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Mixed Strong Form Representation Particle Method for Solids and Structures

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Abstract. In this paper, a generalized particle system (GPS) method, a general method to describe multiple strong form representation based particle methods is described. Gradient, divergence, and Laplacian operators used in various strong form based particle method such as moving particle semi-implicit (MPS) method, smooth particle hydrodynamics (SPH), and peridynamics, can be described by the GPS method with proper selection of parameters. In addition, the application of mixed formulation representation to the GPS method is described. Based on Hu-Washizu principle and Hellinger-Reissner principle, the mixed form refers to the method solving multiple primary variables such as displacement, strain and stress, simultaneously in the FEM method; however for convenience in employing FEM with particle methods, a simple representation in construction only is shown. It is usually applied to finite element method (FEM) to overcome numerical errors including locking issues. While the locking issues do not arise in strong form based particle methods, the mixed form representation in construction only concept applied to GPS method can be the first step for fostering coupling of multi-domain problems, coupling mixed form FEM and mixed form representation GPS method; however it is to be noted that the standard GPS particle method and the mixed for representation construction GPS particle method are equivalent. Two dimensional simple bar and beam problems are presented and the results from mixed form GPS method is comparable to the mixed form FEM results.

Keywords: Particle method, Mixed form, Structural mechanics/dynamics.

1. Introduction

The finite element method (FEM) is, in simple terms, an approximation of an analytical solution, and therefore, some numerical problems that give incorrect solutions occurs under certain conditions. one of the common numerical errors in the finite element method is locking where FEM exhibits an overly stiff behavior introducing false stress and producing incorrect displacement solution.

There are numerous solution to these issues, one of which is called mixed form or sometimes referred to as hybrid form of the finite element method [1, 2]. In traditional FEM, the displacement is first solved and then the stress is calculated in post processing using the computed displacement. Therefore, the method is susceptible to artificial stress in locking problems. A mixed form in finite element method refers to an extension of FEM where the mathematical models involve several quantities that need to be solved simultaneously; for example, Hu-Washizu principle [3] takes displacement, strain, and stress as primary variables and Hellinger-Reissner principle [4] was developed to solve for displacement and stress simultaneously. As stress is no longer solely bounded by the displacement solution, the mixed form approach can resolve those issues.

Alternative to FEM, a large amount of research on the developments of mesh-free methods has been conducted to tackle various engineering applications, notably for crack propagation and large deformation analyses. Some of the widely known

mesh-free weak form based methods include the element free Galerkin (EFG) method [5, 6] and the meshless local Petrov-Galerkin (MLPG) method [7, 8]. In addition, there are also strong form based particle methods including moving particle semi-implicit (MPS) method [9], and smooth particle hydrodynamics (SPH) method [10]. While most of the weak form based mesh-free methods require a construction of background mesh, the strong form based particle methods are meshless in the way of discretizing a body into collection of particles. These strong form particle methods are widely used for fluid flow problems; in recent development, Shimada et al. [11] presented the MPS method implemented with unified explicit time integration algorithms, called the explicit GS4-II family of algorithms [12, 13, 14] which ensure a second-order time accuracy in all the unknowns with particular attention, for solving the incompressible fluids with free surfaces. However, these methods can be extended to solid mechanics problems as well. Chikazawa et al. [15] applied MPS method to elastic structures by interpreting the governing equation into interaction among particles using MPS method definition of gradient and Laplacian operators. Taking the common concept among these particle methods involving the idea of discretizing the system into collection of particles and computing each particle's behaviour based on the influence of their neighboring particles, a generalized particle system (GPS) method is developed to generalize formulation of these different particle methods using Taylor series expansion. Not only the GPS method can describe the discretization method of existing particle methods such as MPS, SPH and peridynamics, it can also introduce new conditions depending on the selection parameter.

To be on par with the finite element method, the mixed form representation concept can also be applied to the GPS method. Although, locking issues do not pertain to the particle methods as there is no interpolation approximation, we anticipate analogous advantages with mixed form approach in certain area simply from the viewpoint of fostering coupling multiple domains in a mixed representation. Unlike FEM where field variables and stress are independent, in this paper the mixed form GPS representation is fundamentally identical to the classical particle method representation; and the field variables and stresses are dependent. One of the possible uses may be found in fostering coupling of multiple domain problems where FEM is coupled with different particle methods for each domain. Likewise, the mixed form particle representation can easily be coupled with mixed form FEM with matching number of degrees of freedom for analysis purposes. The objective is to simply foster coupling domains but not provide new physics between classical particle methods and the mixed form representation of particle methods. This paper is the first attempt towards addressing such representations and approaches. The paper is structured as the following. The GPS method and its derivations is first introduced in Section 2. In Section 3, the mixed form concept for FEM is reviewed, then the mixed form concept extended to the GPS method is demonstrated. In Section 4, the numerical results of various problems are analyzed. And finally, conclusions are proposed in Section 5.

2. Generalized Particle System (GPS) Method

In this section, a general particle based mathematical framework for continuum fields of which the governing equations include gradient, divergence and Laplacian, are given in an integral formulation, and the corresponding discretized formulations can be used in both Eulerian and Lagrangian descriptions.

2.1 Gradient, Divergence and Laplacian of Classical Physical Field

This section summarizes the main idea used for the derivations of the gradient, divergence and Laplacian of a field property. The standard weighted residual method and the Taylor Expansion are exploited to achieve the objective of this work. A physical field can be thought of as the assignment of a physical quantity at each point in space and time. Consider a domain in Euclidean space, E . Let $\mathbf{X} \in \Omega_0 \subset E$ denotes the geometric position vector of a certain position in the domain and $\underline{\mathbf{X}} \in \Omega_0 \subset E$ denotes another point which is close to position \mathbf{X} as shown in Figure 1(a). Therefore, any physical quantity at each point in space and time can be defined as $\phi(\mathbf{X}, t) : \Omega_0 \times I \rightarrow E$. Define $\Omega_x \subset \Omega_0$ as a domain the center point position vector \mathbf{X} , then we have

$$\phi(\mathbf{X}, t) = \lim_{V_{\Omega_x} \rightarrow 0} \frac{\int_{V_{\Omega_x}} \phi(\underline{\mathbf{X}}, t) dV}{V_{\Omega_x}} \tag{1}$$

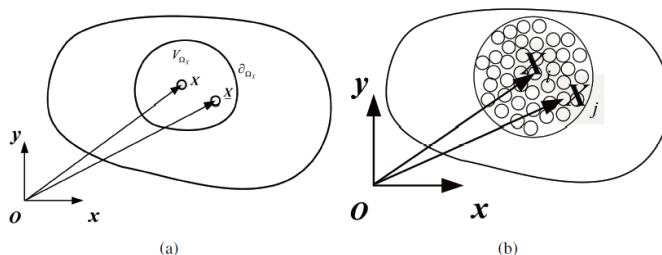


Fig. 1. An illustration of a (a) Continuous domain, (b) Discretized domain.

