_2 / A_{22} \end{bmatrix}. \quad (31)$$

Being $A_{11} = C \cdot \|W_i\|_{L^1}$ and $A_{22} = Ch \cdot \|DW_i\|_{L^1}$, the error introduced neglecting e'_1 and e'_2 for the evaluation of $B(x)$ and its first derivative, equal to e'_1/A_{11} and e'_2/A_{22} respectively, is $O(h^2)$ in both cases.

On the other hand, for particles close to the boundary, both functions $W_i(x)$ and $DW_i(x)$ are not completely developed; we thus have that $e'_1 = \|W_i\|_{L^1} \cdot O(h^2)$ and $e'_2 = \|DW_i\|_{L^1} \cdot O(h^2)$. Moreover, close to the boundary, terms A_{12} and A_{21} do not vanish; hence the error introduced on $B(x_i)$ and $DB(x_i)$ neglecting e'_1 and e'_2 can be evaluated as

$$\begin{aligned}
 & \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}^{-1} \begin{bmatrix} e'_1 \\ e'_2 \end{bmatrix} \\
 & \cong \left(\begin{bmatrix} \|W_i\|_{L^1} & 0 \\ 0 & \|DW_i\|_{L^1} \end{bmatrix} \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & h \end{bmatrix} \right)^{-1} \begin{bmatrix} \|W_i\|_{L^1} \cdot O(h^2) \\ \|DW_i\|_{L^1} \cdot O(h^2) \end{bmatrix} \\
 & = \begin{bmatrix} 1 & 0 \\ 0 & h^{-1} \end{bmatrix} \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix}^{-1} \begin{bmatrix} \|W_i\|_{L^1}^{-1} & 0 \\ 0 & \|DW_i\|_{L^1}^{-1} \end{bmatrix} \begin{bmatrix} \|W_i\|_{L^1} \cdot O(h^2) \\ \|DW_i\|_{L^1} \cdot O(h^2) \end{bmatrix} \\
 & = \begin{bmatrix} O(h^2) \\ O(h) \end{bmatrix},
 \end{aligned} \tag{32}$$

where C_{11} , C_{12} , C_{21} and C_{22} represent constant terms. As a consequence, the evaluation of $DB(x_i)$ is affected by an error of order h^2 inside the domain and of order h close to the boundary. Trying to evaluate also the second derivative of the function $B(x)$, the procedure can be in principle reiterated. Unfortunately, this operation causes a propagation of the error, making the formulation not converging.

3.5 Modified FPM formulation

To overcome the problems highlighted above and to have a converging solution also for the second derivative, a slightly different procedure is here proposed and discussed. In case the values of $B(x_i)$ do not represent real unknowns, the system can be rearranged to introduce also the second derivatives. In fact, introducing the Taylor's expansion for $B(x)$ up to the second order, multiplying it once by $W_i(x)$ and once by $DW_i(x)$, and integrating, the following relationships are obtained

$$\begin{aligned}
 & DB(x_i) \left[\int_{\Omega} (x-x_i) W_i(x) d\Omega \right] + \frac{1}{2} D^2 B(x_i) \left[\int_{\Omega} (x-x_i)^2 W_i(x) d\Omega \right] \\
 & = \int_{\Omega} [B(x) - B(x_i)] W_i(x) d\Omega + e''_1,
 \end{aligned} \tag{33}$$

$$\begin{aligned}
 & DB(x_i) \left[\int_{\Omega} (x-x_i) DW_i(x) d\Omega \right] + \frac{1}{2} D^2 B(x_i) \left[\int_{\Omega} (x-x_i)^2 DW_i(x) d\Omega \right] \\
 & = \int_{\Omega} [B(x) - B(x_i)] DW_i(x) d\Omega + e''_2,
 \end{aligned} \tag{34}$$

where terms e_1'' and e_2'' represent the errors due to series truncation. Then, defining

