

Peridynamic theory and coupling with finite element method for
discontinuities analysis

by

Qibang Liu

B.S., Huazhong University of Science and Technology, China, 2013

AN ABSTRACT OF A DISSERTATION

submitted in partial fulfillment of the
requirements for the degree

DOCTOR OF PHILOSOPHY

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KANSAS STATE UNIVERSITY
Manhattan, Kansas

2022

Abstract

Peridynamics (PD) is a nonlocal continuum theory and is better suited for failure analysis of solids compared with conventional continuum mechanics. However, published bond-based and state-based PD theories and numerical implementations suffer from some drawbacks, including the need for surface correction and volume correction and computational inefficiency. The research presented in this dissertation focuses on advancing the theory of PD, overcoming existing drawbacks of PD, and applying PD in the deformation and failure analysis of solids.

To remove the drawback of the need for a surface correction and a volume correction, a revised non-ordinary state-based PD (RNOSBPD) theory is proposed in this study. For spherical interaction domains, RNOSBPD recovers the original non-ordinary state-based PD (NOSBPD). However, for interaction domains of arbitrary shapes, RNOSBPD remains valid, eliminating the need for a surface or volume correction. Compared with the finite element method (FEM), PD is computationally expensive because of the nature of nonlocal interactions. A new approach for coupling PD with FEM based on the weighted residual method (WRM) is proposed. This new coupling approach is straightforward, and special techniques such as overlapping regions, interface elements, or fictitious nodes published in the literature for coupling PD with FEM are not needed.

Failure analysis frequently involves the investigation of crack propagation. A quasi-static simulation method using our coupled PD-FEM is pioneered to study crack propagation efficiently. The failure criterion in the simulation is based on the maximum circumferential tensile stress. A new numerical method is proposed to evaluate the stress intensity factors using the interaction integral based on the J-integral and to determine the onset of crack propagation and direction of crack growth.

Since it is impractical to store a full global stiffness matrix and to implicitly solve PD in 3D, a new PD model for 3D problems is proposed and presented, in which the global stiffness matrix is stored in a Compressed Sparse Row (CSR) format based on Message Passing Interface (MPI), and the system equations are solved by parallel computing by a Parallel Direct Sparse Solver (PDSS), also based on MPI.

To further improve the computational efficiency of PD, an Enriched Finite Element Method using Peridynamics (EFEM-PD) is proposed, following a similar concept of element enrichment of extended finite element method (XFEM). In EFEM-PD, the FEM model is enriched adaptively with PD equations in regions containing cracks. An adaptive algorithm is implemented with the dual goals of meshing regions with cracks using PD equations while minimizing PD interactions to maximize computational efficiency.

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Acknowledgments

I would like to thank:

- My advisor Dr. Jack Xin for his great guidance, help, and support in my entire study.
- Dr. Youqi Wang for her great guidance, help, and firm support.
- Dr. Bacim Alali for his teaching me on Peridynamics.
- Dr. Jeff Ma for his guidance and help.
- Dr. Jack Xin, Dr. Youqi Wang, Dr. Liang-Wu Cai, Dr. Raj Pal, and Dr. Bacim Alali for their valuable time and serving on my committee.
- All my professors at Kansas State University and Huazhong University of Science and Technology (China) for their guidance.
- My wife for her endless love and support, and my newborn baby for his coming.
- Finally, my parents for their encouragement and help.

Dedication

Dedicated to my wife and my son.

Chapter 1

Introduction

1.1 What is peridynamics?

The analysis and prediction of material behaviors may be conducted at different time and length scales, ranging from angstrom and sub-picoseconds for the vibrations of atomic bonds to millimeters and seconds for deformation of continuum media. Molecular Dynamics (MD) is the mainly atomistic technique in which positions of atoms and molecules are determined typically using the Verlet algorithm [2], which is derived from Newton's equation of motion. MD has been used widely to study material behaviors, including the analysis of crack propagation [3]. MD simulations illustrate the interactions between components and conformational dynamics in the atomistic scale and play a key role in understanding molecular mechanisms. However, they are computationally expensive, and macroscale behavior is challenging to address at the MD level. At the macroscale, material behaviors are generally studied by classical continuum mechanics (CCM), which relies on derivatives of variables. In CCM, the material points interaction is local, which means the material point $\mathbf{x}$ only interacts with its immediate neighbors $\mathbf{x}'$, which satisfy that $|\mathbf{x}' - \mathbf{x}| < \delta \rightarrow 0$, as presented in Fig. 1.1. The internal force at point $\mathbf{x}$, $\mathbf{L}(\mathbf{x})$, has a form of derivatives as

$$\mathbf{L}(\mathbf{x}) = \mathbf{L}^{ccm}(\mathbf{x}, t) = \nabla \cdot \boldsymbol{\sigma}(\mathbf{x}, t) \quad (1.1)$$

in which $\boldsymbol{\sigma}$ represents the first Piola–Kirchhoff stress. The equation of motion is derived based on Newton’s law:

$$\rho \ddot{\mathbf{u}}(\mathbf{x}, t) = \mathbf{L}(\mathbf{x}, t) + \mathbf{b}(\mathbf{x}, t), \quad (1.2)$$

where ρ is the mass density, $\ddot{\mathbf{u}}$ is the acceleration, $\mathbf{b}$ is the external force vector.

Despite of CCM being well established and having been successfully employed to study behaviors of deformable bodies, the mathematical framework of CCM is in some ways ill-suited to model discontinue problems since the derivatives concerning spatial coordinates in CCM are undefined where discontinuities occur.

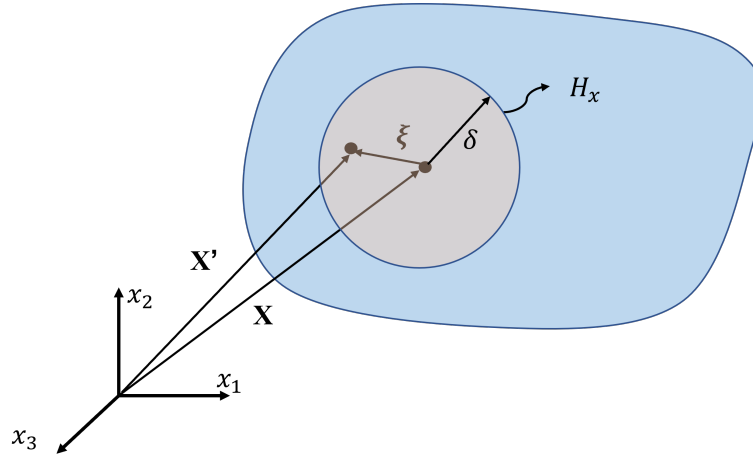


Fig. 1.1: Interaction between material points $\mathbf{x}'$ and $\mathbf{x}$, where the distance between the two points is $|\mathbf{x}' - \mathbf{x}| < \delta$. For CCM, the radius δ is infinitesimal, while for PD, δ is a finite length.

In light of the inadequacies of the CCM, Silling [4] proposed a nonlocal continuum model named *peridynamics* (PD) derived from Greek root *peri-* for *near* and *dynami-* for *force*. PD assumes the material point $\mathbf{x}$ interacts with its neighbors $\mathbf{x}'$ within a spherical domain $H_x = \{\mathbf{x}' \in H_x : |\mathbf{x}' - \mathbf{x}| < \delta\}$, where δ is called the *horizon* and is a finite length, rather than infinitesimal as defined in CCM, as shown in Fig. 1.1. The summation of these interactions is expressed in an integral form rather than a derivative form, as

$$\mathbf{L} = \mathbf{L}^{pd}(\mathbf{x}, t) = \int_{H_x} \mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi}) dV_{x'}, \quad (1.3)$$

where $\boldsymbol{\xi} = \mathbf{x}' - \mathbf{x}$ is called a bond and represents the initial relative position of points $\mathbf{x}'$ and $\mathbf{x}$, $\boldsymbol{\eta} = \mathbf{u}' - \mathbf{u}$ represents the relative displacement of bond $\boldsymbol{\xi}$, and $\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi})$ represents a pairwise force density vector for bond $\boldsymbol{\xi}$. As described in Eq. (1.3), PD employs spatial integration rather than derivatives in its formulation, which makes it is better suited for discontinuity analysis of structures, since the integration equation in PD remains valid at discontinuities.

1.2 PD fundamentals

The PD theory is based on the summation of interactions within neighborhood H_x of material point $\mathbf{x}$ as shown in Fig. 1.1. The first introduced PD theory is the bond-based PD [4] in which a single PD material parameter, the bond constants c , is employed to analyze isotropic materials, resulting in a restriction of a fixed Poisson's ratio of 1/4 [5–7]. Subsequently, Silling et al. [8] introduced the ordinary state-based PD (OSBPD) and non-ordinary state-based PD (NOSBPD) theories to remove the restriction. In this section, these PD fundamentals are introduced.

1.2.1 Bond-based PD

The essential of PD theory is to construct the pairwise force density $\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi})$. For bond-based PD (BBPD), a significant restriction on $\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi})$ is based on Newton's Third Law: the force on point $\mathbf{x}$ due to point $\mathbf{x}'$ equals the force on $\mathbf{x}'$ due to point $\mathbf{x}$ with opposite direction. Therefore,

$$\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi}) = -\mathbf{f}(-\boldsymbol{\eta}, -\boldsymbol{\xi}) \quad (1.4)$$

Eq. (1.4) is called linear admissibility condition of $\mathbf{f}$ which ensures conservation of linear momentum.

To ensures conservation of angular linear momentum, the form of $\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi})$ is restricted by

$$(\boldsymbol{\eta} + \boldsymbol{\xi}) \times \mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi}) = 0. \quad (1.5)$$

Eq. (1.5) is called angular admissibility condition on $\mathbf{f}$. Based on the restrictions of Eqs. (1.4) and (1.5), the most general form of $\mathbf{f}$ is derived as

$$\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi}) = F(\boldsymbol{\eta}, \boldsymbol{\xi})(\boldsymbol{\eta} + \boldsymbol{\xi}), \quad (1.6)$$

in which $F(\boldsymbol{\eta}, \boldsymbol{\xi})$ is a scalar valued function and satisfies

$$F(\boldsymbol{\eta}, \boldsymbol{\xi}) = -F(-\boldsymbol{\eta}, -\boldsymbol{\xi}) \quad (1.7)$$

For a linear elastic isotropic solid, the pairwise force density is generally defined as

$$\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi}) = cs \frac{\boldsymbol{\eta} + \boldsymbol{\xi}}{|\boldsymbol{\eta} + \boldsymbol{\xi}|}, \quad (1.8)$$

where s is the bond stretch defined as

$$s = \frac{|\boldsymbol{\eta} + \boldsymbol{\xi}| - |\boldsymbol{\xi}|}{|\boldsymbol{\xi}|}. \quad (1.9)$$

c is bond constants and is derived by equating the summation of the energy density of bonds to strain energy density of a large homogeneous body under isotropic extension as

$$\frac{1}{2}\boldsymbol{\sigma} : \boldsymbol{\varepsilon} = \frac{1}{2} \int_{H_x} \frac{1}{2} \mathbf{f} \cdot \boldsymbol{\eta} dV_{x'}, \quad (1.10)$$

which leads to the bond constant as

$$c = \frac{18\kappa}{\pi\delta^4}, \quad (1.11)$$

in which κ is the bulk modulus of material. For CCM, representing a homogeneous isotropic material requires two independent parameters, such as the pair constants (E, ν) , (λ, ν) , or (E, μ) , in which E is Young's modulus, μ is shear modulus, ν is Poisson's ratio, λ is the lame's constant. While in BBPD, only one material constant c is used to represent the material, which is very restrictive on material properties. In fact, BBPD requires that

Poisson's ratio is $\nu = 1/4$ for 3D and $\nu = 1/3$ for 2D [4–7].

Note that the general form Eq. (1.8) is a nonlinear function of $\mathbf{u}$ since the bond stretch is a nonlinear function. By assuming small deformations, i.e., $\eta \ll 1$, a linear constitutive PD model was derived as [4, 9]

$$\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi}) = \frac{c}{|\boldsymbol{\xi}|^3} (\boldsymbol{\xi} \otimes \boldsymbol{\xi}) \boldsymbol{\eta} \quad (1.12)$$

1.2.2 State-based PD

As discussed in Section 1.2.1, the original BBPD requires the Poisson's ratio ν be 1/3 for 2D and be 1/4 for 3D. To remove this restriction, Silling et al. [8] proposed a state-based PD (SBPD).

The essence of the SBPD is a mathematical object called *state* which is similar to a mapping. Silling et al. [8] defined that an image of a vector, $\boldsymbol{\xi} = \mathbf{x}' - \mathbf{x}$, under the state $\underline{\mathbf{A}}$ is a tensor, written as $\underline{\mathbf{A}}\langle\boldsymbol{\xi}\rangle$. The reference vector position state called the bond is defined as:

$$\underline{\mathbf{X}}\langle\boldsymbol{\xi}\rangle = \boldsymbol{\xi} = \mathbf{x}' - \mathbf{x}. \quad (1.13)$$

The deformation vector is the deformed state of the bond defined as

$$\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle = \boldsymbol{\eta} + \boldsymbol{\xi}, \quad (1.14)$$

here $\boldsymbol{\eta} = \mathbf{u}' - \mathbf{u}$ is the relative displacement of the bond $\boldsymbol{\xi}$. Within the framework of SBPD, the bond force density is defined as

$$\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi}) = \underline{\mathbf{T}}[\mathbf{x}, t]\langle\boldsymbol{\xi}\rangle - \underline{\mathbf{T}}[\mathbf{x}', t]\langle-\boldsymbol{\xi}\rangle \quad (1.15)$$

in which $\underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle$ represents the force state. The SBPD is further divided into ordinary SBPD (OSBPD) or non-ordinary SBPD (NOSBPD). A material is called ordinary when the force state $\underline{\mathbf{T}}$ is parallel to the deformed bond $\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle = \boldsymbol{\eta} + \boldsymbol{\xi}$, otherwise, the material is called

non-ordinary. For instance, the force state of linear elastic isotropic material in the OSBPD framework is given by [8],

$$\underline{\mathbf{T}}[\mathbf{x}, t]\langle \boldsymbol{\xi} \rangle = \left(\frac{3\kappa\omega(|\boldsymbol{\xi}|)|\boldsymbol{\xi}|}{m}\theta + \frac{15\mu}{m}\omega(|\boldsymbol{\xi}|)e^d \right) \frac{\boldsymbol{\eta} + \boldsymbol{\xi}}{|\boldsymbol{\eta} + \boldsymbol{\xi}|}, \quad (1.16)$$

in which $\omega(|\boldsymbol{\xi}|)$ represents the influence function, κ is the bulk modulus, and μ is the shear modulus. m , θ , and e^d are defined as follows,

$$m = \int_{H_x} \omega(|\boldsymbol{\xi}|)|\boldsymbol{\xi}|^2 dV_{x'}, \quad (1.17)$$

$$\theta = \frac{3}{m} \int_{H_x} \omega(|\boldsymbol{\xi}|)|\boldsymbol{\xi}|(|\boldsymbol{\eta} + \boldsymbol{\xi}| - |\boldsymbol{\xi}|) dV_{x'}, \quad (1.18)$$

$$e^d = (|\boldsymbol{\eta} + \boldsymbol{\xi}| - |\boldsymbol{\xi}|) - \frac{\theta|\boldsymbol{\xi}|}{3}. \quad (1.19)$$

Furthermore, in the corresponding model of NOSBPD, the force state can be defined by the stress tensor as [8]

$$\underline{\mathbf{T}}[\mathbf{x}, t]\langle \boldsymbol{\xi} \rangle = \omega(|\boldsymbol{\xi}|)\boldsymbol{\sigma}(\mathbf{x})\boldsymbol{\mathcal{S}}^{-1}(\mathbf{x})\boldsymbol{\xi}, \quad (1.20)$$

where $\boldsymbol{\sigma}$ is the first Piola-Kirchhoff stress tensor and $\boldsymbol{\mathcal{S}}(\mathbf{x})$ is the shape tensor defined as

$$\boldsymbol{\mathcal{S}}(\mathbf{x}) = \int_{H_x} \omega(|\boldsymbol{\xi}|)(\boldsymbol{\xi} \otimes \boldsymbol{\xi}) dV_{x'}. \quad (1.21)$$

in which $\omega(|\boldsymbol{\xi}|)$ represents the influence function.

It is worthy to note that the bond-based PD can be described by the force state as

$$\underline{\mathbf{T}}[\mathbf{x}, t]\langle \boldsymbol{\xi} \rangle = \frac{1}{2}cs \frac{\boldsymbol{\eta} + \boldsymbol{\xi}}{|\boldsymbol{\eta} + \boldsymbol{\xi}|}. \quad (1.22)$$

Comparison between Eqs. (1.16), (1.20) and (1.22) reveals the differences between the BBPD, OSBPD, and NOSBPD lie in the magnitude and direction of the interaction force states between the materials points. For BBPD, the force states $\underline{\mathbf{T}}[\mathbf{x}]\langle \boldsymbol{\xi} \rangle$ and $\underline{\mathbf{T}}[\mathbf{x}']\langle -\boldsymbol{\xi} \rangle$ have equal magnitudes and are parallel to the deformed relative position vector, while for OSBPD,

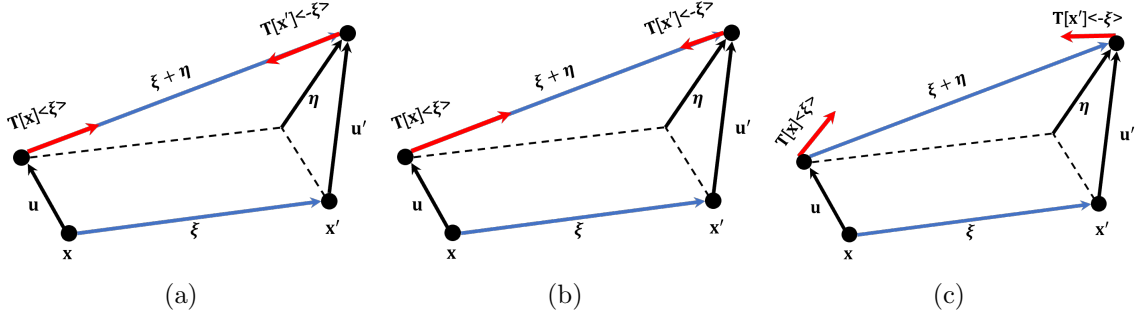


Fig. 1.2: Illustration of BBPD, OSBPD, and NOSBPD: (a) BBPD, the force state $\underline{\mathbf{T}}[\mathbf{x}]\langle\xi\rangle$ and $\underline{\mathbf{T}}[\mathbf{x}']\langle-\xi\rangle$ have same magnitudes as well as being parallel to the deformed relative position vector; (b) OSBPD, the force states have unequal magnitudes yet being parallel to the deformed relative position vector; (c) NOSBPD, the force states have unequal magnitudes and are in arbitrary directions.

their directions are parallel to the deformed relative position vector yet their magnitudes may be different. For NOSBPD, their magnitudes are unequal, and their directions are non-parallel, as seen in Fig. 1.2.

1.3 Surface effect of PD

Both the bond-based PD and the state-based PD are derived based on the assumptions that the interaction horizon is a spherical domain and the material point $\mathbf{x}$ is far from the domain boundary. For material points near the domain boundary, the horizon is truncated and is not a complete sphere, as shown in Fig. 1.3. For these truncated horizons, a surface correction is required [6, 10]

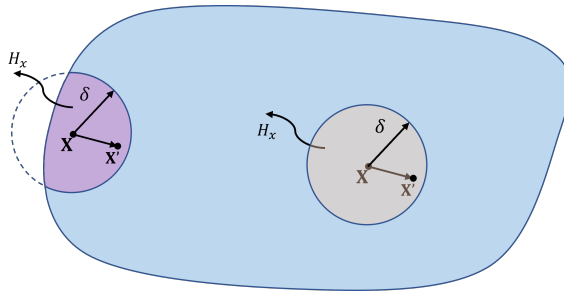


Fig. 1.3: A material point is near domain boundary with a truncated horizon (purple) and a material point is far away from domain boundary with a full horizon (light yellow).

Many surface correction methods have been proposed, and they can be divided into two categories [10]. The first category is modifying the bond force within the truncated horizon by applying a correction factor [11, 12], such as the conical micro-modulus function [13–15], the energy method [6, 16, 17]. The second category is introducing a fictitious layer with thickness δ along the boundary of domain [18, 19].

1.4 Numerical implementation of PD

The equation of motion in PD is generally solved by using numerical techniques with time and spatial integration. The time integration can be conducted by explicit dynamic method or adaptive explicit dynamic method. The spatial integral is usually performed using a simple one-point quadrature of a meshless scheme [20] which requires a volume correction procedure to improve integration accuracy [21–23].

1.4.1 Meshless method for PD

Numerical integration plays a crucial role in the accuracy of numerical PD models. Most published work on PD to date employs a simple meshless cubic cell method with a one-point quadrature for the cells [20]. In this method, the body is discretized into uniformly-sized cubic cells, and the center of each cubic cell is designated as a material point. The bond force on material point $\mathbf{x}_{(i)}$ ($i = 1, 2, \dots$), is integrated over all cubic cells within the horizon, $H_{x_{(i)}}$, of $\mathbf{x}_{(i)}$ and the integration over each cubic cell is approximated by multiplying the cell volume and the integrand evaluated at the cell center, as shown in Fig. 1.4.

The discretized form of equation of motion at each material point, $\mathbf{x}_{(i)}$, in PD is expressed as

$$\rho \ddot{\mathbf{u}}_{(i)} = \sum_m \mathbf{f}(\mathbf{u}_{(m)} - \mathbf{u}_{(i)}, \mathbf{x}_{(m)} - \mathbf{x}_{(i)}) V_{(m)} + \mathbf{b}_{(i)}. \quad (1.23)$$

in which $\mathbf{x}_{(m)}$ represents the point interacts with point $\mathbf{x}_{(i)}$ and is called family member, and $V_{(m)}$ is the cell volume of point $\mathbf{x}_{(m)}$.

This one-point integration is simple and computationally efficient, but with the drawback

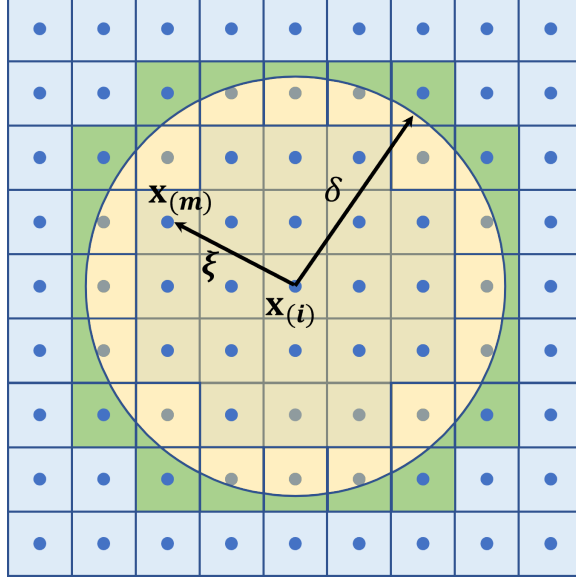


Fig. 1.4: Spatial discretization of meshless method.

of low accuracy. For material points located near the boundary of the horizon whose cells intersect the horizon boundary, only partial cell volume (the yellow part shown in Fig. 1.4) located within the horizon contributes to integration. A volume correction procedure is required to account for such partial contributions. The first and simplest volume correction method is by introducing a linear correction factor as:

$$V'_{(m)} = \begin{cases} \left(\frac{\delta - |\xi|}{2r} + \frac{1}{2} \right) V_{(m)}, & (\delta - r) < |\xi| < \delta \\ V_{(m)}, & |\xi| < (\delta - r) \end{cases} \quad (1.24)$$

in which $V'_{(m)}$ is the corrected volume and r is the half cell size $\frac{\Delta}{2}$. Some other more accurate, yet maybe computational expensive, correction method can be found in [21, 24–26].

1.4.2 Time integration

The time integration of the PD equation of motion is generally performed by explicit forward difference scheme. The equation of motion at time step n is written as

$$\rho_{(i)} \ddot{\mathbf{u}}_{(i)}^n = \sum_m \mathbf{f}^n (\mathbf{u}_{(m)}^n - \mathbf{u}_{(i)}^n, \mathbf{x}_{(m)} - \mathbf{x}_{(i)}) V'_{(m)} + \mathbf{b}_{(i)}. \quad (1.25)$$

The iteration of the explicit time integration scheme can be expressed as

$$\mathbf{u}_{(i)}^{n+1} = \ddot{\mathbf{u}}_{(i)}^n \Delta t^2 + 2\mathbf{u}_{(i)}^n - \mathbf{u}_{(i)}^{n-1}, \quad (1.26)$$

where Δt is the time step size. The explicit scheme is straightforward but conditionally stable. The requirement on time step size Δt for stability can be found in [6, 20].

1.4.3 Adaptive dynamic relaxation for PD

Although the peridynamic theory is in an essentially dynamic form, it still can be applied to solve static or quasi-static problems by the dynamic relaxation method, which introduces artificial damping to the system. The artificial damping can be adaptively modified by using an adaptive dynamic relaxation (ADR) scheme as presented by Kilic and Madenci [27]. Within the framework of ADR, the equation of motion is rewritten at time step n as

$$\ddot{\mathbf{U}}^n + c^n \dot{\mathbf{U}}^n = \mathbf{M}^{-1} \mathbf{F}^n, \quad (1.27)$$

in which $\mathbf{U}$ contains the displacement of the collocation points, $\mathbf{F}$ is composed of internal interaction and external body forces, and the fictitious damping coefficient c^n is determined by [27]

$$c^n = 2\sqrt{\frac{(\mathbf{U}^n)^T \mathbf{K}^n \mathbf{U}^n}{(\mathbf{U}^n)^T \mathbf{U}^n}}, \quad (1.28)$$

in which $\mathbf{K}^n$ is the diagonal local stiffness matrix defined in [27].

1.5 Failure criteria

PD theory describes damages by irreversible bond breakage, which is the non-local interaction of two material points. Thus, an appropriate failure criterion is crucial to determine bond breakage in failure analysis by PD. In PD, the bond status is expressed by the parameter μ defined as

$$\mu = \begin{cases} 1, & \text{unbroken bond} \\ 0, & \text{broken bond.} \end{cases} \quad (1.29)$$

The first proposed failure criterion was the critical stretch criterion [20], in which the bond is treated as broken when the bond stretch s reaches the critical stretch s_0 . The critical stretch s_0 is determined by the material fracture energy G_0 as

$$s_0 = \sqrt{\frac{5G_0}{9\kappa\delta}}, \quad (1.30)$$

where κ is the bulk modulus and δ is the horizon. Based on the energy density ω stored in a deformed bond, Foster et al. [28] proposed the critical energy density criterion, in which the critical energy density ω_0 is also determined by the material fracture energy G_0 as

$$\omega_0 = \frac{4G_0}{\pi\delta^4}. \quad (1.31)$$

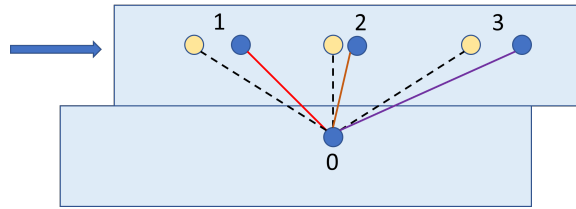


Fig. 1.5: Deformation of PD bonds under shearing mode. Dash lines represent the undeformed bonds and solid lines represent deformed bonds.

Although the critical stretch and critical energy density criteria were commonly used for damage analysis, they are inadequate for pure mode *II* or mode *II* dominant fracture problems [29]. As shown in Fig. 1.5, three bonds are deformed under mode *II* loading

with black dash lines representing the un-deformed bonds. At deformed state, the stretch of bond 0-1 is negative, and that of bond 0-3 is positive. Between the bond 0-1 and bond 0-2, a bond 0-2 exists with zero stretch. Therefore, Bonds 0-1 and 0-2 will not break in the critical stretch criterion. Also, Bond 0-2 will not break in the critical energy density criterion. To remove this inadequacy, Zhang and Qiao [29] proposed a critical skew criterion for quantitative OSBPD analysis of mode *II* fracture.

Since non-ordinary state-based PD (NOSBPD) recovers the concept of non-local stress and strain, an equivalent strain criterion [30] and a maximum principal stress criterion [31] were employed to perform failure analysis by NOSBPD. However, the criterion based on stress and strain may depend strongly on mesh size, as the stress and strain fields near the crack tip exhibit singular behavior.

1.6 Coupling PD with finite element method

The finite element method has been one of the most popular and successful numerical tools for studying structure behaviors for decades due to its computational robustness and efficiency. Despite its widespread applications, the FEM suffers from drawbacks for handling displacement discontinuities as in the cases of cracked bodies and other defects, since the FEM is formulated within the framework of classical continuum mechanics, in which the governing equations require the derivatives of displacements and become invalid at displacement discontinuities. Instead of relying on derivatives of displacements, PD theory bases the force density on an integration form, making it suitable for analyzing structures containing discontinuities. Unfortunately, PD is computationally expensive due to a large number of nonlocal interactions and generally highly refined mesh. Thus, coupling PD with FEM is an appealing choice for taking advantage of these two methods. However, most published coupling methods are not straightforward because FEM allows surface and volume constraints whereas the PD theory considers only volume constraints. These coupling methods commonly require a transition zone to transfer displacements and force information between the PD and the FEM regions.

Macek and Silling [11] coupled PD with FEM by using embedded elements which are available in finite element (FE) analysis code. Kilic and Madenci [32] introduced a coupling method using overlapping regions in which both PD and FE equations are utilized. Agwai et al. [33] coupled PD with FEM using a sub-domain method, where the global modeling is performed using FEM while the PD theory is employed for the sub-modeling and failure prediction. A morphing strategy to couple PD with FEM based on energy equivalence was proposed and was employed for 1D and 2D problems by Lubineau et al. [34]. Liu and Hong [35] introduced interface elements and coupling forces to bridge the PD and FEM. Some adaptive approaches which can transform FEM nodes into peridynamic nodes for coupling PD with FEM were developed in [36–38]. Zaccariotto et al. [39] introduced fictitious FEM nodes and fictitious PD nodes to couple PD with FEM. Bie et al. [40] proposed an approach to couple PD with node-based smoothed finite element which requires no transition region. Zaccariotto et al. [41] also employed a splicing method proposed by Silling et al. [42] to couple PD with FEM and applied this coupling approach to solving 1D, 2D and 3D problems in static and dynamic conditions. Sun and Fish [43] proposed a coupling approach based on a partial superposition of FEM and PD solutions for static and quasi-static problems. To couple PD with FEM, the Arlequin method [44] is used in [45] to impose the mechanical compatibility between finite element and peridynamic sub-regions. Dong et al. [46] proposed a stability-enhanced PD element to couple PD with FEM, in which the stiffness matrix of the PD element is derived to establish the global stiffness matrix. Pagani and Carrera [47] proposed a technique to couple 3D peridynamics with 1D high-order finite elements using Lagrange multipliers. Shen et al. [48] introduced truss elements to bridge finite element (FE) sub-regions and PD sub-regions to couple PD with FEM.

1.7 Research scope and dissertation organization

Peridynamics (PD) is a nonlocal continuum theory based on a framework of integral governing equations and is well suited for failure analysis of solids. However, PD suffers from some drawbacks in its present form, including the need for surface correction and volume

correction, and computational inefficiency. The current research focuses on advancing the theory of PD by removing its drawbacks and applying PD for the deformation and failure analysis of solids.

The organization of this dissertation follows a special format approved by the Department of Mechanical and Nuclear Engineering, Kansas State University. Chapter 1 gives an overview of the theory of Peridynamics and the scope of the current research. Each chapter from Chapter 2 to Chapter 5 consists of a paper published in peer-reviewed scholarly journals or submitted for publication. The final chapter, Chapter 6, presents the final conclusions for this dissertation.

To remove the drawback of the need for a surface correction and a volume correction, a revised non-ordinary state-based PD (RNOSBPD) theory is proposed in Chapter 2. For spherical interaction domains, RNOSBPD recovers the original NOSBPD. However, for interaction domains of arbitrary shapes, RNOSBPD is still valid, eliminating the need for a surface or volume correction. Compared with the finite element method (FEM), PD is computationally expensive because of the nature of nonlocal interactions. A new approach is proposed for coupling PD with the finite element method (FEM) based on the weighted residual method (WRM). This new coupling approach is straightforward, and special techniques such as overlapping regions, interface elements, or fictitious nodes published in the literature for coupling PD with FEM are not needed.

Failure analysis frequently involves the investigation of crack propagation. Using our proposed method of coupling PD with FEM, a pioneering quasi-static simulation method to study crack propagation efficiently is presented in Chapter 3. The failure criterion in the simulation is based on the maximum circumferential tensile stress. A new numerical method is proposed to evaluate the stress intensity factors using the interaction integral based on the J-integral and to determine the trigger of crack propagation and direction of crack growth.

Solving 3D Peridynamics problems directly and implicitly is impractical for most current computers because storing and inverting the huge global stiffness matrix is very demanding computationally. A new PD model for 3D is proposed and presented in Chapter 4, in which the global stiffness matrix is stored in a Compressed Sparse Row (CSR) format based on

Message Passing Interface (MPI), and the system equations are solved by parallel computing by a Parallel Direct Sparse Solver (PDSS), also based on MPI.

To further improve the computational efficiency of PD, a new Enriched Finite Element Method using Peridynamics (EFEM-PD), following a similar concept of element enrichment of extended finite element method (XFEM), is presented in Chapter 5. In EFEM-PD, the FEM model is enriched adaptively with PD equations in regions containing cracks. An adaptive algorithm is implemented with the dual goals of meshing regions with cracks using PD equations while minimizing PD interactions to maximize computational efficiency.

Chapter 2

Revised non-ordinary state-based peridynamics and a new framework for coupling with finite element method ¹

Abstract

In this chapter, we present a revised non-ordinary state-based peridynamics (RNOSBPD), which works for the arbitrary interaction domain and does not require surface correction and volume correction. For the spherical interaction domain, RNOSBPD recovers non-ordinary state-based peridynamics (NOSBPD) of the published work. This current work also presents a new approach to couple the RNOSBPD with FEM (RNOSBPD-FEM). This new coupling approach is straightforward and is easily introduced into commercial finite element codes. With this coupling method, special techniques, such as overlapping regions,

¹This chapter was published on *Engineering Fracture Mechanics*.

Liu, Q., Xin, X. J. (2021). Revised non-ordinary state-based peridynamics and a new framework for coupling with finite element method. *Engineering Fracture Mechanics*, 242, 107483. <https://doi.org/10.1016/j.engfracmech.2020.107483>

interface elements, or fictitious nodes, that have published in the literature for coupling PD with FEM are not needed. Four static applications are performed and the results show the accuracy and efficiency of the RNOSBPD-FEM.

2.1 Introduction

The ability to predict the failure mechanisms of solids is fundamental to theories for structural integrity. Since classical continuum theory utilizes spatial derivatives in its formulation and assumes the material is continuous as it deforms, it is inherently difficult to predict failure of the material. In light of the inadequacies of the classical continuum theory, Peridynamics (PD), based on non-local interactions, was first introduced by Silling [4]. AS PD theory employs spatial integrals of displacements rather than derivatives in its formulation, it is better suited for failure analysis of structures.

The first introduced PD theory is the bond-based PD [4] in which a single PD material parameter, the bond constants c , is employed to analyze isotropic materials, resulting in a restriction of a fixed Poisson's ratio of $1/4$ [5–7]. Subsequently, Silling et al. [8] introduced the ordinary state-based PD (OSBPD) and non-ordinary state-based PD (NOSBPD) theories to remove the restriction. To date, the three versions of PD have been successfully applied to various discontinuous problems, such as crack branching and crack propagation in brittle materials [49], dynamics fracture of the homogeneous and inhomogeneous bars [50], damage and failure analysis of composite materials [51] and metallic structures [52, 53], and fracture analysis of glasses [54–56]

In all of works quoted above, the PD theory was derived by equating the classical strain energy at a point to that of PD with a complete circle or sphere interaction domain [6]. These formulas in PD theory, however, are not valid for a point located near a surface because its interaction domain is not a complete circle or sphere. As a result, PD numerical implementation requires a surface correction procedure to account for the surface effect [6, 10]. Furthermore, most published work on PD to date employs a simple meshless method with a one-point quadrature for cells [20]. Such one-point quadrature requires a volume

correction procedure to improve integration accuracy [21–23].

To remove these two drawbacks, this current work presents a revised non-ordinary state-based peridynamics based on the concept of the numerical differential operator which was first proposed by Madenci et al. [57] and lately modified by Madenci et al. [58]. The modified numerical differential operator is based on the least square minimization (LSM), Taylor series expansion (TSE), and the concept of non-local interactions between field points which is the basis of PD. This modified numerical differential operator does not require that the interaction domain be spherical as required in [8]. Based on this numerical differential operator, Madenci et al. [58] presented an explicit PD-least square minimization (PD-LSM) and proved that the PD-LSM recovers NOSBPD by a special example. In this chapter, the presented RNOSBPD is proved theoretically to recover NOSBPD, and by virtue the advantage of the numerical differential operator, the RNOSBPD works for arbitrary interaction domain and does not require surface correction and volume correction.

Compared with the finite element method (FEM), PD is computationally expensive. Thus, coupling PD with FEM is an appealing choice for taking advantage of these two methods. Macek and Silling [11] coupled PD with FEM by using embedded elements which are available in finite element (FE) analysis code. Kilic and Madenci [32] introduced a coupling method using overlapping regions in which both PD and FE equations are utilized. A morphing strategy to couple PD with FEM based on energy equivalence was proposed by Lubineau et al. [34]. Liu and Hong [35] introduced interface elements and coupling forces to bridge the PD and FEM. Zaccariotto et al. [39] introduced fictitious FEM nodes and fictitious PD nodes to couple PD with FEM. Zaccariotto et al. [41] also employed a splice method which was proposed by Silling et al. [42] to couple PD with FEM and applied this coupling approach to solve 1D, 2D and 3D problems in static and dynamic conditions.

The current work presents a new approach based on the weighted residual method (WRM) for coupling RNOSBPD with the finite element method (FEM). The coupled RNOSBPD and Finite Element Method (RNOSBPD-FEM) is developed to take full advantage of the generality of RNOSBPD and the computational efficiency of FEM. In RNOSBPD-FEM, the problem domain is divided into a PD domain and a FEM domain, and both domains are

discretized into uniform or non-uniform elements. With this framework, the coupling between the PD domain and the FEM domain is straightforward, and special techniques, such as overlapping regions, interface elements, or fictitious nodes, that have been employed in the literature for coupling PD with FEM are not needed. Since RNOSBPD-FEM is derived based on WRM and the whole domain is discretized into finite elements, it can be easily introduced into commercial finite element codes, and the formulation can be converted conveniently between RNOSBPD, FEM, and RNOSBPD-FEM. Four applications concerning deformations and stresses are performed, and the results show the accuracy and efficiency of the proposed coupling framework.

The remainder of this chapter is outlined as follows. First, the theory of NOSBPD is reviewed in section 2.2. Next, the new framework of NOSBPD is proposed in section 2.3. Subsequently, the new coupling approach of RNOSBPD with FEM is presented in section 2.4. Four applications concerning deformations and stresses are performed to validate the proposed NOSBPD-FEM in section 2.5. In the end, concluding remarks are summarized in section 2.6.

2.2 Review of non-ordinary state-based peridynamics

In this section, the NOSBPD first proposed by Silling et al. [8] is briefly reviewed. For completeness and conciseness in presentation, relevant formulas essential for understanding NOSBPD are quoted directly from the published work without derivation.

Consider a material point $\mathbf{x}$ in a domain that interacts with its neighbors $\mathbf{x}'$, which is located within a spherical domain, H_x , with a radius of δ , called a horizon. Silling et al. [8] defined that the image of a vector $\boldsymbol{\xi}$ under the state $\underline{\mathbf{A}}$ is a tensor, written as $\underline{\mathbf{A}}\langle\boldsymbol{\xi}\rangle$. The reference vector position state called the bond is defined as:

$$\underline{\mathbf{X}}\langle\boldsymbol{\xi}\rangle = \boldsymbol{\xi} = \mathbf{x}' - \mathbf{x}. \quad (2.1)$$

The deformation vector state is the deformed state of the bond defined as

$$\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle = \boldsymbol{\eta} + \boldsymbol{\xi}, \quad (2.2)$$

here $\boldsymbol{\eta} = \mathbf{u}' - \mathbf{u}$ is the relative displacement of the bond. The non-local deformation gradient at point $\mathbf{x}$ is given by

$$\bar{\mathbf{F}}(\mathbf{x}) = \left[\int_{H_x} \omega(|\boldsymbol{\xi}|) (\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle \otimes \boldsymbol{\xi}) dV_{x'} \right] \boldsymbol{\mathcal{S}}^{-1}. \quad (2.3)$$

where $\omega(|\boldsymbol{\xi}|)$ is a scalar state called the influence function and $\boldsymbol{\mathcal{S}}$ is the shape tensor defined by

$$\boldsymbol{\mathcal{S}}(\mathbf{x}) = \int_{H_x} \omega(|\boldsymbol{\xi}|) (\boldsymbol{\xi} \otimes \boldsymbol{\xi}) dV_{x'}. \quad (2.4)$$

With the non-local deformation gradient Eq. (2.3), we can derive the non-local displacement gradient as

$$u_{k,j} = \left[\int_{H_x} \omega(|\boldsymbol{\xi}|) (u_k(\mathbf{x}') - u_k(\mathbf{x})) \xi_j dV_{x'} \right] \mathcal{S}_{ij}^{-1}, \quad (2.5)$$

The equation of motion in PD is given by

$$\rho \ddot{\mathbf{u}} = \mathbf{L}(\mathbf{x}, t) + \mathbf{b}(\mathbf{x}, t), \quad (2.6)$$

where ρ is the density of the material and $\mathbf{b}$ is externally applied body force density, and $\mathbf{L}$ is non-local internal force density which can be evaluated as

$$\mathbf{L} = \int_{H_x} \{ \underline{\mathbf{T}}[\mathbf{x}, t] \langle \boldsymbol{\xi} \rangle - \underline{\mathbf{T}}'[\mathbf{x}', t] \langle -\boldsymbol{\xi} \rangle \} dV_{x'}, \quad (2.7)$$

with force vector states $\underline{\mathbf{T}}[\mathbf{x}, t] \langle \boldsymbol{\xi} \rangle$ and $\underline{\mathbf{T}}'[\mathbf{x}', t] \langle -\boldsymbol{\xi} \rangle$ defined by

$$\underline{\mathbf{T}}[\mathbf{x}, t] \langle \boldsymbol{\xi} \rangle = \omega(|\boldsymbol{\xi}|) \boldsymbol{\sigma}(\mathbf{x}) \boldsymbol{\mathcal{S}}^{-1}(\mathbf{x}) \boldsymbol{\xi}, \quad (2.8)$$

and

$$\underline{\mathbf{T}}'[\mathbf{x}', t]\langle -\boldsymbol{\xi} \rangle = -\omega(|\boldsymbol{\xi}|)\boldsymbol{\sigma}(\mathbf{x}')\boldsymbol{\mathcal{F}}^{-1}(\mathbf{x}')\boldsymbol{\xi}, \quad (2.9)$$

where $\boldsymbol{\sigma}$ is the first Piola-Kirchhoff stress tensor which can be obtained from classic constitutive law as a function of the non-local deformation gradient. The non-local internal force density $\mathbf{L}$ is evaluated as

$$\mathbf{L}(\mathbf{x}, t) = \int_{H_x} \omega(|\boldsymbol{\xi}|) \{ \boldsymbol{\sigma}(\mathbf{x})\boldsymbol{\mathcal{F}}^{-1}(\mathbf{x}) + \boldsymbol{\sigma}(\mathbf{x}')\boldsymbol{\mathcal{F}}^{-1}(\mathbf{x}') \} \boldsymbol{\xi} dV_{x'}. \quad (2.10)$$

It's worthy noting that for spherical interaction domain, the integration of $\underline{\mathbf{T}}[\mathbf{x}, t]\langle \boldsymbol{\xi} \rangle$ will vanish,

$$\int_{H_x} \underline{\mathbf{T}}[\mathbf{x}, t]\langle \boldsymbol{\xi} \rangle dV_{x'} = 0. \quad (2.11)$$

NOSBPD converges to the traditional continuum elasticity when the interaction domain is spherical and vanishingly small. When the interaction domain is non-spherical, however, NOSBPD with Eqs. (2.7), (2.8) and (2.9) may fail to satisfy equilibrium and does not converge to the traditional continuum elasticity. The revised NOSBPD (RNOSBPD) developed in the current work overcomes the deficiencies of NOSBPD. The formulas for non-local internal force density $\mathbf{L}$ in RNOSBPD are shown to be different from Eqs. (2.7), (2.8) and (2.9). RNOSBPD, to be presented in the next section, satisfies equilibrium for arbitrarily shaped interaction domain and converges to the traditional continuum elasticity in the limit of vanishingly small interaction domain size.