Weighted Residual Method Weighted residual method has been widely used in solving different kinds of ordinary/partial differential equations, in particular using the Galerkin method, which is the fundamental theory of the finite element method. In this work, we exploit the well-known weighted residual method directly to the Taylor expansion series, such that a

generalized approach of developing and investigating strong form particle-based methods can be explored. In mathematics, a Taylor series is a representation of a function as an infinite sum of terms that is calculated from the values of the function's derivatives at a single point. The Taylor series of a general physical quantity $\boldsymbol{\varphi}(\underline{\mathbf{X}})$ about \mathbf{X} at a fixed time t yields

$$\boldsymbol{\varphi}(\underline{\mathbf{X}}, t) = \boldsymbol{\varphi}(\mathbf{X}, t) + \nabla \boldsymbol{\varphi}(\mathbf{X}, t)(\underline{\mathbf{X}} - \mathbf{X}) + O(\|\underline{\mathbf{X}} - \mathbf{X}\|^2) \tag{2}$$

Where $\Delta \boldsymbol{\varphi}(\mathbf{X}, t)$ is a second order tensor when $\boldsymbol{\varphi}(\mathbf{X}, t)$ is a vector value. In the view of Eq. (2), omitting the higher order terms, we have the first order Taylor series approximation

$$\boldsymbol{\varphi}(\underline{\mathbf{X}}, t) - \boldsymbol{\varphi}(\mathbf{X}, t) \cong \nabla \boldsymbol{\varphi}(\mathbf{X}, t)(\underline{\mathbf{X}} - \mathbf{X}) \tag{3}$$

Define a residual with regards to Eq. (3), \mathbf{R} as

$$\mathbf{R} = \boldsymbol{\varphi}(\underline{\mathbf{X}}, t) - \boldsymbol{\varphi}(\mathbf{X}, t) - \nabla \boldsymbol{\varphi}(\mathbf{X}, t)(\underline{\mathbf{X}} - \mathbf{X}) \tag{4}$$

According to the standard weighted residual method, we introduce a weight function¹, \mathbf{C} , and minimize the residual, Eq. (4) by multiplying the weight function \mathbf{C} and integrating over the domain $\Omega_{\mathbf{X}}$ which yields

$$\int_{\Omega_{\mathbf{X}}} \mathbf{R} \mathbf{C} dV = 0 \tag{5}$$

The objective of the implementation of weighted residual method is to explore the gradient value for both vector and scalar values. The weight function \mathbf{C} provides a wide scope of constructing various particle-based methods. The selection of the weight function \mathbf{C} will be explained in later section of the paper.

Gradient Recall the residual \mathbf{R} in Eq. (4) and the weighted residual, $\mathbf{R} \mathbf{C}$, with respect to a vector property $\boldsymbol{\varphi}$ is

$$(\mathbf{R} \mathbf{C})_{\mathbf{X} \underline{\mathbf{X}}} = (\boldsymbol{\varphi}(\underline{\mathbf{X}}, t) - \boldsymbol{\varphi}(\mathbf{X}, t)) \otimes \mathbf{C} - \nabla \boldsymbol{\varphi}(\mathbf{X}, t)_{\mathbf{X} \underline{\mathbf{X}}} (\underline{\mathbf{X}} - \mathbf{X}) \otimes \mathbf{C} \tag{6}$$

Where \mathbf{C} is a vector with size of geometric dimension of a problem; for example, \mathbf{C} is two by one vectors for 2-D problems. We postulate that Eq. (6) is the exact relationship between a point \mathbf{X} and one of its neighboring point $\underline{\mathbf{X}}$ located in the domain $\Omega_{\mathbf{X}}$ in terms of the weighted residual, $(\mathbf{R} \mathbf{C})_{\mathbf{X} \underline{\mathbf{X}}}$. Therefore, integrating the equation presented above over the domain $\Omega_{\mathbf{X}}$ yields the following formulations

$$\int_{V_{\Omega_{\mathbf{X}}}} (\mathbf{R} \mathbf{C})_{\mathbf{X} \underline{\mathbf{X}}} dV = \int_{V_{\Omega_{\mathbf{X}}}} [(\boldsymbol{\varphi}(\underline{\mathbf{X}}, t) - \boldsymbol{\varphi}(\mathbf{X}, t)) \otimes \mathbf{C}] - [\nabla \boldsymbol{\varphi}(\mathbf{X}, t)_{\mathbf{X} \underline{\mathbf{X}}} (\underline{\mathbf{X}} - \mathbf{X}) \otimes \mathbf{C}] dV = 0 \tag{7}$$

By treating $(\boldsymbol{\varphi}(\underline{\mathbf{X}}, t) - \boldsymbol{\varphi}(\mathbf{X}, t)) \otimes \mathbf{C}$ and $\nabla \boldsymbol{\varphi}(\mathbf{X}, t)_{\mathbf{X} \underline{\mathbf{X}}} (\underline{\mathbf{X}} - \mathbf{X}) \otimes \mathbf{C}$ in the integral presented above as field properties in the domain $\Omega_{\mathbf{X}}$, the following formulations can be obtained

$$\frac{1}{V_{\Omega_{\mathbf{X}}}} \int_{V_{\Omega_{\mathbf{X}}}} [(\boldsymbol{\varphi}(\underline{\mathbf{X}}, t) - \boldsymbol{\varphi}(\mathbf{X}, t)) \otimes \mathbf{C}] dV = \int_{V_{\Omega_{\mathbf{X}}}} \nabla \boldsymbol{\varphi}(\mathbf{X}, t)_{\mathbf{X} \underline{\mathbf{X}}} [(\underline{\mathbf{X}} - \mathbf{X}) \otimes \mathbf{C}] dV \tag{8}$$

Hence, the gradient of a vector can be obtained as

$$\nabla \boldsymbol{\varphi}(\mathbf{X}, t) = \lim_{V_{\Omega_{\mathbf{X}}} \rightarrow 0} \left(\int_{V_{\Omega_{\mathbf{X}}}} (\boldsymbol{\varphi}(\underline{\mathbf{X}}, t) - \boldsymbol{\varphi}(\mathbf{X}, t)) \otimes \mathbf{C} dV \right) \lim_{V_{\Omega_{\mathbf{X}}} \rightarrow 0} \left(\int_{V_{\Omega_{\mathbf{X}}}} (\underline{\mathbf{X}} - \mathbf{X}) \otimes \mathbf{C} dV \right)^{-1} \tag{9}$$

Eq. (9) implies that the proposed gradient operator can converge to the classical continuous field value when the $\Omega_{\mathbf{X}}$ is an infinitesimal domain and the weight function \mathbf{C} is selected properly.

Divergence By representing the divergence model as nabla operator, ∇ , the dot product with some physical quantity, $\boldsymbol{\varphi}$, the divergence model can be written as following,

$$\nabla \cdot \boldsymbol{\varphi}(\mathbf{X}, t) = \nabla^T \boldsymbol{\varphi} = \lim_{V_{\Omega_{\mathbf{X}}} \rightarrow 0} \left(\int_{V_{\Omega_{\mathbf{X}}}} (\boldsymbol{\varphi}(\underline{\mathbf{X}}, t) - \boldsymbol{\varphi}(\mathbf{X}, t))^T \mathbf{C} dV \right) \lim_{V_{\Omega_{\mathbf{X}}} \rightarrow 0} \left(\int_{V_{\Omega_{\mathbf{X}}}} (\underline{\mathbf{X}} - \mathbf{X}) \otimes \mathbf{C} dV \right)^{-1} \tag{10}$$

Laplacian The definition of the Laplacian can be written as

$$\nabla^2 \boldsymbol{\varphi}(\mathbf{X}, t) = \nabla \cdot \nabla \boldsymbol{\varphi}(\mathbf{X}, t) \tag{11}$$

¹ In this work, the weight function used in the weighted residual method is defined as \mathbf{C} , and the weight function for describing the influence generated from neighbouring particle is defined as \mathbf{W} .