$$\begin{aligned} A_{11} &= \int_{\Omega} (x - x_i) W_i(x) \, d\Omega, & A_{12} &= \frac{1}{2} \int_{\Omega} (x - x_i)^2 W_i(x) \, d\Omega, \\ A_{21} &= \int_{\Omega} (x - x_i) DW_i(x) \, d\Omega, & A_{22} &= \frac{1}{2} \int_{\Omega} (x - x_i)^2 DW_i(x) \, d\Omega, \end{aligned} \quad (35)$$

equations (33) and (34) can be re-arranged as

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} DB(x_i) \\ D^2B(x_i) \end{bmatrix} = \begin{bmatrix} \int_{\Omega} [B(x) - B(x_i)] W_i(x) \, d\Omega \\ \int_{\Omega} [B(x) - B(x_i)] DW_i(x) \, d\Omega \end{bmatrix} + \begin{bmatrix} e_1'' \\ e_2'' \end{bmatrix}. \quad (36)$$

In this case, conducting a discussion similar to the previous case, it can be observed that, far from the boundary, given that $W_i(x)$ is a symmetric function, its third-order momentum is null and $e_1'' = \|W_i\|_{L^1} \cdot O(h^4)$, whereas $e_2'' = \|DW_i\|_{L^1} \cdot O(h^3)$. Moreover, due to the symmetry of $W_i(x)$ and to the skew-symmetry of $DW_i(x)$, terms A_{11} and A_{22} vanish, yielding

$$\begin{bmatrix} DB(x_i) \\ D^2B(x_i) \end{bmatrix} = \begin{bmatrix} \int_{\Omega} [B(x) - B(x_i)] DW_i(x) \, d\Omega / A_{21} \\ \int_{\Omega} [B(x) - B(x_i)] W_i(x) \, d\Omega / A_{12} \end{bmatrix} + \begin{bmatrix} e_2'' / A_{21} \\ e_1'' / A_{12} \end{bmatrix}. \quad (37)$$

Given that A_{12} is proportional to $h^2 \cdot \|W_i\|_{L^1}$ and A_{21} is proportional to $h \cdot \|DW_i\|_{L^1}$, the error related to first and second derivative evaluation is $O(h^2)$.

Instead, close to the boundary, functions $W_i(x)$ and $DW_i(x)$ are not completely developed and we have that $e_1'' = \|W_i\|_{L^1} \cdot O(h^3)$ and $e_2'' = \|DW_i\|_{L^1} \cdot O(h^3)$. Terms A_{11} and A_{22} do not vanish and the error introduced neglecting e_1'' and e_2'' can be evaluated as

$$\begin{aligned} & \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}^{-1} \begin{bmatrix} e_1'' \\ e_2'' \end{bmatrix} \\ & \simeq \left(\begin{bmatrix} \|W_i\|_{L^1} & 0 \\ 0 & \|DW_i\|_{L^1} \end{bmatrix} \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix} \begin{bmatrix} h & 0 \\ 0 & h^2 \end{bmatrix} \right)^{-1} \begin{bmatrix} \|W_i\|_{L^1} \cdot O(h^3) \\ \|DW_i\|_{L^1} \cdot O(h^3) \end{bmatrix} \\ & = \begin{bmatrix} h^{-1} & 0 \\ 0 & h^{-2} \end{bmatrix} \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix}^{-1} \begin{bmatrix} \|W_i\|_{L^1}^{-1} & 0 \\ 0 & \|DW_i\|_{L^1}^{-1} \end{bmatrix} \begin{bmatrix} \|W_i\|_{L^1} \cdot O(h^3) \\ \|DW_i\|_{L^1} \cdot O(h^3) \end{bmatrix} \\ & = \begin{bmatrix} O(h^2) \\ O(h) \end{bmatrix}. \end{aligned} \quad (38)$$

Hence, the maximum error related to first and second derivative evaluation is of the order of h^2 far from the boundary and of the order of h close to it.

4 A Novel Second-Order FPM Formulation

Aiming at obtaining in the whole domain a second-order accurate estimate of the second derivative, a novel FPM-based procedure is here proposed. Based on a modification of the kernel functions, this method is able to overcome the reduction of accuracy occurring close to the boundary. The basic idea to achieve this goal is to construct kernel functions satisfying particular conditions, taking their basis from the error evaluation procedure conducted in the previous section.