2.3 Revised non-ordinary state-based peridynamics

In this section, we present a revised NOSBPD (RNOSBPD) based on the essential PD concept of non-local interactions between field points, Taylor series expansion (TSE), and least square minimization (LSM) for numerical differentiation. RNOSBPD works for arbitrary interaction domain and does not require surface correction and volume correction.

According to the non-local interaction of PD theory, the function $f(\mathbf{x})$ at point $\mathbf{x}$ is

affected by $f(\mathbf{x}')$ at the point $\mathbf{x}'$ within the interaction domain, H_x , of point $\mathbf{x}$. The value of $f(\mathbf{x}')$ can be approximately evaluated as

$$f(\mathbf{x}') = f(\mathbf{x}) + f_{,x_i}(\mathbf{x})\xi_i + R, \quad (2.12)$$

here $\mathbf{x}' = \mathbf{x} + \boldsymbol{\xi}$, $\xi_i = x'_i - x_i$, R is the reminder, and $f_{,x_i}(\mathbf{x}) = \frac{\partial f(\mathbf{x})}{\partial x_i}$ ($i = 1, 2, 3$). The weighted error ϵ from the approximation in Eq. (2.12), within the interaction domain of $\mathbf{x}$, can be evaluated as

$$\epsilon = \int_{H_x} \omega(|\boldsymbol{\xi}|) R^2 dV_{x'} = \int_{H_x} \omega(|\boldsymbol{\xi}|) [f(\mathbf{x}') - f(\mathbf{x}) - f_{,x_i}(\mathbf{x})\xi_i]^2 dV_{x'}. \quad (2.13)$$

To minimize the error ϵ , we demand

$$\frac{\partial \epsilon}{\partial f_{,x_i}} = 0. \quad (2.14)$$

This requirement leads to the 1st-order differential of $f(\mathbf{x})$ as

$$f_{,x_i} = \left[\int_{H_x} \omega(|\boldsymbol{\xi}|) (f(\mathbf{x}') - f(\mathbf{x})) \xi_j dV_{x'} \right] \mathcal{S}_{ij}^{-1}, \quad (2.15)$$

here $\mathcal{S}$ is the shape tensor as defined in Eq. (2.4).

Replacing the $f(\mathbf{x})$ in Eq. (2.15) by displacement components u_k leads to the non-local displacement gradient,

$$u_{k,j}^{pd} = \left[\int_{H_x} \omega(|\boldsymbol{\xi}|) (u_k(\mathbf{x}') - u_k(\mathbf{x})) \xi_j dV_{x'} \right] \mathcal{S}_{ij}^{-1}, \quad (2.16)$$

or equivalently,

$$\nabla \mathbf{u}^{pd} = \left[\int_{H_x} \omega(|\boldsymbol{\xi}|) (\boldsymbol{\eta} \otimes \boldsymbol{\xi}) dV_{x'} \right] \mathcal{S}^{-1}. \quad (2.17)$$

Note that Eq. (2.17) is identical to Eq. (2.5). With the non-local displacement gradient, $\nabla \mathbf{u}^{pd}$, we can obtain the non-local stress, $\boldsymbol{\sigma}^{pd}$, by the constitutive law of classical continuum

mechanics. Replacing $f(\mathbf{x})$ in Eq. (2.15) by non-local stress components σ_{mi}^{pd} leads to the non-local internal force vector,

$$\sigma_{mi,i}^{pd} = \left[\int_{H_x} \omega(|\boldsymbol{\xi}|) \left(\sigma_{mi}^{pd}(\mathbf{x}') - \sigma_{mi}^{pd}(\mathbf{x}) \right) \xi_j dV_{x'} \right] \mathcal{S}_{ij}^{-1}, \quad (2.18)$$

or equivalently,

$$\mathbf{L}^{pd} = \nabla \cdot \boldsymbol{\sigma}^{pd} = \int_{H_x} (\mathbf{t}'(\boldsymbol{\xi}, \boldsymbol{\eta}) - \mathbf{t}(\boldsymbol{\xi}, \boldsymbol{\eta})) dV_{x'} = \int_{H_x} \omega(|\boldsymbol{\xi}|) \{ \boldsymbol{\sigma}^{pd}(\mathbf{x}') - \boldsymbol{\sigma}^{pd}(\mathbf{x}) \} \boldsymbol{\mathcal{S}}^{-1}(\mathbf{x}) \boldsymbol{\xi} dV_{x'}, \quad (2.19)$$

here the force states $\mathbf{t}'(\boldsymbol{\xi}, \boldsymbol{\eta})$ and $\mathbf{t}(\boldsymbol{\xi}, \boldsymbol{\eta})$ are defined as follows,

$$\mathbf{t}'(\boldsymbol{\xi}, \boldsymbol{\eta}) = \omega(|\boldsymbol{\xi}|) \boldsymbol{\sigma}^{pd}(\mathbf{x}') \boldsymbol{\mathcal{S}}^{-1}(\mathbf{x}) \boldsymbol{\xi}, \quad (2.20)$$

$$\mathbf{t}(\boldsymbol{\xi}, \boldsymbol{\eta}) = \omega(|\boldsymbol{\xi}|) \boldsymbol{\sigma}^{pd}(\mathbf{x}) \boldsymbol{\mathcal{S}}^{-1}(\mathbf{x}) \boldsymbol{\xi}, \quad (2.21)$$

Note that the process above to derive the displacement gradient and the internal force vector in RNOSBPD does not require that the interaction domain be spherical as required in NOSBPD [8]. In fact, RNOSBPD works for arbitrary interaction domains, and it does not require surface correction and volume correction. Comparison between Eq. (2.10) and Eq. (2.19) clearly reveals the differences in the definition of non-local internal force vector for NOSBPD and RNOSBPD. For the specified spherical interaction domain, because the integration of $\mathbf{T}[\mathbf{x}, t] \langle \boldsymbol{\xi} \rangle$ over the interaction domain will vanish and $\boldsymbol{\mathcal{S}}(\mathbf{x}') = \boldsymbol{\mathcal{S}}(\mathbf{x})$, Eq. (2.10) and Eq. (2.19) become identical. Thus, the RNOSBPD recovers the NOSBPD theory for the spherical domain. For the non-spherical domain, however, Eq. (2.19) and Eq. (2.10) are different, and RNOSBPD is still valid and converges to traditional continuum elasticity for vanishingly small interaction domain, while NOSBPD breaks down and does not satisfy equilibrium. For example, consider a 1D bar under uniaxial tension σ and for the point $\mathbf{x}$ at the left boundary of the bar (Fig. 2.1), since the influence function $\omega(\boldsymbol{\xi})$ is non-negative [8], and from Eq. (2.4) and Eq. (2.7), we conclude that the internal force $L(\mathbf{x}) > 0$, so that point $\mathbf{x}$ is not balanced by NOSBPD, but for RNOSBPD, $L(\mathbf{x})$ is equal to zero.

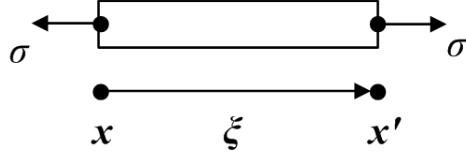


Fig. 2.1: Bond ξ of 1D bar under tension σ .

The energy density at point $\mathbf{x}$ from the force state $\mathbf{t}(\xi, \eta)$ can be evaluated as follows,

$$\begin{aligned}
 U &= \frac{1}{2} \int_{H_x} \mathbf{t} \cdot \eta dV_{x'} \\
 &= \frac{1}{2} \int_{H_x} \omega(|\xi|) \sigma_{ij}^{pd} \mathcal{S}_{jk}^{-1} \xi_k \eta_i dV_{x'} \\
 &= \frac{1}{2} \sigma_{ij}^{pd} \left(\int_{H_x} \omega(|\xi|) \xi_k \eta_i dV_{x'} \right) \mathcal{S}_{jk}^{-1} \\
 &= \frac{1}{2} \sigma_{ij}^{pd} u_{i,j}^{pd} = \frac{1}{2} \sigma_{ij}^{pd} \varepsilon_{ij}^{pd}.
 \end{aligned} \tag{2.22}$$

Thus, only the force state $\mathbf{t}(\xi, \eta)$ has a contribution to the strain energy. To describe the damage of the material, Silling and Askari [20] introduce a bond state parameter μ which is defined as

$$\mu(\xi) = \begin{cases} 1, & \text{unbroken,} \\ 0, & \text{broken.} \end{cases} \tag{2.23}$$

If the bond is broken, the energy in the bond will be released to create a new fracture surface. For pre-existing crack, if a bond crosses the crack, the bond is irreversibly broken. For crack propagation, the criterion for bond breakage is flexible and some of the published failure criteria can be found in [20, 29, 31, 59, 60]. With the bond state parameter, it ensures that damaged bonds are excluded from the calculation of $\nabla \mathbf{u}^{pd}$, that the force state $\mathbf{t}(\xi, \eta)$ takes on a value of 0 at damaged bonds, as described in [8]. Thus, the non-local displacement gradient in Eq. (2.17) can be modified as

$$\nabla \mathbf{u}^{pd} = \left[\int_{H_x} \mu \omega(|\xi|) (\eta \otimes \xi) dV_{x'} \right] \mathcal{S}^{-1}. \tag{2.24}$$

With the representations of this modified non-local displacement gradient and the bond state parameter, the energy density at point $\mathbf{x}$ becomes

$$\begin{aligned} U &= \frac{1}{2} \int_{H_x} \mu \mathbf{t} \cdot \boldsymbol{\eta} dV_{x'} = \frac{1}{2} \sigma_{ij}^{pd} \left(\int_{H_x} \mu \omega(|\boldsymbol{\xi}|) \xi_k \eta_i dV_{x'} \right) \mathcal{S}_{jk}^{-1} \\ &= \frac{1}{2} \sigma_{ij}^{pd} u_{i,j}^{pd} = \frac{1}{2} \sigma_{ij}^{pd} \varepsilon_{ij}^{pd}. \end{aligned} \quad (2.25)$$

2.4 A new coupling approach of RNOSBPD with FEM

A new framework for coupling RNOSBPD with FEM is presented in this section. In this framework, the problem domain is divided into a PD domain and a FEM domain, both of which are discretized into uniform or non-uniform elements. Shared nodes on the interface between the PD domain and the FEM domain play a dual role, governed by the theory of PD on one side and by the theory of elasticity on the other. A similar method to divide the domain was applied in [41]. The weighted residual method is applied to PD equations of motion over the PD domain and elasticity equations of motion over the FEM domain, and the resultant governing equations combine PD and theory of elasticity in a unified way. When the FEM domain shrinks to zero, the formulation fully recovers the RNOSBPD, and when the PD domain shrinks to zero, the formulation becomes the traditional FEM. When the PD domain and the FEM domain both exist, the formulation represents a coupling between RNOSBPD and FEM. We refer to the numerical model developed in this work as RNOSBPD-FEM, which does not need special techniques, such as overlapping region, interface elements, and fictitious nodes as published in the literature.

In section 2.4.1, the discretization of PD domain is presented, and the volume of integration for each family node in the interaction domain is explained. In section 2.4.2, the discretization of the problem domain into a PD domain and a Finite Element Method (FEM) domain is introduced. In section 2.4.3, a framework is developed for coupling PD and FEM in a unified way, in which the governing equations are obtained by applying the weighted residual method (WRM) to the equations of motion from both PD and FEM in a unified way.

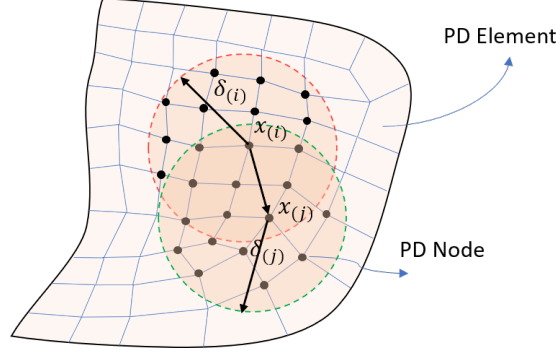


Fig. 2.2: PD domain discretization and the interactions between node $x_{(i)}$ and its family members.

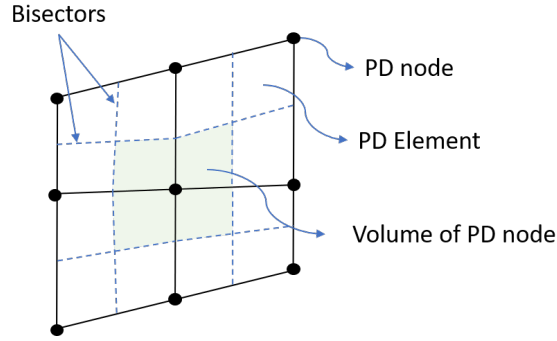


Fig. 2.3: Volume of PD node.

2.4.1 Discretization of PD domain

The RNOSBPD model of a domain can be discretized with traditional finite elements (named as PD element herein) by using commercial software, such as ANSYS due to its robust meshing ability.

As shown in Fig. 2.2, a 2D PD domain is discretized into PD elements and each PD element contains 4 PD nodes. As shown in Fig. 2.3, each PD element is divided into 4 volume parts by two bisectors, and the volume of each PD node is the summation of quarter volumes of all elements connected to the node. It is worth noting that the PD node may not locate at the center of its volume, especially for these nodes locating on the boundary of the domain. Besides, if the domain is discretized with 3 nodes elements, we can treat the 3 node element as 4 node element with the third and fourth nodes collapsed together.

As shown in Fig. 2.2, the internal force vector at PD node $x_{(i)}$ is achieved by including its interactions with other PD nodes (called family members), $x_{(j)}$, in the interaction domain.

The interaction domain of node $\mathbf{x}_{(i)}$ depends on its horizon size $\delta_{(i)}$ and can be an arbitrary shape for RNOSBPD. The horizon size $\delta_{(i)}$ of node $\mathbf{x}_{(i)}$ is specified as $\delta_{(i)} = m\Delta_{(i)}$, with m being a constant and the characteristic length $\Delta_{(i)}$ which depends on the area $A_{(i)}$ or volume $V_{(i)}$ occupied by PD node $\mathbf{x}_{(i)}$. Studies on selecting values of m can be found in [61, 62] and $\Delta_{(i)}$ is defined as [60]

$$\Delta_{(i)} = \begin{cases} \sqrt{A_{(i)}}, & \text{2-D} \\ \sqrt[3]{V_{(i)}}, & \text{3-D} \end{cases}. \quad (2.26)$$

Thus, each PD node has its own horizon size and family members. For non-uniform discretization, the rule to determine family members of node $\mathbf{x}_{(i)}$ is suggested by Hu et al. [60] as

$$H_{\mathbf{x}_{(i)}} = \left\{ \mathbf{x}_{(j)} \in H_{\mathbf{x}_{(i)}} : |\mathbf{x}_{(j)} - \mathbf{x}_{(i)}| \leq \delta_{(i)} \cup |\mathbf{x}_{(j)} - \mathbf{x}_{(i)}| \leq \delta_{(j)} \right\}, \quad (2.27)$$

which ensures that the bond between nodes $\mathbf{x}_{(i)}$ and $\mathbf{x}_{(j)}$ is a paired interaction for either interaction domain.

For node $\mathbf{x}_{(i)}$, there are $N_{(i)}$ family members within its interaction domain and the displacement set of these nodes is

$$\mathbf{u}^{(i)} = \begin{bmatrix} u_{1(i)} & u_{2(i)} & u_{1(2)} & u_{2(2)} & \cdots & u_{1(m)} & u_{2(m)} & \cdots & u_{1(N_{(i)})} & u_{2(N_{(i)})} \end{bmatrix}^T, \quad (2.28)$$

here, the subscript (m) represents the m -th family member node $\mathbf{x}_{(m)}$ within the interaction domain of node $\mathbf{x}_{(i)}$ and its first member is $\mathbf{x}_{(i)}$.

Following a procedure similar to [63], we obtain the discrete form of strain vector at node $\mathbf{x}_{(i)}$ from Eq. (2.24) as follows,

$$\{\varepsilon\}_{(i)}^{pd} = [\varepsilon_x \quad \varepsilon_y \quad \gamma_{xy}]^T = \mathbf{S}^{(i)} \mathbf{A}^{(i)} \mathbf{u}^{(i)}, \quad (2.29)$$

where $\mathbf{S}^{(i)}$ and $\mathbf{A}^{(i)}$ are defined as follows,

$$\mathbf{S}^{(i)} = \begin{bmatrix} \mathcal{S}_{11}^{-1} & 0 & \mathcal{S}_{21}^{-1} & 0 \\ 0 & \mathcal{S}_{12}^{-1} & 0 & \mathcal{S}_{22}^{-1} \\ \mathcal{S}_{12}^{-1} & \mathcal{S}_{11}^{-1} & \mathcal{S}_{22}^{-1} & \mathcal{S}_{21}^{-1} \end{bmatrix}, \quad (2.30)$$

$$\mathbf{A}^{(i)} = \begin{bmatrix} -\sum_{m=2}^{N(i)} \mu_{(im)} \omega_{(im)} \xi_{1(im)} V_{(m)} \mathbf{I}_{2 \times 2} & \mu_{(i2)} \omega_{(i2)} \xi_{1(i2)} V_{(2)} \mathbf{I}_{2 \times 2} & \cdots & \mu_{(iN(i))} \omega_{(iN(i))} \xi_{1(iN(i))} V_{(N(i))} \mathbf{I}_{2 \times 2} \\ -\sum_{m=2}^{N(i)} \mu_{(im)} \omega_{(im)} \xi_{2(im)} V_{(m)} \mathbf{I}_{2 \times 2} & \mu_{(i2)} \omega_{(i2)} \xi_{2(i2)} V_{(2)} \mathbf{I}_{2 \times 2} & \cdots & \mu_{(iN(i))} \omega_{(iN(i))} \xi_{2(iN(i))} V_{(N(i))} \mathbf{I}_{2 \times 2} \end{bmatrix}. \quad (2.31)$$

where the subscript (im) represents the bond between node $\mathbf{x}_{(i)}$ and its m -th family member, and $\mathbf{I}_{2 \times 2}$ represents a identity matrix with size 2×2 . From Eq. (2.29), the discrete form of stress vector at node $\mathbf{x}_{(i)}$ is

$$\{\sigma\}_{(i)}^{pd} = \mathbf{D} \mathbf{S}^{(i)} \mathbf{A}^{(i)} \mathbf{u}^{(i)}, \quad (2.32)$$

here, $\mathbf{D}$ is material stiffness matrix of elasticity material. For plane stress problem,

$$\mathbf{D} = \frac{E}{1 - \nu^2} \begin{bmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & \frac{1-\nu}{2} \end{bmatrix}, \quad (2.33)$$

and for plane strain problem,

$$\mathbf{D} = \frac{E}{(1 - 2\nu)(1 + \nu)} \begin{bmatrix} 1 - \nu & \nu & 0 \\ \nu & 1 - \nu & 0 \\ 0 & 0 & \frac{1-2\nu}{2} \end{bmatrix}. \quad (2.34)$$

Also, from Eq. (2.19), we obtain the discrete form of the internal force vector at node $\mathbf{x}_{(i)}$

as

$$\mathbf{L}_{(i)}^{pd} = \sum_{m=2}^{N_{(i)}} [\mathbf{C}'_{(im)} \mathbf{u}^{(m)} - \mathbf{C}_{(im)} \mathbf{u}^{(i)}], \quad (2.35)$$

where $\mathbf{C}'_{(im)}$ and $\mathbf{C}_{(im)}$ are defined as follows,

$$\mathbf{C}'_{(im)} = \mathbf{Q}_{(im)} \mathbf{D} \mathbf{S}^{(m)} \mathbf{A}^{(m)}, \quad (2.36)$$

$$\mathbf{C}_{(im)} = \mathbf{Q}_{(im)} \mathbf{D} \mathbf{S}^{(i)} \mathbf{A}^{(i)}, \quad (2.37)$$

$$\mathbf{Q}_{(im)} = \begin{bmatrix} Q_1 & 0 & Q_2 \\ 0 & Q_2 & Q_1 \end{bmatrix}, \quad (2.38)$$

$$Q_1 = (\mathcal{S}_{11}^{-1} \xi_{1(im)} + \mathcal{S}_{12}^{-1} \xi_{2(im)}) \omega_{(im)} V_{(m)}, \quad (2.39)$$

$$Q_2 = (\mathcal{S}_{21}^{-1} \xi_{1(im)} + \mathcal{S}_{22}^{-1} \xi_{2(im)}) \omega_{(im)} V_{(m)}. \quad (2.40)$$

It is worth noting that the influence function $\omega(|\boldsymbol{\xi}|)$ may affect the accuracy in numerical implementation. In this chapter, we specify the influence function as a Gaussian distribution in the form of

$$\omega(|\boldsymbol{\xi}|) = e^{-\left(\frac{|\boldsymbol{\xi}|}{a\delta}\right)^2}, \quad (2.41)$$

here, a is a constant and we define it as a *non-local factor*. The effect of a will be studied in section 2.5.2.

2.4.2 Discretization of RNOSBPD-FEM domain

To couple RNOSBPD with traditional FEM, the whole problem domain is divided into a FEM domain and a PD domain, and both domains are discretized into elements, as shown in Fig. 2.4. To distinguish, the elements in the PD domain are called PD elements and elements in the FEM domain are still called finite elements. Note that PD nodes on the interface of the PD domain and the FEM domain are also nodes of the finite element, and the interaction domains of these PD nodes are only determined from the PD domain, and

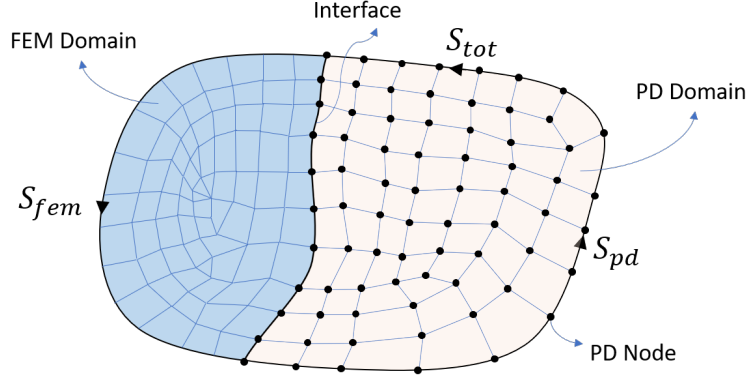


Fig. 2.4: The coupling PD with FEM.

the volumes of these PD nodes are calculated only from the PD elements.

Consider a 2-D discrete domain that contains N nodes, of which N^{pd} are PD nodes. For the i -th PD node $\mathbf{x}_{(i)}$, its displacement vector is $\mathbf{u}_{(i)} = [u_{1(i)} \quad u_{2(i)}]^T$. The displacement set of all nodes (global displacement vector) is expressed as

$$\mathbf{u}_g = \begin{bmatrix} \mathbf{u}_u \\ \mathbf{u}_p \end{bmatrix}, \quad (2.42)$$

here $\mathbf{u}_u$ is the set of all unknown displacement components and $\mathbf{u}_p$ is the set of prescribed displacement components. The displacement vector of the PD node $\mathbf{x}_{(i)}$ can be expressed as

$$\mathbf{u}_{(i)} = \mathbf{M}_{(i)} \mathbf{u}_g, \quad (2.43)$$

here, $\mathbf{M}_{(i)}$ is the mapping matrix from $\mathbf{u}_g$ to $\mathbf{u}_{(i)}$, with size $2 \times 2N$. The displacement set of the family members of the PD node $\mathbf{x}_{(i)}$, $\mathbf{u}^{(i)}$, can be expressed by global displacement vector as

$$\mathbf{u}^{(i)} = \mathbf{M}^{(i)} \mathbf{u}_g, \quad (2.44)$$

here, $\mathbf{M}^{(i)}$ is the mapping matrix from $\mathbf{u}_g$ to $\mathbf{u}^{(i)}$, with size $2N_{(i)} \times 2N$ and it can be specified as follows: if the k -th component of $\mathbf{u}^{(i)}$ and the j -th component of $\mathbf{u}_g$ are same, $M_{kj}^{(i)} = 1$, otherwise $M_{kj}^{(i)} = 0$. Thus, there is one and only one component equal to 1 in each row of

$\mathbf{M}^{(i)}$.

The mapping matrices can be used for the matrix assembling procedure. For example, if $\mathbf{B} = \mathbf{M}_{(p)}^T \mathbf{A} \mathbf{M}^{(i)}$, the assembling procedure to obtain matrix $\mathbf{B}$ from $\mathbf{A}$ is as follows: we first initialize all components of $\mathbf{B}$ as zero, then go through all components of $\mathbf{M}_{(p)}$ and $\mathbf{M}^{(i)}$, if $M_{kj}^{(i)} = 1$ and $M_{mn(p)} = 1$, then $B_{nj} = A_{mk}$ ($n, j \in 1, 2, 3, \dots, 2N$, $m \in 1, 2$, and $k \in 1, 2, 3, \dots, 2N_{(i)}$).

Substituting Eq. (2.44) into Eq. (2.32) and Eq. (2.35), leads to the non-local stress vector and internal force vector by global displacement vector as below,

$$\{\sigma\}_{(i)}^{pd} = \mathbf{D} \mathbf{S}^{(i)} \mathbf{A}^{(i)} \mathbf{M}^{(i)} \mathbf{u}_g, \quad (2.45)$$

$$\mathbf{L}_{(i)}^{pd} = \sum_{m=2}^{N_{(i)}} \left[\mathbf{C}'_{(im)} \mathbf{M}^{(m)} - \mathbf{C}_{(im)} \mathbf{M}^{(i)} \right] \mathbf{u}_g. \quad (2.46)$$

2.4.3 Governing Equations of RNOSBPD-FEM

For a coupled model, both the PD domain and the FEM domain exist. Applying the WRM on the equations of motion and the boundary conditions over the whole problem domain leads to

$$\int_{V_{tot}} \delta \mathbf{u}^T (\mathbf{L} + \mathbf{b} - \rho \ddot{\mathbf{u}}) dV - \int_{S_{tot}} \delta \mathbf{u}^T (\boldsymbol{\sigma} \mathbf{n} - \mathbf{T}) dS = 0, \quad (2.47)$$

where $\mathbf{T}$ is the external traction force on the surface boundary, $\mathbf{n}$ is the unit normal vector of the boundary, V_{tot} and S_{tot} are the volume and surface of the whole domain respectively, and $\delta(\bullet)$ represents a virtual value. Within the FEM domain, applying the Gauss theorem to Eq. (2.47) leads to

$$\begin{aligned} & \int_{V_{fem}} [\delta \mathbf{u}^T \rho \ddot{\mathbf{u}} + \delta(\{\epsilon\}^T) \{\sigma\}] dV + \int_{V_{pd}} \delta \mathbf{u}^T (\rho \ddot{\mathbf{u}} - \mathbf{L}^{pd}) dV + \int_{S_{pd}} \delta \mathbf{u}^T \boldsymbol{\sigma}^{pd} \mathbf{n} dS = \\ & \int_{S_{tot}} \delta \mathbf{u}^T \mathbf{T} dS + \int_{V_{fem}} \delta \mathbf{u}^T \mathbf{b} dV + \int_{V_{pd}} \delta \mathbf{u}^T \mathbf{b} dV, \end{aligned} \quad (2.48)$$

where V_{fem} and V_{pd} represent the volume of the FEM domain and PD domain respectively, and S_{pd} represents the boundary of the PD domain.

The virtual internal work by the internal force of the PD domain, δU_B^{pd} , can be expressed as

$$\delta U_B^{pd} = - \int_{V_{pd}} \delta \mathbf{u}^T \mathbf{L}^{pd} dV = - \sum_{i=1}^{N^{pd}} \delta \mathbf{u}_{(i)}^T \mathbf{L}_{(i)}^{pd} V_{(i)} \quad (2.49)$$

Substituting Eq. (2.43) and Eq. (2.46) into Eq. (2.49) leads to

$$\delta U_B^{pd} = \delta \mathbf{u}_g^T \mathbf{K}_b^{pd} \mathbf{u}_g, \quad (2.50)$$

where $\mathbf{K}_b^{pd} = - \sum_{i=1}^{N^{pd}} \sum_{m=2}^{N_{(i)}} \left[\mathbf{M}_{(i)}^T \mathbf{C}'_{(im)} \mathbf{M}^{(m)} - \mathbf{M}_{(i)}^T \mathbf{C}_{(im)} \mathbf{M}^{(i)} \right]$.

Two adjacent PD nodes on the boundary of the PD domain, S_{pd} , define a PD boundary element (PDBE). As shown in Fig. 2.5, Madenci et al. [31, 64] assume that the displacement and traction vary linearly between the two end nodes, $\mathbf{x}_{(\ell_1)}$ and $\mathbf{x}_{(\ell_2)}$, of the ℓ -th PDBE as

$$\mathbf{u}_{(\ell)} = (1 - s) \mathbf{u}_{(\ell_1)} + s \mathbf{u}_{(\ell_2)}, \quad (2.51)$$

and

$$\mathbf{t}_{(\ell)}^{pd} = (1 - s) \mathbf{t}_{(\ell_1)}^{pd} + s \mathbf{t}_{(\ell_2)}^{pd}, \quad (2.52)$$

where s is the local coordinate of the ℓ -th PDBE with a unit normal vector $\mathbf{n}_{(\ell)}$ and length $\Gamma_{(\ell)}$.

The traction at the two end nodes of ℓ -th PDBE can be expressed as

$$\mathbf{t}_{(\ell_i)}^{pd} = \boldsymbol{\sigma}_{(\ell_i)}^{pd} \mathbf{n}_{(\ell)} = \mathbf{N}_{(\ell)} \{\boldsymbol{\sigma}\}_{(\ell_i)}^{pd} \quad (2.53)$$

where $\mathbf{N}_{(\ell)}$ is defined as

$$\mathbf{N}_{(\ell)} = \begin{bmatrix} n_{1(\ell)} & 0 & n_{2(\ell)} \\ 0 & n_{2(\ell)} & n_{1(\ell)} \end{bmatrix}. \quad (2.54)$$

With this representation of $\mathbf{u}_{(\ell)}$ and $\mathbf{t}_{(\ell)}^{pd}$, the virtual internal work associated with PD domain

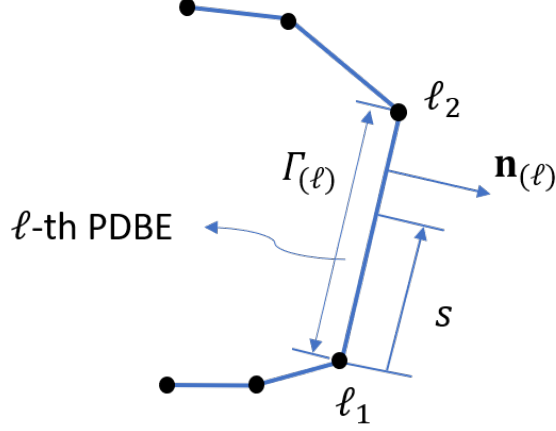


Fig. 2.5: PD boundary elements.

boundary, δU_S^{pd} , can be evaluated as

$$\delta U_S^{pd} = \int_{S_{pd}} \delta \mathbf{u}^T \boldsymbol{\sigma}^{pd} \mathbf{n} dS = \int_{S_{pd}} \delta \mathbf{u}^T \mathbf{t}^{pd} dS = \sum_{\ell=1}^{N_S^{pd}} \left(\Gamma_{(\ell)} \int_0^1 \delta \mathbf{u}_{(\ell)}^T \mathbf{t}_{(\ell)}^{pd} ds \right), \quad (2.55)$$

here, N_S^{pd} is the number of PD BE. Substituting Eqs. (2.43), (2.45), (2.51), (2.52) and (2.53) into Eq. (2.55), leads to

$$\delta U_S^{pd} = \delta \mathbf{u}_g^T \mathbf{K}_s^{pd} \mathbf{u}_g, \quad (2.56)$$

where $\mathbf{K}_s^{pd}$ is defined as

$$\begin{aligned} \mathbf{K}_s^{pd} = & \sum_{\ell=1}^{N_S^{pd}} \Gamma_{(\ell)} \left[\left(\frac{1}{3} \mathbf{M}_{(\ell_1)} + \frac{1}{6} \mathbf{M}_{(\ell_2)} \right) \mathbf{N}_{(\ell)} \mathbf{D} \mathbf{S}^{(\ell_1)} \mathbf{A}^{(\ell_1)} \mathbf{M}^{(\ell_1)} \right] \\ & + \sum_{\ell=1}^{N_S^{pd}} \Gamma_{(\ell)} \left[\left(\frac{1}{6} \mathbf{M}_{(\ell_1)} + \frac{1}{3} \mathbf{M}_{(\ell_2)} \right) \mathbf{N}_{(\ell)} \mathbf{D} \mathbf{S}^{(\ell_2)} \mathbf{A}^{(\ell_2)} \mathbf{M}^{(\ell_2)} \right]. \end{aligned} \quad (2.57)$$

The virtual work by the inertia force in the PD domain, δU_I^{pd} , can be evaluated as

$$\delta U_I^{pd} = \int_{V_{pd}} \delta \mathbf{u}^T \rho \ddot{\mathbf{u}} dV = \delta \mathbf{u}_g^T \mathbf{M}^{pd} \ddot{\mathbf{u}}_g, \quad (2.58)$$

where $\mathbf{M}^{pd} = \sum_{i=1}^{N^{pd}} \rho \mathbf{M}_{(i)}^T \mathbf{M}_{(i)} V_{(i)}$.

Similarly, the virtual work by the external body force $\mathbf{b}$ in the PD domain, δW_B^{pd} , can be evaluated as

$$\delta W_B^{pd} = \int_{V_{pd}} \delta \mathbf{u}^T \mathbf{b} dV = \delta \mathbf{u}_g^T \mathbf{F}_b^{pd}, \quad (2.59)$$

where $\mathbf{F}_b^{pd} = \sum_{i=1}^{N^{pd}} \mathbf{M}_{(i)}^T \mathbf{b}_{(i)} V_{(i)}$.

The virtual strain energy of the FEM domain, δU^{fem} , can be evaluated by the traditional FEM as

$$\delta U^{fem} = \int_{V_{fem}} \delta(\{\epsilon\}^T) \{\sigma\} dV = \delta \mathbf{u}_g^T \mathbf{K}^{fem} \mathbf{u}_g. \quad (2.60)$$

Similarly, the virtual work by the inertial force in the FEM domain, δU_I^{fem} , the virtual work by the external body force in the FEM domain, δW_B^{fem} , and the virtual work by the external traction force of the whole domain, δW_S , can be evaluated by traditional FEM as follows:

$$\delta U_I^{fem} = \int_{V_{fem}} \delta \mathbf{u}^T \rho \ddot{\mathbf{u}} dV = \delta \mathbf{u}_g^T \mathbf{M}^{fem} \ddot{\mathbf{u}}_g, \quad (2.61)$$

$$\delta W_B^{fem} = \int_{V_{fem}} \delta \mathbf{u}^T \mathbf{b} dV = \delta \mathbf{u}_g^T \mathbf{F}_b^{fem}, \quad (2.62)$$

$$\delta W_S = \int_{S_{tot}} \delta \mathbf{u}^T \mathbf{T} dS = \delta \mathbf{u}_g^T \mathbf{F}_s. \quad (2.63)$$

As the traditional FEM is a mature technology, the details to obtain the $\mathbf{K}^{fem}$, $\mathbf{M}^{fem}$, $\mathbf{F}_b^{fem}$ and $\mathbf{F}_s$ are not shown here for conciseness.

Substituting Eqs. (2.50), (2.56), (2.58), (2.59), (2.60), (2.61), (2.62) and (2.63) into Eq. (2.48), we derive the governing equation of this coupling model as follows,

$$\mathbf{M} \ddot{\mathbf{u}}_g + \mathbf{K} \mathbf{u}_g = \mathbf{F}, \quad (2.64)$$

where the global equivalent nodal mass $\mathbf{M}$ is defined as

$$\mathbf{M} = \mathbf{M}^{pd} + \mathbf{M}^{fem}, \quad (2.65)$$

the global stiffness matrix $\mathbf{K}$ is defined as

$$\mathbf{K} = \mathbf{K}_b^{pd} + \mathbf{K}_s^{pd} + \mathbf{K}^{fem} \quad (2.66)$$

and the global equivalent nodal force $\mathbf{F}$ is defined as

$$\mathbf{F} = \mathbf{F}_b^{pd} + \mathbf{F}_b^{fem} + \mathbf{F}_s, \quad (2.67)$$

here, $\mathbf{M}$, $\mathbf{K}$ and $\mathbf{F}$ can be obtained by the assembling procedure as described previously. When $V_{pd} = 0$, Eq. (2.64) represents a pure traditional FEM model and when $V_{fem} = 0$, it represents a pure PD model. Thus, the formulation converts easily between RNOSBPD, FEM, and RNOSBPD-FEM. Besides, Eq. (2.64) can be decomposed as

$$\begin{bmatrix} \mathbf{M}_{uu} & \mathbf{M}_{up} \\ \mathbf{M}_{pu} & \mathbf{M}_{pp} \end{bmatrix} \begin{bmatrix} \ddot{\mathbf{u}}_u \\ \ddot{\mathbf{u}}_p \end{bmatrix} + \begin{bmatrix} \mathbf{K}_{uu} & \mathbf{K}_{up} \\ \mathbf{K}_{pu} & \mathbf{K}_{pp} \end{bmatrix} \begin{bmatrix} \mathbf{u}_u \\ \mathbf{u}_p \end{bmatrix} = \begin{bmatrix} \mathbf{F}_u \\ \mathbf{F}_p \end{bmatrix}. \quad (2.68)$$

As $\mathbf{u}_p$ is the prescribed displacement constraint, Eq. (2.68) can be reduced to

$$\mathbf{M}_{uu}\ddot{\mathbf{u}}_u + \mathbf{K}_{uu}\mathbf{u}_u = \mathbf{F}_u - \mathbf{M}_{up}\ddot{\mathbf{u}}_p - \mathbf{K}_{up}\mathbf{u}_p \quad (2.69)$$

We develop a standalone program to implement RNOSBPD-FEM to perform the examples in section 2.5. The source code can be freely accessed via figshare [65]. RNOSBPD-FEM also can be easily introduced into commercial finite element codes, such as ANSYS, ABAQUS, by adding a routine to obtain $\mathbf{K}_b^{pd}$, $\mathbf{K}_s^{pd}$ and $\mathbf{M}^{pd}$, and to assemble them to global stiffness matrix $\mathbf{K}$ and global equivalent nodal mass $\mathbf{M}$, respectively.

2.5 Numerical results

To demonstrate the capability of this proposed RNOSBPD-FEM, four static plane stress examples concerning displacements and stresses are conducted in this section. These problem

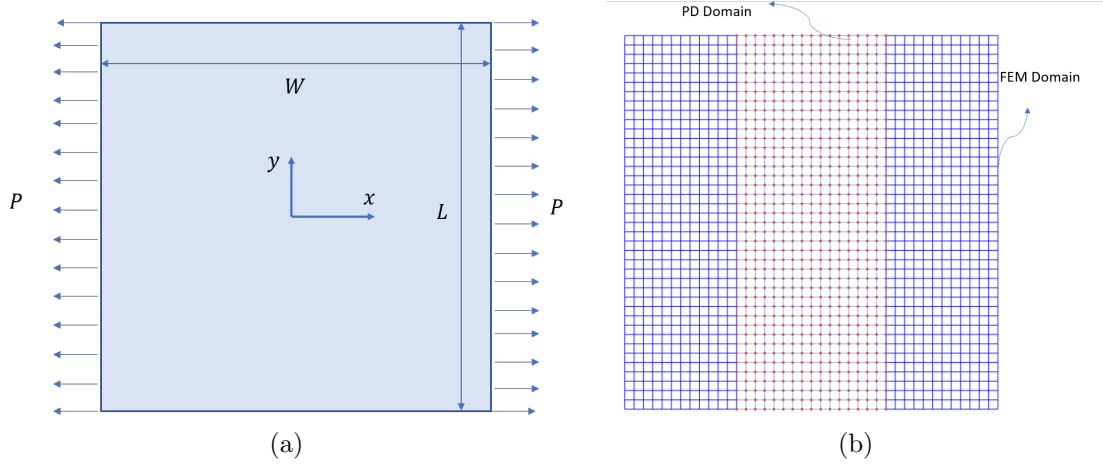


Fig. 2.6: The plate under uniaxial tension: (a) Geometry and loading, (b) Uniform meshes.

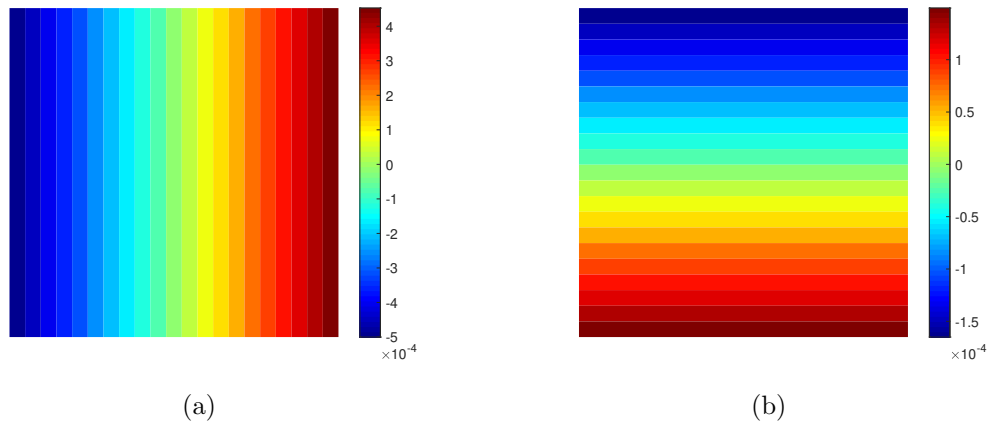


Fig. 2.7: Displacement results from the plate under uniaxial tension: (a) u_x , (b) u_y .

domains are discretized into 4 node elements. The nodal stresses in the FEM domain and the PD domain are calculated by the FEM formulation and the PD equation, Eq. (2.32), respectively. For the interface of FEM domain and PD domain, the nodal stresses are calculated by the average of FEM and PD formulations.

The first three examples concern three isotropic square plates of size 1 m by 1 m. Their Young's modulus, density and Poisson's ratio are specified as $E = 70$ GPa, $\rho = 2700$ kg/m³ and $\nu = 0.33$, respectively. The fourth is a square plate of size 150 mm by 150 mm, and is made of a brittle polymer called polymethylmethacrylate (PMMA) whose Young's modulus, density and Poisson ratio are $E = 2.94$ GPa, $\rho = 1200$ kg/m³ and $\nu = 0.38$, respectively.