In order to obtain the micro Laplacian relationship between the center point \mathbf{X} and its neighboring point $\underline{\mathbf{X}}$, we reconstruct a micro gradient between two points via taking advantage of Eq.(9). One may notice that it is convenient to find the micro gradient from Eq.(6) by setting the $(\mathbf{RC})_{\mathbf{X}\underline{\mathbf{X}}}$ as 0, which yields

$$\nabla \boldsymbol{\varphi}(\mathbf{X},t)_{\mathbf{X}\underline{\mathbf{X}}} = [(\boldsymbol{\varphi}(\underline{\mathbf{X}},t) - \boldsymbol{\varphi}(\mathbf{X},t)) \otimes \mathbf{C}] [(\underline{\mathbf{X}} - \mathbf{X}) \otimes \mathbf{C}]^{-1} \tag{12}$$

However, the rank of matrix $[(\underline{\mathbf{X}} - \mathbf{X}) \otimes \mathbf{C}]$ is '1', which is not available for the calculation of the inverse when the gradient is carried over from the vector gradient calculation. To circumvent the problem mentioned above, a property $\mathbf{A} = (\underline{\mathbf{X}} - \mathbf{X}) \otimes \mathbf{C}$ is introduced and it can be replaced by its average value within an infinitesimal domain via exploiting Eq. (1),

$$\mathbf{A}_{\mathbf{X}\underline{\mathbf{X}}_{\text{avg}}} = \frac{1}{V_{\Omega_x}} \lim_{V_{\Omega_x} \rightarrow 0} \int_{\Omega_x} [(\underline{\mathbf{X}} - \mathbf{X}) \otimes \mathbf{C}] dV \tag{13}$$

Therefore, an alternative micro gradient of a vector is given by taking advantage of the average property, Eq. (13).

$$\nabla \boldsymbol{\varphi}(\mathbf{X},t)_{\mathbf{X}\underline{\mathbf{X}}} = [(\boldsymbol{\varphi}(\underline{\mathbf{X}},t) - \boldsymbol{\varphi}(\mathbf{X},t)) \otimes \mathbf{C}] (\mathbf{A}_{\mathbf{X}\underline{\mathbf{X}}_{\text{avg}}})^{-1} \tag{14}$$

Consequently, the micro Laplacian can be obtained via combining Gauss's Theorem and the gradient formulations. A micro divergence $\nabla \cdot \boldsymbol{\varphi}(\mathbf{X},t)_{\mathbf{X}\underline{\mathbf{X}}}$ is,

$$(\nabla \cdot \boldsymbol{\varphi}(\mathbf{X},t))_{\mathbf{X}\underline{\mathbf{X}}} V_{\underline{\mathbf{X}}} = \boldsymbol{\varphi}(\underline{\mathbf{X}},t) \cdot \mathbf{n}_{\mathbf{X}\underline{\mathbf{X}}} S_{\underline{\mathbf{X}}} \tag{15}$$

Where $S_{\underline{\mathbf{X}}} = V_{\underline{\mathbf{X}}} / |\underline{\mathbf{X}} - \mathbf{X}|$. As will be explained in later section, we can also replace $\mathbf{n}_{\mathbf{X}\underline{\mathbf{X}}}$ with \mathbf{C} . Substituting $S_{\underline{\mathbf{X}}}$ into Eq. (15) yields

$$\nabla \cdot \boldsymbol{\varphi}(\mathbf{X},t)_{\mathbf{X}\underline{\mathbf{X}}} = \mathbf{C} \cdot (\boldsymbol{\varphi}(\underline{\mathbf{X}},t) - \boldsymbol{\varphi}(\mathbf{X},t)) \tag{16}$$

Therefore, the Laplacian of $\boldsymbol{\varphi}(\mathbf{X},t)$ becomes,

$$(\nabla \cdot \nabla \boldsymbol{\varphi}(\mathbf{X},t))_{\mathbf{X}\underline{\mathbf{X}}} |\underline{\mathbf{X}} - \mathbf{X}| = [(\boldsymbol{\varphi}(\underline{\mathbf{X}},t) - \boldsymbol{\varphi}(\mathbf{X},t)) \otimes \mathbf{C}] (\mathbf{A}_{\mathbf{X}\underline{\mathbf{X}}_{\text{avg}}})^{-1} \cdot \mathbf{C} \tag{17}$$

Hence the following Laplacian formulations can be obtained as:

$$\nabla^2 \boldsymbol{\varphi}(\mathbf{X},t) = \nabla \cdot \nabla \boldsymbol{\varphi}(\mathbf{X},t) = \lim_{V_{\Omega_x} \rightarrow 0} \int_{\Omega_x} \frac{[(\boldsymbol{\varphi}(\underline{\mathbf{X}},t) - \boldsymbol{\varphi}(\mathbf{X},t)) \otimes \mathbf{C}] \mathbf{A}_{\mathbf{X}\underline{\mathbf{X}}_{\text{avg}}}^{-1} \cdot \mathbf{C}}{|\underline{\mathbf{X}} - \mathbf{X}|} dV \tag{18}$$

2.2 Gradient, Divergence and Laplacian of a Discretized System

In this section, the gradient, divergence and Laplacian of a vector $\boldsymbol{\varphi}(\mathbf{X},t)$ is given in the discretized system, and the formulations given below are simple to program in practical numerical simulations. Consider a domain Ω_{x_i} in the n_{dim} -dimensional Euclidean space, $E^{n_{\text{dim}}}$, in which n_{dim} denotes the number of dimension, generated from spatial discretization, for example, grids, particles, or elements, etc². Define the physical property $\boldsymbol{\varphi}$ located at i^{th} particle as $\boldsymbol{\varphi}_i$ while j^{th} particle refers to the neighboring particle within the influence domain, Ω_{x_i} . And the particle i has volume V_i . Figure 1(b) gives the discretized configuration in the domain Ω_{x_i} . According to the Gradient, Divergence and Laplacian operators listed in the previous subsection, the discretized formulations are listed as following:

Gradient

$$\nabla \boldsymbol{\varphi}_i = \left[\sum_{j \in \Omega_{x_i}} (\boldsymbol{\varphi}_j - \boldsymbol{\varphi}_i) \otimes \mathbf{C}_j V_j \right] \left[\sum_{j \in \Omega_{x_i}} (\mathbf{X}_j - \mathbf{X}_i) \otimes \mathbf{C}_j V_j \right]^{-1} \tag{19}$$

Divergence

$$\nabla \cdot \boldsymbol{\varphi}_i = \left[\sum_{j \in \Omega_{x_i}} (\boldsymbol{\varphi}_j - \boldsymbol{\varphi}_i) \cdot \mathbf{C}_j V_j \right] \left[\sum_{j \in \Omega_{x_i}} (\mathbf{X}_j - \mathbf{X}_i) \otimes \mathbf{C}_j V_j \right]^{-1} \tag{20}$$

² In this report, the particle is used as the element to discretize the domain.