Similarly to RKPM, we define:

$$K_i(x) = C_i(x) \cdot W_i(x), \quad (39)$$

where $W_i(x)$ are the classical Gaussian kernel functions and

$$C_i(x) = a \left(\frac{x - x_i}{h} \right)^3 + b \frac{x - x_i}{h} + c \quad (40)$$

are polynomials to be determined by the following conditions:

$$\begin{aligned} \int_{\Omega} K_i(x) \, d\Omega &= 1, \\ \int_{\Omega} (x - x_i) K_i(x) \, d\Omega &= 0, \\ \int_{\Omega} (x - x_i)^3 K_i(x) \, d\Omega &= 0, \end{aligned} \quad (41)$$

with $i = 1, 2, \dots, N$, i.e. for each particle. Imposing the above conditions directly in the discrete setting, we obtain

$$\begin{aligned} \sum_{j=1}^N K_i(x_j) \Delta\Omega_j &= 1, \\ \sum_{j=1}^N (x_j - x_i) K_i(x_j) \Delta\Omega_j &= 0, \\ \sum_{j=1}^N (x_j - x_i)^3 K_i(x_j) \Delta\Omega_j &= 0. \end{aligned} \quad (42)$$

The choice of the polynomial (40) guarantees that the linear system given by (42) for the determination of the coefficients a , b , and c is nonsingular for all i . Instead, a quadratic polynomial $C_i(x) = a((x - x_i)/h)^2 + b(x - x_i)/h + c$ would give a singular or close to singular system when x_i is far from the boundary. Moreover, observe that the Gaussian kernel functions on an infinite domain naturally verify the previous conditions, therefore $K_i(x) = W_i(x)$ far from the boundary. So, only kernel functions close to the boundary $\partial\Omega$ are effectively modified.

Then, as in the modified FPM formulation, projecting the Taylor's series expansion against the functions $K_i(x)$ and $DK_i(x)$, the following algebraic linear system in terms of the derivatives of $B(x)$ is obtained for each particle:

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} DB(x_i) \\ D^2B(x_i) \end{bmatrix} = \begin{bmatrix} \int_{\Omega} [B(x) - B(x_i)] K_i(x) d\Omega \\ \int_{\Omega} [B(x) - B(x_i)] DK_i(x) d\Omega \end{bmatrix} + \begin{bmatrix} e_1''' \\ e_2''' \end{bmatrix}, \quad (43)$$

where A_{11} and A_{12} are the first and second momenta of K_i , A_{21} and A_{22} are the first and second momenta of DK_i (see for example equations (35)); finally, e_1''' and e_2''' represent the errors due to series truncation. As a consequence of conditions (41), or (42), we have $A_{11} = 0$, $e_1''' = \|K_i\|_{L^1} \cdot O(h^4)$, and, as usual, $e_2''' = \|DK_i\|_{L^1} \cdot O(h^3)$, for every i . Thus, the error on the evaluation of the first and second derivative of B is

$$\begin{aligned} & \begin{bmatrix} 0 & A_{12} \\ A_{21} & A_{22} \end{bmatrix}^{-1} \begin{bmatrix} e_1''' \\ e_2''' \end{bmatrix} \\ & \cong \left(\begin{bmatrix} \|K_i\|_{L^1} & 0 \\ 0 & \|DK_i\|_{L^1} \end{bmatrix} \begin{bmatrix} 0 & C_{12} \\ C_{21} & C_{22} \end{bmatrix} \begin{bmatrix} h & 0 \\ 0 & h^2 \end{bmatrix} \right)^{-1} \begin{bmatrix} \|K_i\|_{L^1} \cdot O(h^4) \\ \|DK_i\|_{L^1} \cdot O(h^3) \end{bmatrix} \\ & = \begin{bmatrix} h^{-1} & 0 \\ 0 & h^{-2} \end{bmatrix} \begin{bmatrix} -C_{22}C_{12}^{-1}C_{21}^{-1} & C_{21}^{-1} \\ C_{12}^{-1} & 0 \end{bmatrix} \begin{bmatrix} \|K_i\|_{L^1}^{-1} & 0 \\ 0 & \|DK_i\|_{L^1}^{-1} \end{bmatrix} \begin{bmatrix} \|K_i\|_{L^1} \cdot O(h^4) \\ \|DK_i\|_{L^1} \cdot O(h^3) \end{bmatrix} \\ & = \begin{bmatrix} O(h^2) \\ O(h^2) \end{bmatrix}. \end{aligned} \quad (44)$$

It is therefore clear that the employed conditions allow to obtain at least a second-order error everywhere in the domain.