2.5.1 Square Plate under uniaxial tension

As shown in Fig. 2.6, a plate is subjected to uniaxial tension $P = 70$ MPa along the vertical edges. The whole domain is discretized with uniform grids and the grid size is $\Delta = 0.025$ m. The region $-0.2 \text{ m} \leq x \leq 0.2 \text{ m}$ is specified as PD domain. The interaction domain of each PD node is determined by $\delta_{(i)} = 3\Delta_{(i)}$. The non-local factor is specified as $a = 1/4.5$ and it does not affect the accuracy in this example, because the RNOSBPD is derived based on 1-st order Taylor series expansion which can predict exactly the mechanical behaviors of this example.

Fig. 2.7 shows the displacement results from RNOSBPD-FEM. As expected, the displacements u_x varies linearly along the horizontal direction and u_y varies linearly along the vertical direction. Although not shown here, for both RNOSBPD and RNSBPD-FEM, the magnitude of the relative errors of the displacement results of each node is about 10^{-15} , which is up to machine precision, comparing to the analytical results of $u_x = \frac{P}{E}x$ and $u_y = -\nu\frac{P}{E}y$.

To better quantify the improvement of the computational efficiency of the proposed coupling method, we track the computing time T of varied FEM area fraction, A_{fem}/A , where A_{fem} and A are the area of the FEM domain and the whole domain, respectively. The computing time ratio, T/T_{pd} , where T_{pd} is the computing time when $V_{fem} = 0$, is plotted in Fig. 2.8. As it shows, the computing time decreases dramatically with the increase of the

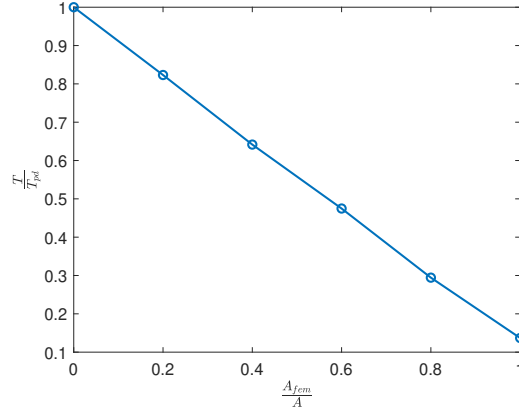


Fig. 2.8: The computing time ratio with different FEM area fractions.

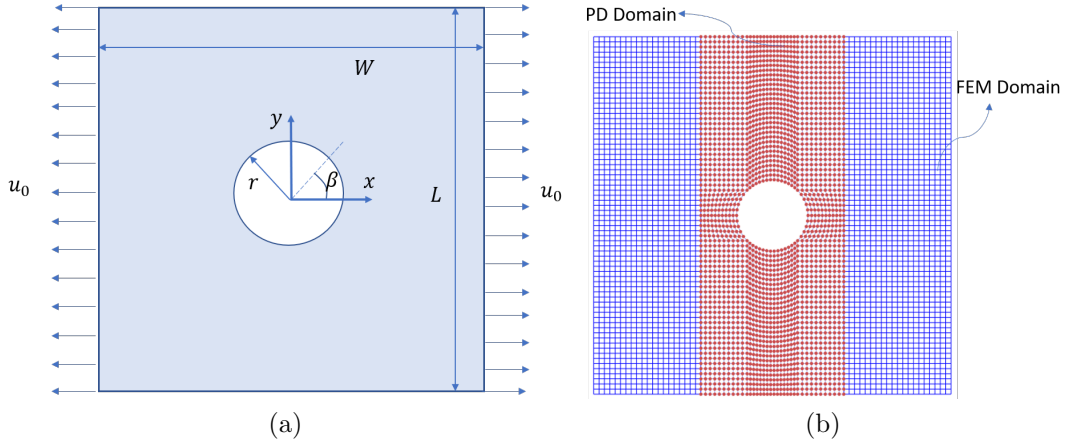


Fig. 2.9: The plate with a hole under displacement loading: (a) Geometry and loading, (b) Non-uniform meshes.

area of the FEM domain.

2.5.2 Square plate with a hole under displacement loading

A square plate with a central hole, as shown in Fig. 2.9, is under a displacement loading $u_0 = 5 \times 10^{-5}$ m. The radius of the hole is $r = 0.1$ m. The whole model is constructed by nonuniform discretization with a total of 5270 nodes and 5100 elements. The region $-0.2 \text{ m} \leq x \leq 0.2 \text{ m}$ is discretized with 2430 PD elements and 2300 PD nodes. The interaction domain of each PD node is determined by $\delta_{(i)} = 4\Delta_{(i)}$ and the non-local factor is specified as $a = 1/4.25$.

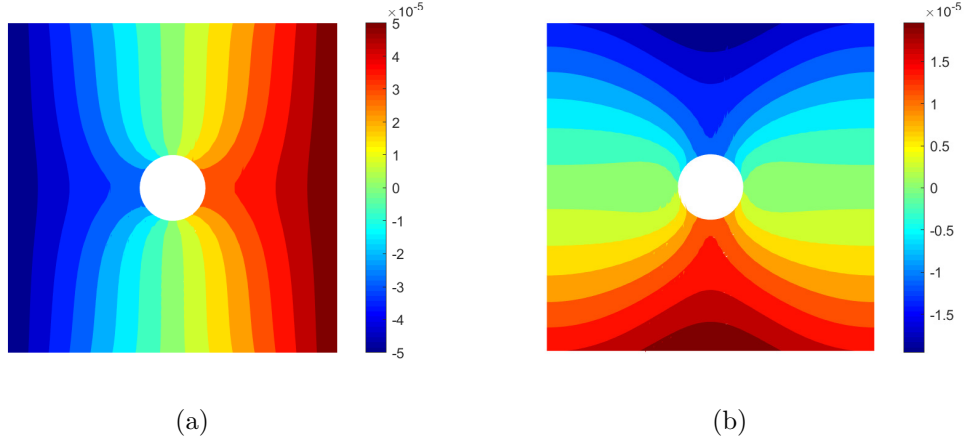


Fig. 2.10: Displacement results from plate with a hole by RNOSBPD-FEM: (a) u_x , (b) u_y .

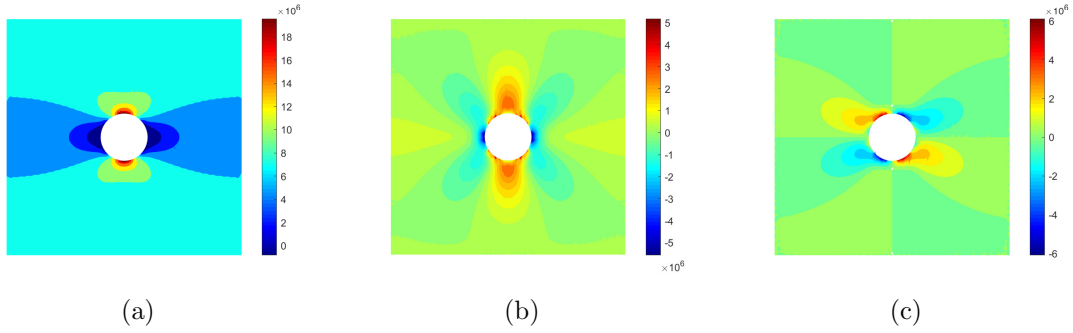


Fig. 2.11: Stress results from plate with a hole: (a) σ_x , (b) σ_y , (c) σ_{xy} .

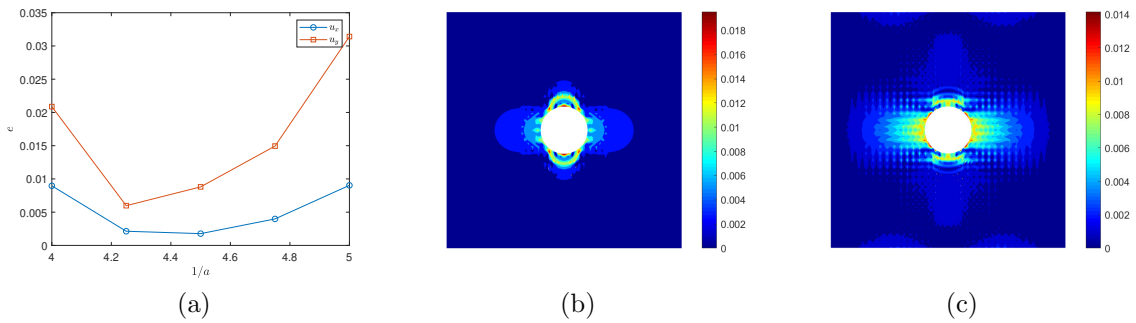


Fig. 2.12: The relative errors e between FEM and PD: (a) global error between FEM and RNOSBPD-FEM with varied non-local factor a ; (b) Error distribution of u_x between FEM and RNOSBPD-FEM with $a = 1/4.25$; (c) Error distribution of u_x between FEM and RNOSBPD with $a = 1/4.25$

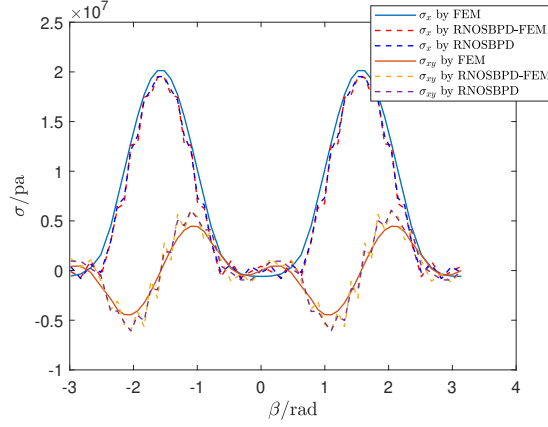


Fig. 2.13: Comparison of PD with FEM for stresses along the edge of the hole.

Fig. 2.10 and Fig. 2.11 show the displacement and stress results by RNOSBPD-FEM, respectively. To study the effect of the influence function, we perform the simulation of this example by RNOSBPD-FEM with varied non-local factor a , and compare the displacement results with traditional FEM. The global relative errors between the two methods are calculated using a measure proposed by Mukherjee and Mukherjee [66] as follows,

$$e = \frac{1}{|u|_{max}^{(r)}} \sqrt{\frac{1}{N} \sum_{i=1}^N [u_i^{(r)} - u_i^{(pd)}]^2}, \quad (2.70)$$

here the superscript (r) represents reference which is FEM in this work, the superscript (pd) represents RNOSBPD-FEM or pure RNOSBPD approach, and N represents the total number of nodes in the domain.

Fig. 2.12a shows the effect of the influence function. As depicted, RNOSBPD-FEM with non-local factor $a = 1/4.25$ leads to more accurate results. Note that the effect of a maybe mesh size dependent. Fig. 2.12b and Fig. 2.12c show the distribution of the relative errors of RNOSBPD-FEM and pure RNOSBPD comparing to FEM, and both show the position of largest errors are at the edge of the hole. Fig. 2.13 shows the normal stresses σ_x and shear stresses σ_{xy} of the RNOSBPD-FEM, RNOSBPD, and FEM along the edge of the hole. As shown, the results of the 3 methods are in good agreement.

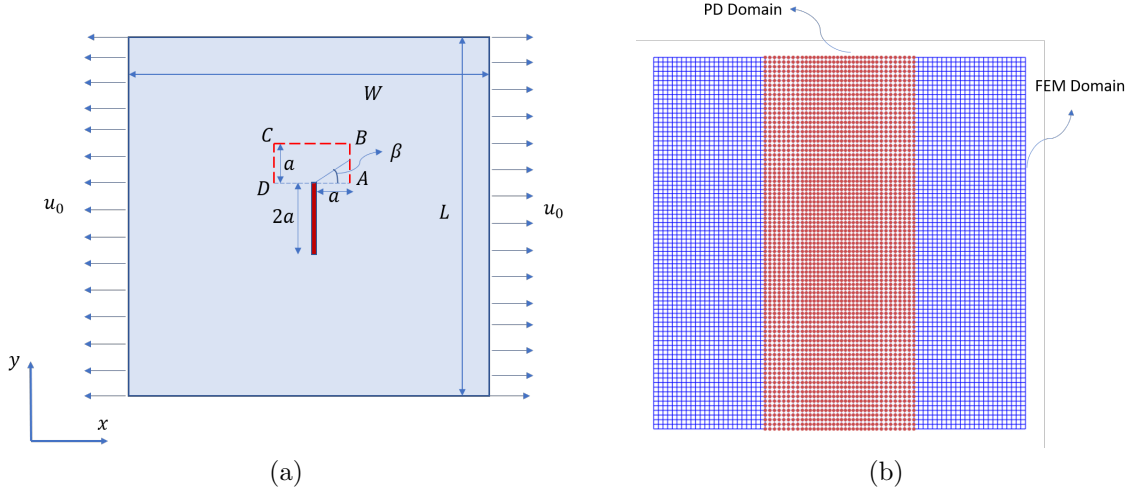


Fig. 2.14: The plate with a pre-existing crack under displacement loading: (a) Geometry and loading, (b) Non-uniform meshes.

2.5.3 Plate with a pre-existing crack under displacement loading

As shown in Fig. 2.14, a square plate with a pre-existing crack is subjected to displacement loading $u_0 = 5 \times 10^{-5}$ m. The length of the crack is $2a = 0.2$ m. The whole domain is constructed by non-uniform discretization with a total of 7140 nodes and 6972 elements. The region $-0.2 \text{ m} \leq x \leq 0.2 \text{ m}$ is specified as the PD domain and is discretized with 3060 PD nodes and 2940 elements. The horizon size is specified as $\delta_{(i)} = 4\Delta_{(i)}$ and the non-local factor is specified as $a = 1/4.5$.

Fig. 2.15 shows the displacements from RNOSBPD-FEM and Fig. 2.16 shows the stress results from RNOSBPD-FEM. Fig. 2.17 shows the displacements of u_x and u_y , the normal stresses, σ_x , and the shear stresses, σ_{xy} , of the RNOSBPD-FEM, RNOSBPD, and FEM along the path $A - B - C - D$ (Fig. 2.14a), where the coordinates of the key points of the path are $A (0.1, 0.1)$ m, $B (0.1, 0.2)$ m, $C (-0.1, 0.2)$ m and $D (-0.1, 0.1)$ m. As Fig. 2.17 shown, the results of the 3 methods are in good agreement.

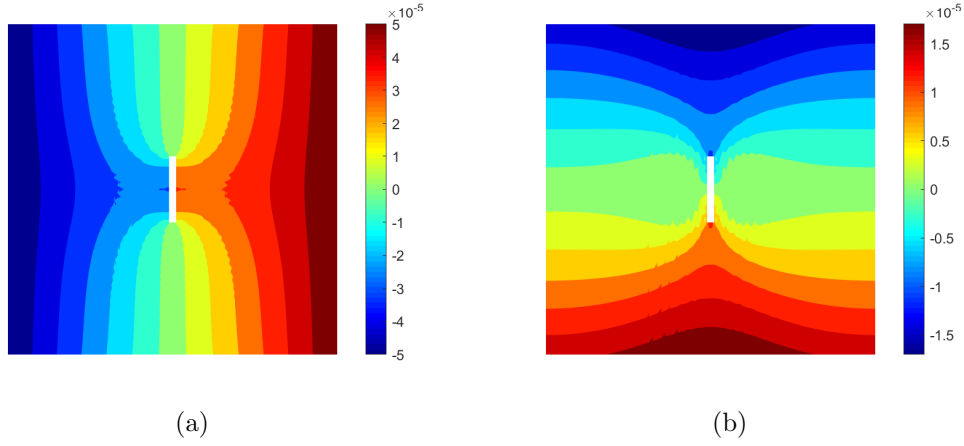


Fig. 2.15: Displacement results from the plate with a pre-existing crack: (a) u_x , (b) u_y .

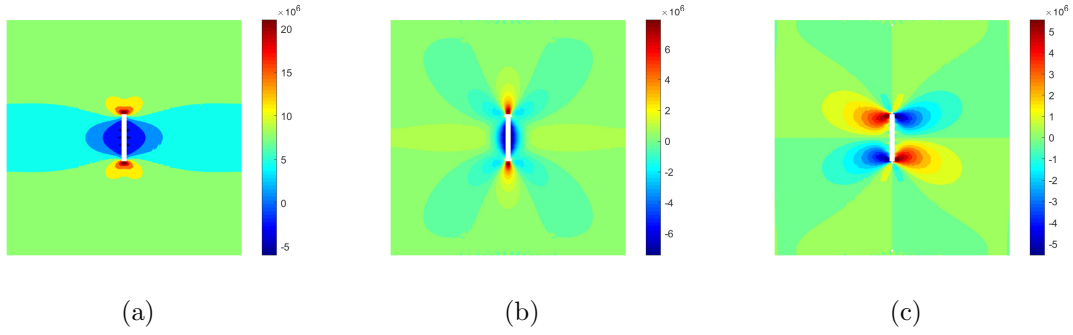


Fig. 2.16: Stress results from the plate with a pre-existing crack: (a) σ_x , (b) σ_y , (c) σ_{xy} .

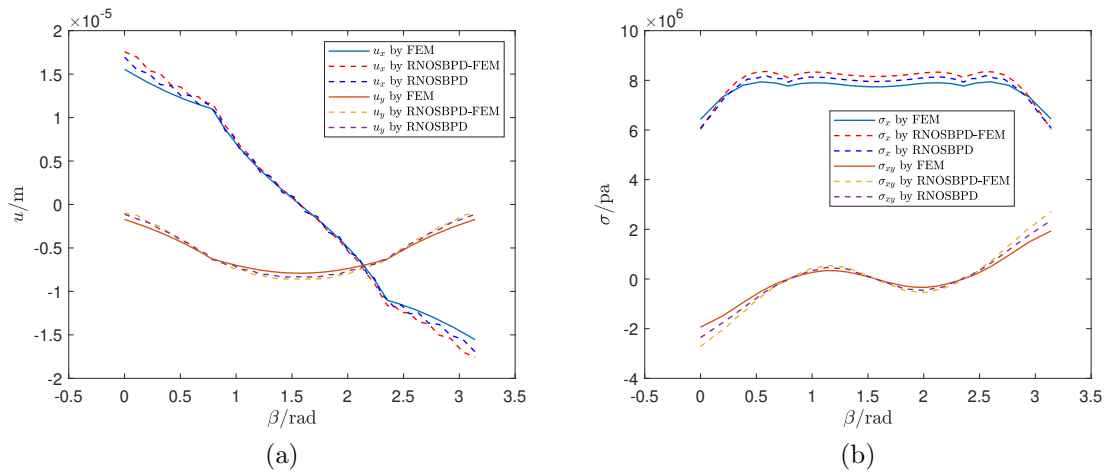


Fig. 2.17: Comparison of PD with FEM for displacement and stress solutions along the path $A - B - C - D$.

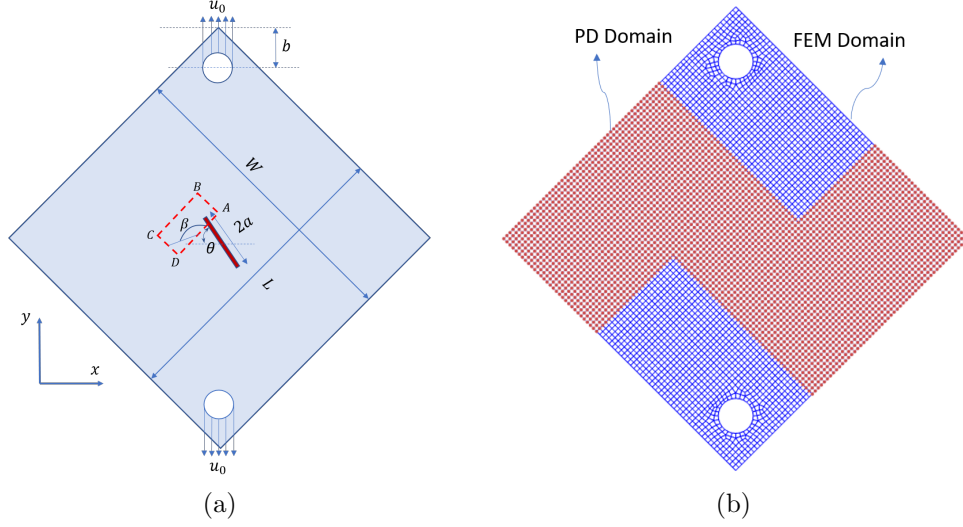


Fig. 2.18: The diagonal plate with an inclined pre-existing crack under displacement loading: (a) Geometry and loading, (b) Non-uniform meshes.

2.5.4 A diagonal plate with an inclined pre-existing crack under displacement loading

As shown in Fig. 2.18, a diagonal plate with an inclined crack is under displacement loading. The inclined angle of the crack is $\theta = 62.5^\circ$ and the crack length is $2a = 45$ mm. The displacement loading $u_0 = 5 \times 10^{-5}$ m is applied to the hole with a radius of 4 mm. The distance between the center of the hole and the corner of the plate is specified as $b = 25$ mm. The whole domain is discretized with a total of 5785 nodes and 5607 elements. The PD domain is discretized with uniform elements with length $\Delta = 2$ mm and it contains 3603 PD nodes and 3450 PD elements. The horizon size and the non-local factor are specified as $\delta_{(i)} = 3\Delta_{(i)}$ and $a = 1/4.5$, respectively.

Fig. 2.19 shows the displacement results of the whole domain from RNOSBPD-FEM and Fig. 2.20 shows the displacements of u_x and u_y , the normal stresses, σ_y , and the shear stresses, σ_{xy} , of the RNOSBPD-FEM and FEM along the path $A - B - C - D$ (Fig. 2.18a), where the coordinates of the key points of the path are A (7.425, 28.64) mm, B (-13.79, 49.85) mm, C (-49.85, 13.79) mm and D (-13.79, 49.85) mm. As Fig. 2.20 shown, the results of the 2 methods are in good agreement.

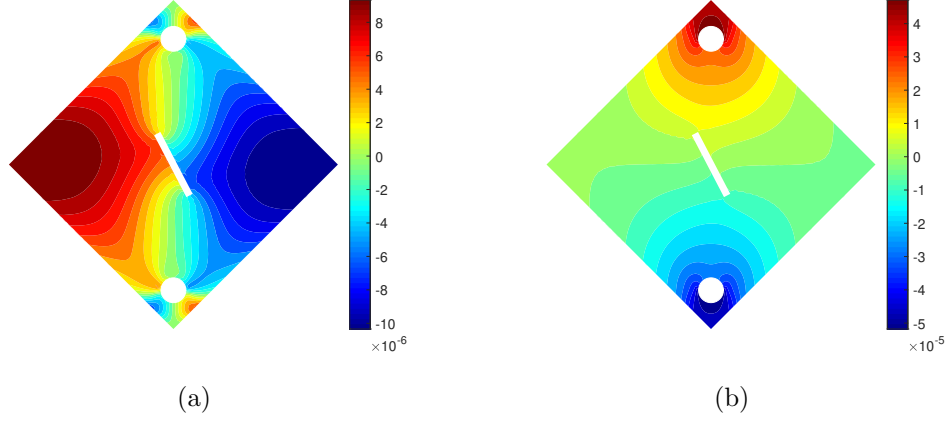


Fig. 2.19: Displacement results from the diagonal plate with a pre-existing inclined crack: (a) u_x , (b) u_y .

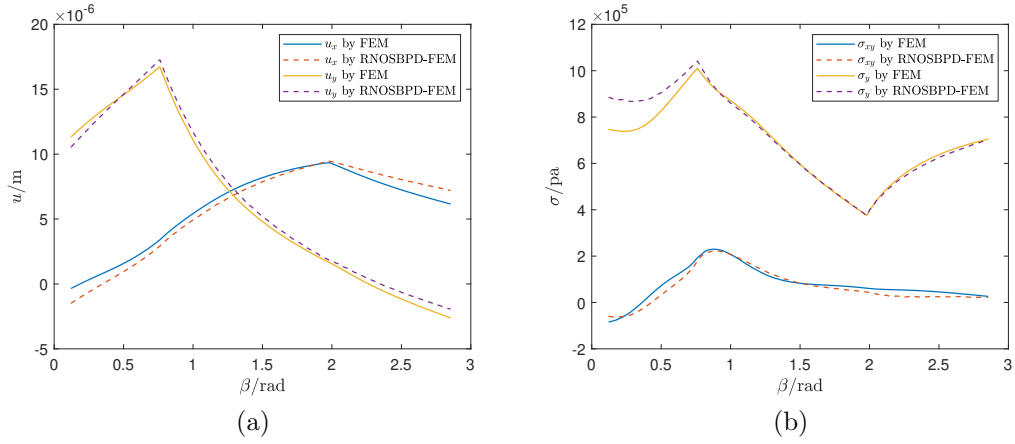


Fig. 2.20: Comparison of PD with FEM for displacement and stress solutions along the path A – B – C – D of the diagonal plate.

2.6 Conclusion

In this chapter, we present a new framework of NOSBPD based on the least square minimization, Taylor series expansion, and the concept of non-local interactions. This revised NOSBPD (RNOSBPD) works for arbitrary interaction domains and doesn't require surface correction and volume correction. For the spherical interaction domain, RNOSBPD recovers NOSBPD published in the literature. This current work also presents a new approach based on WRM to couple the proposed RNOSBPD with FEM (RNOSBPD-FEM). This new coupling approach is straightforward and special techniques, such as overlapping regions, interface elements, or fictitious nodes, that have published in the literature for coupling PD with FEM are not needed. Since RNOSBPD-FEM is derived based on WRM which is also employed to derive the governing equations of FEM, and the whole domain is discretized into elements, this coupling approach is easily introduced into commercial finite element codes, and the formulation can be converted conveniently between RNOSBPD, FEM, and RNOSBPD-FEM. Four static applications concerning deformations and stresses are performed and the results show the accuracy and efficiency of the RNOSBPD-FEM.

Chapter 3

Simulating quasi-static crack propagation by coupled peridynamics least square minimization with finite element method²

Abstract

In this work, we present an innovative simulation method for quasi-static crack propagation in mixed-mode, within a new framework of coupled peridynamics least square minimization and finite element method (PDLSM-FEM). As the inertia effect is neglected for quasi-static problems, the governing equations for PDLSM-FEM can be solved implicitly without iterations. Displacements and stresses from PDLSM-FEM are used to compute the interaction integral, an extended version of the J -integral. The stress intensity factors (SIFs) are derived from the interaction integral and used in the maximum circumferential tensile stress failure

²This chapter was published on *Engineering Fracture Mechanics*.

Liu, Q., Xin, X. J., Ma, J., and Wang, Y. (2021). Simulating quasi-static crack propagation by coupled peridynamics least square minimization with finite element method. *Engineering Fracture Mechanics*, 252, 107862. <https://doi.org/10.1016/j.engfracmech.2021.107862>

criterion to predict the onset of crack propagation and the direction of propagation. New contributions in this work include the following: (1) developing a new framework for coupling PDLSP and FEM; (2) pioneering a quasi-static method for simulating crack propagation in peridynamics; (3) developing an element-based approach for selecting the interaction integral contour; and (4) proposing and implementing an innovative method for handling peridynamic bond breakage and crack growth. Quasi-static crack propagation simulation in this work provides a computationally efficient way to find the shape of the crack, and the current PDLSP-FEM model is straightforward and can be easily introduced into commercial finite element codes. Three numerical examples are carried out, and the results show that the proposed method evaluates SIFs accurately and captures crack growth as expected.

3.1 Introduction

Many problems of fundamental importance in solid mechanics involve pre-existing and propagating discontinuities such as cracks. As classical continuum theory employs spatial derivatives in its formulation and assumes the material is continuous as it deforms, it is inherently difficult to predict discontinuous behaviors such as failure of materials and structures. In light of the inadequacies of the classical continuum theory, Peridynamics (PD), which is based on non-local interactions and employs spatial integrals, was first introduced by Silling [4]. PD theory is better suited for failure analysis of materials and structures because its governing equations are defined by integral equations and remain valid at fracture surfaces.

PD theory has been extended from bond-based theory [4], which has a restriction of a fixed Poisson's ratio of $1/4$ [5–7], to the state-based one [8], which has no restriction on the value of Poisson's ratio. To date, both the bond-based and state-based PD theories have been successfully applied to various discontinuous problems, such as ice craters by impact [67], the interaction between sea ice and wide vertical structures [68], dynamic response of ceramics tiles under impact loading [69]. In all of the works quoted above, both bond-based and state-based PD theories were derived by equating the classical strain energy at a material point to that of PD with a complete circle or sphere interaction domain [6]. These formulas

in PD theory, however, are not valid for a point located near a surface because its interaction domain is not a complete circle or sphere [10]. Furthermore, most published work on PD to date employs a simple meshless method with a one-point quadrature for cells. Such one-point quadrature requires a volume correction procedure to improve integration accuracy [24]. To remove these two drawbacks, Madenci et al. [58] proposed a PD least squares minimization (PDLSPM), and Liu and Xin [70] proposed a revised non-ordinary state-based PD (RNOSBPD). Both methods were derived by Taylor series expansion and the concept of non-local interactions of PD. Comparing to the finite element method (FEM), PD is computationally expensive. Thus, techniques for coupling PD with FEM were proposed to take advantage of these two methods, such as overlapping regions [32], morphing strategy [34], fictitious nodes [39], splice method [36], adaptive coupling approach [71], and weighted residual method [70]. Besides, some other techniques, such as dual-horizon PD model [25] and multi-horizon PD model [72] were also proposed to improve the computational efficiency of PD.

PD theory describes damages by irreversible breakage of a bond, which is the non-local interaction of two material points. Thus, an appropriate failure criterion is very important to determine bond breakage in failure analysis by PD. The first failure criterion called critical stretch criterion is based on bond stretch [20] and the critical stretch value is derived by the interaction formulas of bond-based PD. Recently, Zhang and Qiao [59] proposed a model for the calculation of the critical stretch in ordinary state-based PD (OSBPD). Based on the energy density stored in a deformed bond, the critical energy density criterion was proposed by Foster et al. [28] and later was applied to plastic deformation by Madenci and Oterkus [73]. Zhang and Qiao [29] discussed the limitations of the critical stretch and energy density criteria for pure mode *II* or mode *III* dominant fracture analysis and proposed a criterion named critical skew for quantitative OSBPD analysis of mode *II* fracture. Since non-ordinary state-based PD (NOSBPD) recovers the concept of non-local stress and strain, an equivalent strain criterion [30] and a maximum principal stress criterion [31] were employed to perform failure analysis by NOSBPD. However, the criterion that is based on stress and strain may depend strongly on mesh size, as the stress and strain fields near the crack

tip exhibit singular behavior.

In general, PD is computationally expensive due to a large number of non-local interactions, much-refined mesh, and PD-based codes written in terms of dynamic equilibrium even for static problems. Typically, static problems in PD are solved by adopting an explicit dynamic relaxation method [27] that determines steady-state solutions for a dynamic system by introducing fictitious mass and damping matrices. The explicit dynamic relaxation method is commonly preferred because it does not require large-matrix operations. Although implicit method requires matrix inversion, the stiffness matrix of a FEM model is symmetric and sparse and its inversion is relatively easier and fast computationally. In comparison, mesh refinement in PD increases the size of the stiffness matrix $\mathbf{K}$ and a large number of non-local interactions leads to a denser $\mathbf{K}$, both of which significantly increase the computational cost to solve for $\mathbf{K}^{-1}$. Coupling PD with FEM makes it easier to employ the implicit method to solve fracture problems since FEM nodes interact only with nodes in the same element and neighboring elements, making the number of interactions much smaller than that of a full PD model. Furthermore, FEM enables a much coarser mesh at regions far from the crack tips. Comparing to the explicit method, the implicit method of coupled PD with FEM does not need a large number of iterations for solution, and equilibrium is guaranteed if convergence is reached, thus it is more efficient for static problems [74].

In this work, we propose a new framework for coupling peridynamics least square minimization with finite element method (PDLSSM-FEM) based on the weighted residual method, and conduct PDLSSM-FEM simulations for quasi-static crack propagation under mixed-mode loading. As the inertia effects is neglected in quasi-static simulation, the current model provides an efficient way to find the shape of the crack. The PDLSSM-FEM is straightforward and can be easily introduced into commercial finite element codes. A numerical method for the interaction integral (I -integral), an extended version of the J -integral, to calculate the stress intensity factors (SIFs) is proposed and implemented. Failure is based on the criterion of maximum circumferential tensile stress [75]. The crack growth direction θ_c are determined by maximizing the circumferential tensile stress with respect to the orientation, and crack propagation is triggered when the equivalent SIF K_{eq} of mixed-mode loading reaches the

critical value of material fracture toughness K_{Ic} . As the J -integral is path independent, the proposed method is much more reliable and accurate than using near-tip stresses directly from the PD model which are sensitive to mesh refinement and less accurate. New contributions in this work include the following: (1) developing a new framework for coupling PDLSTM and FEM; (2) pioneering a quasi-static method for simulating crack propagation in peridynamics; (3) developing an element-based approach for selecting the interaction integral contour; and (4) proposing and implementing an innovative method for handling peridynamic bond breakage and crack growth.

The remainder of this paper is outlined as follows. First, the theory of PDLSTM is reviewed in Section 3.2. A new technique for coupling PDLSTM with FEM based on the weighted residual method is developed and presented in Section 3.3, with more details presented in Appendix A. Next, the quasi-static crack growth simulation model for mixed-mode loading is proposed in Section 3.4. Three applications are performed to validate the proposed simulation model in Section 3.5. Finally, concluding remarks are summarized in Section 3.6.

3.2 Peridynamics least square minimization (PDLSTM)

In this section, the peridynamics least square Minimization (PDLSTM) first developed by Madenci et al. [58] is briefly reviewed for completeness. PDLSTM employs the concept of PD interactions and LSM in conjunction with the Taylor series expansion. More detailed formulas essential for understanding PDLSTM can be found in [58].

In PD, the equation of motion is given by

$$\rho \ddot{\mathbf{u}} = \mathbf{L}(\mathbf{x}, t) + \mathbf{b}(\mathbf{x}, t), \quad (3.1)$$

where ρ is the mass density, $\ddot{\mathbf{u}}$ is the acceleration, $\mathbf{b}$ is the external force vector, and $\mathbf{L}$ is the internal force vector. The internal force at point $\mathbf{x}$ is evaluated by the integration of bond force between points $\mathbf{x}$ and $\mathbf{x}'$ over the interaction domain H_x of point $\mathbf{x}$, as shown in Fig. 3.1. Note that the interaction domain H_x can be of a arbitrary shape, and not required to

be a spherical or circle.

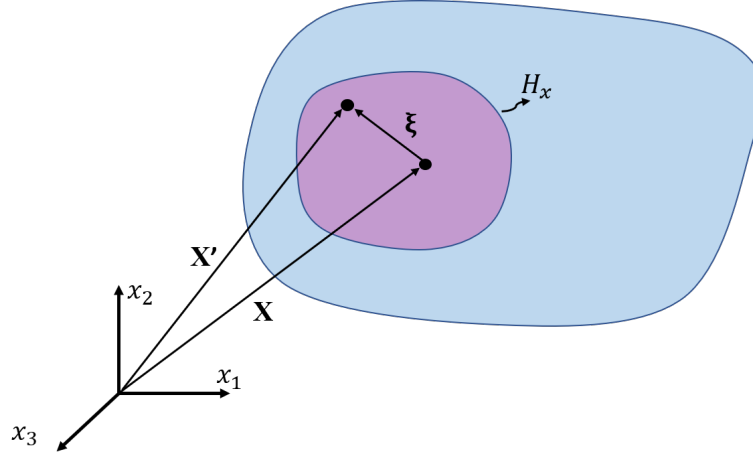


Fig. 3.1: Bond between point $\mathbf{x}'$ and $\mathbf{x}$ in the interaction domain H_x .

For a linear isotropic material response, the non-local internal force vector can be expressed as

$$\mathbf{L}^{pd} = \int_{H_x} \omega(|\boldsymbol{\xi}|) \mathbf{G} \boldsymbol{\eta} dV_{x'}, \quad (3.2)$$

and the non-local displacement gradient is

$$\nabla \mathbf{u}^{pd} = \int_{H_x} \omega(|\boldsymbol{\xi}|) \boldsymbol{\eta} \otimes \mathbf{g} dV_{x'}, \quad (3.3)$$

where $\boldsymbol{\xi} = \mathbf{x}' - \mathbf{x}$ and $\boldsymbol{\eta} = \mathbf{u}(\mathbf{x}') - \mathbf{u}(\mathbf{x})$ are the relative position and relative displacement of points $\mathbf{x}'$ and $\mathbf{x}$, respectively, and $\omega(|\boldsymbol{\xi}|)$ is the weight function. According to the classical continuum mechanics, the stress tensor can be expressed as

$$\boldsymbol{\sigma}^{pd} = \lambda \text{tr}(\nabla \mathbf{u}^{pd}) \mathbf{I} + \mathcal{G} [\nabla \mathbf{u}^{pd} + (\nabla \mathbf{u}^{pd})^T]. \quad (3.4)$$

with λ representing Lamé's material constant and $\mathcal{G}$ representing shear modulus. The matrix

$\mathbf{G}$ in Eq. (3.2) is defined as

$$\mathbf{G} = \begin{bmatrix} (\lambda + \mathcal{G})d_1 + \mathcal{G}(d_1 + d_2 + d_3) & (\lambda + \mathcal{G})d_4 & (\lambda + \mathcal{G})d_5 \\ (\lambda + \mathcal{G})d_4 & (\lambda + \mathcal{G})d_2 + \mathcal{G}(d_1 + d_2 + d_3) & (\lambda + \mathcal{G})d_6 \\ (\lambda + \mathcal{G})d_5 & (\lambda + \mathcal{G})d_6 & (\lambda + \mathcal{G})d_3 + \mathcal{G}(d_1 + d_2 + d_3) \end{bmatrix}, \quad (3.5)$$

The vector $\mathbf{g} = [g_1 \ g_2 \ g_3]^T$ in Eq. (3.3) and $\mathbf{d} = [d_1 \ d_2 \ d_3 \ d_4 \ d_5 \ d_6]^T$ in Eq. (3.5) are defined as

$$\begin{bmatrix} \mathbf{g} \\ \mathbf{d} \end{bmatrix} = \mathbf{A}^{-1} \hat{\boldsymbol{\xi}}, \quad (3.6)$$

where

$$\hat{\boldsymbol{\xi}} = [\xi_1 \ \xi_2 \ \xi_3 \ \xi_1^2 \ \xi_2^2 \ \xi_3^2 \ \xi_1\xi_2 \ \xi_1\xi_3 \ \xi_2\xi_3]^T, \quad (3.7)$$

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix}, \quad (3.8)$$

$$\mathbf{A}_{11} = \int_{H_x} \omega(|\boldsymbol{\xi}|) \begin{bmatrix} \xi_1^2 & \xi_1\xi_2 & \xi_1\xi_3 \\ \xi_1\xi_2 & \xi_2^2 & \xi_2\xi_3 \\ \xi_1\xi_3 & \xi_2\xi_3 & \xi_3^2 \end{bmatrix} dV_{x'}, \quad (3.9)$$

$$\mathbf{A}_{12} = \int_{H_x} \omega(|\boldsymbol{\xi}|) \begin{bmatrix} \frac{\xi_1^3}{2} & \frac{\xi_1\xi_2^2}{2} & \frac{\xi_1\xi_3^2}{2} & \xi_1^2\xi_2 & \xi_1^2\xi_3 & \xi_1\xi_2\xi_3 \\ \frac{\xi_1^2\xi_2}{2} & \frac{\xi_2^3}{2} & \frac{\xi_2\xi_3^2}{2} & \xi_1\xi_2^2 & \xi_1\xi_2\xi_3 & \xi_2^2\xi_3 \\ \frac{\xi_1^2\xi_3}{2} & \frac{\xi_2^2\xi_3}{2} & \frac{\xi_3^3}{2} & \xi_1\xi_2\xi_3 & \xi_1\xi_3^2 & \xi_2\xi_3^2 \end{bmatrix} dV_{x'}, \quad (3.10)$$

$$\mathbf{A}_{21} = \int_{H_x} \omega(|\boldsymbol{\xi}|) \begin{bmatrix} \xi_1^3 & \xi_1^2\xi_2 & \xi_1^2\xi_3 \\ \xi_1\xi_2^2 & \xi_2^3 & \xi_2^2\xi_3 \\ \xi_1\xi_3^2 & \xi_2\xi_3^2 & \xi_3^3 \\ \xi_1^2\xi_2 & \xi_1\xi_2^2 & \xi_1\xi_2\xi_3 \\ \xi_1^2\xi_3 & \xi_1\xi_2\xi_3 & \xi_1\xi_3^2 \\ \xi_1\xi_2\xi_3 & \xi_2^2\xi_3 & \xi_2\xi_3^2 \end{bmatrix} dV_{x'}, \quad (3.11)$$

$$\mathbf{A}_{22} = \int_{H_x} \omega(|\boldsymbol{\xi}|) \begin{bmatrix} \frac{\xi_1^4}{2} & \frac{\xi_1^2 \xi_2^2}{2} & \frac{\xi_1^2 \xi_3^2}{2} & \xi_1^3 \xi_2 & \xi_1^3 \xi_3 & \xi_1^2 \xi_2 \xi_3 \\ \frac{\xi_1^2 \xi_2^2}{2} & \frac{\xi_2^4}{2} & \frac{\xi_2^2 \xi_3^2}{2} & \xi_1 \xi_2^3 & \xi_1 \xi_2^2 \xi_3 & \xi_2^3 \xi_3 \\ \frac{\xi_1^2 \xi_3^2}{2} & \frac{\xi_2^2 \xi_3^2}{2} & \frac{\xi_3^4}{2} & \xi_1 \xi_2 \xi_3^2 & \xi_1 \xi_3^3 & \xi_2 \xi_3^3 \\ \frac{\xi_1^3 \xi_2}{2} & \frac{\xi_1 \xi_2^3}{2} & \frac{\xi_1 \xi_2 \xi_3^2}{2} & \xi_1^2 \xi_2^2 & \xi_1^2 \xi_2 \xi_3 & \xi_1 \xi_2^2 \xi_3 \\ \frac{\xi_1^3 \xi_3}{2} & \frac{\xi_1 \xi_2^2 \xi_3}{2} & \frac{\xi_1 \xi_3^3}{2} & \xi_1^2 \xi_2 \xi_3 & \xi_1^2 \xi_3^2 & \xi_1 \xi_2 \xi_3^2 \\ \frac{\xi_1^2 \xi_2 \xi_3}{2} & \frac{\xi_2^3 \xi_3}{2} & \frac{\xi_2 \xi_3^3}{2} & \xi_1 \xi_2^2 \xi_3 & \xi_1 \xi_2 \xi_3^2 & \xi_2^2 \xi_3^2 \end{bmatrix} dV_{x'}. \quad (3.12)$$

Note that for the 2D case, the vector $\mathbf{g}$ and $\mathbf{d}$ are reduced to $\mathbf{g} = [g_1 \ g_2]^T$ and $\mathbf{d} = [d_1 \ d_2 \ d_3]^T$, respectively, and all the components with ξ_3 in matrix $\mathbf{A}$ and vector $\hat{\boldsymbol{\xi}}$ will be deleted. For plane strain problems, the matrix $\mathbf{G}$ is reduced to

$$\mathbf{G} = \begin{bmatrix} (\lambda + \mathcal{G})d_1 + \mathcal{G}(d_1 + d_2) & (\lambda + \mathcal{G})d_3 \\ (\lambda + \mathcal{G})d_3 & (\lambda + \mathcal{G})d_2 + \mathcal{G}(d_1 + d_2) \end{bmatrix}, \quad (3.13)$$

and for plane stress problems,

$$\mathbf{G} = \begin{bmatrix} \frac{E}{2(1-\nu)}d_1 + \mathcal{G}(d_1 + d_2) & \frac{E}{2(1-\nu)}d_3 \\ \frac{E}{2(1-\nu)}d_3 & \frac{E}{2(1-\nu)}d_2 + \mathcal{G}(d_1 + d_2) \end{bmatrix}, \quad (3.14)$$

here ν is Poisson's ratio, E is Young's modulus.