Laplacian

$$\nabla^2 \varphi_i = \frac{1}{V_{\Omega_{X_i}}} \sum_{j \in \Omega_{X_i}} \frac{[(\varphi_j - \varphi_i) \otimes \mathbf{C}_j] (\mathbf{A}_{ij})^{-1} \cdot \mathbf{C}_j}{|\mathbf{X}_j - \mathbf{X}_i|} V_j \quad (21)$$

2.3 Selection of the Arbitrary Weight Function C

By selecting different \mathbf{C} , various existing particle method approaches can be obtained, and these particle-based methods have first order accuracy as the derivation is under the framework of the first order Taylor expansion series. In order to obtain the optimal \mathbf{C} , the least squares weighted residual technique is exploited via minimizing the L^2 error of Taylor approximation. Introducing an Error Ξ of the first order Taylor approximation within the domain Ω_x

$$\Xi_x = \int_{\Omega_x} [\varphi_{xx} - \nabla \varphi(\underline{\mathbf{X}} - \mathbf{X})]^2 W_{xx} dV \quad (22)$$

Where $\varphi_{xx} = \varphi_x - \varphi_x$.

To minimize the error Ξ_x and get the best approximation, the Least Squares Technique is exploited by introducing $\frac{\partial \Xi_x}{\partial \nabla \varphi_x} = 0$:

$$\begin{aligned} \frac{\partial}{\partial \nabla \varphi_x} \int_{\Omega_x} [\varphi_{xx} - \nabla \varphi_x(\underline{\mathbf{X}} - \mathbf{X})]^2 W_{xx} dV &= 0 \\ 2 \int_{\Omega_x} [\varphi_{xx} - \nabla \varphi_x(\underline{\mathbf{X}} - \mathbf{X})] \frac{\partial [\varphi_{xx} - \nabla \varphi_x(\underline{\mathbf{X}} - \mathbf{X})]}{\partial \nabla \varphi_x} W_{xx} dV &= 0 \\ \int_{\Omega_x} \varphi_{xx} \otimes (\underline{\mathbf{X}} - \mathbf{X}) W_{xx} dV - \nabla \varphi_x \int_{\Omega_x} (\underline{\mathbf{X}} - \mathbf{X}) \otimes (\underline{\mathbf{X}} - \mathbf{X}) dV &= 0 \end{aligned} \quad (23)$$

Therefore, the optimal gradient operator can be obtained from Eq. (23) and this gradient operator maintains the best approximation of

$$\nabla \varphi_x = \left[\int_{\Omega_x} \varphi_{xx} \otimes (\underline{\mathbf{X}} - \mathbf{X}) W_{xx} dV \right] \left[\int_{\Omega_x} (\underline{\mathbf{X}} - \mathbf{X}) \otimes (\underline{\mathbf{X}} - \mathbf{X}) W_{xx} dV \right]^{-1} \quad (24)$$

According to Eq. (24), the optimal \mathbf{C} is $(\underline{\mathbf{X}} - \mathbf{X})$, which minimizes the L^2 error of Taylor approximation. Recall the micro weighted residual equation Eq. (6), substituting $\mathbf{C} = (\underline{\mathbf{X}} - \mathbf{X})$ yields

$$(\mathbf{RC})_{xx} = (\varphi(\underline{\mathbf{X}}, t) - \varphi(\mathbf{X}, t)) \otimes (\underline{\mathbf{X}} - \mathbf{X}) - \nabla \varphi(\mathbf{X}, t) (\underline{\mathbf{X}} - \mathbf{X}) \otimes (\underline{\mathbf{X}} - \mathbf{X}) \quad (25)$$

where the $(\underline{\mathbf{X}} - \mathbf{X})$ is equivalent to \mathbf{n}_{ij} as the norm of vector $(\underline{\mathbf{X}} - \mathbf{X})$, and can be canceled on both sides of the Eq. (25) if we set $(\mathbf{RC})_{xx} = 0$. Therefore, we propose the weight function \mathbf{C} used in the generalized particle-based method as $\mathbf{C} = \vartheta \mathbf{n}_{ij}$,

where ϑ is a scalar value. Changing the scalar value ϑ to 1, $|\underline{\mathbf{X}} - \mathbf{X}|$ or $\frac{dW(X_{ij})}{dX_{ij}}$ obtains the differential operators in

MPS method, Peridynamics or the Total Lagrangian SPH method, respectively; moreover, with different values of ϑ , we can achieve new variants of particle-based methods. Recovering the operators for the MPS method is explained in the remark below.

Remark 2.1

Moving Particle System/Semi-implicit: As mentioned before, the proposed calculus is a general approach to obtain the gradient, divergence and Laplacian of physical properties. Also by changing the weight function \mathbf{C} , the proposed method can obtain different particle-based methods. In the derivation presented below; the weighted average approach is applied by introducing a weighting function W_{ij} . By selecting the arbitrary $\mathbf{C} = \mathbf{n}_{ij}$, the gradient and Laplacian in terms of the original MPS method can be derived from the proposed approach as well. Suppose the φ is a scalar value, and recall Taylor expansion series of a scalar value Eq. (2); consequently, by substituting $\mathbf{C} = \mathbf{n}_{ij}$ and $\mathbf{n}_{ij} = (\mathbf{X}_j - \mathbf{X}_i) / |\mathbf{X}_j - \mathbf{X}_i|$ in the discretized system yields,

$$(\varphi_j - \varphi_i) \mathbf{n}_{ij} = [\nabla \varphi_{ij} \cdot (\mathbf{X}_j - \mathbf{X}_i)] \mathbf{n}_{ij} \quad (26)$$

And



$$\frac{(\varphi_j - \varphi_i) \mathbf{n}_{ij}}{|\mathbf{X}_j - \mathbf{X}_i|} = (\mathbf{n}_{ij} \otimes \mathbf{n}_{ij}) \nabla \varphi_{ij} \tag{27}$$

By discretizing Eq. (13) and Eq. (14), we have

$$\mathbf{A}_{ij} = \frac{1}{V_{\Omega_{X_i}}} \sum_{j \in \Omega_{X_i}} (\mathbf{n}_{ij} \otimes \mathbf{n}_{ij}) V_j = \frac{\sum_{j \in \Omega_{X_i}} (\mathbf{n}_{ij} \otimes \mathbf{n}_{ij}) W_{ij} V_j}{\underbrace{V_{\Omega_{X_i}} \sum_{j \in \Omega_{X_i}} W_{ij}}_{\text{Normalized Weighted Average } A}} \tag{28}$$

And the micro gradient relationship between \mathbf{X}_i and \mathbf{X}_j is given as

$$\nabla \varphi_{ij} = \left[\frac{\sum_{k \in \Omega_{X_j}} (\mathbf{n}_{jk} \otimes \mathbf{n}_{jk}) W_{jk} V_k}{V_{\Omega_{X_j}} \sum_{k \in \Omega_{X_j}} W_{jk}} \right]^{-1} \frac{(\varphi_j - \varphi_i) \mathbf{n}_{ij}}{|\mathbf{X}_j - \mathbf{X}_i|} \tag{29}$$