5 Numerical Tests

To assess the performance of the discussed formulations, the following three different sets of numerical tests are performed:

- Derivative test: second derivatives of known functions are evaluated via particle formulations and the results are compared with the exact solution. The order of convergence of the obtained solutions is determined as well.
- Elastic static test: the displacements of an elastic rod are determined via particle procedures, given boundary conditions and body load; results are then compared with the exact solution and the order of convergence of the obtained solutions is determined as well.

- Elastic vibration test: again referring to an elastic rod, the eigenvalue problem is addressed, determining the errors related to numerically obtained spectra.

Such tests have been conducted using the different SPH-based approaches discussed in previous sections, i.e., in particular:

- original formulation (see section 3.1 for more details);
- Chen and Beraun's formulation (see section 3.2);
- first and second-order RKPM (see section 3.3);
- modified FPM (see section 3.5);
- novel second-order FPM (see section 4).

All tests are carried out on the domain $\Omega = [0, 1]$, with a uniformly spaced particle discretization. A Gaussian function, with h equal to the distance between two consecutive particles, is considered as the basic kernel function.

5.1 Derivative test

The aim of this first test is to evaluate the approximation, obtained through the discussed formulations, of the second derivative $f''(x)$ of a given functions $f(x)$, here assumed here to be $f(x) = e^x$.

To evaluate convergence orders, the infinity norm (i.e., the maximum of the absolute value) of the difference between the exact and the numerical solution is computed for each investigated formulation. These values are plotted in logarithmic scale, as a function of the number of particles, in Figures 1; the slope of the obtained curves indicates the order of convergence. It can be observed that the original formulation, the RKPM, and the Chen and Beraun's formulations appear to be not converging. This happens because the infinity norm of the error is governed by the maximum error in the domain, which occurs on the boundary. On the contrary, in the FPM formulations the infinity norm of the error decreases as the particle number increases. In particular, it is possible to see that the modified FPM shows a first-order convergence, while the novel FPM approach shows, as expected, a second-order convergence. Moreover, to test the robustness of the novel formulation, a random perturbation of maximum amplitude $\delta/4$ (where δ is the distance between two consecutive particles) has been applied to the particle distribution. Also in this case a second-order convergence is obtained.

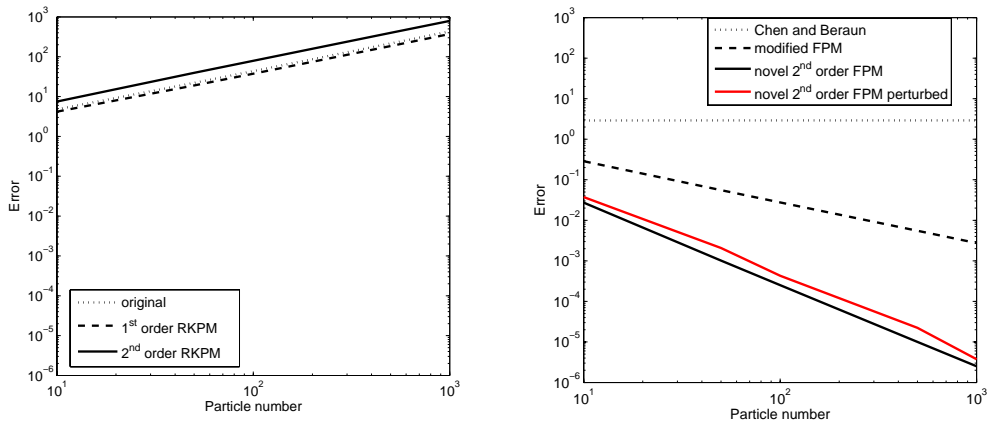


Figure 1: Infinity norm error in the second derivative approximation versus particle number for an exponential function.