3.3 Coupled peridynamics least square minimization and finite element method

Compared to FEM, PD is computationally expensive. To increase computational efficiency, a new framework for coupling PD with FEM is proposed in this work to take advantage of these two methods. A numerical method base on PDLSP-FEM is then applied to model quasi-static crack propagation. For completeness and brevity in presentation, the formulation of coupled PDLSP-FEM is outlined succinctly in this section, with more lengthy details

presented in Appendix A.

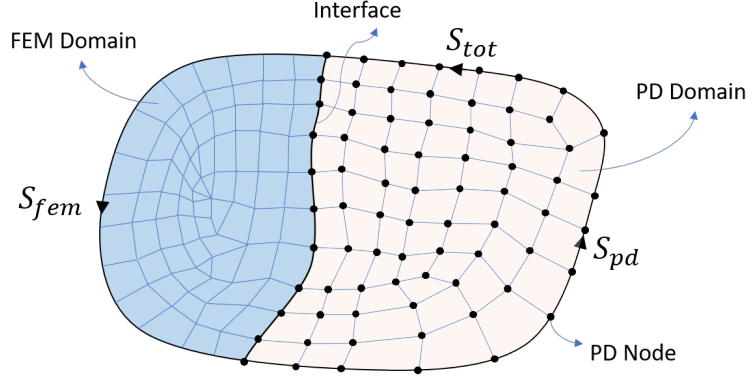


Fig. 3.2: A coupled PD-FEM model.

The coupled PDLSM-FEM is based on the weighted residual method (WRM) with the problem domain divided into a PD domain and a FEM domain, both of which are discretized into uniform or non-uniform elements, as illustrated in Fig. 3.2. To distinguish, the elements in the PD domain are called PD elements, and elements in the FEM domain are still called finite elements. Note that PD nodes on the interface of the PD domain and the FEM domain are also nodes of the finite element, and the interaction domains of these PD nodes are only determined from the PD domain, and the volumes of these PD nodes are calculated only from the PD elements. This method of coupling is straightforward and is easily introduced into commercial finite codes. The formulation of the coupling framework can be converted conveniently between pure PDLSM, pure FEM, and coupled PDLSM-FEM.

Applying the WRM on the equilibrium equations and the boundary conditions over the whole problem domain leads to

$$\int_{V_{tot}} \delta \mathbf{u}^T (\mathbf{L} + \mathbf{b} - \rho \ddot{\mathbf{u}}) dV - \int_{S_{tot}} \delta \mathbf{u}^T (\boldsymbol{\sigma} \mathbf{n} - \mathbf{T}) dS = 0, \quad (3.15)$$

where $\mathbf{T}$ is the external traction on the surface boundary, $\mathbf{n}$ is the unit normal vector of the boundary, V_{tot} and S_{tot} are the volume and surface of the whole domain respectively, and $\delta(\bullet)$ represents a virtual value. For the PD domain V_{pd} , the internal force vector takes on the

integral form of Eq. (3.2), and for the FEM domain V_{fem} , it takes on the differential form of

$$\mathbf{L} = \nabla \cdot \boldsymbol{\sigma}. \quad (3.16)$$

For the surface of the PD domain, S_{pd} , the stress in the item $\delta \mathbf{u}^T \boldsymbol{\sigma} \mathbf{n}$ is derived based on the integral form of Eq. (3.3), and for the surface of the FEM domain, S_{fem} , $\delta \mathbf{u}^T \boldsymbol{\sigma} \mathbf{n}$ is canceled by applying Gauss theorem as

$$\int_{V_{fem}} \delta \mathbf{u}^T \mathbf{L} dV - \int_{S_{fem}} \delta \mathbf{u}^T \boldsymbol{\sigma} \mathbf{n} dS = - \int_{V_{fem}} \nabla \delta \mathbf{u} : \boldsymbol{\sigma} dV. \quad (3.17)$$

It is shown in the Appendix A that Eq. (3.15) can be transformed into the final governing equation for PDLSM-FEM as follows:

$$\mathbf{M} \ddot{\mathbf{u}}_g + \mathbf{K} \mathbf{u}_g = \mathbf{F}, \quad (3.18)$$

where $\mathbf{u}_g$, $\mathbf{M}$, $\mathbf{K}$ and $\mathbf{F}$ represent the global nodal displacement vector, the global equivalent nodal mass matrix, the global stiffness matrix, and the global equivalent nodal force, respectively. Details of the derivation are presented in Appendix A. For quasi-static crack propagation, the acceleration vector $\ddot{\mathbf{u}}_g$ is negligibly small, and Eq. (3.18) is reduced to

$$\mathbf{K} \mathbf{u}_g = \mathbf{F}, \quad (3.19)$$

which is the system equation to be solved implicitly in the current quasi-static crack propagation simulation. Comparing to explicit dynamic relaxation method, directly and implicitly solving Eq. (3.19) avoids a large number of iterations and is highly computationally efficient.

3.4 Quasi-static crack propagation simulation

In this section, we present an innovative quasi-static solution of crack growth problems based on the PDLSM-FEM technique and the linear elastic fracture mechanics (LEFM).

The proposed method is an efficient way to simulate crack propagation when comparing to dynamic simulations. The crack propagation criterion is based on the maximum circumferential tensile stress evaluated from Stress Intensity Factors (SIFs), which are computed from the interaction integral (I -integral) of J -integral. As the J -integral is path independent, the proposed method is much more reliable and accurate than using near-tip stresses directly from the PD model which are sensitive to mesh refinement and are less accurate. In subsection 3.4.1, the I -integral proposed by Yau et al. [76] to calculate SIFs is briefly reviewed. After that, we present the numerical integration of I -integral in subsection 3.4.2 and the failure criterion for quasi-static crack propagation in subsection 3.4.3. Finally, the simulation process is summarized in subsection 3.4.4

3.4.1 Stress intensity factors and interaction integral

In LEFM, the stress and displacement fields near the crack tip region can be evaluated by SIFs as follows. For mode I loading,

$$\begin{cases} u_x = \frac{K_I(1+\nu)}{E} \sqrt{\frac{r}{2\pi}} \cos \frac{\theta}{2} (\kappa - 1 + 2 \sin^2 \frac{\theta}{2}), \\ u_y = \frac{K_I(1+\nu)}{E} \sqrt{\frac{r}{2\pi}} \sin \frac{\theta}{2} (\kappa + 1 - 2 \cos^2 \frac{\theta}{2}). \end{cases} \quad (3.20)$$

$$\begin{cases} \sigma_x = \frac{K_I}{\sqrt{2\pi r}} \cos \frac{\theta}{2} (1 - \sin \frac{\theta}{2} \sin \frac{3\theta}{2}), \\ \sigma_y = \frac{K_I}{\sqrt{2\pi r}} \cos \frac{\theta}{2} (1 + \sin \frac{\theta}{2} \sin \frac{3\theta}{2}), \\ \sigma_{xy} = \frac{K_I}{\sqrt{2\pi r}} \sin \frac{\theta}{2} \cos \frac{\theta}{2} \cos \frac{3\theta}{2} \end{cases} \quad (3.21)$$

For mode II loading,

$$\begin{cases} u_x = \frac{K_{II}(1+\nu)}{E} \sqrt{\frac{r}{2\pi}} \sin \frac{\theta}{2} (\kappa + 1 + 2 \cos^2 \frac{\theta}{2}), \\ u_y = -\frac{K_{II}(1+\nu)}{E} \sqrt{\frac{r}{2\pi}} \cos \frac{\theta}{2} (\kappa - 1 - 2 \sin^2 \frac{\theta}{2}). \end{cases} \quad (3.22)$$

$$\begin{cases} \sigma_x = -\frac{K_{II}}{\sqrt{2\pi r}} \sin \frac{\theta}{2} \left(2 + \cos \frac{\theta}{2} \cos \frac{3\theta}{2}\right), \\ \sigma_y = \frac{K_{II}}{\sqrt{2\pi r}} \sin \frac{\theta}{2} \cos \frac{\theta}{2} \cos \frac{3\theta}{2}, \\ \sigma_{xy} = \frac{K_{II}}{\sqrt{2\pi r}} \cos \frac{\theta}{2} \left(1 - \sin \frac{\theta}{2} \sin \frac{3\theta}{2}\right) \end{cases} \quad (3.23)$$

in which ν is the Poisson ratio and the constant κ is defined as $\kappa = (3 - \nu)/(1 + \nu)$ for plane stress and $\kappa = (3 - 4\nu)$ for plane strain problems. Since these field variables are expressed in terms of SIFs, accurate evaluation of the SIFs for the analysis of fracture behavior is important. Different techniques have been proposed in the literature for evaluating SIFs. In this study, SIFs are computed based on the J -integral:

$$J = \int_{\Gamma} \left(w \mathcal{D}_{1j} - \sigma_{ij} \frac{\partial u_i}{\partial x_1} \right) n_j d\Gamma, \quad (3.24)$$

in which $w = \frac{1}{2} \sigma_{ij} \varepsilon_{ij}$ is the strain energy density, n_j is the unit outward normal vector to the contour Γ of integration, $\mathcal{D}$ is the Kronecker delta, and coordinates (x_1, x_2) are taken to be the local crack tip coordinates with the x_1 axis parallel to the crack faces. For general 2D mixed-mode problems, the J -integral is related to SIFs as

$$J = \frac{K_I^2}{E^*} + \frac{K_{II}^2}{E^*}, \quad (3.25)$$

where E^* is defined as

$$E^* = \begin{cases} E, & \text{plane stress,} \\ \frac{E}{1-\nu^2}, & \text{plane strain.} \end{cases} \quad (3.26)$$

in which E is Young's modulus and ν is the Poisson ratio. To evaluate SIFs, we employ the I -integral based on J -integral which was first proposed by Yau et al. [76]. Consider two states of a cracked body, that is, the present state (1) called by $(u_i^{(1)}, \varepsilon_{ij}^{(1)}, \sigma_{ij}^{(1)})$ and an auxiliary state (2) denoted by $(u_i^{(2)}, \varepsilon_{ij}^{(2)}, \sigma_{ij}^{(2)})$, the J -integral for the sum of states (1) and

(2) is:

$$J^{(1+2)} = \int_{\Gamma} \left(\frac{1}{2} \left(\sigma_{km}^{(1)} + \sigma_{km}^{(2)} \right) \left(\varepsilon_{km}^{(1)} + \varepsilon_{km}^{(2)} \right) \mathcal{D}_{1j} - \left(\sigma_{ij}^{(1)} + \sigma_{ij}^{(2)} \right) \frac{\partial}{\partial x_1} \left(u_i^{(1)} + u_i^{(2)} \right) \right) n_j d\Gamma. \quad (3.27)$$

Expanding and rearranging terms gives

$$J^{(1+2)} = J^{(1)} + J^{(2)} + I^{(1,2)}, \quad (3.28)$$

where $I^{(1,2)}$ is called the interaction integral (I -integral) for states (1) and (2), defined as

$$I^{(1,2)} = \int_{\Gamma} \left(w^{(1,2)} \mathcal{D}_{1j} - \sigma_{ij}^{(1)} \frac{\partial u_i^{(2)}}{\partial x_1} - \sigma_{ij}^{(2)} \frac{\partial u_i^{(1)}}{\partial x_1} \right) n_j d\Gamma, \quad (3.29)$$

where $w^{(1,2)}$ is the interaction strain energy defined by

$$w^{(1,2)} = \sigma_{ij}^{(1)} \varepsilon_{ij}^{(2)} = \sigma_{ij}^{(2)} \varepsilon_{ij}^{(1)}. \quad (3.30)$$

The J -integral definition in Eq. (3.25) can be written by the combined states (1) and (2) as

$$J^{(1+2)} = J^{(1)} + J^{(2)} + \frac{2}{E^*} \left(K_I^{(1)} K_I^{(2)} + K_{II}^{(1)} K_{II}^{(2)} \right), \quad (3.31)$$

Equating Eq. (3.28) and Eq. (3.31) leads to

$$I^{(1,2)} = \frac{2}{E^*} \left(K_I^{(1)} K_I^{(2)} + K_{II}^{(1)} K_{II}^{(2)} \right). \quad (3.32)$$

Making the choice of auxiliary state (2) as the pure mode I asymptotic fields with $K_I^{(2)} = 1$ and $K_{II}^{(2)} = 0$ gives SIF of mode I for state (1) in terms of the interaction integral

$$K_I^{(1)} = \frac{E^*}{2} I_{mode \ I}^{(1)}. \quad (3.33)$$

Similarly, making auxiliary state (2) as the pure mode II asymptotic fields with $K_I^{(2)} = 0$

and $K_{II}^{(2)} = 1$ gives SIF of mode II for state (1) as

$$K_{II}^{(1)} = \frac{E^*}{2} I_{mode\ II}^{(1)}. \quad (3.34)$$

3.4.2 Numerical Integration of I-Integral

SIFs are the most important parameters for the analysis of linear fracture behavior. To evaluate SIFs, we present an innovative method of numerical integration of I -integral over a path of PD nodes in this subsection.

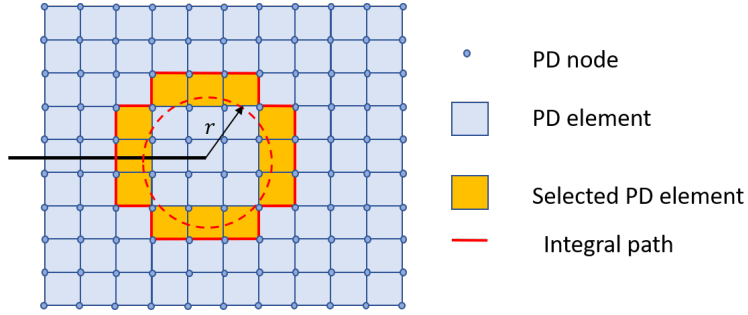


Fig. 3.3: Contour of the I -integral.

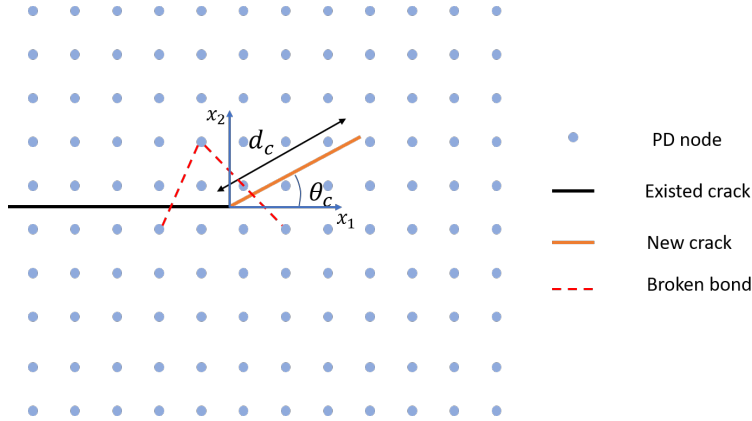


Fig. 3.4: Schematic of crack growth.

To determine the I -integral contour, we propose the following guiding principle: (1) the integral contour should stay outside of and yet follow closely a base circle with desired size centered at the crack tip; (2) the selection of contour segments should allow easy and automatic implementation in the simulation; (3) the union of all contour segments must

form a continuous path; and (4) no part of the contour goes inside the base circle.

To determine the contour, the PD domain is first discretized into 4-noded PD elements (quadrilateral elements), as illustrated in Fig. 3.3. A base circle with a specified radius r is defined, shown by the red dot line in the figure. Next, PD elements forming the contour are selected based on this criterion: the selected elements must have either 2 or 3 nodes outside the base circle (yellow elements in the figure). Connecting consecutively all outside the base circle nodes of the selected elements forms the integral contour, as illustrated by the solid red lines in the figure. Although not shown herein, if the domain is discretized with 3-noded PD elements (triangle elements), we can treat these 3-noded elements as 4-noded elements with the fourth node and third node collapsed together. Note that, although we have the PD element concept here, the numerical implementation of PDLsM in the PD domain is a meshless method, rather than an element-based method. With the segments of the contour from each selected PD element, the value of interaction integral $I^{(1,2)}$ can be evaluated as

$$I^{(1,2)} = \sum_{e=1}^{N_{se}} \sum_{p=1}^{1 \text{ or } 2} (F_{(p)} + F_{(p+1)}) \frac{l_p}{2}, \quad (3.35)$$

where l_p is the length of the segment between nodes (p) and $(p+1)$, N_{se} is the number of selected PD elements, and $F_{(p)}$ denotes the integrand at node (p) as:

$$F_{(p)} = \left(w^{(1,2)} \mathcal{D}_{1j} - \sigma_{ij}^{(1)} \frac{\partial u_i^{(2)}}{\partial x_1} - \sigma_{ij}^{(2)} \frac{\partial u_i^{(1)}}{\partial x_1} \right) n_j, \quad (3.36)$$

here the normal vector $\mathbf{n}$ can be determined by right-hand rule as:

$$\mathbf{n} = \begin{cases} \frac{x_{2(p)} - x_{2(p+1)}}{l_p} \mathbf{i} + \frac{x_{1(p+1)} - x_{1(p)}}{l_p} \mathbf{j}, & z > 0, \\ \frac{x_{2(p+1)} - x_{2(p)}}{l_p} \mathbf{i} + \frac{x_{1(p)} - x_{1(p+1)}}{l_p} \mathbf{j}, & z < 0. \end{cases} \quad (3.37)$$

in which z is defined as below

$$z = (x_{1(p+1)} - x_{1(p)}) (x_{2(p+1)} - x_{2(t)}) - (x_{2(p+1)} - x_{2(p)}) (x_{1(p+1)} - x_{1(t)}), \quad (3.38)$$

where $x_{1(t)}$ and $x_{2(t)}$ are coordinates of the crack tip. The displacement, strain, and stress fields of state (1), that is, $u_i^{(1)}$, $\varepsilon_{ij}^{(1)}$, and $\sigma_{ij}^{(1)}$ are obtained by the PDLMS-FEM technique, while these field variables of the auxiliary state (2) are evaluated from LEFM formulas as in the Eqs. (3.20), (3.21), (3.22) and (3.23) with $K_I^{(2)} = 1$, $K_{II}^{(2)} = 0$ or $K_I^{(2)} = 0$, $K_{II}^{(2)} = 1$. With the displacement, strain, and stress fields of state (1) and of the auxiliary state (2), the value of $F_{(p)}$ at each node (p) on the integral path is evaluated by Eq. (3.36), and then the I -integral $I^{(1,2)}$ is evaluated by Eq. (3.35). As described in section 3.4.1, assumed values of $K_I^{(2)} = 1$ and $K_{II}^{(2)} = 0$ lead to $I_{mode\ I}^{(1)} = I^{(1,2)}$, and assumed values of $K_I^{(2)} = 0$ and $K_{II}^{(2)} = 1$ lead to $I_{mode\ II}^{(1)} = I^{(1,2)}$. With the values of $I_{mode\ I}^{(1)}$ and $I_{mode\ II}^{(1)}$, SIFs are evaluated by Eq. (3.33) and Eq. (3.34). Note that a transformation from global coordinates to local coordinates is needed to evaluate the SIFs.

3.4.3 Crack propagation criterion

In crack propagation simulation, three propagation conditions need to be determined at each load step: (a) onset of propagation, i.e., whether or not the crack will propagate; (b) direction of propagation, i.e., along which direction the crack will propagate; and (c) amount of propagation, i.e., how long the crack will propagate. Criteria for conditions (a) and (b) are related to the underlying physics of crack propagation, while condition (c) is only an issue that needs to be dealt with in the numerical simulation.

For a general mixed-mode case, various criteria have been published by researchers to determine the first two conditions, such as the maximum energy release rate [75], the minimum strain energy density criteria [77], the maximum circumferential tensile stress [75]. In this study, the maximum circumferential tensile stress theory is employed to determine the crack propagation direction. Based on this theory, the hoop stress reaches its maximum value on the plane of zero shear stress. For LEFM, the size of plastic zone at the crack tip is negligible and the singular term solutions of stresses at the crack tip are used to determine the crack propagation angle θ_c , which is defined as the angle between the line of crack and the crack growth direction (Fig. 3.4). The value of θ_c is determined by requiring the shear

stress to become zero, and is found to be

$$\theta_c = \begin{cases} 2 \tan^{-1} \left(\frac{K_I}{4K_{II}} - \frac{1}{4} \sqrt{\left(\frac{K_I}{K_{II}} \right)^2 + 8} \right) & \text{for } K_{II} > 0, \\ 2 \tan^{-1} \left(\frac{K_I}{4K_{II}} + \frac{1}{4} \sqrt{\left(\frac{K_I}{K_{II}} \right)^2 + 8} \right) & \text{for } K_{II} < 0, \end{cases} \quad (3.39)$$

For a crack to propagate, the maximum circumferential tensile stress must reach a critical value. This results in an equivalent SIF in mixed-mode condition as

$$K_{eq} = K_I \cos^3 \frac{\theta_c}{2} - \frac{3}{2} K_{II} \cos \frac{\theta_c}{2} \sin \theta_c. \quad (3.40)$$

with θ_c determined by Eq. (3.39). If $K_{eq} > K_{Ic}$, in which K_{Ic} is the fracture toughness, the crack will propagate in the direction of θ_c , as shown in Fig. 3.4.

Most published criteria deal with only conditions (a) and (b), i.e., the onset of propagation and direction of propagation, and do not address condition (c), i.e., the amount of crack propagation. In the physical world, how much the crack will propagate depends on the body geometry and loading mechanism. If crack growth is unstable, once the propagation is triggered, K_{eq} will remain larger than K_{Ic} , and the crack will propagate in an unstable manner until ultimate failure. If crack growth is stable, once the crack starts to propagate, K_{eq} will drop below K_{Ic} , and crack growth will stop. Crack growth therefore is infinitesimal in stable growth, and a load increase is needed for further crack growth.

In numerical simulation, once the criterion for crack propagation is met, a somewhat arbitrary yet reasonable amount of crack growth must be assumed in each load step. The assumed crack growth amount is ultimately limited to the resolution of the numerical model. Since the fine PD elements near the crack tip represent the limit of the model resolution, we propose that the crack propagation amount should be comparable to the minimum characteristic length $\Delta_{min} = \sqrt{A_{min}}$ of PD nodes (A_{min} represents minimum PD node's area), for example α times the Δ_{min} , with α in the range of 0.5 to 1.5.

In the simulation, we implement the technique to model crack growth as following. We

pre-define the amount of crack growth d_c based on the PD elements size in each load step. Whenever the condition $K_{eq} > K_{Ic}$ is reached, the crack will propagate an amount d_c along the direction of θ_c . All bonds crossing the path of d_c will be treated as broken with their bond status parameter μ updated from 1 to 0.

Depending on the value of d_c and the level of load increment, it is possible that in stable crack propagation, after the crack propagates one d_c , several load increments are needed before K_{eq} rises above K_{Ic} again. On the other hand, in unstable crack propagation, once the propagation is triggered, K_{eq} remains above K_{Ic} no matter how much the crack propagates. In this case, the load level is kept unchanged, and the crack will continue to propagate in increment of d_c in our simulation.

3.4.4 Step by step simulation process and flowchart

The simulation process is described step by step here to present a whole picture view of our model. A small load in terms of prescribed displacements is applied to the domain firstly, and the global stiffness $\mathbf{K}$ and global equivalent nodal force $\mathbf{F}$ are computed as described in Appendix A. Then the displacement field $\mathbf{U} = \mathbf{K}^{-1}\mathbf{F}$, and the field of strain and stress are solved. The strain and stress of the PD domain are obtained by Eq. (A.3) and Eq. (A.5), respectively. In the FEM domain, strain and stress are calculated by FEM formulas and for the PD-FEM interface, the nodal stresses and strains are calculated by the average of FEM and PD formulations. With the fields of displacement, strain, and stress, the SIFs, K_I and K_{II} are calculated according to Eqs. (3.33), (3.34), (3.35), and (3.36) for each crack tip. Next, the crack growth direction θ_c and equivalent SIF K_{eq} are obtained by Eq. (3.39) and Eq. (3.40), respectively. If $K_{eq} > K_{Ic}$, the crack will grow along the direction θ_c by length d_c , with the new crack represented by a fictitious segment from the old crack tip to the new crack tip. All bonds passing through the new crack will be broken, so that the bond status parameter μ of these bonds will be updated, as well as the global stiffness $\mathbf{K}$, which becomes more compliant. If $K_{eq} < K_{Ic}$, the load will be increased by small increments until K_{eq} exceeds K_{Ic} , and the simulation goes to the next iteration. Fig. 3.5 shows the flowchart

of the quasi-static crack propagation simulation. In the simulation, K_{eq} and θ_c for each crack tip are obtained and then the positions of new crack tips are determined, therefore this simulation method can handle multiple cracks.

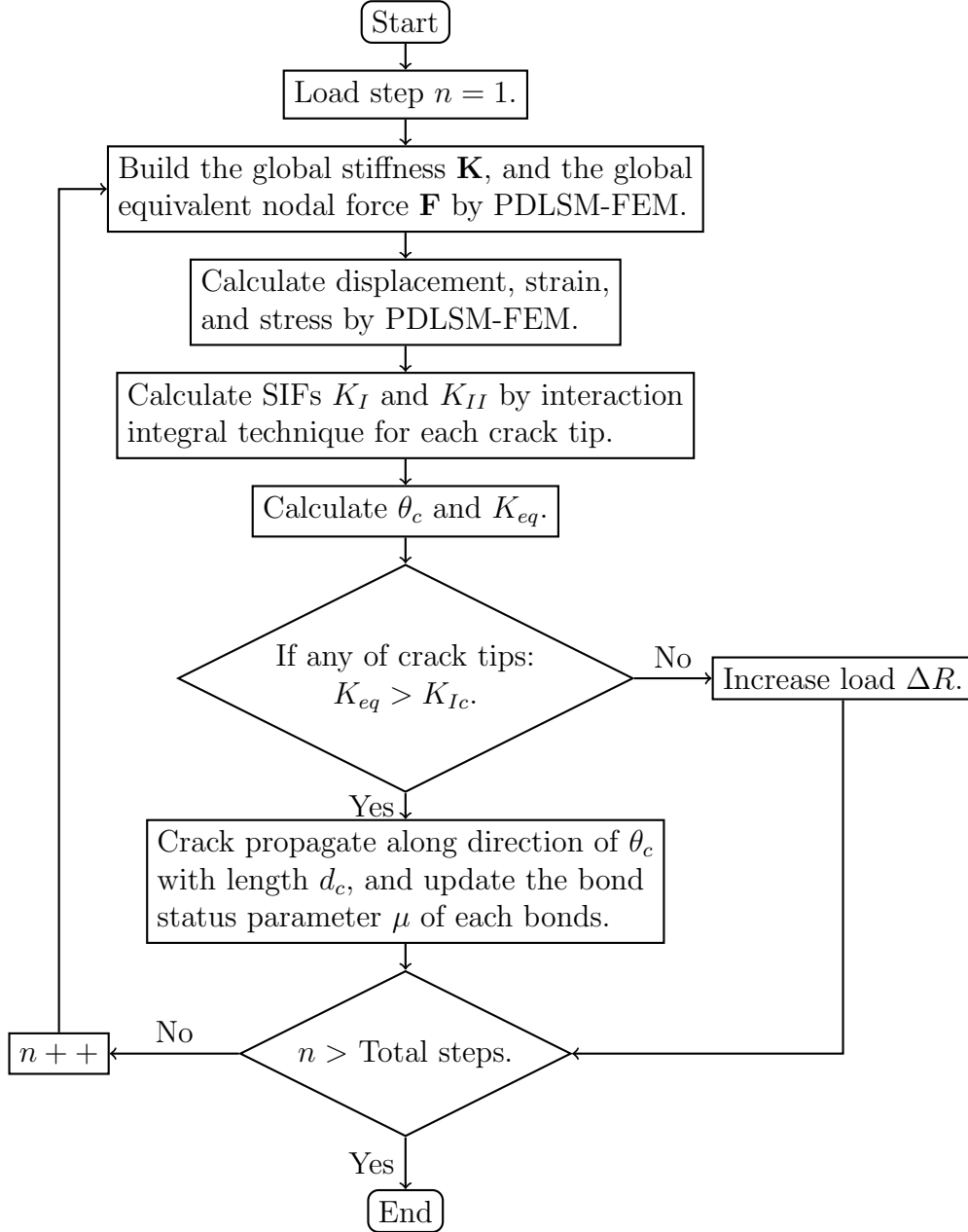


Fig. 3.5: Flowchart of crack propagation simulation.

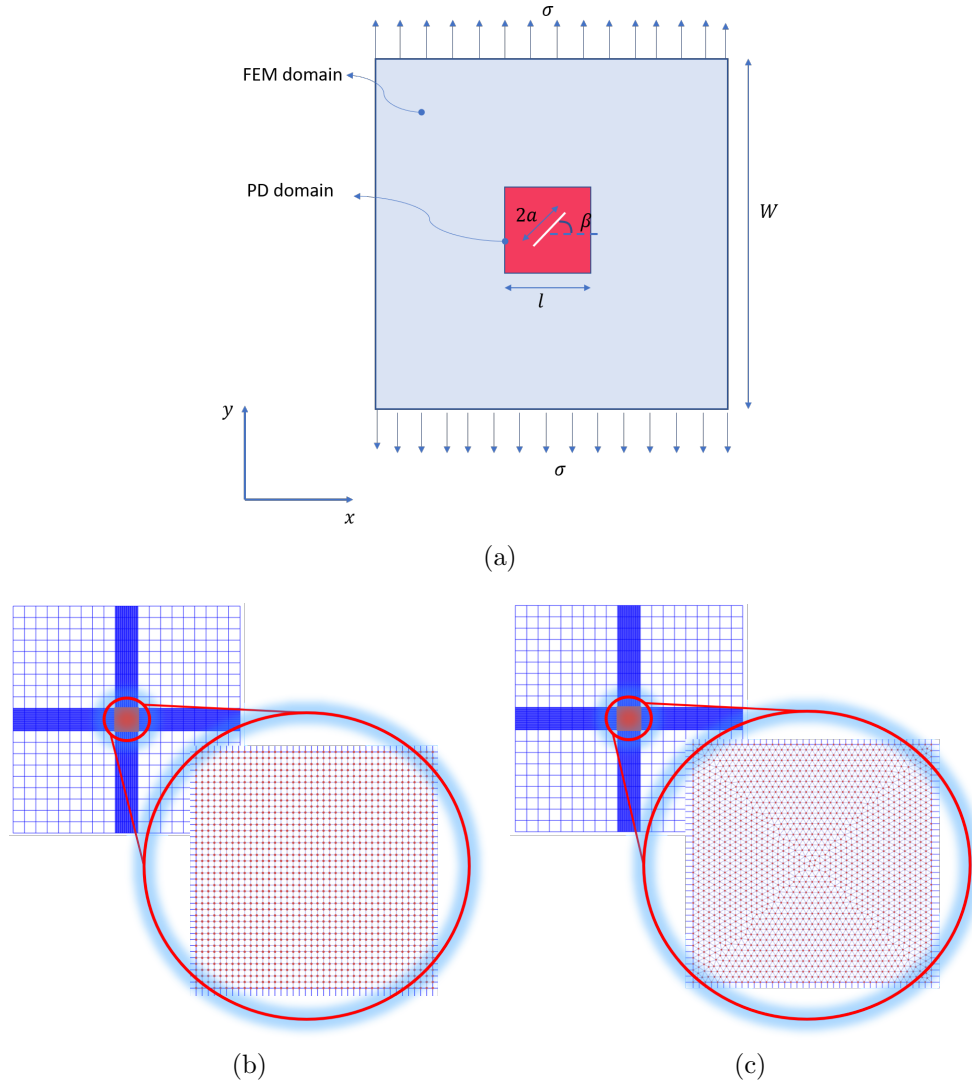


Fig. 3.6: Infinite plate with a central inclined crack: (a) Geometry, (b) 4-noded PD elements, (c) 3-noded PD elements.

3.5 Numerical results

To demonstrate the capability of the simulation model developed in this work, three plane stress examples are conducted and presented in this section. The first example is an infinite plate with an inclined crack at its center subjected to uniform far-field tension, in mixed-mode loading. The second and third examples are a disk-shaped plate and a diagonal plate with a pre-existing crack under displacement loading. In the first example, we investigate the SIFs of the infinite plate and compare the results against analytical solutions to demonstrate the accuracy of the proposed method, and a similar simulation by X-FEM can be found in [78]. In the second and third examples, we simulate the quasi-static crack growth of the two plates to show the capability of the proposed method to simulate crack propagation.

Note that the influence function $\omega(|\boldsymbol{\xi}|)$ may affect the accuracy in numerical implementation. In this paper, we specify the influence function as a Gaussian distribution in the form of

$$\omega(|\boldsymbol{\xi}|) = e^{-\left(\frac{|\boldsymbol{\xi}|}{\mathcal{a}\delta(i)}\right)^2}, \quad (3.41)$$

here, $\mathcal{a}$ is a constant and we define it as a *non-local factor*.

3.5.1 An infinite plate with an inclined crack for verifying SIFs

As shown in Fig. 3.6a, a square plate with a central inclined crack is under uniform tension $\sigma = 70$ Mpa. The material constants of the plate are specified as Young's modulus $E = 70$ GPa, Poisson's ratio $\nu = 0.33$. The edge length of the plate is $W = 1$ m, and the crack length is defined as $2a = 40$ mm. As the ratio $W/a = 50$ is sufficiently large, we can approximately treat this plate as an infinite plate. At the center of the plate, a small square sub-domain with size $l = 0.1$ m is defined as a PD domain, and the remaining part is defined as a FEM domain. The FEM domain is discretized as coarse 4-noded mesh, and the PD domain is discretized as very fine 4-noded PD elements (total of 1521) as shown in Fig. 3.6b, or discretized as very fine 3-noded PD elements (total of 3450) as shown in Fig. 3.6c. The

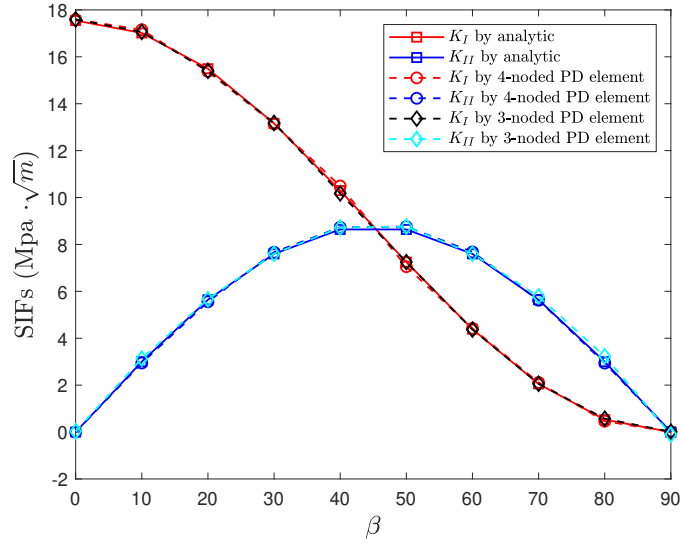


Fig. 3.7: Comparison of SIFs between the numerical and analytical solutions at various crack angle β .

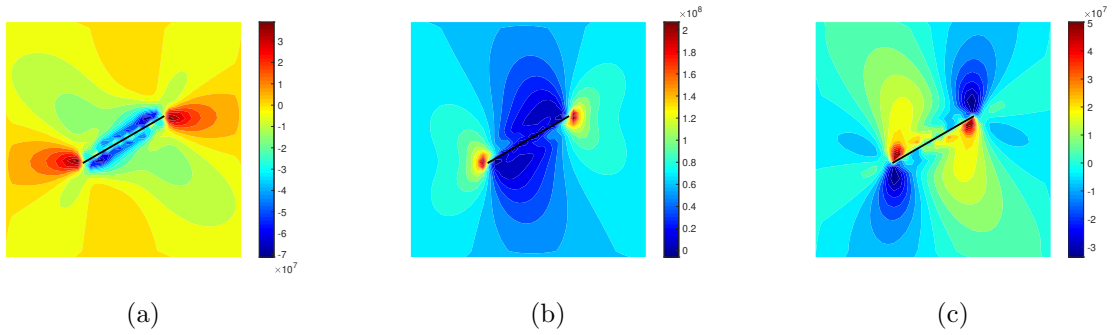


Fig. 3.8: Stress distributions for PD domain of the infinite plate with an inclined crack at angle $\beta = 30^\circ$: (a) σ_{xx} , (b) σ_{yy} , (c) σ_{xy} .

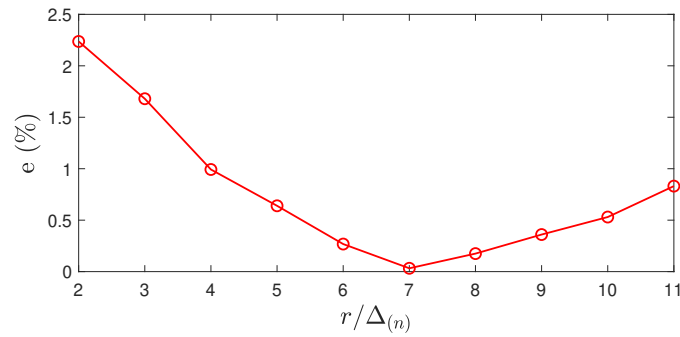


Fig. 3.9: Relative errors of SIF K_I of model I with various integration radius r .

analytical solution of this example with SIFs defined for modes I and II as [79]

$$\begin{cases} K_I = \sigma \sqrt{\pi a} \cos^2 \beta, \\ K_{II} = \sigma \sqrt{\pi a} \cos \beta \sin \beta. \end{cases} \quad (3.42)$$

The PDLISM-FEM analysis is performed with non-local factor $\varpi = 1/3$ for 4-noded PD elements and $\varpi = 1/4$ for 3-noded PD elements. The radius of the based circle for the I -integral path is defined as $r = m_r \Delta_{(n)}$, where $m_r = 6$ and $\Delta_{(n)}$ is the characteristic length of the node which is nearest to the crack tip. The horizon size is specified as $\delta_{(i)} = 4\Delta_{(i)}$. Fig. 3.7 shows the evaluations of SIFs K_I and K_{II} at various crack angle β for the numerical and theoretical solutions. Obviously, the relative error is almost negligible and a remarkable agreement can be seen between the theoretical values and numerical results by 4-noded and 3-noded PD models. Fig. 3.8 shows the stress results by PDLISM-FEM analysis with 4-noded PD elements for the infinite plate with an inclined $\beta = 30^\circ$ crack. Finally, the effect of integration radius $r = m_r \Delta_{(n)}$ on evaluation SIF K_I by 4-noded PD elements for pure mode I ($\beta = 0$) is studied and the results are shown in Fig. 3.9. As it shows, for $m_r = 2$, the relative error is the largest with value $e = 2.24\%$ and for $m_r \geq 4$, the relative error is less than 1%.

3.5.2 A disk-shaped plate under displacement loading

This example is to simulate crack propagation of a disk-shaped plate. As shown in Fig. 3.10a, a disk-shaped plate with a pre-existing crack is under displacement loading with $u_1 = 0$ and u_2 increasing from zero with incremental $\Delta u_2 = 5.106 \times 10^{-6}$ m. The dimension of the plate is $W = 106.9$ mm, $a_0 = 44.3$ mm and thickness $B = 50$ mm. The material constants of the plate are Young's modulus $E = 33.5$ GPa, Poisson's ration $\nu = 0.3$, and fracture toughness $K_{Ic} = 1.09$ MPa $\sqrt{\text{m}}$. The whole plate is modeled by non-uniform discretization with a total of 5893 nodes and 5730 elements. The region of -10.7 mm $< y < 10.7$ mm is discretized with 1980 PD nodes and 1869 4-noded PD elements. The minimum characteristic length is

$\Delta_{min} = 1.2$ mm and the crack growth length for each step is specified as $d_c = 1$ mm. The horizon size is $\delta_{(i)} = 4\Delta_{(i)}$, and the radius of the base circle for I -integral is $r = 6\Delta_{(n)}$. The non-local factor is $\varrho = 1/4$ in this example.

Fig. 3.11 shows the crack propagation and stress distributions of the disk-shaped plate at various load steps. As it shows, the crack propagates along the central horizontal line as expected and the stresses are concentrated at the crack tip. When the crack tip is far from the boundary of the domain (load step $n = 6$ and $n = 24$), the stress fields near the crack tip are similar to the analytical solutions.

Fig. 3.12a shows the SIF K_I at various load steps. As it shows, the crack starts to propagate at load step $n = 6$ and after that, the SIF K_I decreases. When $K_I < K_{Ic}$, the displacement loading increases with Δu_2 . Fig. 3.12b shows the reaction force at various displacement loading. As it shows, the reaction force decreases overall after crack growth due to the increased structural compliance. Note that the increase of reaction force is due to an increase in displacement loading.

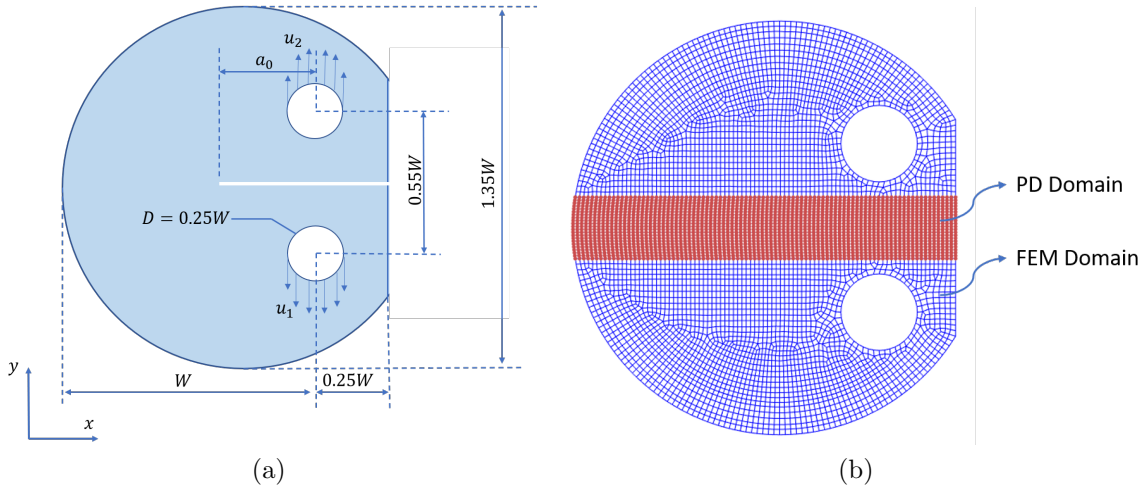


Fig. 3.10: A disk-shaped plate under displacement loading: (a) Geometry, (b) non-uniform mesh.