Gradient Operator: Introducing the weighting function W_{ij} and supposing $V_i = V_j$ and $V_{\Omega_{X_i}} = V_{\Omega_{X_j}}$ yields

$$\begin{aligned} \nabla \varphi_i &= \frac{1}{V_{\Omega_{X_i}} \sum_{j \in \Omega_{X_i}} W_{ij}} \sum_{j \in \Omega_{X_i}} \left[\frac{\sum_{k \in \Omega_{X_j}} (\mathbf{n}_{jk} \otimes \mathbf{n}_{jk}) W_{jk} V_k}{V_{\Omega_{X_j}} \sum_{k \in \Omega_{X_j}} W_{jk}} \right]^{-1} \frac{(\varphi_j - \varphi_i) \mathbf{n}_{ij}}{|\mathbf{X}_j - \mathbf{X}_i|} W_{ij} V_j \\ &= \frac{1}{\sum_{j \in \Omega_{X_i}} W_{ij}} \sum_{j \in \Omega_{X_i}} \left[\frac{\sum_{k \in \Omega_{X_j}} (\mathbf{n}_{jk} \otimes \mathbf{n}_{jk}) W_{jk}}{\sum_{k \in \Omega_{X_j}} W_{jk}} \right]^{-1} \frac{(\varphi_j - \varphi_i) \mathbf{n}_{ij}}{|\mathbf{X}_j - \mathbf{X}_i|} W_{ij} \end{aligned} \tag{30}$$

It is worth noting that for a general particle within a uniformly distributed system, the weighted average matrix \mathbf{A}_{jk} is a diagonal matrix. Consequently, $\mathbf{A}_{jk} = d\mathbf{I}$, where \mathbf{I} is identity matrix and d equals to dimensional number. Therefore, Eq. (30) recovers the gradient calculation in the traditional MPS method, and can be rewritten as

$$\nabla \varphi_i = \frac{d}{n_0} \sum_{j \in \Omega_{X_i}} \frac{(\varphi_j - \varphi_i)}{|\mathbf{X}_j - \mathbf{X}_i|^2} (\mathbf{X}_j - \mathbf{X}_i) W_{ij} \tag{31}$$

Where $n_0 = \sum_j W_{ij}$.

Laplacian operator: Recall the micro gradient of a vector Eq. (6) and follow a similar procedure as the MPS gradient derivation, we obtain

$$\begin{aligned} (\varphi_j - \varphi_i) \otimes \mathbf{n}_{ij} &= \nabla \varphi_{ij} (\mathbf{X}_j - \mathbf{X}_i) \otimes \mathbf{n}_{ij} \\ \nabla \varphi_{ij} &= \frac{(\varphi_j - \varphi_i) \otimes \mathbf{n}_{ij}}{|\mathbf{X}_j - \mathbf{X}_i|} \left[\frac{\sum_{k \in \Omega_{X_j}} (\mathbf{n}_{jk} \otimes \mathbf{n}_{jk}) W_{jk} V_k}{V_{\Omega_{X_j}} \sum_{k \in \Omega_{X_j}} W_{jk}} \right]^{-1} \end{aligned} \tag{32}$$

According to Eq. (17), the micro Laplacian in terms of the MPS method can be obtained as

$$\nabla \cdot \nabla \varphi_{ij} |\mathbf{X}_j - \mathbf{X}_i|^2 = (\varphi_j - \varphi_i) \otimes \mathbf{n}_{ij} \left[\frac{\sum_{k \in \Omega_{X_j}} (\mathbf{n}_{jk} \otimes \mathbf{n}_{jk}) W_{jk} V_k}{V_{\Omega_{X_j}} \sum_{k \in \Omega_{X_j}} W_{jk}} \right]^{-1} \cdot \mathbf{n}_{ij} \tag{33}$$

Introducing the weighting function W_{ij} and supposing $V_i = V_j$ and $V_{\Omega_{X_i}} = V_{\Omega_{X_j}}$ yields

$$\nabla^2 \varphi_i = \frac{\sum_{j \in \Omega_{X_i}} (\varphi_j - \varphi_i) \otimes \mathbf{n}_{ij} \left[\frac{\sum_{k \in \Omega_{X_j}} (\mathbf{n}_{jk} \otimes \mathbf{n}_{jk}) W_{jk} V_k}{V_{\Omega_{X_j}} \sum_{k \in \Omega_{X_j}} W_{jk}} \right]^{-1} \cdot \mathbf{n}_{ij} W_{ij} V_j / (\sum_{j \in \Omega_{X_i}} W_{ij})}{\sum_{j \in \Omega_{X_i}} \|\mathbf{X}_j - \mathbf{X}_i\|^2 W_{ij} V_j / (\sum_{j \in \Omega_{X_i}} W_{ij})} \tag{34}$$



$$= \frac{\left[\frac{V_K \sum_{k \in \Omega_{x_j}} (\mathbf{n}_{jk} \otimes \mathbf{n}_{jk}) \mathcal{W}_{jk}}{V_{\Omega_{x_j}} \sum_{k \in \Omega_{x_j}} \mathcal{W}_{jk}} \right]^{-1} \sum_{j \in \Omega_{x_i}} (\boldsymbol{\varphi}_j - \boldsymbol{\varphi}_i) \otimes \mathbf{n}_{ij} \cdot \mathbf{n}_{ij} \mathcal{W}_{ij} / \left(\sum_{j \in \Omega_{x_i}} \mathcal{W}_{ij} \right)}{\underbrace{\sum_{j \in \Omega_{x_i}} |\mathbf{X}_j - \mathbf{X}_i|^2 \mathcal{W}_{ij} V_j / \left(\sum_{j \in \Omega_{x_i}} \mathcal{W}_{ij} \right)}_{\lambda_0}} \quad (34\text{-cont.})$$

Therefore, the Laplacian operator in terms of the traditional MPS method can be obtained as

$$\nabla^2 \boldsymbol{\varphi}_i = \frac{V_{\Omega_{x_j}} / V_K d}{\lambda_0 n_0} \sum_{j \in \Omega_{x_i}} (\boldsymbol{\varphi}_j - \boldsymbol{\varphi}_i) \mathcal{W}_{ij} \quad (35)$$

Where $\lambda_0 = \left(\sum_{j \in \Omega_{x_i}} |\mathbf{X}_j - \mathbf{X}_i|^2 \mathcal{W}_{ij} \right) / \left(\sum_{j \in \Omega_{x_i}} \mathcal{W}_{ij} \right)$, d is dimensional number, and the ratio $V_{\Omega_{x_j}} / V_K$ depends on the discretization of the system. In the MPS method, the ratio is set as 2. It is worth noting that the traditional MPS method does not deal with the divergence operator as it was originally designed under the frame of Lagrangian description; and the gradient operator in the conventional MPS method is not consistent with the Laplacian operator from the perspective of the divergence theorem, whereas the proposed method fulfills the divergence theorem.

3. Mixed Form

Mixed formulation refers to a certain approach to handle a set of differential equations for solving a numerical problem. In general, it is called mixed formulation when all the variables, such as displacement or stress, are independently approximated. For an example in elasticity, we have the governing equation and constitutive relation as following

$$\begin{aligned} \frac{d\boldsymbol{\sigma}}{dx} + \mathbf{b} &= 0 \\ \boldsymbol{\sigma} - E \frac{du}{dx} &= 0 \end{aligned} \quad (36)$$

If we combine the two equations and let u be the only independent variable, we get

$$\frac{d}{dx} \left[E \frac{du}{dx} \right] + \mathbf{b} = 0 \quad (37)$$

Which corresponds to the traditional displacement formulation? Now the most general mixed form of equation can be written as

$$\begin{aligned} \nabla \cdot \boldsymbol{\sigma} + \mathbf{b}_i &= 0 && \text{(equilibrium)} \\ \boldsymbol{\sigma} &= \mathbf{D} \boldsymbol{\varepsilon} && \text{(constitutive)} \\ \boldsymbol{\varepsilon} &= \nabla u && \text{(strain definition)} \end{aligned} \quad (38)$$

and these equation will be simultaneously solved. In this section, we will look at how mixed form is achieved for both FEM and GPS method.