5.2 Elastic static test

The aim of this test is to address the static problem for an elastic rod (assumed to have unitary length and axial stiffness), determining the axial displacement u at particle positions given an axial body load f , and comparing the obtained results with the exact solution. The second order differential equation governing the problem is

$$-u'' = f, \quad (45)$$

with appropriate boundary conditions. In particular, we consider $f = e^x$, a clamped end for $x = 0$ and a traction-free condition for $x = 1$. So, we impose $u(0) = u'(1) = 0$ and the corresponding exact solution is $u = -e^x + ex + 1$.

Also in this case, the infinity norm of the difference between the exact and the numerical solution is evaluated for each investigated formulation, to study the order of convergence for the different formulations, and the results are reported in Figure 2. It can be observed that the FPM formulations present a second-order convergence, whereas Chen and Beraun's procedure is characterized by a first-order convergence. Instead, original formulation and first- and second-order RKPM are not convergent at all¹. We finally highlight the better performance, in terms of global error, of the novel FPM formulation with respect to the modified FPM in the second test case.

¹ In Figure 2 (left), it may seem that original formulation and first-order RKPM converge with order one, but, indeed, employing a larger number of particles makes clear that convergence is lost, as it happens for second-order RKPM.

Also in this test, the same perturbation of the particle distribution used for the previous case has been also considered for the novel FPM formulation. As it can be observed in Figure 2 (right) a second-order convergence is obtained, even in this case.

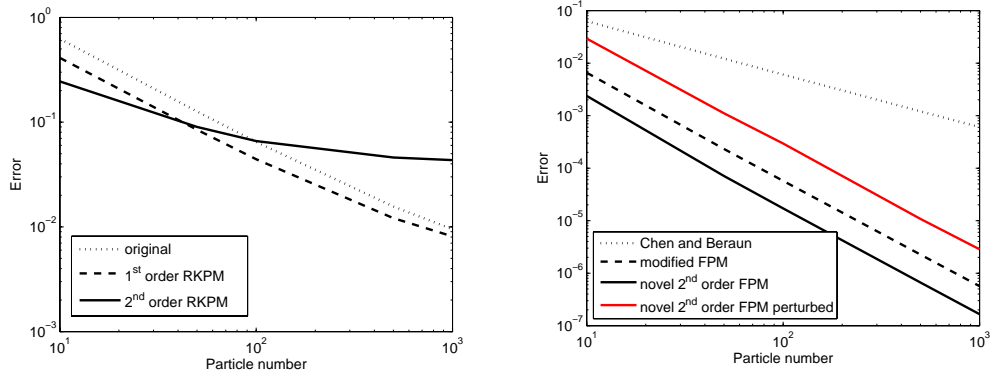


Figure 2: Displacement infinity norm error versus particle number for an exponential load, imposing a Dirichlet and a Neumann homogeneous boundary conditions.

5.3 Elastic vibration test

Also in this test we refer to an elastic rod, which is assumed to have unitary axial stiffness and density, with homogeneous Dirichlet boundary conditions:

$$x(0) = x(1) = 0. \quad (46)$$

The governing equation of the corresponding dynamic problem is

$$\frac{\partial^2 x}{\partial X^2} + \frac{\partial^2 x}{\partial t^2} = 0, \quad (47)$$

where X and x are the initial and the current configuration of the element, respectively.

In a stationary problem the following equation holds

$$\frac{\partial^2 x}{\partial t^2} = \omega^2 x, \quad (48)$$

where ω is the vibration frequency of the rod; hence, we may write

$$\frac{\partial^2 x}{\partial X^2} + \omega^2 x = 0, \quad (49)$$

and the solution of this differential equation is given by

$$x = \sin(\omega X). \quad (50)$$

Thus, imposing boundary conditions, we may find natural frequencies as

$$\omega_n = \pi n, \quad (51)$$

where n is a positive integer.