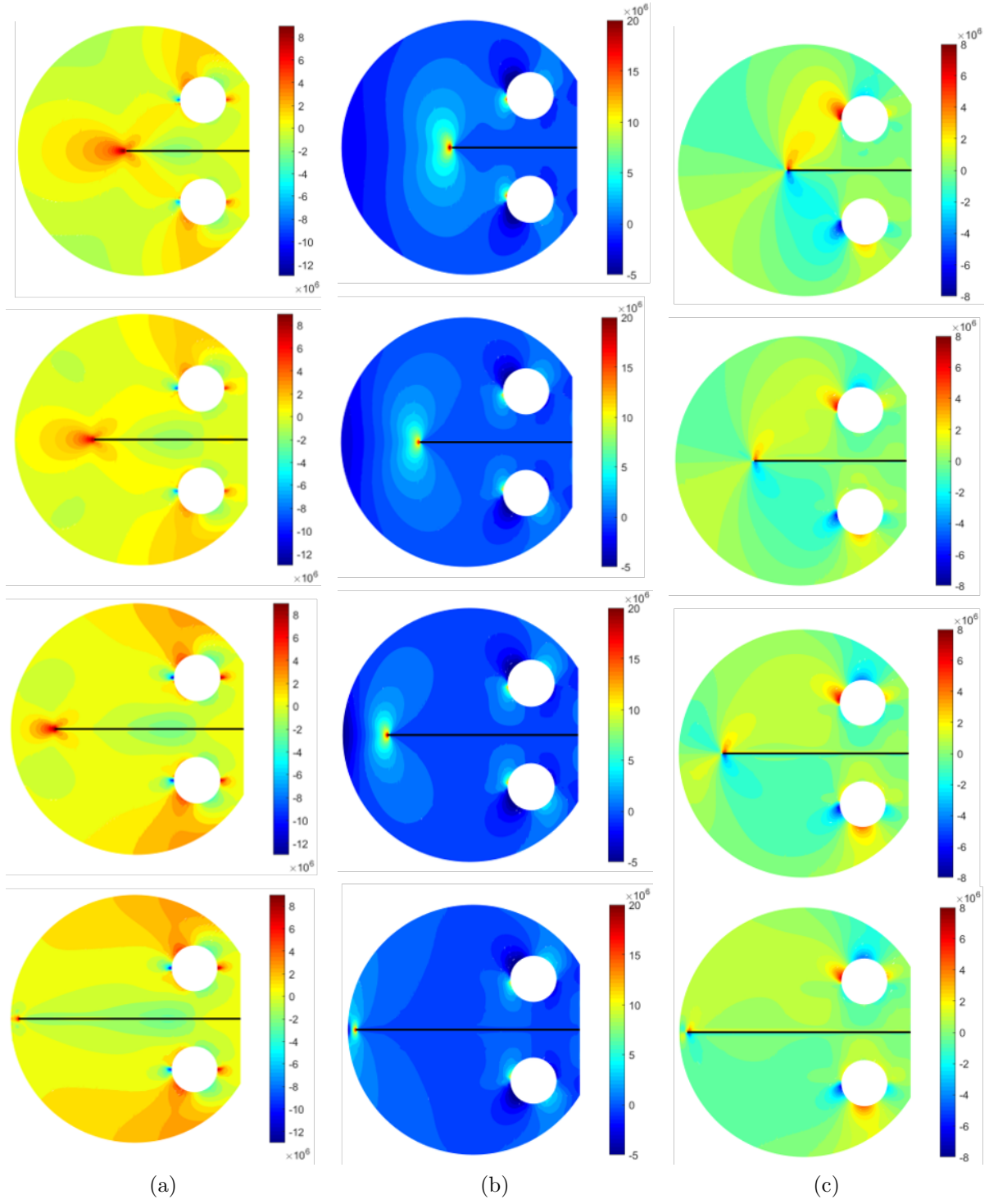


Fig. 3.11: Crack propagation and stress distributions of the disk-shaped plate at load step $n = 6, n = 24, n = 48$ and $n = 72$: (a) σ_{xx} , (b) σ_{yy} , (c) σ_{xy} .

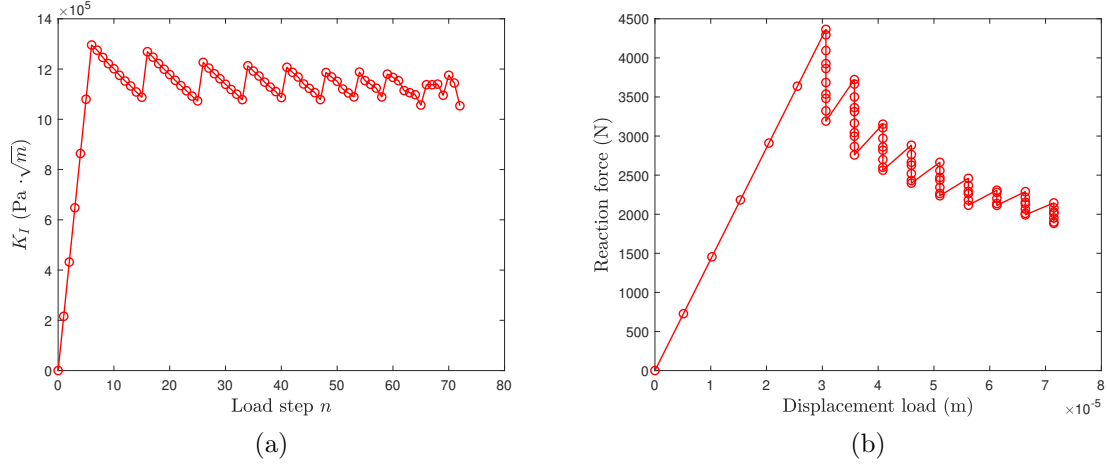


Fig. 3.12: The reaction force and SIF K_I of the disk-shaped plate during crack growth: (a) SIF K_I at various load steps n , (b) Reaction force at various displacement loading.

3.5.3 A diagonal plate under displacement loading

This example is to simulate crack propagation of a diagonal plate with a pre-existing inclined crack. As shown in Fig. 3.13a, a diagonal plate with size $150 \text{ mm} \times 150 \text{ mm} \times 5 \text{ mm}$ is under displacement loading with $u_1 = 0$ and u_2 increasing from zero with incremental $\Delta u_2 = 1.689 \times 10^{-4} \text{ m}$. The crack inclined angle is $\beta = 62.5^\circ$ and its length is specified as $2a = 45 \text{ mm}$. The radius of the loading hole is $r = 8 \text{ mm}$ and the distance between the center of the hole and the corner of the plate is specified as $b = 25 \text{ mm}$. This plate is made of a brittle polymer called polymethylmethacrylate (PMMA) whose Young's modulus, Poisson ratio, and fracture toughness are $E = 2.94 \text{ GPa}$, $\nu = 0.38$, and $K_{Ic} = 1.33 \text{ MPa}$, respectively. As shown in Fig. 3.13b, the whole domain is discretized with a total of 5785 nodes and 5607 elements. The PD domain is discretized with uniform elements with size of 2 mm and it contains 3603 PD nodes and 3450 4-noded PD elements. The horizon size is specified as $\delta_{(i)} = 3\Delta_{(i)}$ and the radius of the base circle for the I -integral is $r = 6\Delta_{(n)}$. The non-local factor is $\alpha = 1/4$ in this example. The crack growth length for each step in this simulation is specified as $d_c = 1 \text{ mm}$.

Fig. 3.14 shows the stress distributions of the diagonal plate at various load steps. As it shows, the stresses are concentrated at the crack tip. Fig. 3.15 shows the SIFs and the

reaction force of the diagonal plate during crack propagation. The crack of the plate starts to grow at load step $n = 5$, in which the equivalent SIF is $K_{eq} = 1.331 \text{ Mpa} \approx K_{Ic}$, and the critical reaction force $P = 3362 \text{ N}$, which is close to the experiment result $P_{cr} = 3192 \text{ N}$ [1]. Fig. 3.15b shows the reaction force decreases due to crack growth. As Fig. 3.15a shows, before the crack growth ($n < 5$), the plate is under pure mode II loading as $K_I \approx 0$. After the crack growth but before the 30-th loading step, the plate is under mix-mode loading and the changing of the sign of K_{II} makes the crack propagate with a zigzag shape. After the 30-th loading step, $K_{II} \approx 0$ and the plate is under pure mode I loading. Fig. 3.16 shows the crack path of the diagonal plate which is in good agreement with the experimental observation.

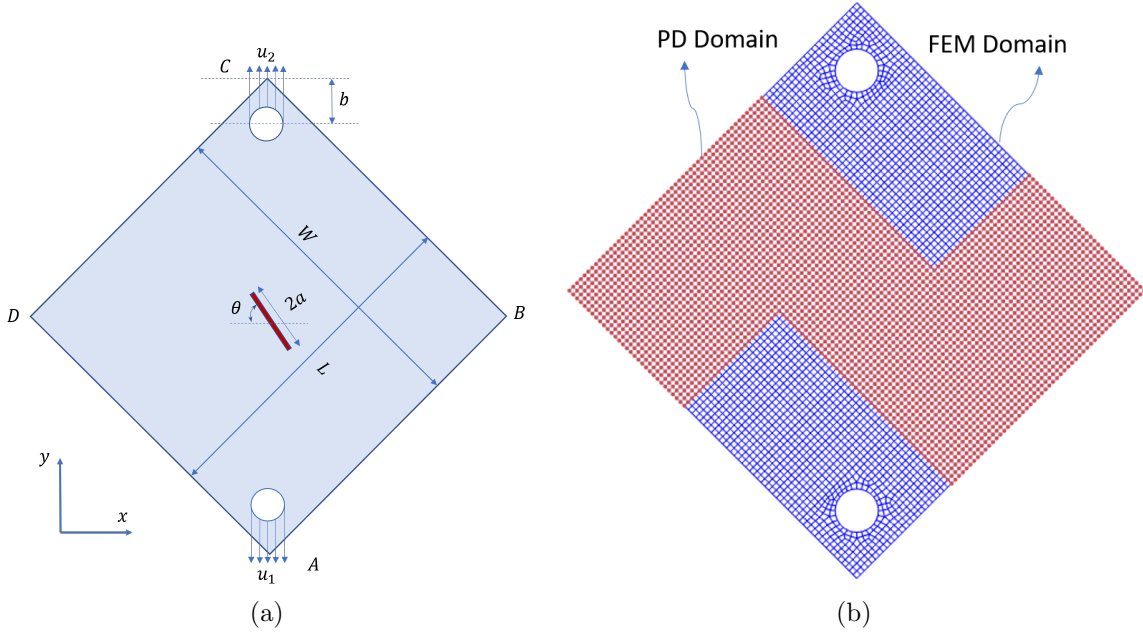


Fig. 3.13: A diagonal plate under displacement loading: (a) Geometry, (b) non-uniform mesh.

3.6 Conclusions

In this paper, we develop a framework for coupling peridynamics least square minimization and finite element method (PDLSP-FEM) based on the weighted residual method, and a

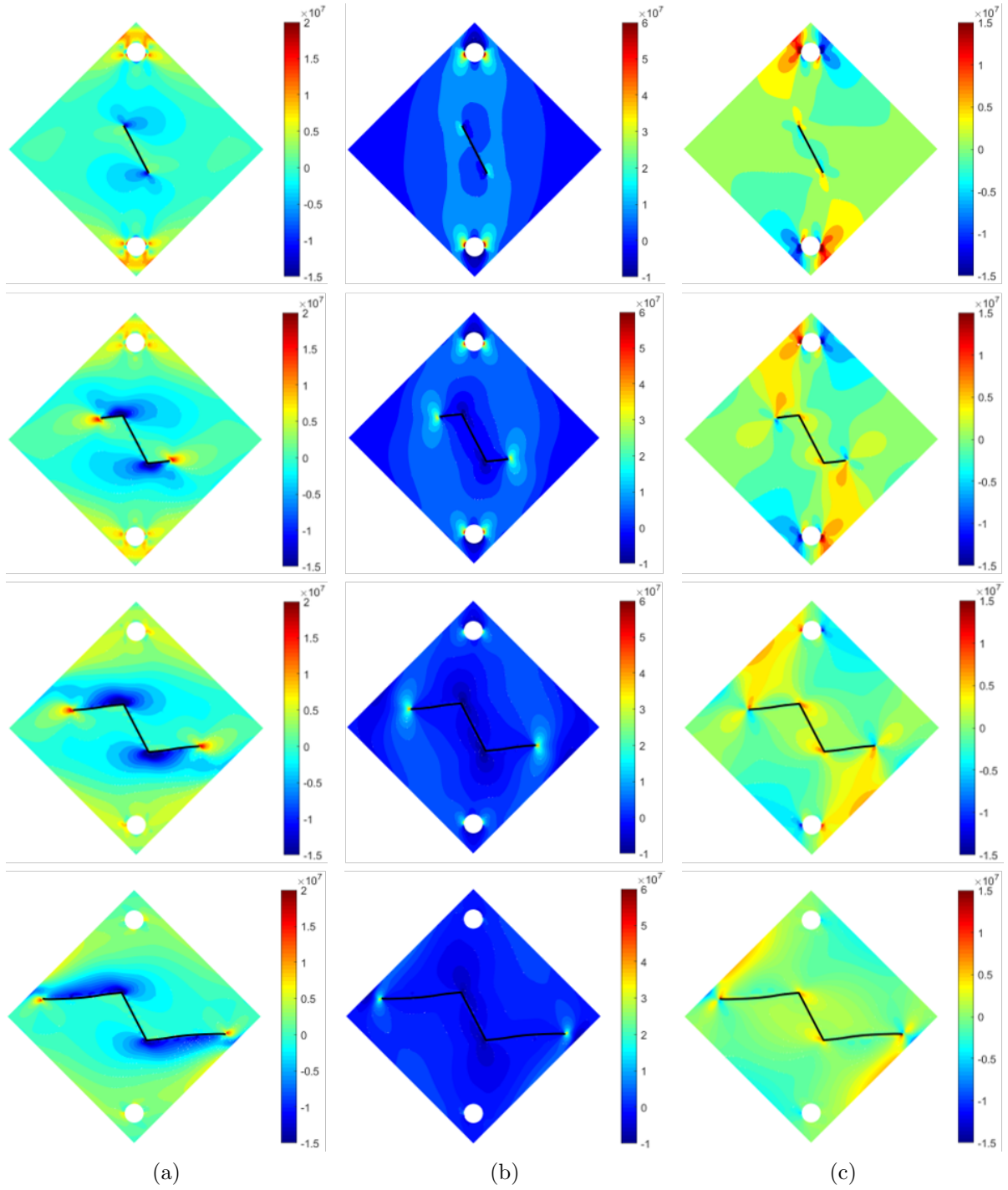


Fig. 3.14: Crack propagation and stress distributions of the diagonal plate at load step $n = 5$, $n = 24$, $n = 48$ and $n = 72$: (a) σ_{xx} , (b) σ_{yy} , (c) σ_{xy} .

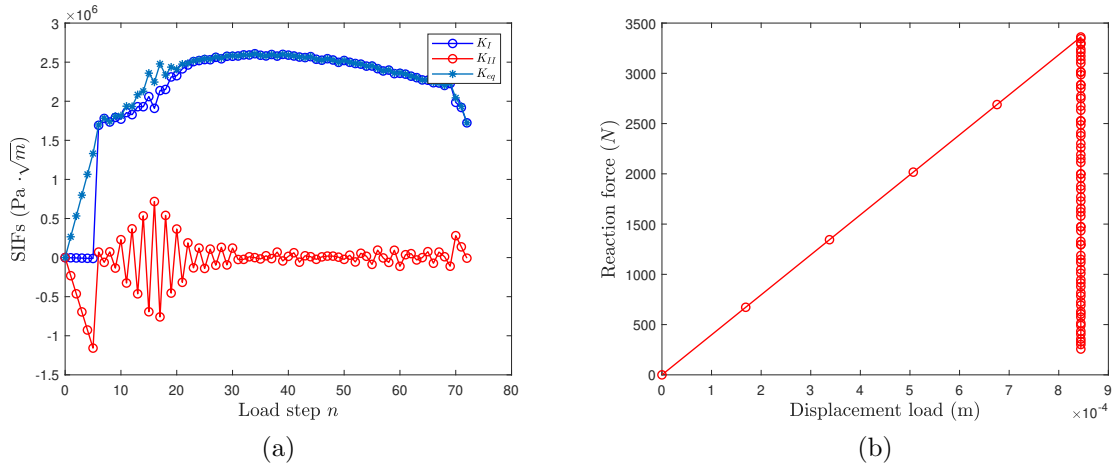


Fig. 3.15: The reaction force and SIFs of the diagonal plate during crack growth: (a) SIFs at various load steps n , (b) Reaction force at various displacement loading.

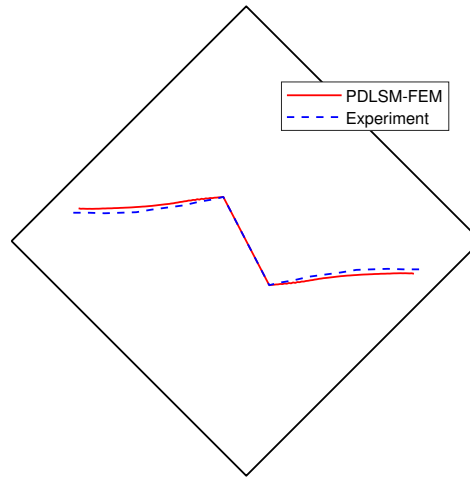


Fig. 3.16: Comparison of crack growth path by PDLSM-FEM against experiment observation [1].

quasi-static crack propagation simulation method for mixed-mode loading. Compared with other PD methods, PDLSM does not require surface correction and volume correction. The PDLSM-FEM provides a unified way to couple PDLSM and FEM, and can be easily introduced into commercial finite element codes. The quasi-static crack propagation simulation method provides an efficient way to find the shape of the crack. The interaction integral of J -integral is applied to calculate the stress intensity factors (SIFs) in mixed mode loading. The criterion of the maximum circumferential tensile stress is utilized to predict the onset of crack propagation and direction of propagation. As the J -integral is path independent, the proposed method avoids using the near tip stresses from PDLSM-FEM which are sensitive to mesh refinement and therefore less accurate. New contributions in this work include the following: (1) developing a new framework for coupling PDLSM and FEM; (2) pioneering a quasi-static method for simulating crack propagation in peridynamics; (3) developing an element-based approach for selecting the interaction integral contour; and (4) proposing and implementing an innovative method for handling peridynamic bond breakage and crack growth. One infinite plate with an inclined central crack under far-field tension is performed to calculate its displacement, stress, strain fields, and SIFs. The comparison of the SIFs between numerical and analytical solutions shows a good accuracy of the proposed method. Crack propagations in a disk-shaped plate and a diagonal plate under displacement loading are simulated, and the results show the capacity of the proposed method to model crack growth efficiently and satisfactorily.

Appendix A

PDLSM-FEM in 2D

The formulas of coupled PDLSM-FEM are rather lengthy, therefore only the outline is presented in the main text. For completeness, detailed formulas are given here in this Appendix.

A.1 Discretization of PD domain

The PDLSM model of a domain can be discretized with elements (named as PD element herein) by using commercial software, such as ANSYS due to its robust meshing ability. As illustrated in Fig. A.1, a 2D PD domain is discretized into PD elements and each PD

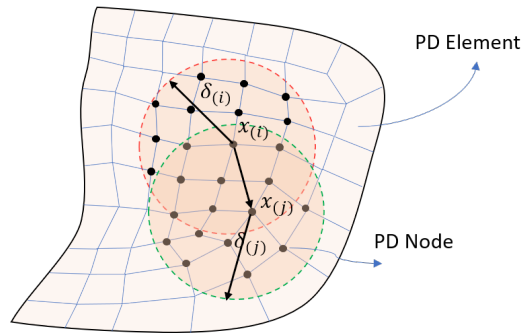


Fig. A.1: PD domain discretization and interactions between node $x_{(i)}$ and its family members.

element contains 4 PD nodes. Each PD element is divided into 4 parts with equal volume, and each part will count toward the volume of the associated node. Although not shown

here, if the domain is discretized with 3-noded elements, a similar method will be used. It is worth noting that the PD node may not locate at the center of its volume, especially for these nodes locating on the boundary of the domain.

As shown in Fig. A.1, the internal force vector at PD node $\mathbf{x}_{(i)}$ is calculated by including the interactions with its family members, $\mathbf{x}_{(j)}$, in the interaction domain. The interaction domain of node $\mathbf{x}_{(i)}$ depends on its horizon size $\delta_{(i)}$. The horizon size $\delta_{(i)}$ of node $\mathbf{x}_{(i)}$ is specified as $\delta_{(i)} = m\Delta_{(i)}$, with m being an constant and the characteristic length $\Delta_{(i)} = \sqrt{A_{(i)}}$, which depends on the area $A_{(i)}$ occupied by PD node $\mathbf{x}_{(i)}$. For non-uniform discretization, the rule to determine family members of node $\mathbf{x}_{(i)}$ is suggested by Hu et al. [60] as

$$H_{\mathbf{x}_{(i)}} = \left\{ \mathbf{x}_{(j)} \in H_{\mathbf{x}_{(i)}} : |\mathbf{x}_{(j)} - \mathbf{x}_{(i)}| \leq \delta_{(i)} \cup |\mathbf{x}_{(j)} - \mathbf{x}_{(i)}| \leq \delta_{(j)} \right\}, \quad (\text{A.1})$$

which ensures that the bond between nodes $\mathbf{x}_{(i)}$ and $\mathbf{x}_{(j)}$ is a paired interaction for either interaction domain. For node $\mathbf{x}_{(i)}$, there are $N_{(i)}$ family members within its interaction domain and the displacement set of these nodes is

$$\mathbf{u}^{(i)} = \begin{bmatrix} u_{1(i)} & u_{2(i)} & u_{1(2)} & u_{2(2)} & \cdots & u_{1(m)} & u_{2(m)} & \cdots & u_{1(N_{(i)})} & u_{2(N_{(i)})} \end{bmatrix}^T, \quad (\text{A.2})$$

here, the subscript (m) represents the m -th family member node $\mathbf{x}_{(m)}$ within the interaction domain of node $\mathbf{x}_{(i)}$ and the first family member is itself, $\mathbf{x}_{(i)}$. From Eq. (3.3), we obtain the discrete form of strain vector at node $\mathbf{x}_{(i)}$ as

$$\{\varepsilon\}_{(i)}^{pd} = [\varepsilon_x \quad \varepsilon_y \quad \gamma_{xy}]^T = \mathbf{C}^{(i)} \mathbf{u}^{(i)}, \quad (\text{A.3})$$

$$\mathbf{C}^{(i)} = \begin{bmatrix} -\sum_{m=2}^{N(i)} \mu_{(im)} \omega_{(im)} g_{1(im)} V_{(m)} & 0 & \mu_{(i2)} \omega_{(i2)} g_{1(i2)} V_{(2)} \\ 0 & -\sum_{m=2}^{N(i)} \mu_{(im)} \omega_{(im)} g_{2(im)} V_{(m)} & 0 \\ -\sum_{m=2}^{N(i)} \mu_{(im)} \omega_{(im)} g_{2(im)} V_{(m)} & -\sum_{m=2}^{N(i)} \mu_{(im)} \omega_{(im)} g_{1(im)} V_{(m)} & \mu_{(i2)} \omega_{(i2)} g_{2(i2)} V_{(2)} \\ 0 & \cdots & \mu_{(iN(i))} \omega_{(iN(i))} g_{1(iN(i))} V_{(N(i))} & 0 \\ \mu_{(i2)} \omega_{(i2)} g_{2(i2)} V_{(2)} & \cdots & 0 & \mu_{(iN(i))} \omega_{(iN(i))} g_{2(iN(i))} V_{(N(i))} \\ \mu_{(i2)} \omega_{(i2)} g_{1(i2)} V_{(2)} & \cdots & \mu_{(iN(i))} \omega_{(iN(i))} g_{2(iN(i))} V_{(N(i))} & \mu_{(iN(i))} \omega_{(iN(i))} g_{1(iN(i))} V_{(N(i))} \end{bmatrix}, \quad (\text{A.4})$$

where the subscript (im) represents the bond between node $\mathbf{x}_{(i)}$ and its m -th family member. From Eq. (A.3), the discrete form of stress vector at node $\mathbf{x}_{(i)}$ is

$$\{\sigma\}_{(i)}^{pd} = \mathbf{D} \mathbf{C}^{(i)} \mathbf{u}^{(i)}, \quad (\text{A.5})$$

here, $\mathbf{D}$ is material stiffness matrix of elasticity material. For plane stress problem,

$$\mathbf{D} = \frac{E}{1 - \nu^2} \begin{bmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & \frac{1-\nu}{2} \end{bmatrix}, \quad (\text{A.6})$$

and for plane strain problem,

$$\mathbf{D} = \frac{E}{(1 - 2\nu)(1 + \nu)} \begin{bmatrix} 1 - \nu & \nu & 0 \\ \nu & 1 - \nu & 0 \\ 0 & 0 & \frac{1-2\nu}{2} \end{bmatrix}. \quad (\text{A.7})$$

From Eq. (3.2), we obtain the discrete form of the internal force vector at node $\mathbf{x}_{(i)}$ as

$$\mathbf{L}_{(i)}^{pd} = \mathbf{H}^{(i)} \mathbf{u}^{(i)}, \quad (\text{A.8})$$

$$\mathbf{H}^{(i)} = \begin{bmatrix} -\sum_{m=2}^{N_{(i)}} \mu_{(im)} \omega_{(im)} \mathbf{G}_{(im)} V_{(m)} & \mu_{(i2)} \omega_{(i2)} \mathbf{G}_{(i2)} V_{(2)} & \cdots & \cdots & \mu_{(iN_{(i)})} \omega_{(iN_{(i)})} \mathbf{G}_{(iN_{(i)})} V_{(N_{(i)})} \end{bmatrix}. \quad (\text{A.9})$$

The bond status parameter $\mu_{(im)}$ in Eq. (A.4) and Eq. (A.9) is determined by the failure criteria.

A.2 Discretization of PDL-SM-FEM domain

To couple PDL-SM with FEM, the whole problem domain is divided into a FEM domain and a PD domain, and both domains are discretized into elements, as shown in Fig. 3.2. To distinguish, elements in the PD domain are called PD elements and elements in the FEM domain are still called finite elements. Note that PD nodes on the PD-FEM interface are also nodes of the finite element, and the interaction domains of these PD nodes are only determined from the PD domain, and the volumes of these PD nodes are calculated only from the PD elements.

Consider a 2-D discrete domain that contains N nodes, of which N^{pd} are PD nodes. For the i -th PD node $\mathbf{x}_{(i)}$, its displacement vector is $\mathbf{u}_{(i)} = [u_{1(i)} \quad u_{2(i)}]^T$ and can be expressed as

$$\mathbf{u}_{(i)} = \mathbf{M}_{(i)} \mathbf{u}_g, \quad (\text{A.10})$$

here, $\mathbf{u}_g$ is the displacement set of all nodes (global displacement vector) and $\mathbf{M}_{(i)}$ is the mapping matrix from $\mathbf{u}_g$ to $\mathbf{u}_{(i)}$, with size $2 \times 2N$. The displacement set of the family members of the PD node $\mathbf{x}_{(i)}$, $\mathbf{u}^{(i)}$, can be expressed by global displacement vector as

$$\mathbf{u}^{(i)} = \mathbf{M}^{(i)} \mathbf{u}_g, \quad (\text{A.11})$$

here, $\mathbf{M}^{(i)}$ is the mapping matrix from $\mathbf{u}_g$ to $\mathbf{u}^{(i)}$, with size $2N_{(i)} \times 2N$, and it can be specified as follows: if the k -th component of $\mathbf{u}^{(i)}$ and the j -th component of $\mathbf{u}_g$ are same, $M_{kj}^{(i)} = 1$, otherwise $M_{kj}^{(i)} = 0$. The matrix $\mathbf{M}_{(i)}$ is determined in a similar way. Substituting Eq. (A.11) into Eq. (A.5) and Eq. (A.8), leads to the non-local stress vector and internal force vector

expressed in terms of the global displacement vector as below,

$$\{\sigma\}_{(i)}^{pd} = \mathbf{DC}^{(i)} \mathbf{M}^{(i)} \mathbf{u}_g, \quad (\text{A.12})$$

$$\mathbf{L}_{(i)}^{pd} = \mathbf{H}^{(i)} \mathbf{M}^{(i)} \mathbf{u}_g. \quad (\text{A.13})$$

A.3 Governing Equations of PDLMS-FEM

Applying the WRM to the equilibrium equations and the boundary conditions over the whole problem domain leads to the governing equation for PDLMS-FEM as expressed in Eq. (15) in the main text. Within the FEM domain, applying the Gauss theorem to Eq. (3.15) leads to

$$\begin{aligned} & \int_{V_{fem}} [\delta \mathbf{u}^T \rho \ddot{\mathbf{u}} + \delta(\{\epsilon\}^T) \{\sigma\}] dV + \int_{V_{pd}} \delta \mathbf{u}^T (\rho \ddot{\mathbf{u}} - \mathbf{L}^{pd}) dV + \int_{S_{pd}} \delta \mathbf{u}^T \boldsymbol{\sigma}^{pd} \mathbf{n} dS = \\ & \int_{S_{tot}} \delta \mathbf{u}^T \mathbf{T} dS + \int_{V_{fem}} \delta \mathbf{u}^T \mathbf{b} dV + \int_{V_{pd}} \delta \mathbf{u}^T \mathbf{b} dV, \end{aligned} \quad (\text{A.14})$$

where V_{fem} and V_{pd} represent the volume of the FEM domain and PD domain respectively, and S_{pd} represents the boundary of the PD domain. The virtual internal work by the internal force of the PD domain, δU_B^{pd} , can be expressed as

$$\delta U_B^{pd} = - \int_{V_{pd}} \delta \mathbf{u}^T \mathbf{L}^{pd} dV = \delta \mathbf{u}_g^T \mathbf{K}_b^{pd} \mathbf{u}_g, \quad (\text{A.15})$$

where $\mathbf{K}_b^{pd} = - \sum_{i=1}^{N^{pd}} \mathbf{M}_{(i)}^T \mathbf{H}_{(i)} \mathbf{M}^{(i)} V_{(i)}$. Two adjacent PD nodes on the boundary of the PD domain, S_{pd} , define a PD boundary element (PDBE). As shown in Fig. A.2, it is assumed that the displacement and traction force vary linearly between the two end nodes, $\mathbf{x}_{(\ell_1)}$ and $\mathbf{x}_{(\ell_2)}$, of the ℓ -th PDBE as

$$\mathbf{u}_{(\ell)} = (1 - s) \mathbf{u}_{(\ell_1)} + s \mathbf{u}_{(\ell_2)}, \quad (\text{A.16})$$

and

$$\mathbf{t}_{(\ell)}^{pd} = (1 - s)\mathbf{t}_{(\ell_1)}^{pd} + s\mathbf{t}_{(\ell_2)}^{pd}, \quad (\text{A.17})$$

where s is the local coordinate of the ℓ -th PDBE with a unit normal vector $\mathbf{n}_{(\ell)}$ and length $\Gamma_{(\ell)}$. The traction force at the two end nodes of ℓ -th PDBE can be expressed as

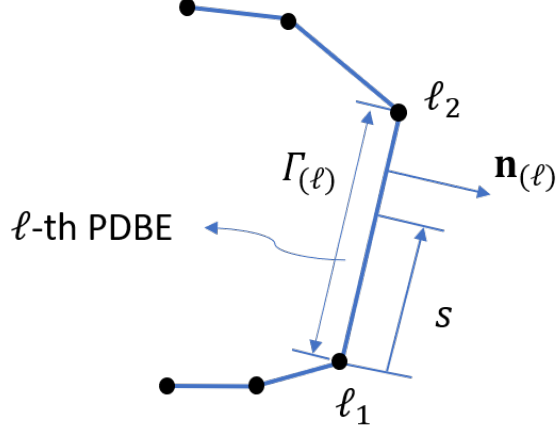


Fig. A.2: PD boundary elements.

$$\mathbf{t}_{(\ell_i)}^{pd} = \boldsymbol{\sigma}_{(\ell_i)}^{pd} \mathbf{n}_{(\ell)} = \mathbf{N}_{(\ell)} \{\sigma\}_{(\ell_i)}^{pd} \quad (\text{A.18})$$

where $\mathbf{N}_{(\ell)}$ is defined as

$$\mathbf{N}_{(\ell)} = \begin{bmatrix} n_{1(\ell)} & 0 & n_{2(\ell)} \\ 0 & n_{2(\ell)} & n_{1(\ell)} \end{bmatrix}. \quad (\text{A.19})$$

With this representation of $\mathbf{u}_{(\ell)}$ and $\mathbf{t}_{(\ell)}^{pd}$, the virtual internal work associated with PD domain boundary, δU_S^{pd} , can be evaluated as

$$\delta U_S^{pd} = \int_{S_{pd}} \delta \mathbf{u}^T \boldsymbol{\sigma}^{pd} \mathbf{n} dS = \int_{S_{pd}} \delta \mathbf{u}^T \mathbf{t}^{pd} dS = \delta \mathbf{u}_g^T \mathbf{K}_s^{pd} \mathbf{u}_g, \quad (\text{A.20})$$

where $\mathbf{K}_s^{pd}$ is defined as

$$\mathbf{K}_s^{pd} = \sum_{\ell=1}^{N_S^{pd}} \Gamma_{(\ell)} \left[\left(\frac{1}{3} \mathbf{M}_{(\ell_1)} + \frac{1}{6} \mathbf{M}_{(\ell_2)} \right) \mathbf{N}_{(\ell)} \mathbf{D} \mathbf{C}^{(\ell_1)} \mathbf{M}^{(\ell_1)} + \left(\frac{1}{6} \mathbf{M}_{(\ell_1)} + \frac{1}{3} \mathbf{M}_{(\ell_2)} \right) \mathbf{N}_{(\ell)} \mathbf{D} \mathbf{C}^{(\ell_2)} \mathbf{M}^{(\ell_2)} \right], \quad (\text{A.21})$$

in which N_S^{pd} is the number of PDBE. The virtual work by the inertia force in the PD domain, δU_I^{pd} , can be evaluated as

$$\delta U_I^{pd} = \int_{V_{pd}} \delta \mathbf{u}^T \rho \ddot{\mathbf{u}} dV = \delta \mathbf{u}_g^T \mathbf{M}^{pd} \ddot{\mathbf{u}}_g, \quad (\text{A.22})$$

where $\mathbf{M}^{pd} = \sum_{i=1}^{N_S^{pd}} \rho \mathbf{M}_{(i)}^T \mathbf{M}_{(i)} V_{(i)}$. Similarly, the virtual work by the external body force $\mathbf{b}$ in the PD domain, δW_B^{pd} , can be evaluated as

$$\delta W_B^{pd} = \int_{V_{pd}} \delta \mathbf{u}^T \mathbf{b} dV = \delta \mathbf{u}_g^T \mathbf{F}_b^{pd}, \quad (\text{A.23})$$

where $\mathbf{F}_b^{pd} = \sum_{i=1}^{N_S^{pd}} \mathbf{M}_{(i)}^T \mathbf{b}_{(i)} V_{(i)}$. The virtual strain energy of the FEM domain, δU^{fem} , can be evaluated by FEM as

$$\delta U^{fem} = \int_{V_{fem}} \delta(\{\epsilon\}^T) \{\sigma\} dV = \delta \mathbf{u}_g^T \mathbf{K}^{fem} \mathbf{u}_g. \quad (\text{A.24})$$

Similarly, the virtual work by the inertial force in the FEM domain, δU_I^{fem} , the virtual work by the external body force in the FEM domain, δW_B^{fem} , and the virtual work by the external traction force of the whole domain, δW_S , can be evaluated by FEM as follows:

$$\delta U_I^{fem} = \int_{V_{fem}} \delta \mathbf{u}^T \rho \ddot{\mathbf{u}} dV = \delta \mathbf{u}_g^T \mathbf{M}^{fem} \ddot{\mathbf{u}}_g, \quad (\text{A.25})$$

$$\delta W_B^{fem} = \int_{V_{fem}} \delta \mathbf{u}^T \mathbf{b} dV = \delta \mathbf{u}_g^T \mathbf{F}_b^{fem}, \quad (\text{A.26})$$

$$\delta W_S = \int_{S_{tot}} \delta \mathbf{u}^T \mathbf{T} dS = \delta \mathbf{u}_g^T \mathbf{F}_s. \quad (\text{A.27})$$

As FEM is a mature technology, the details to obtain the $\mathbf{K}^{fem}$, $\mathbf{M}^{fem}$, $\mathbf{F}_b^{fem}$ and $\mathbf{F}_s$ are not shown here for conciseness. Substituting Eqs. (A.22), (A.23), (A.24), (A.25), (A.26) and

(A.27) into Eq. (A.14) leads to the governing equation of this coupling model,

$$\mathbf{M}\ddot{\mathbf{u}}_g + \mathbf{K}\mathbf{u}_g = \mathbf{F}, \quad (\text{A.28})$$

where the global equivalent nodal mass $\mathbf{M}$ is defined as

$$\mathbf{M} = \mathbf{M}^{pd} + \mathbf{M}^{fem}, \quad (\text{A.29})$$

the global stiffness matrix $\mathbf{K}$ is defined as

$$\mathbf{K} = \mathbf{K}_b^{pd} + \mathbf{K}_s^{pd} + \mathbf{K}^{fem} \quad (\text{A.30})$$

and the global equivalent nodal force $\mathbf{F}$ is defined as

$$\mathbf{F} = \mathbf{F}_b^{pd} + \mathbf{F}_b^{fem} + \mathbf{F}_s, \quad (\text{A.31})$$

here, $\mathbf{M}$, $\mathbf{K}$ and $\mathbf{F}$ can be obtained by the assembling procedure as described previously. When $V_{pd} = 0$, Eq. (A.28) represents a pure traditional FEM model and when $V_{fem} = 0$, it represents a pure PD model. Thus, the formulation converts easily between PDLSM, FEM, and PDLSM-FEM.

Chapter 4

Coupled Peridynamics Least Square Minimization with Finite Element Method in 3D and implicit solutions by Message Passing Interface³

Abstract

In this work, we present a new framework to couple peridynamics least squares minimization with finite element method (PDLSM-FEM) for three-dimensional (3D) problems based on the weighted residual method (WRM). In PDLSM-FEM, the problem domain is divided into a PD domain and a FEM domain, and both domains are discretized into uniform or non-uniform elements. Within this framework, the coupling between the PD domain and the FEM domain is straightforward, and the formulation can be converted conveniently between PDLSM, FEM, and PDLSM-FEM. To directly and implicitly solve for displacements, we

³This chapter was published on *Journal of Peridynamics and Nonlocal Modeling*.
Liu, Q., Xin, X. J., and Ma, J. (2021). Coupled Peridynamics Least Square Minimization with Finite Element Method in 3D and Implicit Solutions by Message Passing Interface. *Journal of Peridynamics and Nonlocal Modeling*. <https://doi.org/10.1007/s42102-021-00060-3>

present an algorithm to assemble the global stiffness matrix in a compressed sparse row (CSR) format by the message passing interface (MPI) technique. The system equations are solved by the parallel direct sparse solver (PDSS) of the Intel Math Kernel Library (MKL). Three static examples are performed and the results show the proposed PDLsm-FEM can substantially reduce computational cost in terms of model efficiency and memory usage. Comparison between PDLsm-FEM results and FEM results using ANSYS demonstrates the good accuracy of the proposed PDLsm-FEM.

4.1 Introduction

Many problems of fundamental importance in solid mechanics involve pre-existing and propagating discontinuities such as cracks. As classical continuum theory employs spatial derivatives in its formulation and assumes the material is continuous as it deforms, it is inherently difficult to predict discontinuous behaviors such as failure of materials and structures. In light of the inadequacies of the classical continuum theory, Peridynamics (PD), which is based on non-local interactions and employs spatial integrals, was first introduced by Silling [4]. PD theory is better suited for failure analysis of materials and structures because its governing equations are defined by integral equations and remain valid at fracture surfaces.

The first introduced PD theory is the bond-based PD (BBPD) [4] in which a single PD material parameter, the bond constants c , is employed to analyze isotropic materials, resulting in a restriction of a fixed Poisson's ratio of $1/4$ [6]. Subsequently, Silling et al. [8] introduced the ordinary state-based PD (OSBPD) and non-ordinary state-based PD (NOSBPD) to remove the restriction. Both bond-based and state-based PD theories were derived by equating the classical strain energy at a material point to that of PD with a complete circle or sphere interaction domain [6]. These formulas in PD theory, however, are not valid for a point located near a surface because its interaction domain is not a complete circular or spherical [10]. Furthermore, most published work on PD to date employs a simple meshless method with a one-point quadrature for cells. Such one-point quadrature requires a volume correction procedure to improve integration accuracy [24]. To remove these two

drawbacks, Madenci et al. [58] proposed a PD least squares minimization (PDLSPM), and Liu and Xin [70] proposed a revised non-ordinary state-based PD (RNOSBPD). Both methods were derived by Taylor series expansion and the concept of non-local interactions of PD. To date, the PD theories have been not only applied to various structural discontinuous problems, such as damage and failure analysis of composite materials [51], metallic structures [53], ice craters [67], ceramics tiles [69], and glasses [54–56], but also extended to the analysis of heat conduction [80, 81], fluid flow [82, 83], electro-mechanical behavior [84], thermal and electrical transport processes of thermoelectric materials [85], and many others.

Compared with the finite element method (FEM), PD is computationally expensive. Thus, coupling PD with FEM is an appealing choice for taking advantage of these two methods. Kilic and Madenci [32] introduced a coupling method using overlapping regions in which both BBPD and FE equations are utilized. Agwai et al. [33] coupled BBPD with FEM using a sub-domain method, where the global modeling is performed using FEM while the PD theory is employed for the sub-modeling and failure prediction. A morphing strategy to couple BBPD with FEM based on energy equivalence was proposed and was employed for 1D and 2D problems by Lubineau et al. [34]. Liu et al. [35] introduced interface elements and coupling forces to bridge the BBPD and FEM. Some adaptive approaches which can transform FEM nodes into peridynamic nodes for coupling BBPD or OSBPD with FEM were developed in [36–38]. Bie et al. [40] proposed an approach to couple OSBPD with node-based smoothed finite element which requires no transition region. Sun and Fish [43] proposed a coupling approach based on a partial superposition of FEM and PD solutions for static and quasi-static problems. To couple OSBPD with FEM, the Arlequin method [44] is used in [45] to impose the mechanical compatibility between finite element and peridynamic sub-regions. Dong et al. [46] proposed a stability-enhanced PD element to couple NOSBPD with FEM, in which the stiffness matrix of the PD element is derived to establish the global stiffness matrix. Pagani and Carrera [47] proposed a technique to couple 3D peridynamics with 1D high-order finite elements using Lagrange multipliers. Shen et al. [48] introduced truss elements to bridge finite element (FE) sub-regions and PD sub-regions to couple PD with FEM. The authors Liu et al. [86] proposed a straightforward framework to couple

PDLSM with FEM for 2D problems based on weighted residual method.

In general, PD is computationally expensive due to a large number of non-local interactions, much-refined mesh, and PD-based codes written in terms of dynamic equilibrium even for static problems. Typically, static problems in PD are solved by adopting an explicit adaptive dynamic relaxation (ADR) method [27] that determines steady-state solutions for a dynamic system by introducing fictitious mass and damping matrices. The explicit dynamic relaxation method is commonly preferred because it does not require large-matrix operations. Generally, the explicit dynamic relaxation method requires a large number of iterations for each time step to find a convergent solution. An alternative way would be to build the system equations $\mathbf{Ku} = \mathbf{F}$, then directly and implicitly solve the system equations for displacement solutions. Comparing to the explicit ADR method, the implicit method does not need a large number of iterations for solutions, and equilibrium is guaranteed if convergence is reached, thus it is more efficient for static problems. Sun and Sundararaghavan [87] used an implicit scheme to find the solution to a NOSBPD model of crystal plasticity with Newton-Raphson method. Breitenfeld et al. [63] implicitly implemented NOSBPD formulation for quasi-static linearly elastic solids problems. Zaccariotto et al. [88] implemented BBPD within an implicit code for static crack propagation phenomena based on the Newton-Raphson method. Prakash and Stewart [9] presented an algorithm that used coordinate and neighbor information to directly generate the sparse matrices based on BBPD formulas and solve the system equations for 2D static or quasi-static problems, which was shown much faster than the ADR method. Although the implicit method requires matrix inversion, the stiffness matrix of a FEM model is symmetric and sparse and its inversion is relatively easier and fast computationally. In comparison, mesh refinement in PD increases the size of the stiffness matrix $\mathbf{K}$ and a large number of non-local interactions leads to a denser $\mathbf{K}$, both of which significantly increase the computational cost to solve for $\mathbf{K}^{-1}$. Coupling PD with FEM makes it easier to employ the implicit method to solve fracture problems since FEM nodes interact only with nodes in the connecting elements, making the number of interactions much smaller than that of a full PD model. Furthermore, FEM enables a much coarser mesh at regions far from the crack tips. Ni et al. [74] presented a static solution of

crack propagation problems by implicitly solving a coupled BBPD with FEM. In some of the works for coupling PD with FEM quoted above, the implicit method was used to solve static problems for taking advantage of these two methods [34, 37, 38, 46–48, 86].