3.1 Two Field Mixed Formulation using FEM

Two field mixed form of solving for displacement and stress is derived from Hellinger-Reissner variational principle. In depth mathematical formulation is explained in [4]. In this paper, only the application is briefly reviewed. First, the weak form of the equation of motion is derived using the virtual work principle and written as

$$\int_{\Omega} \delta \boldsymbol{\varepsilon}^T \boldsymbol{\sigma} d\Omega - \int_{\Omega} \delta \mathbf{u}^T \mathbf{b} d\Omega - \int_{\Gamma_t} \delta \mathbf{u}^T \bar{\mathbf{t}} d\Gamma = 0 \quad (39)$$

And secondly, the approximate integral form of the constitutive relation is written as

$$\boldsymbol{\sigma} = \mathbf{D} \boldsymbol{\varepsilon} \quad (40)$$

$$\int_{\Omega} \delta \boldsymbol{\sigma}^T (\nabla u - \mathbf{D}^{-1} \boldsymbol{\sigma}) d\Omega = 0 \quad (41)$$

We can then replace variables with product of shape function N as following

$$\begin{aligned} N_u \hat{\boldsymbol{\delta}} u &\text{ for } \boldsymbol{\delta} u \\ \mathbf{B}_u \hat{\boldsymbol{\delta}} u &\equiv \nabla N_u \hat{\boldsymbol{\delta}} u \text{ for } \boldsymbol{\delta} \boldsymbol{\varepsilon} \\ N_{\sigma} \hat{\boldsymbol{\delta}} \boldsymbol{\sigma} &\text{ for } \boldsymbol{\delta} \boldsymbol{\sigma} \end{aligned} \quad (42)$$



Therefore, we can write Eq. (39), and Eq. (41) together in a matrix form

$$\begin{bmatrix} 0 & C^T \\ C & A \end{bmatrix} \begin{Bmatrix} \hat{u} \\ \hat{\sigma} \end{Bmatrix} = \begin{Bmatrix} f_1 \\ f_2 \end{Bmatrix} \tag{43}$$

Where

$$\begin{aligned} A &= -\int_{\Omega} N_{\sigma}^T D^{-1} N_{\sigma} d\Omega \\ C &= \int_{\Omega} N_{\sigma}^T B d\Omega \\ f_1 &= \int_{\Omega} N_u^T b d\Omega + \int_{\Gamma_f} N_u^T \bar{t} dT \\ f_2 &= 0 \end{aligned} \tag{44}$$

For particle methods, the components in the above standard matrix forms become simpler. Instead of using the weak form, the gradient and divergence operators are replaced with discretized approximations in particle methods as discussed in the previous section. Thus the standard matrix form simply represents the governing equation and constitutive law for stress.

3.2 Mixed Form Representation with Dependence of Field Variables and stress for GPS

The traditional formulation of GPS involves discretizing the governing equation with Laplacian term $\nabla \cdot \nabla \phi = \nabla^2 \phi$. Instead of combining the governing equation and constitutive law, we simply discretize the two equations separately as following:

$$\begin{aligned} \rho \ddot{u} + \nabla \cdot \sigma &= f \\ \sigma &= D \nabla u \end{aligned} \tag{45}$$

The gradient and divergence terms are applied to displacement and stress and the two operators can be discretized using the GPS method by applying Eq. (19) and Eq. (20), respectively. However, unlike the mixed form FEM, here in the particle based GPS method, the field variables and stress are dependent; consequently it is simply a form representation in construction only to foster coupling of multiple domains via mixed form FEM to particle methods mimicking such constructions. The discretized terms become the following:

$$\nabla u_i = \left[\sum_{j \in \Omega_{x_i}} (u_j - u_i) \otimes C_j V_j \right] \left[\sum_{j \in \Omega_{x_i}} (r_{ij}) \otimes C_j V_j \right]^{-1} \tag{46}$$

$$\nabla \cdot \sigma_i = \left[\sum_{j \in \Omega_{x_i}} (\sigma_j - \sigma_i)^T C_j V_j \right] \left[\sum_{j \in \Omega_{x_i}} (r_{ij}) \otimes C_j V_j \right]^{-1} \tag{47}$$

The above equations can be rearranged to separate u_i and u_j making it easier to form matrices.

$$\nabla u_i = \sum_j \frac{-C_{ij} V_j}{\sum_k r_{ik} \otimes C_{ik} V_k} u_i + \sum_j \frac{C_{ij} V_j}{\sum_k r_{ik} \otimes C_{ik} V_k} u_j \tag{48}$$

$$\nabla \cdot \sigma_i = \sum_j \sigma_j^T \frac{-C_{ij} V_j}{\sum_k r_{ik} \otimes C_{ik} V_k} + \sum_j \sigma_j^T \frac{C_{ij} V_j}{\sum_k r_{ik} \otimes C_{ik} V_k} \tag{49}$$

After the gradient term and the divergence term have been replaced as suggested, the Eq. (45) can be rearranged to matrix forms.

$$\begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix} \begin{Bmatrix} \ddot{u} \\ \ddot{\sigma} \end{Bmatrix} + \begin{bmatrix} 0 & \nabla \cdot \\ D \nabla & -I \end{bmatrix} \begin{Bmatrix} u \\ \sigma \end{Bmatrix} = \begin{Bmatrix} f \\ 0 \end{Bmatrix} \tag{50}$$

Where M is diagonal mass matrix and I is identity matrix. A simple 1-D structure as shown in Figure 2 will be used as an example and provide proof of concept for mixed formulation mimicked in the GPS method.

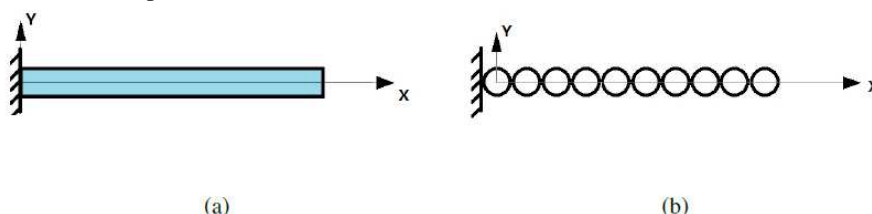


Fig.2. (a) Geometry of simple 1-D bar and (b) its particle discretization

Let the influence domain to include just one neighboring particle in each direction; the gradient operator can be represented in matrix forms as following for the 1-D example:

$$\nabla = \begin{bmatrix} \frac{-C_{12}D_2}{D_2} & \frac{C_{12}V_2}{D_1} & 0 & \dots & 0 \\ \frac{C_{21}V_2}{D_2} & (\frac{-C_{21}V_1}{D_2} + \frac{-C_{23}D_3}{D_2}) & \frac{C_{23}V_3}{D_2} & \dots & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \dots & \frac{C_{N-1,N-2}V_{N-2}}{D_{N-1}} & (\frac{-C_{N-1,N-2}V_{N-2}}{D_{N-1}} + \frac{-C_{N-1,N}V_N}{D_{N-1}}) & \frac{C_{N-1,N}V_N}{D_{N-1}} \\ 0 & \dots & \dots & \frac{C_{N,N-1}V_{N-1}}{D_N} & \frac{-C_{N,N-1}V_{N-1}}{D_N} \end{bmatrix} \tag{51}$$

Where N is number of particles and

$$\begin{aligned} D_1 &= |r_{12}|V_2 \\ D_2 &= |r_{21}|V_1 + |r_{23}|V_3 \\ D_{N-1} &= |r_{N-1,N-2}|V_{N-2} + |r_{N-1,N}|V_N \\ D_N &= |r_{N,N-1}|V_{N-1} \end{aligned} \tag{52}$$

It is worth noting that in 1-D problems, the divergence operator is identical to the gradient operator.