The discrete counterpart of (49) is

$$\mathbf{K}\mathbf{x} + \omega^2\mathbf{x} = 0, \quad (52)$$

where \mathbf{K} is the stiffness matrix associated to the second-order discrete derivative (note that, assuming a unitary density, the mass matrix in SPH-based approaches is the identity). Hence, the eigenvalues of \mathbf{K} represent the numerical approximation of ω_n^2 for $n = 1, \dots, N$ with N the number of particles. The ratio between the numerically evaluated vibration frequencies and the corresponding exact ones can be computed for each vibration mode, giving rise to a normalized numerical spectrum.

Figure 3 reports the different normalized numerical spectra computed, employing 100 particles and using the different considered SPH-based methods as well as, for comparison reasons, using the standard linear finite element method (FEM); in particular the lumped mass case for the FEM has been used, given the similarities with the particle methods in the mass discretization approach. It can be observed that the original and RKPM formulations strongly underestimate vibration frequencies, also for lowest modes, presenting a rapidly decreasing spectrum (the original and the first-order RKPM formulation curves overlap in Figure 3). On the contrary, Chen and Beraun's, modified FPM and second-order FPM formulations show very similar results (the three curves overlap in the part of Figure 3 on the right), approximating much better (and in a fashion similar to FEM) the overall spectrum and, in particular, predicting well low frequencies. For comparison purposes, the spectra for higher order formulations of FEM can be found in Hughes (2000) or in Cottrell, Hughes and Reali (2007), Cottrell, Reali, Bazilevs and Hughes (2006) and Hughes, Reali, and Sangalli (2008).

6 Conclusions

In the present work several particle procedures are investigated in one dimension, with the goal of evaluating their performance in the approximation of derivatives and, as a consequence, in the approximation of static and dynamic elasticity problems. In particular, an analysis of the error has been conducted for the original

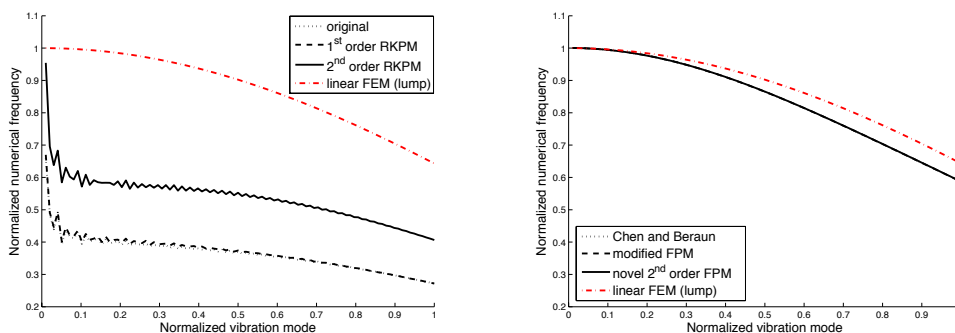


Figure 3: Normalized numerical spectra (using 100 particles).

SPH method, the Chen and Beraun's formulation, the RKPM procedures and a modified FPM formulation. The performed numerical tests reveal that the original and RKPM formulations appear to suffer of lack of accuracy in boundary zones, and perform poorly in frequency analysis. The modified FPM formulation, instead, presents second-order accuracy in approximating second derivatives inside the domain, but only first-order accuracy close to the boundary.

A novel method is also illustrated with the objective of overcoming such boundary deficiencies, coupling the projection procedure of FPM with enhanced kernel functions inspired by RKPM. In this way, second-order accuracy in approximating second derivatives is maintained even close to the boundary. The conducted numerical tests confirm these conclusions and, in particular, the second derivative tests highlight the improved accuracy provided by the proposed formulation. As a final word, it is underlined that the methodology is only presented in one dimension, since the extension to two and three dimensions appeared quite complicated to be implemented and since the purpose of this work is to show in a simple case the performance of the analyzed methods. However, with the same approach authors developed a further method, also based on the projection procedure and on enhanced kernel functions, which has been presented in the two-dimensional case in Asprone, Auricchio and Reali (2010).

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