In this work, we present a new framework to couple PDLSM with FEM (PDLSM-FEM) for 3D problems based on the weighted residual method (WRM), which was used to derive the weak form of PDLSM in [64] for 2D problems. In the paper [64], it discretized the domain by elements and took the center of the elements as the integral points to derive the weak form of pure PDLSM based on WRM and meshless method. In the current work (PDLSM-FEM), the problem domain is divided into a PD domain and a FEM domain, and both domains are discretized into uniform or non-uniform elements. The elements' nodes in the PD domain are treated as integral points, named as PD nodes, whose volumes are calculated from the volume of the connecting elements. To derive the governing equation, the PDLSM formulas and the meshless method are employed in the PD domain, while the FEM formulas and the mesh-based method are employed in the FEM domain. With this framework, the coupling between the PD domain and the FEM domain is straightforward, and the formulation can be converted conveniently between PDLSM, FEM, and PDLSM-FEM. To directly and implicitly solve for displacements, we present an algorithm to assemble the global stiffness matrix $\mathbf{K}$ in a compressed sparse row (CSR) format by message passing interface (MPI) technique. Within the CSR format, only non-zero coefficients of the stiffness matrix, and their row and column indices are stored, rather than the full matrix. The system equations $\mathbf{Ku} = \mathbf{F}$ are solved by the parallel direct sparse solver (PDSS) of Intel Math Kernel Library (MKL). Three examples are performed to demonstrate the computational cost reduction and accuracy of the proposed PDLSM-FEM.

The remainder of this paper is outlined as follows. First, the theory of PDLSM is reviewed in Section 4.2. A new technique for coupling PDLSM with FEM for 3D problems based on the weighted residual method is developed and presented in Section 4.3. Next, the algorithm for assembling the global stiffness matrix in a CSR format is illustrated in Section 4.4. Three applications are performed to validate the computational efficiency and accuracy of PDLSM-FEM in Section 4.5. Finally, concluding remarks are summarized in Section 4.6.

4.2 Peridynamics least square minimization

In this section, the peridynamics least square minimization (PDLSTM) first developed in [58] is briefly reviewed. PDLSTM employs the concept of PD interactions and LSM in conjunction with the Taylor series expansion (TSE). Relevant formulas essential for understanding PDLSTM can be found in [58]. As described in [58], the variation between $f(\mathbf{x}')$ and $f(\mathbf{x})$ can be approximated based on TSE in a 3 dimensional space as

$$f(\mathbf{x}') = \sum_{n=0}^N B^n f(\mathbf{x}) + R(N, \mathbf{x}). \quad (4.1)$$

in which $R(N, \mathbf{x})$ is the remainder and B^n is defined as

$$B^n = \frac{1}{n!} \left(\xi_1 \frac{\partial}{\partial x_1} + \xi_2 \frac{\partial}{\partial x_2} + \xi_3 \frac{\partial}{\partial x_3} \right)^n, \quad (4.2)$$

and $\mathbf{x}' = \mathbf{x} + \boldsymbol{\xi}$ represents the neighbours of point $\mathbf{x}$ within its interaction domain H_x . The weighted error E_x from the approximation in Eq. (4.1) within the interaction domain can be evaluated based on least square minimization as

$$E_x = \int_{H_x} \omega(|\boldsymbol{\xi}|) R^2 dV_{x'} = \int_{H_x} \omega(|\boldsymbol{\xi}|) \left[f(\mathbf{x}') - \sum_{n=0}^N B^n f(\mathbf{x}) \right]^2 dV_{x'}. \quad (4.3)$$

This error can be minimized by requiring its first variation to vanish as $\delta E_x = 0$. For 2nd-order TSE ($N = 2$), this requirement leads to the derivatives of $f(\mathbf{x})$ in a integral form as

$$\begin{aligned} & \left[\frac{\partial}{\partial x_1} \quad \frac{\partial}{\partial x_2} \quad \frac{\partial}{\partial x_3} \quad \frac{\partial^2}{\partial x_1^2} \quad \frac{\partial^2}{\partial x_2^2} \quad \frac{\partial^2}{\partial x_3^2} \quad \frac{\partial^2}{\partial x_1 x_2} \quad \frac{\partial^2}{\partial x_2 x_3} \quad \frac{\partial^2}{\partial x_3 x_1} \right]^T f(\mathbf{x}) = \\ & \int_{H_x} \omega(|\boldsymbol{\xi}|) \begin{bmatrix} \mathbf{g} \\ \mathbf{d} \end{bmatrix} (f(\mathbf{x}') - f(\mathbf{x})) dV'. \end{aligned} \quad (4.4)$$

The vector $\mathbf{g} = [g_1 \ g_2 \ g_3]^T$ and $\mathbf{d} = [d_1 \ d_2 \ d_3 \ d_4 \ d_5 \ d_6]^T$ are defined as

$$\begin{bmatrix} \mathbf{g} \\ \mathbf{d} \end{bmatrix} = \mathbf{A}^{-1} \hat{\boldsymbol{\xi}}, \quad (4.5)$$

where

$$\hat{\boldsymbol{\xi}} = [\xi_1 \ \xi_2 \ \xi_3 \ \xi_1^2 \ \xi_2^2 \ \xi_3^2 \ \xi_1\xi_2 \ \xi_2\xi_3 \ \xi_1\xi_3]^T, \quad (4.6)$$

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix}, \quad (4.7)$$

$$\mathbf{A}_{11} = \int_{H_x} \omega(|\boldsymbol{\xi}|) \begin{bmatrix} \xi_1^2 & \xi_1\xi_2 & \xi_1\xi_3 \\ \xi_1\xi_2 & \xi_2^2 & \xi_2\xi_3 \\ \xi_1\xi_3 & \xi_2\xi_3 & \xi_3^2 \end{bmatrix} dV_{x'}, \quad (4.8)$$

$$\mathbf{A}_{12} = \int_{H_x} \omega(|\boldsymbol{\xi}|) \begin{bmatrix} \frac{\xi_1^3}{2} & \frac{\xi_1\xi_2^2}{2} & \frac{\xi_1\xi_3^2}{2} & \xi_1^2\xi_2 & \xi_1^2\xi_3 & \xi_1\xi_2\xi_3 \\ \frac{\xi_1^2\xi_2}{2} & \frac{\xi_2^3}{2} & \frac{\xi_2\xi_3^2}{2} & \xi_1\xi_2^2 & \xi_1\xi_2\xi_3 & \xi_2^2\xi_3 \\ \frac{\xi_1^2\xi_3}{2} & \frac{\xi_2^2\xi_3}{2} & \frac{\xi_3^3}{2} & \xi_1\xi_2\xi_3 & \xi_1\xi_3^2 & \xi_2\xi_3^2 \end{bmatrix} dV_{x'}, \quad (4.9)$$

$$\mathbf{A}_{21} = \int_{H_x} \omega(|\boldsymbol{\xi}|) \begin{bmatrix} \xi_1^3 & \xi_1^2\xi_2 & \xi_1^2\xi_3 \\ \xi_1\xi_2^2 & \xi_2^3 & \xi_2^2\xi_3 \\ \xi_1\xi_3^2 & \xi_2\xi_3^2 & \xi_3^3 \\ \xi_1^2\xi_2 & \xi_1\xi_2^2 & \xi_1\xi_2\xi_3 \\ \xi_1\xi_2\xi_3 & \xi_2^2\xi_3 & \xi_2\xi_3^2 \\ \xi_1^2\xi_3 & \xi_1\xi_2\xi_3 & \xi_1\xi_3^2 \end{bmatrix} dV_{x'}, \quad (4.10)$$

$$\mathbf{A}_{22} = \int_{H_x} \omega(|\boldsymbol{\xi}|) \begin{bmatrix} \frac{\xi_1^4}{2} & \frac{\xi_1^2 \xi_2^2}{2} & \frac{\xi_1^2 \xi_3^2}{2} & \xi_1^3 \xi_2 & \xi_1^3 \xi_3 & \xi_1^2 \xi_2 \xi_3 \\ \frac{\xi_1^2 \xi_2^2}{2} & \frac{\xi_2^4}{2} & \frac{\xi_2^2 \xi_3^2}{2} & \xi_1 \xi_2^3 & \xi_1 \xi_2^2 \xi_3 & \xi_2^3 \xi_3 \\ \frac{\xi_1^2 \xi_3^2}{2} & \frac{\xi_2^2 \xi_3^2}{2} & \frac{\xi_3^4}{2} & \xi_1 \xi_2 \xi_3^2 & \xi_1 \xi_3^3 & \xi_2 \xi_3^3 \\ \frac{\xi_1^3 \xi_2}{2} & \frac{\xi_1 \xi_2^3}{2} & \frac{\xi_1 \xi_2 \xi_3^2}{2} & \xi_1^2 \xi_2^2 & \xi_1^2 \xi_2 \xi_3 & \xi_1 \xi_2^2 \xi_3 \\ \frac{\xi_1^2 \xi_2 \xi_3}{2} & \frac{\xi_2^3 \xi_3}{2} & \frac{\xi_2 \xi_3^3}{2} & \xi_1 \xi_2^2 \xi_3 & \xi_1 \xi_2 \xi_3^2 & \xi_2^2 \xi_3^2 \\ \frac{\xi_1^3 \xi_3}{2} & \frac{\xi_1 \xi_2^2 \xi_3}{2} & \frac{\xi_1 \xi_3^3}{2} & \xi_1^2 \xi_2 \xi_3 & \xi_1^2 \xi_3^2 & \xi_1 \xi_2 \xi_3^2 \end{bmatrix} dV_{x'}. \quad (4.11)$$

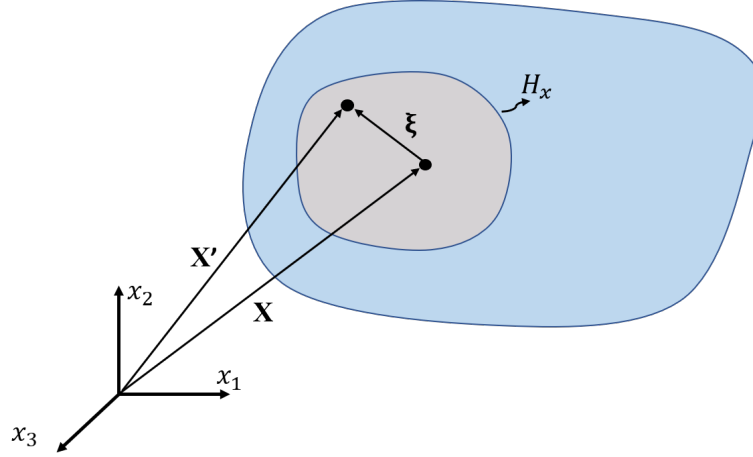


Fig. 4.1: Bond between points $\mathbf{x}'$ and $\mathbf{x}$ in the interaction domain H_x .

The differential operator of Eq. (4.4) can be used to derive the equation of motion in engineering problems by replacing the $f(\mathbf{x})$ as displacement components $u_i(\mathbf{x})$ ($i = 1, 2, 3$), as shown in [64]. In PD, the equation of motion is given by

$$\rho \ddot{\mathbf{u}} = \mathbf{L}^{pd}(\mathbf{x}, t) + \mathbf{b}(\mathbf{x}, t), \quad (4.12)$$

where ρ is the mass density, $\ddot{\mathbf{u}}$ is the acceleration, $\mathbf{b}$ is the external force vector, and $\mathbf{L}$ is the internal force vector. The internal force at point $\mathbf{x}$ is evaluated by the integration of bond force between material points $\mathbf{x}$ and $\mathbf{x}'$ over the interaction domain H_x of the material point $\mathbf{x}$, as shown in Fig. 4.1. According to the classical continuum mechanics (CCM), the internal force vector can be expressed as

$$\mathbf{L}^{pd}(\mathbf{x}, t) = \nabla \cdot \boldsymbol{\sigma}^{pd}(\mathbf{x}, t), \quad (4.13)$$

in which $\boldsymbol{\sigma}^{pd}$ is Cauchy's stress. For a linear isotropic material, the stress tensor can be expressed as

$$\boldsymbol{\sigma}^{pd} = \lambda \text{tr}(\nabla \mathbf{u}^{pd}) \mathbf{I} + \mathcal{G} [\nabla \mathbf{u}^{pd} + (\nabla \mathbf{u}^{pd})^T], \quad (4.14)$$

with λ representing Lamé's material constant and $\mathcal{G}$ representing shear modulus. Replacing the $f(\mathbf{x})$ of Eq. (4.4) by displacement components $u_i(\mathbf{x})$ leads to the non-local displacement gradient as

$$\nabla \mathbf{u}^{pd} = \int_{H_x} \omega(|\boldsymbol{\xi}|) \boldsymbol{\eta} \otimes \mathbf{g} dV_{x'}, \quad (4.15)$$

and the non-local internal force vector as

$$\mathbf{L}^{pd} = \int_{H_x} \omega(|\boldsymbol{\xi}|) \mathbf{G} \boldsymbol{\eta} dV_{x'}, \quad (4.16)$$

where $\boldsymbol{\xi} = \mathbf{x}' - \mathbf{x}$ and $\boldsymbol{\eta} = \mathbf{u}(\mathbf{x}') - \mathbf{u}(\mathbf{x})$ are the relative position and relative displacement of points $\mathbf{x}'$ and $\mathbf{x}$, respectively, and $\omega(|\boldsymbol{\xi}|)$ is the weight function. The matrix $\mathbf{G}$ in Eq. (4.16) is defined as

$$\mathbf{G} = \begin{bmatrix} (\lambda + \mathcal{G})d_1 + \mathcal{G}(d_1 + d_2 + d_3) & (\lambda + \mathcal{G})d_4 & (\lambda + \mathcal{G})d_6 \\ (\lambda + \mathcal{G})d_4 & (\lambda + \mathcal{G})d_2 + \mathcal{G}(d_1 + d_2 + d_3) & (\lambda + \mathcal{G})d_5 \\ (\lambda + \mathcal{G})d_6 & (\lambda + \mathcal{G})d_5 & (\lambda + \mathcal{G})d_3 + \mathcal{G}(d_1 + d_2 + d_3) \end{bmatrix}, \quad (4.17)$$

Note that the derivation of Eq. (4.15) and Eq. (4.16) does not require the interaction domain H_x to be a sphere, as many published PD models required. In fact, the interaction domain H_x can be of arbitrary shape. Thus, the surface effect [10] can be ignored and the volume correction [24] is not required.

4.3 A coupling framework of PDLSM and FEM for 3D problems

A new framework for coupling PDLSM with FEM is presented in this section. In this framework, the problem domain is divided into a PD domain and a FEM domain, both of which are discretized into uniform or non-uniform elements. Shared nodes on the interface between the PD domain and the FEM domain play a dual role, governed by the theory of PD on one side and by the theory of elasticity on the other. The weighted residual method is applied to PD equations of motion over the PD domain and elasticity equations of motion over the FEM domain, and the resultant governing equations combine PD and theory of elasticity in a unified way. When the FEM domain shrinks to zero, the formulation fully recovers the PDLSM and when the PD domain shrinks to zero, the formulation becomes FEM. When the PD domain and the FEM domain both exist, the formulation represents a coupling between PDLSM and FEM. We refer to the numerical model developed in this work as PDLSM-FEM.

4.3.1 Discretization of PD domain

The PDLSM model of a domain can be discretized with elements (named as PD element herein) using commercial software, such as ANSYS due to its robust meshing ability, as shown in Fig. 4.2. For 3D cases, the PD element can be tetrahedron, hexahedron, pyramid, and prism, etc., which are compatible with the elements definition in commercial FEM codes. Each PD element is divided into N_n parts with equal volume V_e/N_n , in which N_n is the number of nodes of the PD element and V_e is the volume of the PD element. Then volume V_e/N_n will be ascribed to each node of the PD element. It is worth noting that the PD node may not locate at the center of its volume, especially for these nodes locating on the boundary of the domain. Although we have the PD element concept here, the numerical implementation of PDLSM in the PD domain is a meshless method, rather than an element-based method.

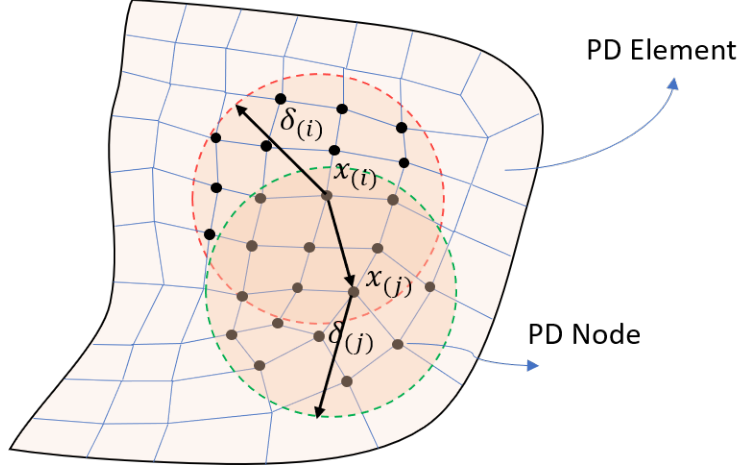


Fig. 4.2: 2D schematic PD domain discretization and the interactions between node $\mathbf{x}_{(i)}$ and its family members.

As shown in Fig. 4.2, the internal force vector at PD node $\mathbf{x}_{(i)}$ is achieved by including the effect of its interactions with other PD nodes (family members), $\mathbf{x}_{(j)}$, in the interaction domain. The interaction domain of node $\mathbf{x}_{(i)}$ depends on its family size $\delta_{(i)}$ and can be of arbitrary shape for PDLMS. The family size $\delta_{(i)}$ of node $\mathbf{x}_{(i)}$ is specified as $\delta_{(i)} = m\Delta_{(i)}$, with the m -ratio being of constant and the characteristic length $\Delta_{(i)}$ depends on volume $V_{(i)}$ occupied by PD node $\mathbf{x}_{(i)}$. $\Delta_{(i)}$ is defined as [60]

$$\Delta_{(i)} = \sqrt[3]{V_{(i)}} \quad (4.18)$$

Thus, each PD node has its own family size and family members. For non-uniform discretization, the rule to determine family members of node $\mathbf{x}_{(i)}$ is suggested in [60] as

$$H_{\mathbf{x}_{(i)}} = \left\{ \mathbf{x}_{(j)} \in H_{\mathbf{x}_{(i)}} : |\mathbf{x}_{(j)} - \mathbf{x}_{(i)}| \leq \delta_{(i)} \cup |\mathbf{x}_{(j)} - \mathbf{x}_{(i)}| \leq \delta_{(j)} \right\}, \quad (4.19)$$

which ensures that the bond between nodes $\mathbf{x}_{(i)}$ and $\mathbf{x}_{(j)}$ is a paired interaction for either interaction domain. For node $\mathbf{x}_{(i)}$, there are $N_{(i)}$ family members within its interaction

domain and the displacement set of these nodes is

$$\mathbf{u}^{(i)} = \left[u_{1(i)} \ u_{2(i)} \ u_{3(i)} \ u_{1(2)} \ u_{2(2)} \ u_{3(2)} \ \cdots \ u_{1(m)} \ u_{2(m)} \ u_{3(m)} \ \cdots \ u_{1(N(i))} \ u_{2(N(i))} \ u_{3(N(i))} \right]^T, \quad (4.20)$$

here, the subscript (m) represents the m -th family member node $\mathbf{x}_{(m)}$ within the interaction domain of node $\mathbf{x}_{(i)}$ and its first member is itself $\mathbf{x}_{(i)}$. From Eq. (3.3), we obtain the discrete form of strain vector at node $\mathbf{x}_{(i)}$ as

$$\{\varepsilon\}_{(i)}^{pd} = [\varepsilon_x \ \varepsilon_y \ \varepsilon_z \ \gamma_{xy} \ \gamma_{yz} \ \gamma_{zx}]^T = \mathbf{C}^{(i)} \mathbf{u}^{(i)}, \quad (4.21)$$

in which the matrix $\mathbf{C}$ is defined as below,

$$\mathbf{C}^{(i)} = \begin{bmatrix} -\sum_{m=2}^{N(i)} C_{1(im)} & 0 & 0 & C_{1(i2)} & 0 & 0 & \cdots \\ 0 & -\sum_{m=2}^{N(i)} C_{2(im)} & 0 & 0 & C_{2(i2)} & 0 & \cdots \\ 0 & 0 & -\sum_{m=2}^{N(i)} C_{3(im)} & 0 & 0 & C_{3(i2)} & \cdots \\ -\sum_{m=2}^{N(i)} C_{2(im)} & -\sum_{m=2}^{N(i)} C_{1(im)} & 0 & C_{2(i2)} & C_{1(i2)} & 0 & \cdots \\ 0 & -\sum_{m=2}^{N(i)} C_{3(im)} & -\sum_{m=2}^{N(i)} C_{2(im)} & 0 & C_{3(i2)} & C_{2(i2)} & \cdots \\ -\sum_{m=2}^{N(i)} C_{3(im)} & 0 & -\sum_{m=2}^{N(i)} C_{1(im)} & C_{3(i2)} & 0 & C_{1(i2)} & \cdots \\ \cdots & C_{1(im)} & 0 & 0 & \cdots & C_{1(iN(i))} & 0 & 0 \\ \cdots & 0 & C_{2(im)} & 0 & \cdots & 0 & C_{2(iN(i))} & 0 \\ \cdots & 0 & 0 & C_{3(im)} & \cdots & 0 & 0 & C_{3(iN(i))} \\ \cdots & C_{2(im)} & C_{1(im)} & 0 & \cdots & C_{2(iN(i))} & C_{1(iN(i))} & 0 \\ \cdots & 0 & C_{3(im)} & C_{2(im)} & \cdots & 0 & C_{3(iN(i))} & C_{2(iN(i))} \\ \cdots & C_{3(im)} & 0 & C_{1(im)} & \cdots & C_{3(iN(i))} & 0 & C_{1(iN(i))} \end{bmatrix}, \quad (4.22)$$

where the subscript (im) represents the bond between node $\mathbf{x}_{(i)}$ and its m -th family member,

and $C_{k(im)}(k = 1, 2, 3)$ are defined as

$$C_{k(im)} = \mu_{(im)}\omega_{(im)}g_{k(im)}V_{(m)}, \quad (4.23)$$

here $\mu_{(im)}$ and $\omega_{(im)}$ are the bond status parameter and the influence function, respectively, and $g_{k(im)}$ is defined in Eq. (4.5). From Eq. (4.21), the discrete form of stress vector at node $\mathbf{x}_{(i)}$ is

$$\{\sigma\}_{(i)}^{pd} = \mathbf{D}\mathbf{C}^{(i)}\mathbf{u}^{(i)}, \quad (4.24)$$

here, $\mathbf{D}$ is material stiffness matrix of elasticity material and is defined as

$$\mathbf{D} = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} (1-\nu) & \nu & \nu & 0 & 0 & 0 \\ \nu & (1-\nu) & \nu & 0 & 0 & 0 \\ \nu & \nu & (1-\nu) & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1-2\nu}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1-2\nu}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1-2\nu}{2} \end{bmatrix}, \quad (4.25)$$

Also, from Eq. (3.2), we obtain the discrete form of the internal force vector at node $\mathbf{x}_{(i)}$ as

$$\mathbf{L}_{(i)}^{pd} = \mathbf{H}^{(i)}\mathbf{u}^{(i)}, \quad (4.26)$$

$$\mathbf{H}^{(i)} = \begin{bmatrix} -\sum_{m=2}^{N(i)} \mu_{(im)}\omega_{(im)}\mathbf{G}_{(im)}V_{(m)} & \mu_{(i2)}\omega_{(i2)}\mathbf{G}_{(i2)}V_{(2)} & \cdots & \mu_{(iN(i))}\omega_{(iN(i))}\mathbf{G}_{(iN(i))}V_{(N(i))} \end{bmatrix}. \quad (4.27)$$

The bond status parameter $\mu_{(im)}$ in Eq. (4.23) and Eq. (4.27) is equal to 1 for unbroken bonds or equal to 0 for broken bonds. The bond status can be determined by the failure criteria which are flexible and some of the published failure criteria can be found in [20, 30, 31, 60].

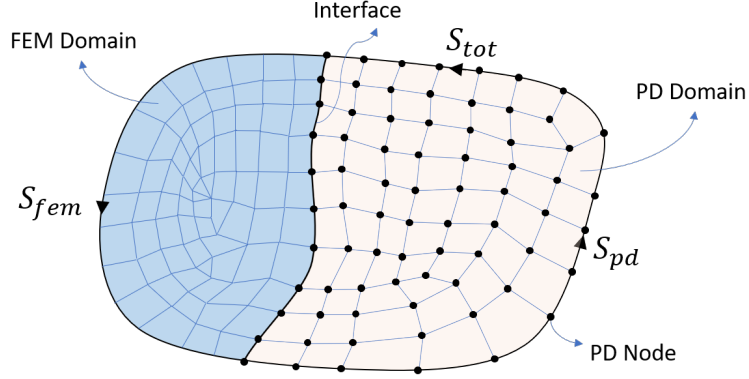


Fig. 4.3: 2D schematic of the coupling PD with FEM.

4.3.2 Discretization of PDLsm-FEM domain

To couple PDLsm with FEM, the whole problem domain is divided into a FEM domain and a PD domain, and both domains are discretized into 3D elements, as shown in Fig. 4.3. For clarification, the elements in the PD domain are called PD elements and elements in the FEM domain are still called finite elements. Note that PD nodes on the PD-FEM interface are also nodes of the finite element, and the volumes of these PD nodes are calculated only from the PD elements. As describe in Section 5.2, PDLsm works for arbitrary interaction domain shape, and does not require surface correction. Thus, the FEM nodes can be either counted or not counted as family members of these PD nodes near the PD-FEM interface. In this work, the interaction domains of PD nodes are only determined from the PD domain but do not count FEM nodes as PD family members. That means, for these PD nodes near PD domain boundary, the interaction domain is truncated by PD domain boundary.

Consider a whole 3D discrete domain that contains N_g nodes, of which N^{pd} are PD nodes. For the i -th PD node $\mathbf{x}_{(i)}$, its displacement vector is $\mathbf{u}_{(i)} = [u_{1(i)} \quad u_{2(i)} \quad u_{3(i)}]^T$. The displacement set of all nodes (global displacement vector) is expressed as

$$\mathbf{u}_g = \begin{bmatrix} \mathbf{u}_u \\ \mathbf{u}_p \end{bmatrix}, \quad (4.28)$$

here $\mathbf{u}_u$ is the set of all unknown displacement components and $\mathbf{u}_p$ is the set of prescribed

displacement components. The displacement vector of the PD node $\mathbf{x}_{(i)}$ can be expressed as

$$\mathbf{u}_{(i)} = \mathbf{M}_{(i)} \mathbf{u}_g, \quad (4.29)$$

here, $\mathbf{M}_{(i)}$ is the mapping matrix from $\mathbf{u}_g$ to $\mathbf{u}_{(i)}$, with size $3 \times 3N_g$, and subscript (i) represents the PD node $\mathbf{x}_{(i)}$.

The displacement set of the family members of the PD node $\mathbf{x}_{(i)}$, $\mathbf{u}^{(i)}$, can be expressed by global displacement vector as

$$\mathbf{u}^{(i)} = \mathbf{M}^{(i)} \mathbf{u}_g, \quad (4.30)$$

here, superscript (i) represents the family members of the PD node $\mathbf{x}_{(i)}$, and $\mathbf{M}^{(i)}$ is the mapping matrix from $\mathbf{u}_g$ to $\mathbf{u}^{(i)}$, with size $3N_{(i)} \times 3N_g$ and it can be specified as follows: if the k -th component of $\mathbf{u}^{(i)}$ and the j -th component of $\mathbf{u}_g$ are the same, $M_{kj}^{(i)} = 1$, otherwise $M_{kj}^{(i)} = 0$. Thus, there is one and only one component equal to 1 in each row of $\mathbf{M}^{(i)}$. Also, $\mathbf{M}_{(i)}$ is determined by a similar way.

The mapping matrices are used for the matrix assembling procedure. For example, if $\mathbf{B} = \mathbf{M}_{(p)}^T \mathbf{A} \mathbf{M}^{(i)}$, the assembling procedure to obtain matrix $\mathbf{B}$ from $\mathbf{A}$ is as follows: we first initialize all components of $\mathbf{B}$ as zero, then go through all components of $\mathbf{M}_{(p)}$ and $\mathbf{M}^{(i)}$, if $M_{kj}^{(i)} = 1$ and $M_{mn(p)} = 1$, then $B_{nj} = A_{mk}$ ($n, j \in 1, 2, 3, \dots, 3N_g$, $m \in 1, 2$, and $k \in 1, 2, 3, \dots, 3N_{(i)}$).

Substituting Eq. (4.30) into Eq. (4.24) and Eq. (4.26), leads to the non-local stress vector and internal force vector by global displacement vector as below,

$$\{\sigma\}_{(i)}^{pd} = \mathbf{D} \mathbf{C}^{(i)} \mathbf{M}^{(i)} \mathbf{u}_g, \quad (4.31)$$

$$\mathbf{L}_{(i)}^{pd} = \mathbf{H}^{(i)} \mathbf{M}^{(i)} \mathbf{u}_g. \quad (4.32)$$

4.3.3 Governing Equations of PDLISM-FEM

For a coupled model, both the PD domain and the FEM domain exist. Applying the WRM on the equilibrium equation and the boundary condition over the whole problem domain leads to

$$\int_{V_{tot}} \delta \mathbf{u}^T (\mathbf{L} + \mathbf{b} - \rho \ddot{\mathbf{u}}) dV - \int_{S_{tot}} \delta \mathbf{u}^T (\boldsymbol{\sigma} \mathbf{n} - \mathbf{T}) dS = 0, \quad (4.33)$$

where $\mathbf{T}$ is the external traction force on the surface boundary, $\mathbf{n}$ is the unit normal vector of the boundary, V_{tot} and S_{tot} are the volume and surface of the whole domain respectively, and $\delta(\bullet)$ represents a virtual value. The virtual work of inner volume forces and of the boundary surface forces are split into PD and FEM contributions as:

$$\int_{V_{tot}} \delta \mathbf{u}^T (\rho \ddot{\mathbf{u}} - \mathbf{L}) dV = \int_{V_{pd}} \delta \mathbf{u}^T (\rho \ddot{\mathbf{u}} - \mathbf{L}^{pd}) dV + \int_{V_{fem}} \delta \mathbf{u}^T (\rho \ddot{\mathbf{u}} - \mathbf{L}^{fem}) dV, \quad (4.34)$$

and

$$\int_{S_{tot}} \delta \mathbf{u}^T \boldsymbol{\sigma} \mathbf{n} dS = \int_{S_{pd}} \delta \mathbf{u}^T \boldsymbol{\sigma}^{pd} \mathbf{n} dS + \int_{S_{fem}} \delta \mathbf{u}^T \boldsymbol{\sigma}^{fem} \mathbf{n} dS, \quad (4.35)$$

where V_{fem} and V_{pd} represent the volume of the FEM domain and PD domain respectively, and S_{pd} and S_{fem} represent the boundary of the PD domain and FEM domain respectively. For the PD domain V_{pd} , the internal force vector, $\mathbf{L}^{pd}$, takes on the integral form of Eq. (4.32) which is based on meshless method. While for the FEM domain V_{fem} , the Gauss integration and element-based method are used, and the internal force vector $\mathbf{L}^{fem}$, takes on the differential form of

$$\mathbf{L}^{fem} = \nabla \cdot \boldsymbol{\sigma}^{fem}. \quad (4.36)$$

For the surface of the PD domain, S_{pd} , the stress in the item of $\delta \mathbf{u}^T \boldsymbol{\sigma}^{pd} \mathbf{n}$ is derived based on the integral form of Eq. (4.31). For the surface of the FEM domain, S_{fem} , the item of

$\delta \mathbf{u}^T \boldsymbol{\sigma}^{fem} \mathbf{n}$ is canceled by applying Gauss theorem as

$$\begin{aligned} \int_{V_{fem}} \delta \mathbf{u}^T \mathbf{L}^{fem} dV &= \int_{V_{fem}} \{ \nabla \cdot (\delta \mathbf{u}^T \boldsymbol{\sigma}^{fem}) - \nabla \delta \mathbf{u} : \boldsymbol{\sigma}^{fem} \} dV \\ &= \int_{S_{fem}} \delta \mathbf{u}^T \boldsymbol{\sigma}^{fem} \mathbf{n} dS - \int_{V_{fem}} \nabla \delta \mathbf{u} : \boldsymbol{\sigma}^{fem} dV. \end{aligned} \quad (4.37)$$

Therefore, Eq. (4.33) becomes to

$$\begin{aligned} \int_{V_{fem}} [\delta \mathbf{u}^T \rho \ddot{\mathbf{u}} + \delta(\{\varepsilon^{fem}\}^T) \{\sigma^{fem}\}] dV &+ \int_{V_{pd}} \delta \mathbf{u}^T (\rho \ddot{\mathbf{u}} - \mathbf{L}^{pd}) dV + \int_{S_{pd}} \delta \mathbf{u}^T \boldsymbol{\sigma}^{pd} \mathbf{n} dS = \\ \int_{S_{tot}} \delta \mathbf{u}^T \mathbf{T} dS &+ \int_{V_{fem}} \delta \mathbf{u}^T \mathbf{b} dV + \int_{V_{pd}} \delta \mathbf{u}^T \mathbf{b} dV. \end{aligned} \quad (4.38)$$

The virtual internal work by the internal force of the PD domain, δU_B^{pd} , is expressed as

$$\delta U_B^{pd} = - \int_{V_{pd}} \delta \mathbf{u}^T \mathbf{L}^{pd} dV = - \sum_{i=1}^{N^{pd}} \delta \mathbf{u}_{(i)}^T \mathbf{L}_{(i)}^{pd} V_{(i)} \quad (4.39)$$

Substituting Eq. (4.29) and Eq. (4.32) into Eq. (4.39) leads to

$$\delta U_B^{pd} = \delta \mathbf{u}_g^T \mathbf{K}_b^{pd} \mathbf{u}_g, \quad (4.40)$$

where $\mathbf{K}_b^{pd} = - \sum_{i=1}^{N^{pd}} \mathbf{M}_{(i)}^T \mathbf{H}_{(i)} \mathbf{M}_{(i)} V_{(i)}$. The boundary of the PD domain S_{pd} is discretized as 4-noded or 3-noded boundary elements, named as PD boundary element (PDBE), by the discretization of the PD domain, as shown in Fig. 4.4. The virtual internal work associated with PD domain boundary, δU_S^{pd} , is evaluated as

$$\delta U_S^{pd} = \int_{S_{pd}} \delta \mathbf{u}^T \boldsymbol{\sigma}^{pd} \mathbf{n} dS = \sum_{e=1}^{N_S^{pd}} \left(\delta U_{S_e}^{pd} \right), \quad (4.41)$$

in which N_S^{pd} is the number of PDBEs, and $\delta U_{S_e}^{pd}$ is the virtual internal work associated with

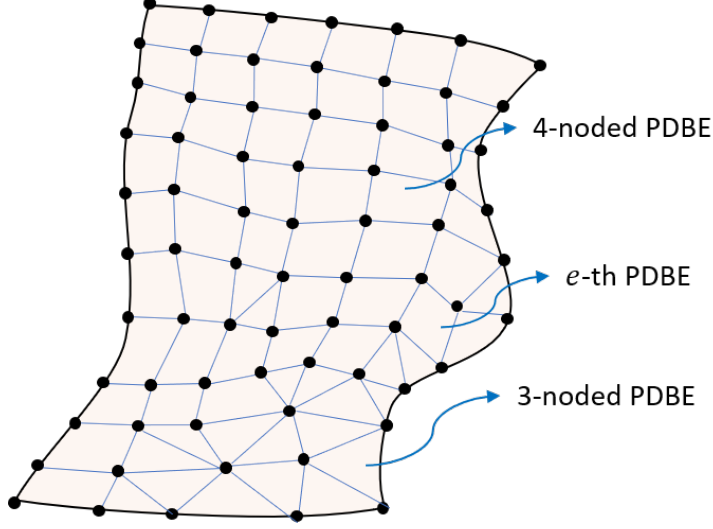


Fig. 4.4: PD boundary element.

the e -th PDBE and is defined as

$$\delta U_{S_e}^{pd} = \int_{S_e} \delta \mathbf{u}^T \boldsymbol{\sigma}^{pd} \mathbf{n} dS \quad (4.42)$$

The stress on the S_e is approximately expressed as

$$\boldsymbol{\sigma}^{pd} = \sum_{i=1} \mathcal{N}_i \boldsymbol{\sigma}_{(e_i)}^{pd}, \quad (4.43)$$

the displacement of S_e is approximately expressed as

$$\mathbf{u}^{pd} = \sum_{i=1} \mathcal{N}_i \mathbf{u}_{(e_i)}^{pd} = \mathcal{N} \mathbf{u}_e, \quad (4.44)$$

and the coordinate of S_e is expressed as

$$\mathbf{x} = \sum_{i=1} \mathcal{N}_i \mathbf{x}_{(e_i)}, \quad (4.45)$$

in which e_i represents the i -th node of the e -th PDBE, and $\mathcal{N}_i$ represent the shape functions,

which are defined as follows. For 4-noded PDBE,

$$\begin{cases} \mathcal{N}_1 = 0.25(1-p)(1-q) \\ \mathcal{N}_2 = 0.25(1+p)(1-q) \\ \mathcal{N}_3 = 0.25(1+p)(1+q) \\ \mathcal{N}_4 = 0.25(1-p)(1+q) \end{cases} \quad (4.46)$$

where $p, q \in [-1, 1]$, are local coordinates. The matrix $\mathcal{N}$ is defined as

$$\mathcal{N} = [\mathcal{N}_1 \mathbf{I} \quad \mathcal{N}_2 \mathbf{I} \quad \mathcal{N}_3 \mathbf{I} \quad \mathcal{N}_4 \mathbf{I}] \quad (4.47)$$

in which $\mathbf{I}$ is a identical matrix with size 3×3 . $\mathbf{u}_e$ is the nodal displacement set of the e -th PDBE and is defined as

$$\mathbf{u}_e = [u_{1(e_1)} \quad u_{2(e_1)} \quad u_{3(e_1)} \cdots u_{1(e_4)} \quad u_{2(e_4)} \quad u_{3(e_4)}]^T \quad (4.48)$$

$\mathbf{u}_e$ is also expressed by the global displacement vector as

$$\mathbf{u}_e = \mathbf{M}_e \mathbf{u}_g \quad (4.49)$$

where $\mathbf{M}_e$ is the mapping matrix from $\mathbf{u}_g$ to $\mathbf{u}_e$ and can be obtained as described previously. The traction applied on the infinitesimal area of the boundary of 4-noded PDBE can be expressed by the local coordinates as

$$\boldsymbol{\sigma}^{pd} \mathbf{n} dS = \boldsymbol{\sigma}^{pd} \left(\frac{\partial \mathbf{x}}{\partial p} \times \frac{\partial \mathbf{x}}{\partial q} \right) dp dq = \bar{\mathbf{N}} \{ \sigma \}^{pd} dp dq \quad (4.50)$$

in which $\overline{\mathbf{N}}$ is defined as

$$\overline{\mathbf{N}} = \begin{bmatrix} \overline{N}_1 & 0 & 0 & \overline{N}_2 & 0 & \overline{N}_3 \\ 0 & \overline{N}_2 & 0 & \overline{N}_1 & \overline{N}_3 & 0 \\ 0 & 0 & \overline{N}_3 & 0 & \overline{N}_2 & \overline{N}_1 \end{bmatrix}. \quad (4.51)$$

here $\overline{N}_1$, $\overline{N}_2$ and $\overline{N}_3$ are defined as

$$\begin{cases} \overline{N}_1 = \frac{\partial x_2}{\partial p} \frac{\partial x_3}{\partial q} - \frac{\partial x_3}{\partial p} \frac{\partial x_2}{\partial q} \\ \overline{N}_2 = \frac{\partial x_3}{\partial p} \frac{\partial x_1}{\partial q} - \frac{\partial x_1}{\partial p} \frac{\partial x_3}{\partial q} \\ \overline{N}_3 = \frac{\partial x_1}{\partial p} \frac{\partial x_2}{\partial q} - \frac{\partial x_2}{\partial p} \frac{\partial x_1}{\partial q} \end{cases} \quad (4.52)$$

For 4-noded PDBE, $\delta U_{S_e}^{pd}$ can be evaluated by Gauss integration as below,

$$\begin{aligned} \delta U_{S_e}^{pd} &= \int_{-1}^1 \int_{-1}^1 \delta \mathbf{u}^T \overline{\mathbf{N}} \{\sigma\}^{pd} dp dq \\ &= \int_{-1}^1 \int_{-1}^1 \delta \mathbf{u}_e^T \mathcal{N}^T \overline{\mathbf{N}} \sum_{i=1}^4 \mathcal{N}_{e_i} \{\sigma\}_{(e_i)}^{pd} dp dq \\ &= \sum_p \sum_q \sum_{i=1}^4 \delta \mathbf{u}_e^T \mathcal{N}^T \overline{\mathbf{N}} \mathcal{N}_{e_i} \{\sigma\}_{(e_i)}^{pd} w_p w_q \\ &= \sum_p \sum_q \sum_{i=1}^4 \delta \mathbf{u}_g^T \mathbf{M}_e^T \mathcal{N}^T \overline{\mathbf{N}} \mathcal{N}_{e_i} \mathbf{D} \mathbf{C}^{(e_i)} \mathbf{M}^{(e_i)} \mathbf{u}_g w_p w_q \\ &= \delta \mathbf{u}_g^T \left(\sum_p \sum_q \sum_{i=1}^4 \mathbf{M}_e^T w_p w_q \mathcal{N}^T \overline{\mathbf{N}} \mathcal{N}_i \mathbf{D} \mathbf{C}^{(e_i)} \mathbf{M}^{(e_i)} \right) \mathbf{u}_g \\ &= \delta \mathbf{u}_g^T \mathbf{K}_{S_e}^{pd} \mathbf{u}_g \end{aligned} \quad (4.53)$$

where w_p and w_q are the weights of Gauss integration, and $\mathbf{K}_{S_e}^{pd}$ is defined as

$$\mathbf{K}_{S_e}^{pd} = \sum_p \sum_q \sum_{i=1}^4 \mathbf{M}_e^T w_p w_q \mathcal{N}^T \overline{\mathbf{N}} \mathcal{N}_i \mathbf{D} \mathbf{C}^{(e_i)} \mathbf{M}^{(e_i)} \quad (4.54)$$

For 3-noded PDBE, a similar way can be employed to evaluate $\mathbf{K}_{S_e}^{pd}$ as

$$\mathbf{K}_{S_e}^{pd} = \mathbf{M}_e^T \sum_{i=1}^3 \left[\left(\int_{S_e} \mathcal{N}^T \mathcal{N}_i dS \right) \bar{\mathbf{N}} \mathbf{DC}^{(e_i)} \mathbf{M}^{(e_i)} \right] \quad (4.55)$$

in which $\mathcal{N}$ is defined as

$$\mathcal{N} = [\mathcal{N}_1 \mathbf{I} \quad \mathcal{N}_2 \mathbf{I} \quad \mathcal{N}_3 \mathbf{I}] \quad (4.56)$$

where $\mathbf{I}$ is an identical matrix with size 3×3 , $\mathcal{N}_i$ is the area coordinates, and the matrix $\bar{\mathbf{N}}$ is defined as Eq. (4.51), in which $\bar{N}_i$ ($i = 1, 2, 3$), are replaced by the unit normal vector components of the PDBE S_e . The integration of $\int_{S_e} \mathcal{N}^T \mathcal{N}_i dS$ can be evaluated by the following exact integration expression as

$$\int_{S_e} \mathcal{N}_1^a \mathcal{N}_2^b \mathcal{N}_3^c dS = \frac{a! b! c!}{(a + b + c + 2)!} 2A_{S_e} \quad (4.57)$$

here A_{S_e} is the area of the triangle.