4. Numerical Examples

4.1 2-D Static Bending (Shear Locking)

A two dimensional plane stress problem using both FEM and GPS is analyzed. As shown in Fig. 3, $L=10\text{ m}$ by $w=1\text{ m}$ beam has a fixed boundary on the left wall and traction load of -10 N/m is applied on the right edge of the structure. The material has Young’s Modulus of 10 MPa , Poisson’s ratio of 0.3 . The structure is discretized into $124\text{ node/particles}$ with $31\text{ nodes/particles}$ along the width and 4 nodes/particles along the height.

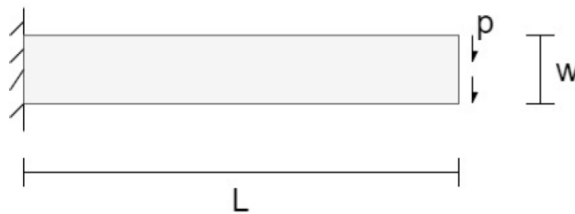


Fig. 3. Diagram of structure for bending problem

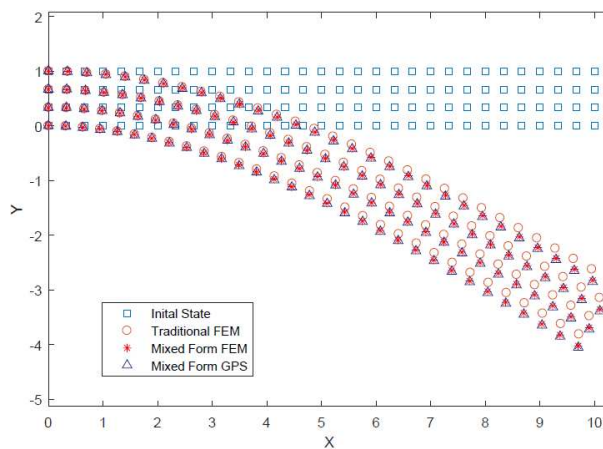


Fig. 4. Deformation comparison among different methods (scaled by 1000)

Table 1. Y displacements at the free end of the beam

Y Displacement [m]	
Traditional FEM	-3.810×10^{-3}
Mixed Form FEM	-4.024×10^{-3}
Mixed Form GPS	-4.052×10^{-3}
Analytical	-4×10^{-3}

As shown in Figure 4, and Table 1, the traditional FEM gives smaller deformation due to shear locking. The mixed form representation of GPS result (field variable and stress are dependent) is more comparable to the mixed form FEM (field variables and stress are independent) result which is free from the locking issue. Von Mises stress contour of the beam (presented in undeformed shape) from the mixed form FEM and mixed form representation of GPS is shown in Figure 5 and the results closely match.

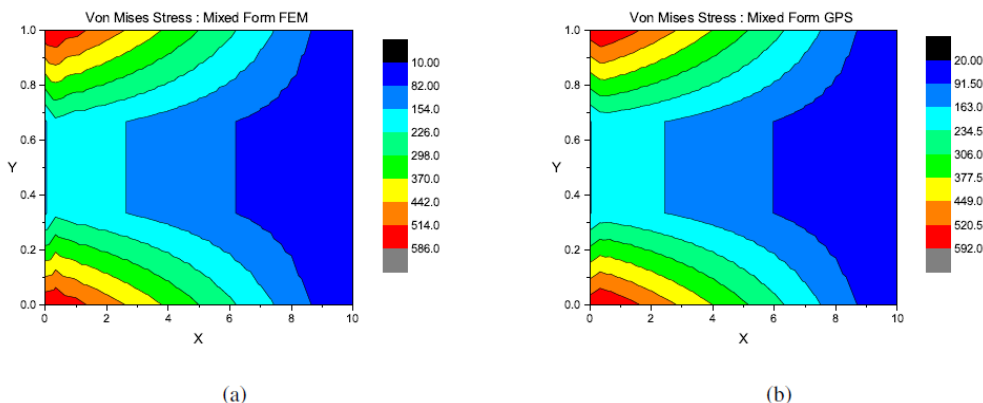


Fig. 5. Von Mises stress contour map of (a) mixed form FEM result and (b) mixed form GPS result

4.2 2-D Beam Bending Dynamic Problem

A beam with the same geometry as the static problem beam is used to illustrate the application of the mixed form representation of the GPS method in plane stress dynamic problem. A cantilever beam of 10 m by 1 m with 1 m thickness is fixed on the left side and is experiencing downward traction, p , of 100000 N/m. It is discretized into 124 particles with 31 particles along the length and 4 particles along the height. The density, ρ , of the beam is set to be 271.2 kg/m³, Young modulus, E , to be 72 GPa, and Poisson's ratio to be 0.3 for the properties of the material. Implicit U0(1,1,0) algorithm from the GS4 time scheme is used to solve the time integration to ensure second order accuracy. Δt for time integration is set to be 60 μs . The time history of y-direction displacement, velocity and acceleration of a node at the free end is evaluated.

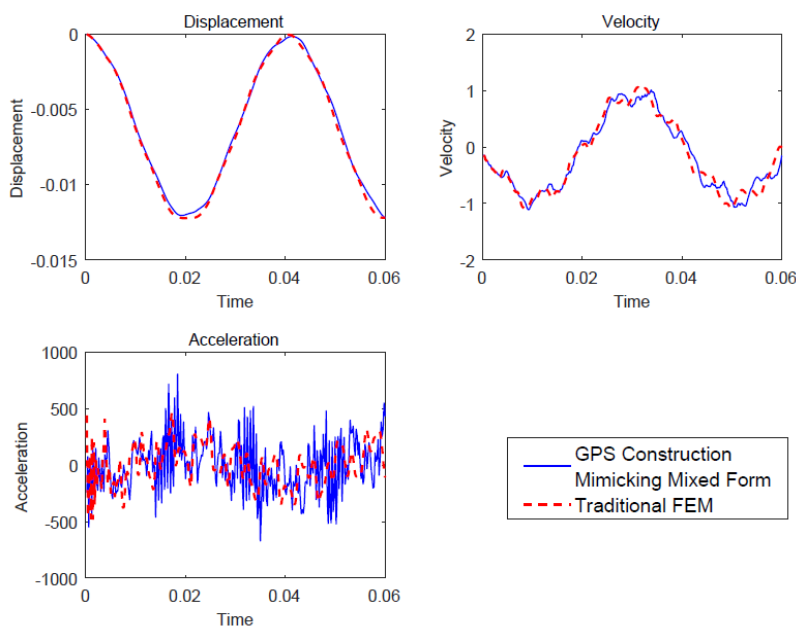


Fig. 6. Time history of displacement, velocity, and acceleration of the particle/node at the free end of the beam