With the representation of $\mathbf{K}_{S_e}^{pd}$, the virtual internal work by the internal force of the PD domain is evaluated as

$$\delta U_S^{pd} = \delta \mathbf{u}_g^T \mathbf{K}_s^{pd} \mathbf{u}_g, \quad (4.58)$$

where $\mathbf{K}_s^{pd}$ is defined as

$$\mathbf{K}_s^{pd} = \sum_{e=1}^{N_S^{pd}} \mathbf{K}_{S_e}^{pd} \quad (4.59)$$

in which N_S^{pd} is number of PDBEs. The virtual work by the inertia force in the PD domain, δU_I^{pd} , can be evaluated as

$$\delta U_I^{pd} = \int_{V_{pd}} \delta \mathbf{u}^T \rho \ddot{\mathbf{u}} dV = \delta \mathbf{u}_g^T \mathbf{M}^{pd} \ddot{\mathbf{u}}_g, \quad (4.60)$$

where $\mathbf{M}^{pd} = \sum_{i=1}^{N^{pd}} \rho \mathbf{M}_{(i)}^T \mathbf{M}_{(i)} V_{(i)}$. Similarly, the virtual work by the external body force $\mathbf{b}$ in

the PD domain, δW_B^{pd} , can be evaluated as

$$\delta W_B^{pd} = \int_{V_{pd}} \delta \mathbf{u}^T \mathbf{b} dV = \delta \mathbf{u}_g^T \mathbf{F}_b^{pd}, \quad (4.61)$$

where $\mathbf{F}_b^{pd} = \sum_{i=1}^{N^{pd}} \mathbf{M}_{(i)}^T \mathbf{b}_{(i)} V_{(i)}$.

The virtual strain energy of the FEM domain, δU^{fem} , can be evaluated by the FEM as

$$\delta U^{fem} = \int_{V_{fem}} \delta(\{\varepsilon^{fem}\}^T) \{\sigma^{fem}\} dV = \delta \mathbf{u}_g^T \mathbf{K}^{fem} \mathbf{u}_g. \quad (4.62)$$

Similarly, the virtual work by the inertial force in the FEM domain, δU_I^{fem} , the virtual work by the external body force in the FEM domain, δW_B^{fem} , and the virtual work by the external traction force of the whole domain, δW_S , can be evaluated by FEM as follows:

$$\delta U_I^{fem} = \int_{V_{fem}} \delta \mathbf{u}^T \rho \ddot{\mathbf{u}} dV = \delta \mathbf{u}_g^T \mathbf{M}^{fem} \ddot{\mathbf{u}}_g, \quad (4.63)$$

$$\delta W_B^{fem} = \int_{V_{fem}} \delta \mathbf{u}^T \mathbf{b} dV = \delta \mathbf{u}_g^T \mathbf{F}_b^{fem}, \quad (4.64)$$

$$\delta W_S = \int_{S_{tot}} \delta \mathbf{u}^T \mathbf{T} dS = \delta \mathbf{u}_g^T \mathbf{F}_s. \quad (4.65)$$

As the FEM is a mature technology, the details to obtain the $\mathbf{K}^{fem}$, $\mathbf{M}^{fem}$, $\mathbf{F}_b^{fem}$ and $\mathbf{F}_s$ are not shown here for conciseness. Substituting Eqs. (4.40), (4.58), (4.60), (4.61), (4.62), (4.63), (4.64) and (4.65) into Eq. (4.38) leads to the governing equation of this coupling model,

$$\mathbf{M} \ddot{\mathbf{u}}_g + \mathbf{K} \mathbf{u}_g = \mathbf{F}, \quad (4.66)$$

where the global equivalent nodal mass $\mathbf{M}$ is defined as

$$\mathbf{M} = \mathbf{M}^{pd} + \mathbf{M}^{fem}, \quad (4.67)$$

the global stiffness matrix $\mathbf{K}$ is defined as

$$\mathbf{K} = \mathbf{K}_b^{pd} + \mathbf{K}_s^{pd} + \mathbf{K}^{fem} \quad (4.68)$$

and the global equivalent nodal force $\mathbf{F}$ is defined as

$$\mathbf{F} = \mathbf{F}_b^{pd} + \mathbf{F}_b^{fem} + \mathbf{F}_s, \quad (4.69)$$

here, $\mathbf{M}$, $\mathbf{K}$ and $\mathbf{F}$ can be obtained by the assembling procedure as described previously. Note that $\mathbf{M}^{pd}$ is a lumped diagonal mass matrix, while $\mathbf{M}^{fem}$ can be either lumped diagonal or consistent mass matrix. For explicit dynamic solutions, using lumped diagonal mass matrix $\mathbf{M}^{fem}$ may be more efficient since it is easier to solve for $\mathbf{M}^{-1}$. When $V_{pd} = 0$, Eq. (4.66) represents a pure FEM model and when $V_{fem} = 0$, it represents a pure PD model. Thus, the formulation converts easily between PDLSP, FEM, and PDLSP-FEM. Besides, Eq. (4.66) can be decomposed as

$$\begin{bmatrix} \mathbf{M}_{uu} & \mathbf{M}_{up} \\ \mathbf{M}_{pu} & \mathbf{M}_{pp} \end{bmatrix} \begin{bmatrix} \ddot{\mathbf{u}}_u \\ \ddot{\mathbf{u}}_p \end{bmatrix} + \begin{bmatrix} \mathbf{K}_{uu} & \mathbf{K}_{up} \\ \mathbf{K}_{pu} & \mathbf{K}_{pp} \end{bmatrix} \begin{bmatrix} \mathbf{u}_u \\ \mathbf{u}_p \end{bmatrix} = \begin{bmatrix} \mathbf{F}_u \\ \mathbf{F}_p \end{bmatrix}. \quad (4.70)$$

As $\mathbf{u}_p$ is the prescribed displacement constraint, Eq. (4.70) reduces to

$$\mathbf{M}_{uu}\ddot{\mathbf{u}}_u + \mathbf{K}_{uu}\mathbf{u}_u = \mathbf{F}_u - \mathbf{M}_{up}\ddot{\mathbf{u}}_p - \mathbf{K}_{up}\mathbf{u}_p \quad (4.71)$$

For static problem, Eq. (4.70) reduces to

$$\mathbf{K}_{uu}\mathbf{u}_u = \mathbf{F}_u - \mathbf{K}_{up}\mathbf{u}_p \quad (4.72)$$

4.4 Assembling stiffness matrix

In this work, the large linear systems of equations are solved by the Parallel Direct Sparse Solver (PDSS) of Intel Math Kernel Library (MKL). PDSS is for cluster interface and is based on message passing interface (MPI) technique. The large sparse matrix is stored in a compressed sparse row (CSR) format which is one of inputs of PDSS. In this section, we present how to assemble the global stiffness matrix in a CSR format by MPI technique. Note that zero-based indexing is employed for arrays in this coding and the program is written in C++ environment.

4.4.1 Initialize data model

As described in Section 4.3, the problem domain is divided into a PD domain and a FEM domain, both of which can be discretized as elements by commercial finite element codes, such as ANSYS. Then the nodes' coordinates, elements' connectivity, essential and natural boundary conditions are read by the program from the input file. The volume of each PD node is calculated from the volume of PD elements. The family members of the PD node $\mathbf{x}_{(i)}$ are stored in a container of `std::vector`, in which the first member is itself $\mathbf{x}_{(i)}$. Each node has 3 degrees of freedom (DOF) and the total number of DOFs is $N_t = 3N_g$, of which N_r are unknown DOFs, and N_p are constrained DOFs. Because constrained DOFs need not be solved, the problem is reduced to Eq. (4.72). To build the Eq. (4.72), a link between the DOFs of each node and the index of $\mathbf{u}_u$ is created as `idx[i][j]`, in which i represents the i -th node, and $j = 0, 1, 2$ represents the DOF. If the DOF is unknown, `idx[i][j]` represents position of the DOF in vector $\mathbf{u}_u$, otherwise `idx[i][j] = -1`. Determination of the 2D array `idx[][]` is shown in Algorithm 1.

Note that `idx[][]` is an alternative to the mapping matrices in Eqs. (4.29), (4.30) and (4.49). For example, in Eq. (4.29),

$$\mathbf{u}_{(i)} = [u_{1(i)} \quad u_{2(i)} \quad u_{3(i)}]^T = \mathbf{M}_{(i)} \mathbf{u}_g, \quad (4.73)$$

Algorithm 1: Determine the array $\text{idx}[\][\]$.

```

1 count  $\leftarrow$  0;
2 for  $i \leftarrow 0$  to  $< N_g$  do
3   for  $j \leftarrow 0$  to 3 do
4     if  $j$ -th DOF of  $i$ -th node is constrained then
5        $\text{idx}[i][j] \leftarrow -1$ ;
6     else
7        $\text{idx}[i][j] \leftarrow \text{count}$ ;
8        $\text{count}++$ ;

```

if DOF $u_{j(i)}$, ($j = 1, 2, 3$) is unknown, the j -th row and $\text{idx}[i][j-1]$ -th column coefficient of $\mathbf{M}_{(i)}$ is $\mathbf{M}_{(i)j, \text{idx}[i][j-1]} = 1$ and other coefficients of $\mathbf{M}_{(i)}$ are zero. Thus, during assembling the stiffness matrix, there is no need to build the mapping matrices.

4.4.2 Create interactive list and determine the non-zero coefficients' indices

It is impractical to store the full stiffness matrix. For example, a 3D domain with 10^5 nodes requires 670.5 gigabytes to store the full stiffness matrix using double precision. Thus, the stiffness matrix is stored in a CSR format, which only stores the non-zero coefficients and their column and row indices information by 3 arrays, $\mathbf{K}[\]$, $\mathbf{ja}[\]$, and $\mathbf{ia}[\]$, respectively. The array $\mathbf{K}[\]$ contains the non-zero coefficients of the matrix corresponding to the indices in $\mathbf{ja}[\]$, which stores the column indices of each non-zero coefficient. The array $\mathbf{K}[\]$ and $\mathbf{ja}[\]$ have the same size. The array $\mathbf{ia}[\]$ has a size of $N_r + 1$, in which N_r is the total number of rows of the matrix. $\mathbf{ia}[i]$ ($0 \leq i < N_r$) points to the first column index of row i in the $\mathbf{ja}[\]$. That is, $\mathbf{ia}[i]$ gives the index of the coefficient in array $\mathbf{K}[\]$ that is the first non-zero coefficient from row i of the matrix. $(\mathbf{ia}[i + 1] - \mathbf{ia}[i])$ gives the number of non-zero coefficients of the row i of the matrix, and the last element $\mathbf{ia}[N_r]$ is taken to be equal to the number of non-zero coefficient in the matrix. To assemble the stiffness matrix, we need to determine the indices of rows and columns of all the non-zero coefficients and store them in the arrays $\mathbf{ia}[\]$ and $\mathbf{ja}[\]$. In this subsection, we present how to obtain the

Algorithm 2: Create interaction list.

```
/* PD node interacting with its family members. */
1 for  $n \leftarrow 0$  to  $< N^{pd}$  do
    /* For each PD node. */
    2 std::vector fami  $\leftarrow$  family member of  $n$ -th PD node;
    3  $i \leftarrow \text{fami.at}(0)$  ; // The 1st family member is itself.
    4 iN[i].assign(fami.begin(), fami.end());
    /* PD node of the PDBE interacting with the nodes of the same PDBE and their
       family members. */
    5 for  $e \leftarrow 0$  to  $< N_S^{pd}$  do
        /* For each PDBE. */
        6 for  $n_1 \leftarrow$  node of the  $e$ -th PDBE do
            7 std::vector fami  $\leftarrow$  the family members of the node  $n_1$ ;
            8 for  $n_2 \leftarrow$  node of the  $e$ -th PDBE do
                9 if  $n_1 \neq n_2$  then
                    10 iN[n2].insert(iN[n2].end(), fami.begin(), fami.end());
            /* Node of the FE interacting with the node of the same FE. */
    11 for  $e \leftarrow 0$  to  $< N^{fe}$  do
        /* For each FE. */
        12 for  $n_1 \leftarrow$  node of the  $e$ -th FE do
            13 for  $n_2 \leftarrow$  node of the  $e$ -th FE do
                14 iN[n1].push_back( $n_2$ );
        /* Delete the duplicated nodes and sort the interaction list in ascending order.
           */
    15 unordered_set<int> inteSet ; // declare a unordered_set
    16 for  $n \leftarrow 0$  to  $< N_g$  do
        /* For each node. */
        17 for  $nid \leftarrow$  node in list iN[n] do
            18 inteSet.insert(nid) ; // store the unique nodes
        19 iN[n].assign(inteSet.begin(), inteSet.end());
        20 sort(iN[n].begin(), iN[n].end()) ; // sort in a ascending order
        21 inteSet.clear();
```

array `ia[]` and `ja[]`.

Create interaction list The row `idx[i][j]` of the stiffness matrix is corresponding to the j -th DOF of i -th node. The non-zero coefficients of row `idx[i][j]` are determined by other nodes which are interacting with the i -th node. Thus, the interaction list `iN[i]` is created to store the nodes which are interacting with the i -th node. `iN[i]` is a standard sequence container `std::vector`, whose size can be changed dynamically. There are 3 interaction types: (1) PD node in the PD domain interacting with its family members; (2) PD node of PDBE interacting with the nodes of the same PDBE and their family members; and (3) FE's nodes interacting with the nodes of the same FE. Note that interaction list `iN[i]` of node i contains itself. The pseudo-code to obtain the interaction list is shown in Algorithm 2.

Algorithm 3: Obtain arrays `ia[]` and `ja[]`

```

1 Initialize ia[] = 0 ; // size of ia is  $N_r + 1$ .
2 std::vector<int> vja ; // declare a vector for ja[].
3 for  $n_1 \leftarrow 0$  to  $< N_g$  do
4     /* For each node. */
5     for  $j_1 \leftarrow 0$  to  $< 3$  do
6         if idx[n1][j1] != -1 then
7             for  $n_2 \leftarrow$  node in list iN[n1] do
8                 for  $j_2 \leftarrow 0$  to  $< 3$  do
9                     if idx[n2][j2] != -1 then
10                        vja.push_back(idx[n2][j2]);
11                        ia[idx[n1][j1]+1]++;
12
13 for  $i \leftarrow 0$  to  $< N_r$  do
14     ia[i+1] = ia[i] + ia[i+1];
15 for  $i \leftarrow 0$  to  $< ia[N_r]$  do
16     ja[i] = vja.at(i);

```

Determine the non-zero coefficients' indices With the interaction list, `iN`, of each node, the row and column information of all the non-zero coefficients of the stiffness matrix $\mathbf{K}_{uu}$ can be determined. The column and row indices information of the non-zero coefficients

are stored in the arrays `ja[]` and `ia[]`. The pseudo-code for obtaining the `ia[]` and `ja[]` is shown in Algorithm 3.

4.4.3 Assembling the stiffness matrix by MPI

With the arrays `ia[]` and `ja[]`, the positions of all non-zero coefficients of the stiffness matrix are known. To find the corresponding position in the array `K[]` of the *row*-th row and *col*-th column coefficient of the stiffness matrix $\mathbf{K}_{uu}$, a function `findCSRIndexOfMat(row, col)` is first built. A binary searching method is employed in this function to take advantage of ascending order of `ja[]` for each row. The assembling procedure of the stiffness matrix is time-consuming, but is independent between each PD node, each PDBE, and each FE. Thus, the MPI technique is applied to assemble the stiffness matrix. Note that, during assembling the stiffness matrix $\mathbf{K}_{uu}$, the item $-\mathbf{K}_{up}\mathbf{u}_p$ is obtained simultaneously and stored in the array `local_F[]`. With the stiffness matrix and equivalent nodal force, the displacements are solved by the PDSS, which is also based on the MPI technique. The pseudo-code for assembling the stiffness matrix is presented in Algorithm 4. For the matrix $\mathbf{K}_s^{pd}$, we only illustrate the assembling procedure for 4-noded PDBE for conciseness, and for 3-noded PDBE, a similar procedure can be used.

4.5 Numerical results and performance evaluation

To demonstrate the capability of this proposed PDLSS-FEM, three static examples concerning displacements and stresses are conducted in this section. In the first example, a block under uniaxial uniform tension at various PD volume fraction, *m*-ratio, and number of cores is analyzed in this section, to better quantify the improvement of the computational cost of the proposed coupling method. The second example concerns a block with a hole at its center under displacement loading, and the third example is a block with a pre-existing crack under displacement loading. For the first and third examples, the material constants are Young's modulus $E = 70$ GPa and Poisson's ratio $\nu = 0.33$. For the second example,

Algorithm 4: Assembling the stiffness matrix

```
/* create a function to find the index of the non-zero coefficient  $K_{uu}$ [row][col]
   in the array  $K[ ]$ , using a binary method. */
1 Function findCSRIndexOfMat(row, col):
2   low = ia[row];
3   up = ia[row+1];
4   while low < up do
5     mid = (low+up)/2;
6     if ja[mid] == col then
7       return mid;
8     else if col < ja[mid] then
9       up = mid;
10    else
11      low = mid + 1;

12 Initialize local_K[ ] = 0 ; // size of local_K[ ] is ia[Nr].
13 Initialize local_F[ ] = 0 ; // size of local_F[ ] is Nr.
14 rank ← rank ID;
15 numProc ← number of cores;
   /* Assemble the matrix  $K_b^{pd}$  */
16 startP = rank * Npd / numProc;
17 endP = (rank + 1) * Npd / numProc;
18 for i ← startP to <endP do
19   std::vector fami ← family member of i-th PD node;
20   n1 = fami.at(0);
21   H[ ][ ] ← matrix (−V(i)H(i)) of the i-th PD node n1;
   /* Start Assembling */
22   for j1 ← 0 to < 3 do
23     if idx[n1][j1] != -1 then
24       for m ← 0 to < fami.size() do
25         n2 = fami.at(m);
26         for j2 ← 0 to < 3 do
27           if idx[n2][j2] != -1 then
28             t = findCSRIndexOfMat(idx[n1][j1], idx[n2][j2]);
29             local_K[t] = local_K[t] + H[j1][3m + j2];
30           else
31             local_F[idx[i][j1]] = local_F[idx[i][j1]] − H[j1][3m + j2]*u[n2][j2];

   /* Assemble the matrix  $K^{fem}$ . */
32 startP = rank * Nfe / numProc;
33 endP = (rank + 1) * Nfe / numProc;
```

```

34 for e ← startP to <endP do
35   Ke ← Element stiffness matrix;
36   /* Start Assembling. Nfe is number of FE, Ne is number of node in FE. */
37   for i1 ← 0 to < Ne do
38     n1 ← the i1-th node of the FE;
39     for j1 ← 0 to < 3 do
40       if idx[n1][j1] != -1 then
41         for i2 ← 0 to < Ne do
42           n2 ← the i2-th node of the FE;
43           for j2 ← 0 to < 3 do
44             if idx[n2][j2] != -1 then
45               t = findCSRIndexOfMat(idx[n1][j1], idx[n2][j2]);
46               local_K[t] = local_K[t] + Ke[3i1 + j1][3i2 + j2];
47             else
48               local_F[idx[n1][j1]] = local_F[idx[n1][j1]] -
49                 Ke[3i1 + j1][3i2 + j2] * u[n2][j2];
50   /* Assemble the matrix Kspd. */
51   startP = rank * NSpd / numProc;
52   endP = (rank + 1) * NSpd / numProc;
53   for e ← startP to <endP do
54     for p ← Gauss points do
55       for q ← Gauss points do
56         for i ← 0 to < 4 do
57           ei ← the i-th node of the PDBe;
58           std::vector fami ← family members of the node ei;
59           eK[ ][ ] ← matrix of (wpwqℳTℳiDC(ei));
60           /* Start Assembling. */
61           for i1 ← 0 to < 4 do
62             n1 ← the i1-th node of the PDBe;
63             for j1 ← 0 to < 3 do
64               if idx[n1][j1] != -1 then
65                 for m ← 0 to < fami.size() do
66                   n2 = fami.at(m);
67                   for j2 ← 0 to < 3 do
68                     if idx[n2][j2] != -1 then
69                       t = findCSRIndexOfMat(idx[n1][j1], idx[n2][j2]);
70                       local_K[t] = local_K[t] + eK[3i1 + j1][3m + j2];
71                     else
72                       local_F[idx[n1][j1]] = local_F[idx[n1][j1]] -
73                         eK[3i1 + j1][3m + j2] * u[n2][j2];

```

```

69 Get the nodal forces from external forces and add to local_F[ ];
    /* Get K[ ] and nodal force F[ ] by the MPI_Allreduce routine of MPI.          */
70 K[ ] ← summation of local_K[ ] by MPI_Allreduce routine;
71 F[ ] ← summation of local_F[ ] by MPI_Allreduce routine;

```

Young's modulus and Poisson's ratio are specified as $E = 200$ GPa and $\nu = 0.3$, respectively.

In these simulations, the nodal stresses in the FEM domain and the PD domain are calculated by the FEM formulation and the PD equation, Eq. (2.32), respectively. For the PD-FEM interface, the nodal stresses are calculated by the average of FEM and PD formulations. All PD bonds that pass through the pre-existing crack are broken. We also analyze the second and third examples by ANSYS. The comparison of the displacement and stress by PDLSE-FEM and ANSYS shows good agreements between the two methods. Note that the influence function $\omega(|\xi|)$ may affect the accuracy in numerical implementation. In this paper, we specify the influence function as a Gaussian distribution in the form of

$$\omega(|\xi|) = e^{-\left(\frac{|\xi|}{c\delta(i)}\right)^2}, \quad (4.74)$$

here, c is a constant and we define it as a *non-local factor*. In this paper, we take $c = 1/4$.

All the PDLSE-FEM simulations are run on the *Moles* computing nodes of the *Beocat* machine at Kansas State University. The *Beocat* machine has 120 *Moles* computing nodes and each node has 32 GB RAM, 2 *Xeon E5-2630 v4* CPU processors with a total of 20 cores, and 2 *Intel I350* network interface controllers.

4.5.1 A block under uniaxial uniform tension

As shown in Fig. 4.5a, a block with size $1 \text{ m} \times 1 \text{ m} \times 0.5 \text{ m}$ is under uniaxial uniform tension $P = 0.7$ MPa. The middle part of the block is specified as PD domain, and the left and right parts are specified as FEM domain, as shown in Fig. 4.5b. The whole domain is discretized with uniform cube mesh with mesh size 25 mm, and it contains a total of 32000 elements and a total of 35301 nodes. To better evaluate the performance of the coupling method,

we simulate the example with various volume fraction of PD domain $v_r = \frac{V_{pd}}{V_{tot}}$. Fig. 4.5b illustrates the meshes for $v_r = 0.4$ with blue PD domain and purple FEM domain. Note that $v_r = 0$ represents a pure FEM model, and $v_r = 1.0$ represents a pure PDLSM model.

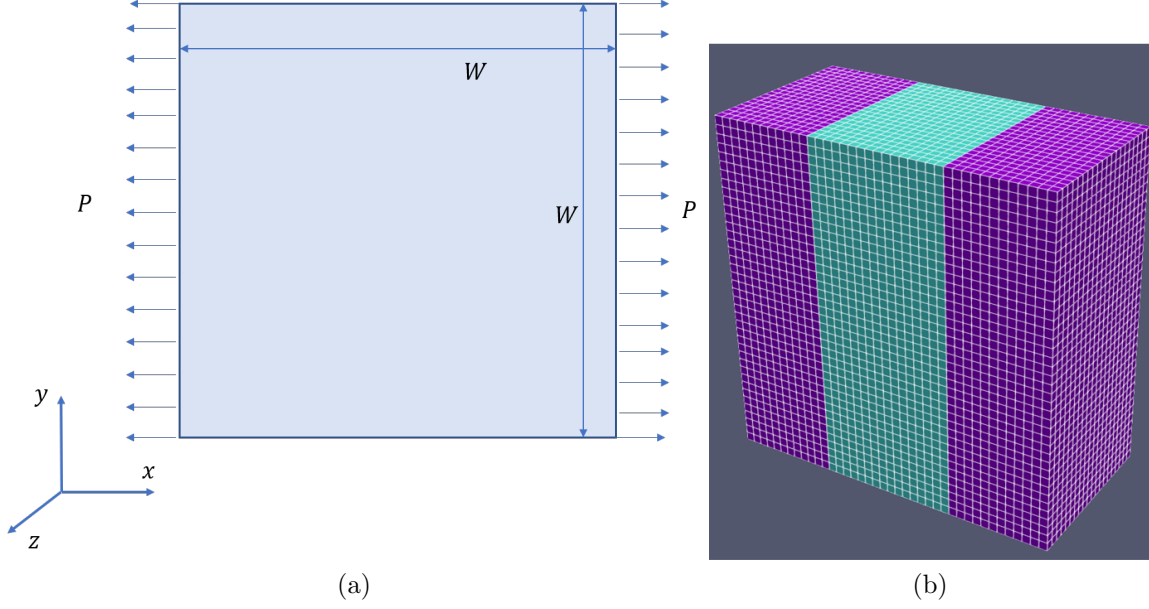


Fig. 4.5: The block with uniaxial uniform tension: (a) Geometry and loading, (b) illustrated uniform meshes for $v_r = 0.4$.

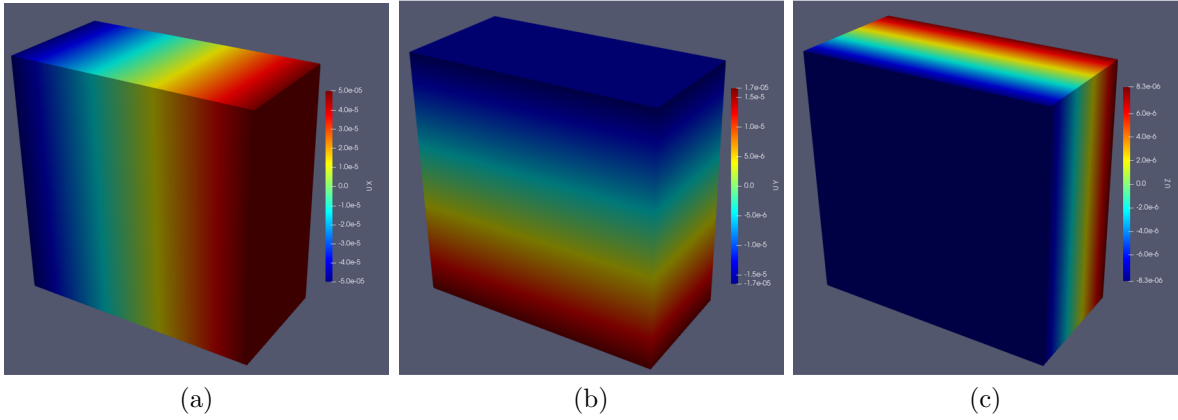


Fig. 4.6: Displacement results of the block under uniaxial uniform tension: (a) u_x , (b) u_y , (c) u_z .

Fig. 4.6 shows the displacement results for $v_r = 0.4$. As expected, the displacements u_x , u_y , and u_z vary linearly along the x -, y -, and z -direction, respectively. Although not shown here, for all the simulations of this example, the magnitude of the relative errors of

the displacement results of each node is up to machine precision, compared to the analytical results of $u_x = \frac{P}{E}x$, $u_y = -\nu\frac{P}{E}y$, and $u_z = -\nu\frac{P}{E}z$, as both PDLSTM and FEM can predict exactly the mechanical behaviors of this example.

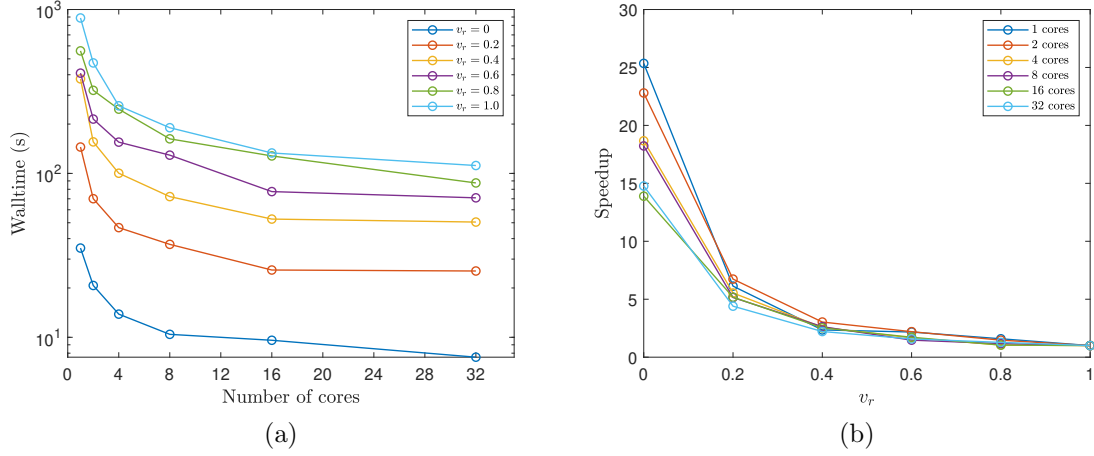


Fig. 4.7: Wall time and speedup of the coupling model for assembling the stiffness matrix and solving the system equations with constant $m = 4$, yet various v_r and various cores.

Fig. 4.7 illustrates the wall time and speedup of the coupling model for assembling the stiffness matrix and solving the system equations, with constant $m = 4$, yet various v_r and various cores. The speedup is defined as the wall time ratio of the coupling model to the pure PD model ($v_r = 1.0$). As Fig. 4.7a shows, the coupling model scales well from 1 to 4 cores, almost linearly, after which, the performance is not improved substantially as the number of cores increases further due to communication between cores. After the number of cores reaches 16, the wall time is almost an constant. Thus, for saving computing resources, we may run the program on up to 16 cores. As shown in Fig. 4.7b, this coupling model improves computational efficiency significantly. The pure FEM model ($v_r = 0$) is 14 – 25 times faster than the pure PD model ($v_r = 1$) and a larger volume of FEM domain saves more computational cost. When $v_r = 0.2$, the coupling model is 4.4 – 6.7 times faster than the pure PD model. Note that we use uniform mesh in this example, but for practical applications of PDLSTM-FEM, we can use very coarse mesh in the FEM domain, which is far from the discontinuous region, and relative finer mesh in the PD domain, where discontinuities occur. This treatment may save much more computational cost compared to treating the whole

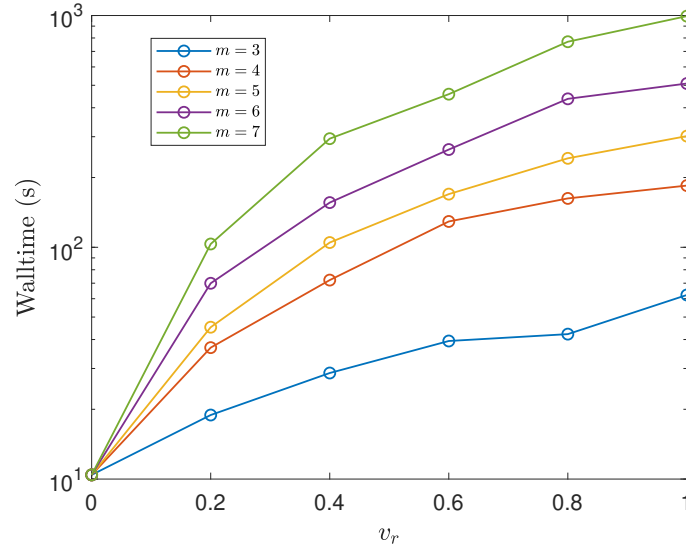


Fig. 4.8: Wall time for assembling the stiffness matrix and solving the system equations with constant 8 cores, yet various v_r and various m -ratio.

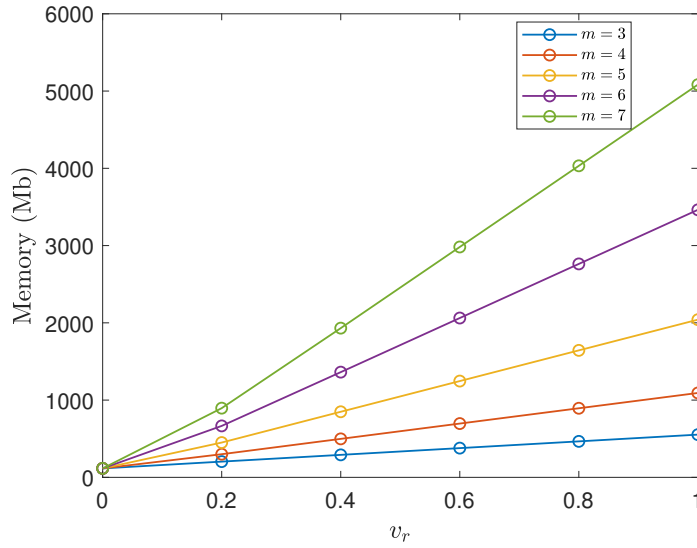


Fig. 4.9: Memories for storing the stiffness matrix in CSR format in each core with various v_r and various m -ratio.

domain as a full PD domain with fine mesh. In general and by comparison, to get results with similar accuracy, PDLSM requires finer mesh than FEM does, due to two reasons: (a) PDLSM assumes that the displacements are in 2nd-order form (see Section 5.2) within the interaction domain H_x , which contains many elements inside, while FEM assumes the displacements are in a 2nd-order form (for 8-noded brick elements) or even higher-order form (depends on element type) within every single element, which is much smaller than the interaction domain of PD; (b) numerical implementation of PD employs the simple meshless method with a one-point quadrature for cells, while FEM employs the element-based method with Gauss integration which is much more accurate than the one-point quadrature method.

Fig. 4.8 shows the wall time for assembling the stiffness matrix and solving the system equations, with constant 8 cores, yet various v_r and various m -ratio. As it shows, increasing m -ratio makes the consuming time increase sharply. When $m = 7$ and $v_r = 1.0$, the run time is 994 s, which is about 96 times more than the pure FEM model with run time 10.4 s. Fig. 4.9 shows the memories for storing the stiffness matrix in CSR format for each core with various v_r and various m -ratio. Note that the data types of the arrays `ia[]` and `ja[]` are `long long int`, and non-zero coefficients are stored by double precision. As it shows, the memory increases almost linearly when increasing PD volume fraction. Increasing the m -ratio makes the memory increase sharply and when m -ratio is larger, slightly increasing m -ratio leads to an enormous increase in the memory usage due to the enormous increase of interaction domain volume. When $m = 7$ and $v_r = 1.0$, the memory usage to store the stiffness matrix is 5083 MB, which is about 43.8 times more than that of the pure FEM model, with a memory usage of 116 MB. In comparison, if the full stiffness matrix was stored for this example, it would have required memory of 83.4 GB for each core. Thus, in general, the proposed coupling PDLSM-FEM greatly reduces computational cost in terms of program run time and memory usage.

4.5.2 A block with a hole under displacement loading

A block with a central hole, as depicted in Fig. 4.10, is under a displacement loading $u_0 = 5 \times 10^{-5}$ m. Due to symmetry, only one-eighth of the box is modeled in this simulation. The symmetrical boundary conditions are applied on the faces $x = 0$, $y = 0$ and $z = 0$. The radius of the hole is $r = 0.1$ m. The length of the model is $L = 0.5$ m and the thickness of the model is $B = 0.25$ m. The whole model utilizes non-uniform discretization with a total of 16480 nodes and 90811 tetrahedron elements. The region $0 \leq x \leq 0.2 \text{ m} \cap 0 \leq y \leq 0.2 \text{ m}$ is discretized with 12009 PD nodes and 66741 tetrahedron PD elements. The interaction domain of each PD node is determined by $\delta_{(i)} = 4\Delta_{(i)}$. Fig. 4.10b illustrates the tetrahedron meshes with blue PD domain and purple FEM domain.

Fig. 4.11 presents the displacement results of the block with a hole by PDLISM-FEM. Fig. 4.12a demonstrates the comparison of u_x and u_y along the edge of the hole at $z = 0$ obtained from PDLISM-FEM and ANSYS. It is clear that u_x and u_y obtained from the proposed method and ANSYS are in excellent agreement. Fig. 4.12b illustrates the comparison of σ_y and σ_z along the edge of the hole at $z = 0$ obtained from the proposed method and ANSYS. It reveals that stresses values obtained from these two methods are in excellent agreement while the σ_y values predicted using the proposed method is slightly lower than that obtained using ANSYS.

4.5.3 A block with a pre-existing crack under displacement loading

As shown in Fig. 4.13a, a block with a pre-existing crack is subjected to displacement loading $u_0 = 5 \times 10^{-5}$ m. The edge length of the block is $L = 1$ m and the thickness of block is $B = 0.1$ m. The length of the crack is $2a = 0.2$ m. A fictitious plane is used to represents the crack and all PD bonds crossing the plane are broken. The whole domain is constructed by non-uniform discretization with a total of 57772 nodes and 51000 hexahedron elements. The region $-0.15 \text{ m} \leq x \leq 0.15 \text{ m}$ is specified as the PD domain and is discretized with 35552 PD nodes and 31000 hexahedron elements. The family size is specified as $\delta_{(i)} = 4\Delta_{(i)}$. Fig.

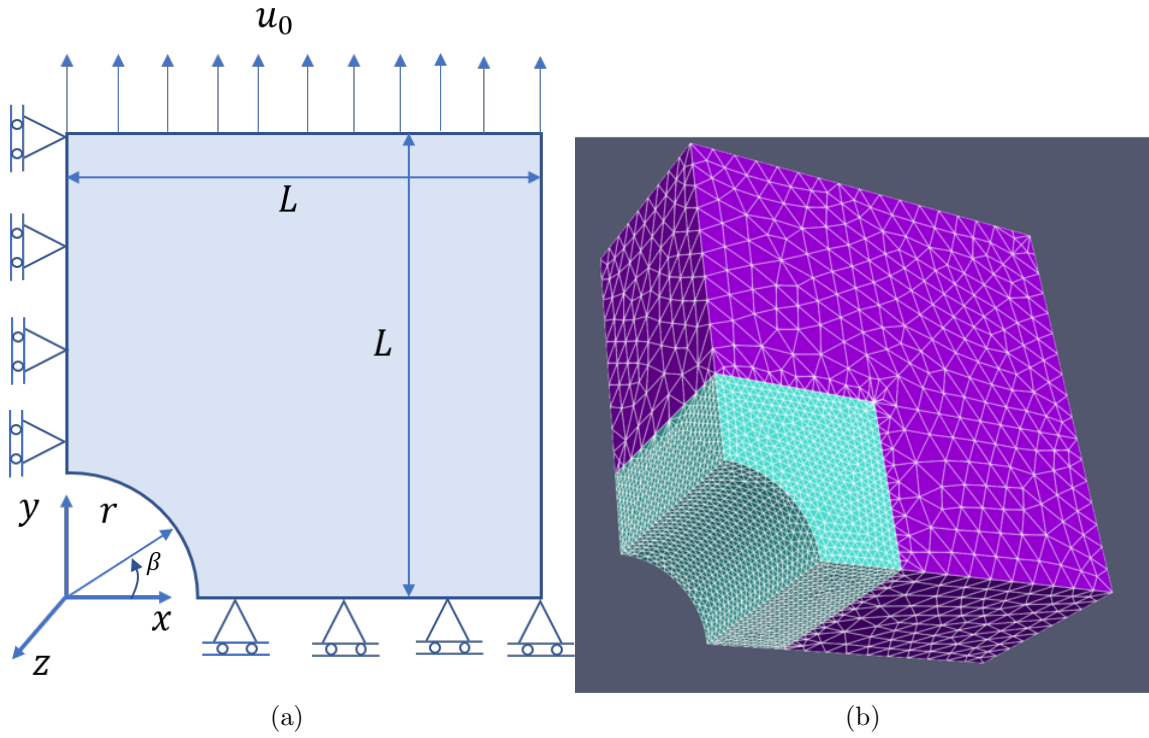


Fig. 4.10: The block with a hole under displacement loading: (a) Geometry and loading, (b) Non-uniform tetrahedron meshes.

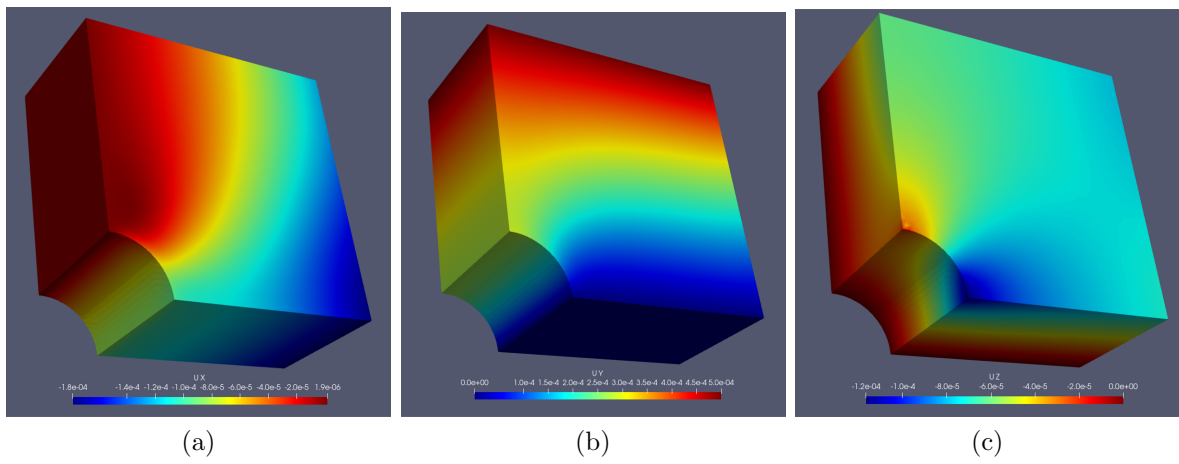


Fig. 4.11: Displacements of the block with a hole: (a) u_x , (b) u_y , (c) u_z .

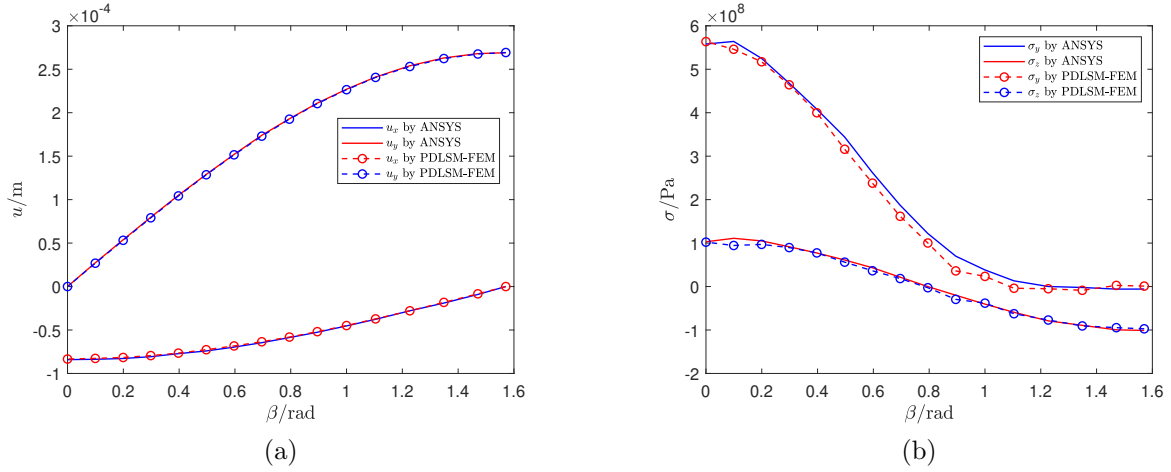


Fig. 4.12: Comparison of PDLSM-FEM with ANSYS for displacement and stress solutions along with the edge of the hole at $z = 0$: (a) Comparison of displacements u_x and u_y , (b) comparison of stresses σ_y and σ_z .