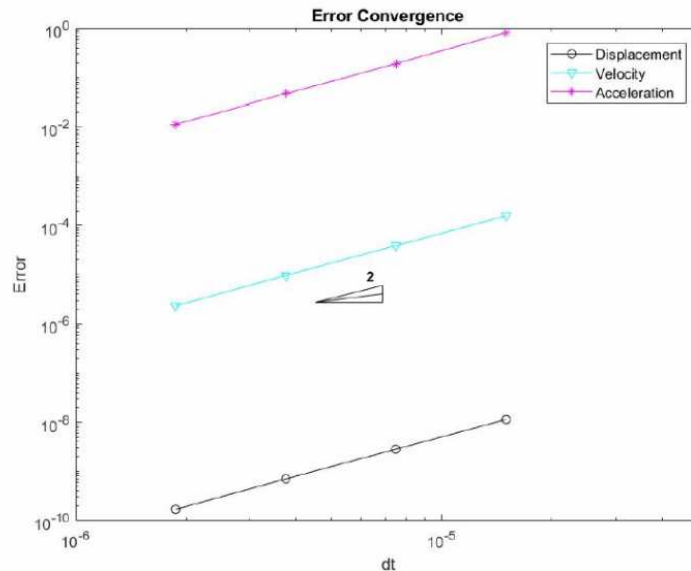


Fig.7. Convergence rate of displacement, velocity, and acceleration from the GPS method mimicking mixed form (log-log scale)

Figure 6 shows time history of displacement, velocity and acceleration for node/particle at the end of the beam. All three variables for the mixed form GPS are in agreement with FEM result. In order to verify the time accuracy of the method, the convergence rate is calculated as following

$$Error = \left| \frac{u - u_{exact}}{u_{exact}} \right| \quad (53)$$

Where solution with fine Δt is taken as u_{exact} . Figure 7 shows the order of convergence for mixed form GPS to be second order accurate.

4.3 2-D Bar in Compression Dynamic Problem

Fig. 8 shows the 2-D geometry for a wave propagation problem. It is a rectangular bar of 10 m by 1 m with 1 m thickness, which is fixed on the left side wall as boundary condition. The bar is compressed from the right side with p , the distributed load, of 10000 N/m. This material has 72 GPa for Young's modulus, 0.3 for Poisson's ratio, and 2712 kg/m³ for density. GPS is implemented with 31 particles in length, and 4 particles in height making it total of 124 particles. Explicit U0(1,1,0) algorithm from the GS4 time scheme algorithm is used to solve the time integration and Δt for time integration is set to be 0.8 μs . The time history of x-direction displacement, velocity and acceleration of a node at the free end is evaluated.

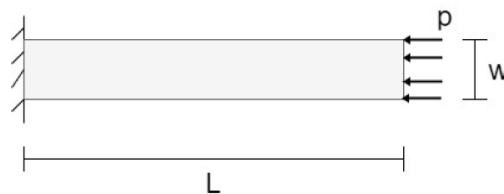
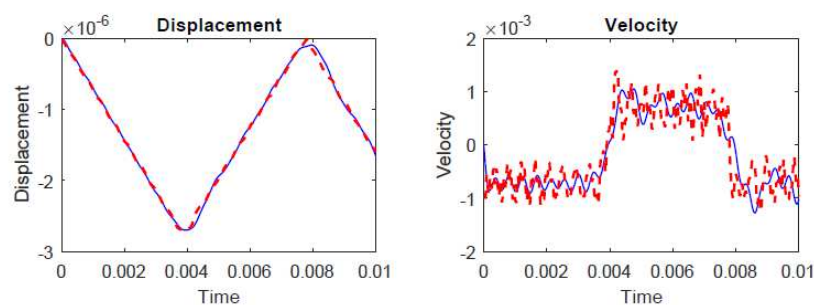


Fig. 8. Diagram of structure for wave propagation problem

As Figure 9 illustrates, the solutions from the two methods match well for displacement, velocity acceleration with slight oscillation differences in velocity and acceleration likely caused by time integration algorithm. Figure 10 displays that the mixed form representation of the GPS method is second order accurate in time in wave propagation type of problems also.



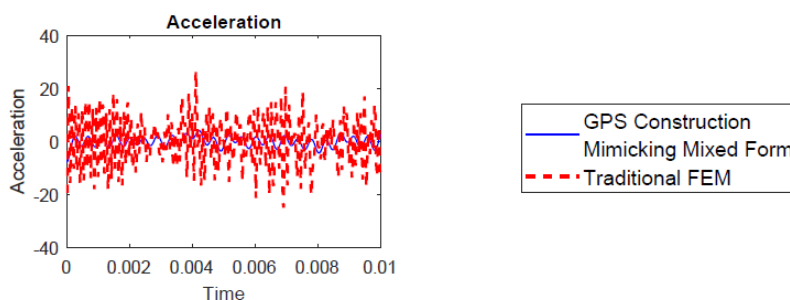


Fig. 9. Time history of displacement, velocity, and acceleration of the particle/node at the free end of the bar

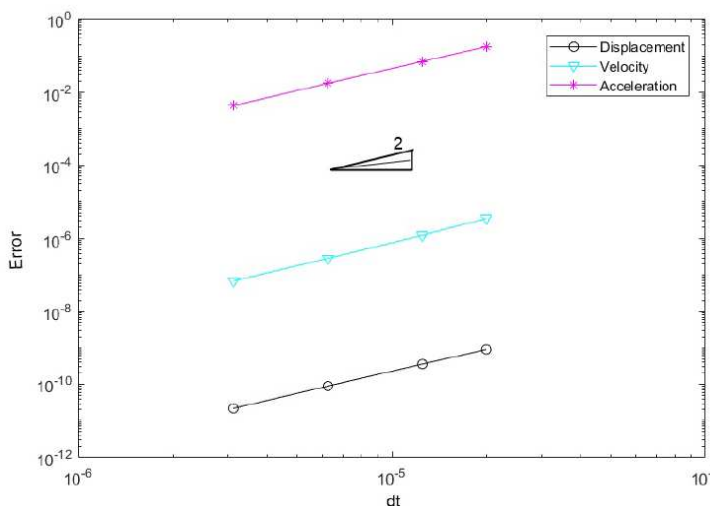


Fig.10. Convergence rate of displacement, velocity, and acceleration from the GPS mimicking mixed form (log-log scale)

5. Conclusions

In this paper, we have proposed a general method to describe multiple strong form based particle methods and application of mixed formulation representation to the generalized method. The mixed form representation of the GPS method can be seen as an extension to the traditional method as it solves for displacement and stress simultaneously. Applying to 2-D simple bar and beam problems, the results from mixed form representation of the GPS method is on par with mixed form FEM results. The mixed form representation in construction only concept applied to GPS method can be the first step for fostering coupling of multi-domain problems, coupling mixed form FEM (displacement - stress independence) and mixed form representation GPS method (displacement-stress dependence); however, it is to be noted that the standard GPS particle method and the mixed for representation construction GPS particle method are equivalent. Although the strong form particle method inherently does not cause locking issue as in FEM, introducing the mixed form representation to the generalized particle method opens further study possibilities including multi-domain coupling method problems utilizing mixed form FEM and mixed form representation of the GPS method.

Conflict of Interest

The authors declare no conflict of interest.

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