4.13b illustrates the hexahedron meshes with blue PD domain and purple FEM domain.

Fig. 4.14 demonstrates the displacements from PDLSM-FEM and Fig. 4.15 presents the deformed shape and stress results of the block. Note that the deformation is magnified 2000 times in Fig. 4.15. As shown in the figures, an obvious discontinuity occurs at the crack position and stresses are concentrated at the crack front. Fig. 4.16 elucidates the displacements of u_x and u_y , the normal stresses, σ_x , and the shear stresses, σ_{xy} , from PDLSM-FEM and ANSYS, along with path $\overline{ABCD}$ as seen in Fig. 4.13a, where the coordinates of the key points of the path are A (0.15, 0.1, 0) m, B (0.15, 0.25, 0) m, C (-0.15, 0.25, 0) m and D (-0.15, 0.1, 0) m. It is observed that for u_x , the proposed method and ANSYS generate very close results for the horizontal segment $\overline{BC}$; for the vertical segments $\overline{AB}$ and $\overline{CD}$, PDLSM-FEM generates slightly larger value than ANSYS. Very interestingly, for u_y , PDLSM-FEM and ANSYS generates very close results on the vertical segments $\overline{AB}$ and $\overline{CD}$; on the horizontal segments $\overline{BC}$, PDLSM-FEM generates slightly larger results. It is very clear that for both stress and displacement, the results by the two methods are in good agreement.

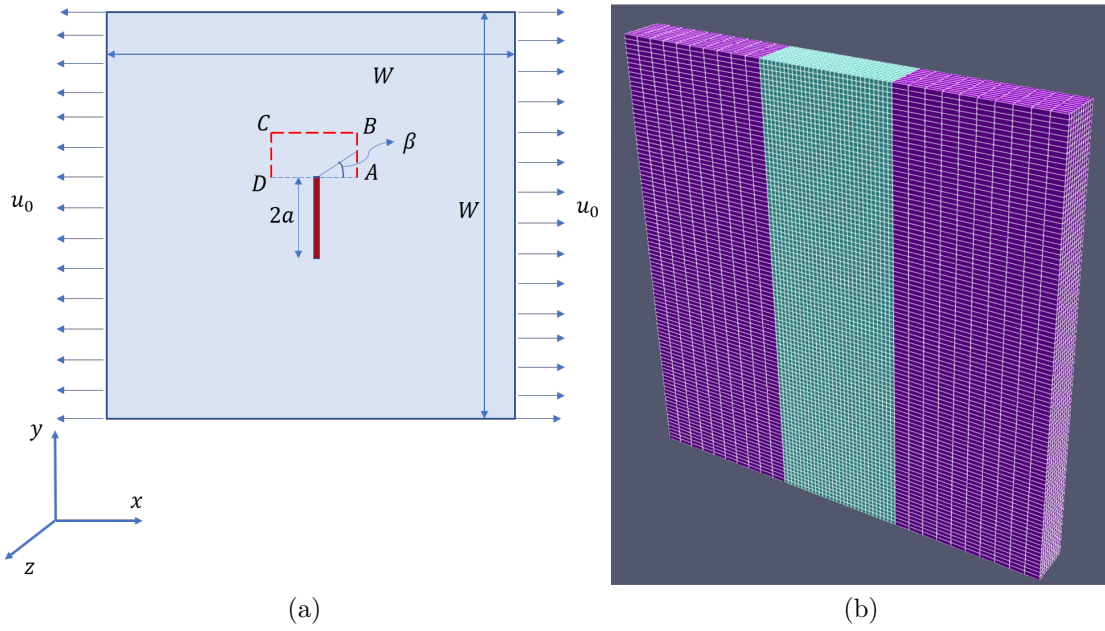


Fig. 4.13: The block with a pre-existing crack under displacement loading: (a) Geometry and loading, (b) Non-uniform hexahedron meshes.

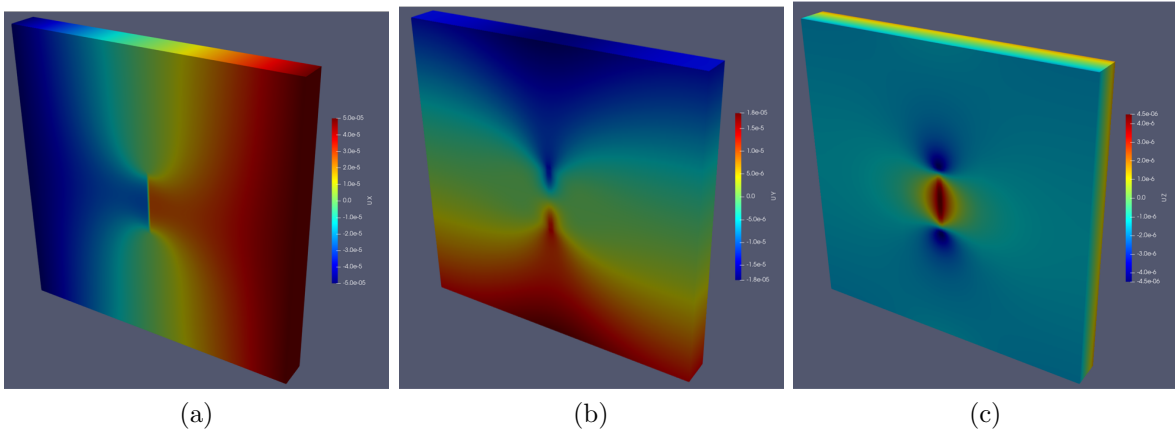


Fig. 4.14: Displacement results from the block with a pre-existing crack: (a) u_x , (b) u_y , (c) u_z .

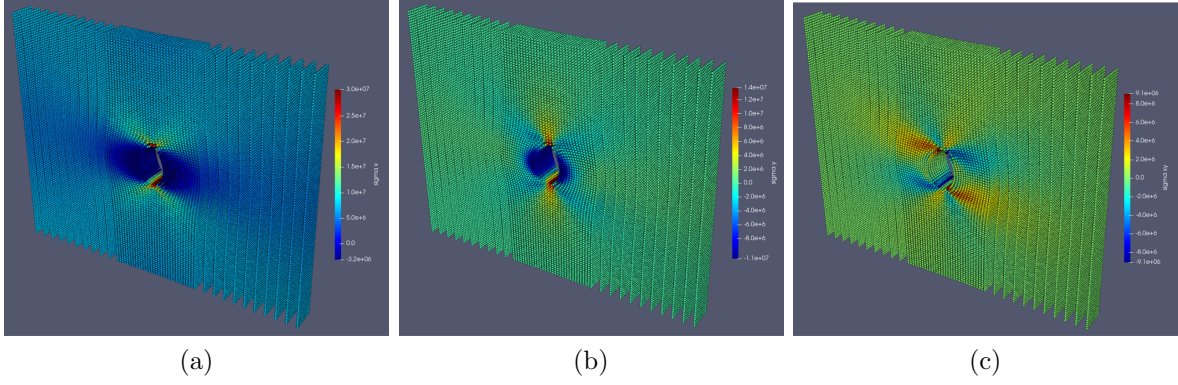


Fig. 4.15: Deformed shape and stress results of the block a with pre-existing crack: (a) σ_x , (b) σ_y , (c) σ_{xy}

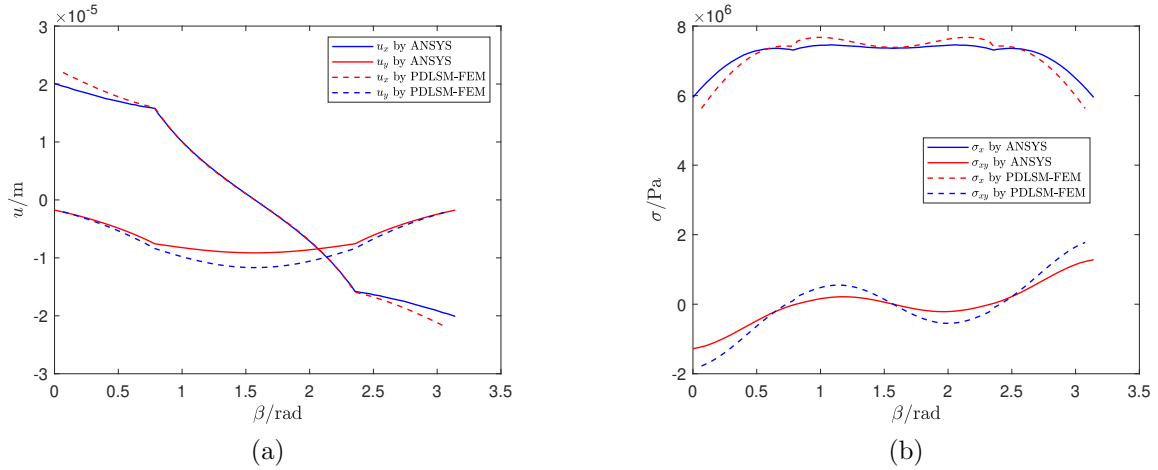


Fig. 4.16: Comparison of PDLSM-FEM with ANSYS for displacement and stress solutions along with the path $\overline{ABCD}$: (a) Comparison of displacements u_x and u_y ; (b) comparison of stresses σ_x and σ_{xy} .

4.6 Conclusions

In this work, we present a new framework to couple PDLSM with FEM (PDLSM-FEM) for 3D problems based on the weighted residual method. In PDLSM-FEM, the problem domain is divided into a PD domain and a FEM domain, and both domains are discretized into uniform or non-uniform elements. The coupling method is straightforward, and the formulation can be converted conveniently between PDLSM, FEM, and PDLSM-FEM. To directly and implicitly solve the 3D problems, we present an algorithm to assemble the global stiffness matrix in a compressed sparse row (CSR) format by message passing interface technique (MPI). Within the CSR format, only non-zero coefficients of the stiffness matrix, and their row and column indices information are stored. The system equations are solved by the parallel direct sparse solver which is also based on MPI. Three static examples are performed to demonstrate the capability of this proposed PDLSM-FEM. For the first example, the magnitude of the relative errors of the displacement results of each node is up to machine precision, compared to the analytical results. The performance evaluation of the first example shows the MPI technique improves the computational efficiency generally and the maximum number of cores is suggested as 16. The performance evaluation also demonstrates that the proposed PDLSM-FEM significantly improves the computational efficiency, which is up to 96 times faster than the pure PDLSM, and significantly saves memory usage, which is up to 43 times less than the pure PDLSM. For the second and third examples, the displacements and stresses are obtained by PDLSM-FEM, and comparison with results using ANSYS demonstrates the proposed PDLSM-FEM has good accuracy.

Chapter 5

Enriching finite element method by peridynamics⁴

Abstract

This study presents an Enriched Finite Element Method by Peridynamics (EFEM-PD) for discontinuity analysis. In EFEM-PD, the Finite Element Method (FEM) is coupled with Peridynamics (PD), which utilizes the PD theory for modeling discontinuities while maximizing the FEM region for computational efficiency. With the framework of EFEM-PD, only elements intersecting with the crack path and their neighboring elements are enriched by the PD equations. The remaining elements are those of conventional FEM. Element stiffness matrix and governing equations in 2-D and 3-D are derived. Numerical integration of interaction integral is proposed and implemented to evaluate the stress intensity factors (SIFs) for 2-D problems. The criterion of maximum hoop tensile stress is employed for failure prediction. New contributions of this work include FEM enriched with PD with adaptivity for minimizing the PD region and the application of EFEM-PD to quasi-static crack propagation analysis. Simulations of three 2-D plane stress plates and one 3-D block with static or quasi-static cracks propagation are performed. Results show the proposed

⁴This chapter was submitted to journal for publish.

EFEM-PD improves computational efficiency substantially and has reasonable accuracy and good capability of crack propagation prediction.

5.1 Introduction

The finite element method has been one of the most popular and successful numerical tools for studying structure behaviors for decades. The FEM requires the domain to be discretized into non-overlapping elements whose displacements are approximated with polynomials. Stress and strain fields then are derived from the displacement approximation based on classical continuum theory. Despite its widespread applications, the FEM suffers from drawbacks for handling displacement discontinuities as in the cases of cracked bodies and other defects, since the FEM is formulated within the framework of classical continuum mechanics, in which the governing equations require the derivatives of displacements and become invalid at displacement discontinuities. Various ways to handle displacement discontinuities such as cracks have been proposed. A typical technique is to remesh repeatedly to match the discontinuities so that the discontinuities, such as cracks, always coincide with element edges and propagate only along the boundaries of neighboring elements. Remeshing, however, is computationally intensive and somewhat cumbersome.

Peridynamics (PD), introduced first by Silling [4], removes the inadequacies of the classical continuum theory. Instead of relying on derivatives of displacements, PD theory takes the force density in an integration form, making it suitable for analyzing structures containing discontinuities. However, the original version of the PD theory requires volume and surface correction to improve simulation accuracy. To remove these requirements, Madenci et al. [58] developed a PD theory based on least-squares minimization.

Since PD is computationally expensive but can handle discontinuities, while FEM is well developed and computationally efficient, coupling PD with FEM is highly desirable for both methods. Sun and Fish [43] devised a method of coupling based on a partial superposition of FEM and PD solutions for static and quasi-static problems. Shen et al. [48] introduced truss elements to bridge finite element (FE) sub-regions and PD sub-regions to couple PD

with FEM. Pagani and Carrera [47] developed a technique to couple 3-D peridynamics with 1-D high-order finite elements using Lagrange multipliers. The authors Liu and Xin [70], Liu et al. [86, 89] proposed a straightforward framework to couple PD with FEM for 2-D and 3-D problems using the weighted residual method. Zaccariotto et al. [36], Wang, Yongwei et al. [37], Tong et al. [38] have developed various adaptive approaches which can transform FEM nodes into PD nodes for coupling PD with FEM.

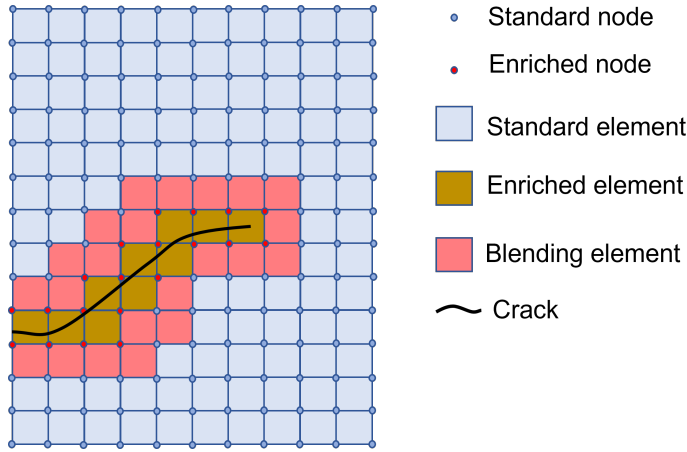


Fig. 5.1: XFEM modeling of a cracked body. The Heaviside function enriches the elements across the crack line. Asymptotic functions enrich elements at the crack tips. Immediately neighboring elements of enriched elements, referred to as blending elements, are partially enriched.

The extended finite element method (XFEM) offers another way of modeling discontinuities. It was first introduced by Belytschko and Black [90], Moës et al. [91], and later utilized in the commercial code of ABAQUS. Based on the concept of partition of unity proposed by Melenk and Babuška [92], XFEM enriches the finite element formulation by the local enrichment function. The nodes of elements containing discontinuities are enhanced using the enrichment function with additional degrees of freedom (DOFs). Asymptotic functions extracted from analytical solutions in conjunction with the Heaviside jump function are utilized to model discontinuities across the crack line [93], as shown in Fig. 5.1. All nodes in enriched elements, referred to as enriched nodes, are augmented with additional DOFs, while nodes in standard elements do not have such additional DOFs. The elements neighboring the enriched elements are referred to as blending elements, which are partially enriched since

they have both enriched nodes and standard nodes.

Following a similar concept of element enrichment, we propose an Enriched Finite Element Method using Peridynamics (EFEM-PD) for discontinuity analysis in this work. In EFEM-PD, the FEM model is enriched adaptively with PD equations in regions containing cracks. An adaptive algorithm is implemented with the dual goals of meshing regions with cracks using PD equations while minimizing the use of PD interactions to maximize computational efficiency. With the framework of EFEM-PD, only elements intersecting with the crack and the neighboring elements are enriched by the PD least-squares minimization (PDLSM) formulation, which is suitable for modeling the failure of structures. The remaining elements are conventional FEM elements. Based on the weighted residual method, we derive the element stiffness matrix and governing equations of the whole domain in 2-D and 3-D. Numerical integration of interaction integral is proposed and implemented to evaluate the stress intensity factors (SIFs) for 2-D problems. The criterion of maximum circumferential tensile stress (MCTS) [75] is used for failure prediction. The crack growth direction θ_c is determined based on MCTS concerning the orientation, and crack starts to grow when the equivalent SIF K_{eq} reaches the fracture toughness K_{Ic} . The enriched elements are adaptively updated based on the current crack configuration and crack propagation.

This paper is organized as follows. First, PDLSM theory is briefly reviewed in Section 5.2, and the model of EFEM-PD is proposed and presented in Section 5.3. After that, the 2-D simulation model of quasi-static crack growth is described in Section 5.4. Next, four examples are performed to demonstrate the proposed EFEM-PD in Section 5.5. Finally, the conclusions are drawn in Section 5.6.

5.2 Peridynamics least-square minimization theory

Since Peridynamics was first introduced by [4], various modifications and improvements to the theory have been proposed in the literature. The PDLSM introduced by [58] has some marked advantages, including allowing arbitrarily shaped interaction domains and eliminating surface correction. In this work, PDLSM is utilized to enrich the FEM model

for regions containing cracks. Detailed PDLMS can be found in [58], but this section briefly reviews the formulation for completeness.

In PD, point $\mathbf{x}$ interacts with its neighbors $\mathbf{x}' = \mathbf{x} + \boldsymbol{\xi}$ within its interaction domain H_x , as illustrated in Fig. 5.2. Based on this nonlocal interaction concept of PD, the 2nd-order Taylor Series Expansion, and the least-squares minimization [58] explicitly derived the nonlocal PDLMS differential operator as follows,

$$\begin{bmatrix} \frac{\partial}{\partial x_1} & \frac{\partial}{\partial x_2} & \frac{\partial}{\partial x_3} & \frac{\partial^2}{\partial x_1^2} & \frac{\partial^2}{\partial x_2^2} & \frac{\partial^2}{\partial x_3^2} & \frac{\partial^2}{\partial x_1 x_2} & \frac{\partial^2}{\partial x_2 x_3} & \frac{\partial^2}{\partial x_3 x_1} \end{bmatrix}^T f(\mathbf{x}) = \int_{H_x} \omega(|\boldsymbol{\xi}|) \begin{bmatrix} \mathbf{g} \\ \mathbf{d} \end{bmatrix} (f(\mathbf{x}') - f(\mathbf{x})) dV'. \quad (5.1)$$

The vectors $\mathbf{g} = [g_1 \ g_2 \ g_3]^T$ and $\mathbf{d} = [d_1 \ d_2 \ d_3 \ d_4 \ d_5 \ d_6]^T$ are defined as follows,

$$\begin{bmatrix} \mathbf{g} \\ \mathbf{d} \end{bmatrix} = \mathbf{A}^{-1} \hat{\boldsymbol{\xi}}, \quad (5.2)$$

where

$$\hat{\boldsymbol{\xi}} = [\xi_1 \ \xi_2 \ \xi_3 \ \xi_1^2 \ \xi_2^2 \ \xi_3^2 \ \xi_1 \xi_2 \ \xi_2 \xi_3 \ \xi_1 \xi_3]^T, \quad (5.3)$$

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix}, \quad (5.4)$$

$$\mathbf{A}_{11} = \int_{H_x} \omega(|\boldsymbol{\xi}|) \begin{bmatrix} \xi_1^2 & \xi_1 \xi_2 & \xi_1 \xi_3 \\ \xi_1 \xi_2 & \xi_2^2 & \xi_2 \xi_3 \\ \xi_1 \xi_3 & \xi_2 \xi_3 & \xi_3^2 \end{bmatrix} dV_{x'}, \quad (5.5)$$

$$\mathbf{A}_{12} = \int_{H_x} \omega(|\boldsymbol{\xi}|) \begin{bmatrix} \frac{\xi_1^3}{2} & \frac{\xi_1 \xi_2^2}{2} & \frac{\xi_1 \xi_3^2}{2} & \xi_1^2 \xi_2 & \xi_1^2 \xi_3 & \xi_1 \xi_2 \xi_3 \\ \frac{\xi_1^2 \xi_2}{2} & \frac{\xi_2^3}{2} & \frac{\xi_2 \xi_3^2}{2} & \xi_1 \xi_2^2 & \xi_1 \xi_2 \xi_3 & \xi_2^2 \xi_3 \\ \frac{\xi_1^2 \xi_3}{2} & \frac{\xi_2^2 \xi_3}{2} & \frac{\xi_3^3}{2} & \xi_1 \xi_2 \xi_3 & \xi_1 \xi_3^2 & \xi_2 \xi_3^2 \end{bmatrix} dV_{x'}, \quad (5.6)$$

$$\mathbf{A}_{21} = \int_{H_x} \omega(|\boldsymbol{\xi}|) \begin{bmatrix} \xi_1^3 & \xi_1^2 \xi_2 & \xi_1^2 \xi_3 \\ \xi_1 \xi_2^2 & \xi_2^3 & \xi_2^2 \xi_3 \\ \xi_1 \xi_3^2 & \xi_2 \xi_3^2 & \xi_3^3 \\ \xi_1^2 \xi_2 & \xi_1 \xi_2^2 & \xi_1 \xi_2 \xi_3 \\ \xi_1 \xi_2 \xi_3 & \xi_2^2 \xi_3 & \xi_2 \xi_3^2 \\ \xi_1^2 \xi_3 & \xi_1 \xi_2 \xi_3 & \xi_1 \xi_3^2 \end{bmatrix} dV_{x'}, \quad (5.7)$$

$$\mathbf{A}_{22} = \int_{H_x} \omega(|\boldsymbol{\xi}|) \begin{bmatrix} \frac{\xi_1^4}{2} & \frac{\xi_1^2 \xi_2^2}{2} & \frac{\xi_1^2 \xi_3^2}{2} & \xi_1^3 \xi_2 & \xi_1^3 \xi_3 & \xi_1^2 \xi_2 \xi_3 \\ \frac{\xi_1^2 \xi_2^2}{2} & \frac{\xi_2^4}{2} & \frac{\xi_2^2 \xi_3^2}{2} & \xi_1 \xi_2^3 & \xi_1 \xi_2^2 \xi_3 & \xi_2^3 \xi_3 \\ \frac{\xi_1^2 \xi_3^2}{2} & \frac{\xi_2^2 \xi_3^2}{2} & \frac{\xi_3^4}{2} & \xi_1 \xi_2 \xi_3^2 & \xi_1 \xi_3^3 & \xi_2 \xi_3^3 \\ \frac{\xi_1^3 \xi_2}{2} & \frac{\xi_1 \xi_2^3}{2} & \frac{\xi_1 \xi_2 \xi_3^2}{2} & \xi_1^2 \xi_2^2 & \xi_1^2 \xi_2 \xi_3 & \xi_1 \xi_2^2 \xi_3 \\ \frac{\xi_1^2 \xi_2 \xi_3}{2} & \frac{\xi_2^3 \xi_3}{2} & \frac{\xi_2 \xi_3^3}{2} & \xi_1 \xi_2^2 \xi_3 & \xi_1 \xi_2 \xi_3^2 & \xi_2^2 \xi_3^2 \\ \frac{\xi_1^3 \xi_3}{2} & \frac{\xi_1 \xi_2^2 \xi_3}{2} & \frac{\xi_1 \xi_3^3}{2} & \xi_1^2 \xi_2 \xi_3 & \xi_1^2 \xi_3^2 & \xi_1 \xi_2 \xi_3^2 \end{bmatrix} dV_{x'}. \quad (5.8)$$

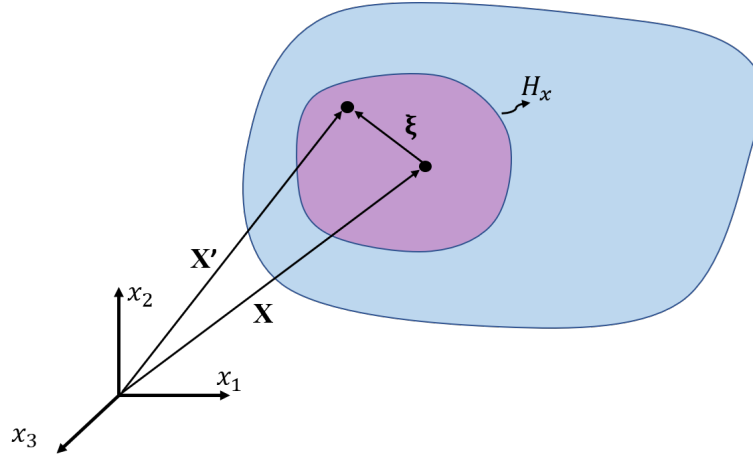


Fig. 5.2: Field point $\mathbf{x}$ interacts with its neighbors $\mathbf{x}'$ within the interaction domain H_x .

The nonlocal differential operator of Eq. (5.1) was employed to derive the equation of motion, as pointed out in [64]. In PD theory, the equation of motion is defined as

$$\rho \ddot{\mathbf{u}} = \mathbf{L}^{pd}(\mathbf{x}, t) + \mathbf{b}(\mathbf{x}, t), \quad (5.9)$$

where $\mathbf{b}$ represents the external body force, $\ddot{\mathbf{u}}$ is the acceleration, $\mathbf{L}$ represents the internal

body force, and ρ is the mass density. The internal body force $\mathbf{L}^{pd}(\mathbf{x}, t)$ is calculated by the summation of bond force density between points $\mathbf{x}$ and $\mathbf{x}'$ over the domain H_x of point $\mathbf{x}$, as illustrated in Fig. 5.2. Based on the classical continuum mechanics, replacing $f(\mathbf{x})$ in Eq. (5.1) by displacement $u_i(\mathbf{x})$, and introducing the bond status parameter μ gives the nonlocal displacement gradient,

$$\nabla \mathbf{u}^{pd} = \int_{H_x} \mu \omega(|\boldsymbol{\xi}|) \boldsymbol{\eta} \otimes \mathbf{g} dV_{x'}, \quad (5.10)$$

and the nonlocal internal force vector,

$$\mathbf{L}^{pd} = \int_{H_x} \mu \omega(|\boldsymbol{\xi}|) \mathbf{G} \boldsymbol{\eta} dV_{x'}, \quad (5.11)$$

where $\omega(|\boldsymbol{\xi}|)$ is the weight function, $\boldsymbol{\xi} = \mathbf{x}' - \mathbf{x}$ is the bond's relative position between $\boldsymbol{\eta} = \mathbf{u}(\mathbf{x}') - \mathbf{u}(\mathbf{x})$ is the bond's, relative displacement, and the bond status parameter μ is defined as

$$\mu = \begin{cases} 1, & \text{unbroken bond,} \\ 0, & \text{broken bond,} \end{cases} \quad (5.12)$$

and the matrix $\mathbf{G}$ is defined as below,

$$\mathbf{G} = \begin{bmatrix} (\lambda + \mathcal{G})d_1 + \mathcal{G}(d_1 + d_2 + d_3) & (\lambda + \mathcal{G})d_4 & (\lambda + \mathcal{G})d_6 \\ (\lambda + \mathcal{G})d_4 & (\lambda + \mathcal{G})d_2 + \mathcal{G}(d_1 + d_2 + d_3) & (\lambda + \mathcal{G})d_5 \\ (\lambda + \mathcal{G})d_6 & (\lambda + \mathcal{G})d_5 & (\lambda + \mathcal{G})d_3 + \mathcal{G}(d_1 + d_2 + d_3) \end{bmatrix}, \quad (5.13)$$

For 2-D problems, the vectors $\mathbf{d}$ and $\mathbf{g}$ are reduced to as $\mathbf{d} = [d_1 \ d_2 \ d_3]^T$ and $\mathbf{g} = [g_1 \ g_2]^T$, respectively, and all the components with ξ_3 in vector $\hat{\boldsymbol{\xi}}$ and matrix $\mathbf{A}$ will be removed. For plane stress cases, the matrix $\mathbf{G}$ is reduced to as

$$\mathbf{G} = \begin{bmatrix} \frac{E}{2(1-\nu)}d_1 + \mathcal{G}(d_1 + d_2) & \frac{E}{2(1-\nu)}d_3 \\ \frac{E}{2(1-\nu)}d_3 & \frac{E}{2(1-\nu)}d_2 + \mathcal{G}(d_1 + d_2) \end{bmatrix}, \quad (5.14)$$

and for plane strain problems,

$$\mathbf{G} = \begin{bmatrix} (\lambda + \mathcal{G})d_1 + \mathcal{G}(d_1 + d_2) & (\lambda + \mathcal{G})d_3 \\ (\lambda + \mathcal{G})d_3 & (\lambda + \mathcal{G})d_2 + \mathcal{G}(d_1 + d_2) \end{bmatrix}, \quad (5.15)$$

here ν is the Poisson's ratio, E is the Young's modulus, $\mathcal{G}$ is the shear modulus, and λ is the Lamé's constant.

An critical, advantageous feature of PDLSE is that during the derivation of Eq. (5.10) and Eq. (5.11), the interaction domain H_x is not required to be a sphere. As a result, the interaction domain for points near or on the boundary can be tailored to stay entirely inside the problem domain without causing any surface effect, and the volume correction, which is typically needed for PD models, is not required for PDLSE.

5.3 Enriched finite element method by peridynamics

Following a similar concept of enrichment in XFEM, which enriches elements and nodes by Heaviside jump function and asymptotic functions, we propose in this section the EFEM-PD in which PDLSE equations enrich the nodes and elements in regions containing cracks to allow for discontinuity analysis.

In the framework of EFEM-PD, the problem domain is meshed into elements, as presented in Fig. 5.3. The elements touched by the crack line are referred to as α -enriched elements. The immediate neighbors of α -enriched elements are referred to as β -enriched elements. The β -enriched elements are centers within the circle or sphere of radius r_β centered at α -enriched elements' centers. The radius r_β is $r_\beta = m_\beta \Delta_{min}$ where Δ_{min} is the minimum element size and m_β is a constant. $m_\beta < 1$ means there are no β -enriched elements.

The nodes of enriched elements are referred to as enriched nodes which are governed by PDLSE equations. As presented in Fig. 5.3, the enriched node $\mathbf{x}$ interacts with its family members, which are located within its interaction domain H_x . Whenever the interaction bond crosses the crack, it will be broken permanently. The un-enriched elements and unen-

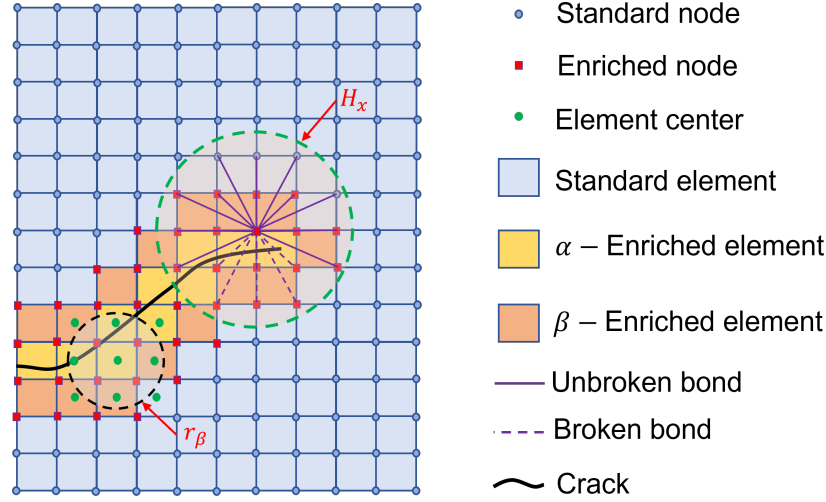


Fig. 5.3: Enriched FEM by PD for modeling of a cracked body. The elements touched by the crack line are α -enriched elements. The β -enriched elements' centers are located within circle r_β centered at α -enriched elements' centers. The node of the enriched element is an enriched node that interacts with its neighbors within its interaction domain H_x .

riched nodes are referred to as standard elements and standard nodes, respectively. Whether an element will be enriched or not depends on the proximity of the element to the current crack location, and the decision for enrichment will be updated adaptively during crack propagation.

Within the standard elements, the conventional FEM is employed, while within enriched elements, the one-point quadrature for the PD equations is employed. To derive the resultant governing equations, the weighted residual method (WRM) is applied to the Neumann boundary conditions and the equations of motion and over the problem body, as shown below,

$$\int_{S_{tot}} \delta \mathbf{u}^T (\boldsymbol{\sigma} \mathbf{n} - \mathbf{T}) dS - \int_{V_{tot}} \delta \mathbf{u}^T (\mathbf{L} + \mathbf{b} - \rho \ddot{\mathbf{u}}) dV = 0, \quad (5.16)$$

where $\mathbf{L}$ represents the internal body force, $\mathbf{T}$ is the external traction, S_{tot} and V_{tot} represent the surface and volume of the whole body, respectively, $\mathbf{n}$ represents the boundary's unit normal vector, and $\delta \mathbf{u}$ represents the admissible displacement. The summation of that of

elements can express the virtual inner work of the domain as

$$\int_{S_{tot}} \delta \mathbf{u}^T \boldsymbol{\sigma} \mathbf{n} dS - \int_{V_{tot}} \delta \mathbf{u}^T \mathbf{L} dV = \sum_{e=1}^N \delta U_e, \quad (5.17)$$

where N is the number of elements in the domain, and δU_e is the virtual inner work of each element and is defined as

$$\delta U_e = \int_{S_e} \delta \mathbf{u}^T \boldsymbol{\sigma} \mathbf{n} dS - \int_{V_e} \delta \mathbf{u}^T \mathbf{L} dV, \quad (5.18)$$

here S_e is the surface of the element and V_e represents the element's volume.

5.3.1 Stiffness matrix of standard element

The global element stiffness matrix $\mathbf{K}_E^{std}$ of each standard element based on conventional FEM formulas is presented in this section. As the conventional FEM is a well-established technology, only necessary formulas are presented in this section for completeness and without derivation for conciseness.

Within each standard element, the internal force is defined in the differential form of

$$\mathbf{L} = \nabla \cdot \boldsymbol{\sigma}. \quad (5.19)$$

Applying Gauss divergence theorem to Eq. (5.18) leads to the virtual inner work as

$$\delta U_e^{std} = \int_{S_e} \delta \mathbf{u}^T \boldsymbol{\sigma} \mathbf{n} dS - \int_{V_e} \delta \mathbf{u}^T \mathbf{L} dV = \int_{V_e} \nabla \delta \mathbf{u} : \boldsymbol{\sigma} dV. \quad (5.20)$$

Based on the conventional FEM formulas, the discrete form of the virtual work of standard elements is expressed as

$$\delta U_e^{std} = \int_{V_e} \nabla \delta \mathbf{u} : \boldsymbol{\sigma} dV = \delta \mathbf{u}_e^T \mathbf{K}_e^{std} \mathbf{u}_e, \quad (5.21)$$

here $\mathbf{u}_e$ is the element's nodal displacement vector, $\mathbf{K}_e^{std}$ is the local element stiffness matrix of the standard element and is defined as

$$\mathbf{K}_e^{std} = \int_{V_e} \mathbf{B}^T \mathbf{D} \mathbf{B} dV, \quad (5.22)$$

in which $\mathbf{D}$ is elasticity matrix and is defined as follows. For 3-D problems,

$$\mathbf{D} = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} (1-\nu) & \nu & \nu & 0 & 0 & 0 \\ \nu & (1-\nu) & \nu & 0 & 0 & 0 \\ \nu & \nu & (1-\nu) & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1-2\nu}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1-2\nu}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1-2\nu}{2} \end{bmatrix}, \quad (5.23)$$

For 2-D plane stress problem,

$$\mathbf{D} = \frac{E}{1-\nu^2} \begin{bmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & \frac{1-\nu}{2} \end{bmatrix}, \quad (5.24)$$

and for 2-D plane strain problem,

$$\mathbf{D} = \frac{E}{(1-2\nu)(1+\nu)} \begin{bmatrix} 1-\nu & \nu & 0 \\ \nu & 1-\nu & 0 \\ 0 & 0 & \frac{1-2\nu}{2} \end{bmatrix}. \quad (5.25)$$

The matrix $\mathbf{B}$ links the strains to the nodal displacements and is defined as

$$\mathbf{B} = \begin{bmatrix} \mathbf{B}_1 & \mathbf{B}_2 & \cdots & \mathbf{B}_{N_e} \end{bmatrix} \quad (5.26)$$

where N_e is the number of element's nodes, and $\mathbf{B}_i$ ($i = 1, 2, \dots, N_e$) is defined as follows.

For 2-D problems,

$$\mathbf{B}_i = \begin{bmatrix} \frac{\partial \mathcal{N}_i}{\partial x_1} & 0 & \frac{\partial \mathcal{N}_i}{\partial x_2} \\ 0 & \frac{\partial \mathcal{N}_i}{\partial x_2} & \frac{\partial \mathcal{N}_i}{\partial x_1} \end{bmatrix}^T, \quad (5.27)$$

and for 3-D problems,

$$\mathbf{B}_i = \begin{bmatrix} \frac{\partial \mathcal{N}_i}{\partial x_1} & 0 & 0 & \frac{\partial \mathcal{N}_i}{\partial x_2} & 0 & \frac{\partial \mathcal{N}_i}{\partial x_3} \\ 0 & \frac{\partial \mathcal{N}_i}{\partial x_2} & 0 & \frac{\partial \mathcal{N}_i}{\partial x_1} & \frac{\partial \mathcal{N}_i}{\partial x_3} & 0 \\ 0 & 0 & \frac{\partial \mathcal{N}_i}{\partial x_3} & 0 & \frac{\partial \mathcal{N}_i}{\partial x_2} & \frac{\partial \mathcal{N}_i}{\partial x_1} \end{bmatrix}^T, \quad (5.28)$$

in which $\mathcal{N}_i$ is the shape function.

The element's nodal displacement vector $\mathbf{u}_e$ can be mapped from the global nodal displacement vector $\mathbf{u}_g$ by a mapping matrix $\mathbf{M}_e$ as

$$\mathbf{u}_e = \mathbf{M}_e \mathbf{u}_g. \quad (5.29)$$

where the mapping matrix $\mathbf{M}_e$ is constructed in the following way: if the k -th DOF of $\mathbf{u}_e$ and the j -th DOF of $\mathbf{u}_g$ are the same, $M_{e(kj)} = 1$, otherwise $M_{e(kj)} = 0$. Therefore, the virtual work of standard elements is transformed into

$$\delta U_e^{std} = \delta \mathbf{u}_g^T \mathbf{M}_e^T \mathbf{K}_e^{std} \mathbf{M}_e \mathbf{u}_g = \delta \mathbf{u}_g^T \mathbf{K}_E^{std} \mathbf{u}_g, \quad (5.30)$$

from which the global element stiffness matrix $\mathbf{K}_E^{std}$ follows

$$\mathbf{K}_E^{std} = \mathbf{M}_e^T \mathbf{K}_e^{std} \mathbf{M}_e. \quad (5.31)$$

5.3.2 Stiffness matrix of enriched element

In this section, the stiffness matrix of the enriched element is formulated based on the PDLSPM. The discrete form of the PDLSPM equations is briefly presented first, and the derivation details can be found in [86, 89]. Next, the stiffness matrix of the enriched element is

derived.

5.3.2.1 Discrete form of PD equations

Consider the i -th enriched node $\mathbf{x}_{(i)}$ has nodal displacement as

$$\mathbf{u}_{(i)} = \begin{cases} [u_{1(i)} & u_{2(i)}]^T, & \text{2-D,} \\ [u_{1(i)} & u_{2(i)} & u_{3(i)}]^T, & \text{3-D.} \end{cases} \quad (5.32)$$

The enriched node $\mathbf{x}_{(i)}$ interacts with its family members which are located within its interaction domain $H_{x_{(i)}}$. Denote $\mathbf{u}^{(i)}$ as the displacement vector of family members of the enriched node $\mathbf{x}_{(i)}$ and define it as

$$\mathbf{u}^{(i)} = \mathbf{u}^{(i)} = \begin{bmatrix} \mathbf{u}_{(i)}^T & \mathbf{u}_{(2)}^T & \mathbf{u}_{(m)}^T & \cdots & \mathbf{u}_{(N_{(i)})}^T \end{bmatrix}^T. \quad (5.33)$$

here, $N_{(i)}$ represents the number of family members, and subscript (m) represents the m th family member $\mathbf{x}_{(m)}$ of node $\mathbf{x}_{(i)}$. The vectors $\mathbf{u}^{(i)}$ and $\mathbf{u}_{(i)}$ can be mapped from the global nodal displacement vector $\mathbf{u}_g$ through two mapping matrices $\mathbf{M}_{(i)}$ and $\mathbf{M}^{(i)}$ as follows,

$$\mathbf{u}^{(i)} = \mathbf{M}^{(i)} \mathbf{u}_g. \quad (5.34)$$

$$\mathbf{u}_{(i)} = \mathbf{M}_{(i)} \mathbf{u}_g. \quad (5.35)$$

From Eq. (5.10), we derive the strain vector of the enriched node $\mathbf{x}_{(i)}$ in a discrete form based on the simple one-point quadrature method as

$$\{\varepsilon\}_{(i)}^{er} = \mathbf{C}^{(i)} \mathbf{u}^{(i)}, \quad (5.36)$$

where the matrix $\mathbf{C}^{(i)}$ is defined as follows. For 2-D problems,

$$\mathbf{C}^{(i)} = \begin{bmatrix} -\sum_{m=2}^{N(i)} C_{1(im)} & 0 & C_{1(i2)} & 0 & \cdots & C_{1(iN(i))} & 0 \\ 0 & -\sum_{m=2}^{N(i)} C_{2(im)} & 0 & C_{2(i2)} & \cdots & 0 & C_{1(iN(i))} \\ -\sum_{m=2}^{N(i)} C_{2(im)} & -\sum_{m=2}^{N(i)} C_{1(im)} & C_{2(i2)} & C_{1(i2)} & \cdots & C_{2(iN(i))} & C_{1(iN(i))} \end{bmatrix}. \quad (5.37)$$

and for 3-D problems,

$$\mathbf{C}^{(i)} = \begin{bmatrix} -\sum_{m=2}^{N(i)} C_{1(im)} & 0 & 0 & C_{1(i2)} & 0 & 0 & \cdots & C_{1(iN(i))} & 0 & 0 \\ 0 & -\sum_{m=2}^{N(i)} C_{2(im)} & 0 & 0 & C_{2(i2)} & 0 & \cdots & 0 & C_{2(iN(i))} & 0 \\ 0 & 0 & -\sum_{m=2}^{N(i)} C_{3(im)} & 0 & 0 & C_{3(i2)} & \cdots & 0 & 0 & C_{3(iN(i))} \\ -\sum_{m=2}^{N(i)} C_{2(im)} & -\sum_{m=2}^{N(i)} C_{1(im)} & 0 & C_{2(i2)} & C_{1(i2)} & 0 & \cdots & C_{2(iN(i))} & C_{1(iN(i))} & 0 \\ 0 & -\sum_{m=2}^{N(i)} C_{3(im)} & -\sum_{m=2}^{N(i)} C_{2(im)} & 0 & C_{3(i2)} & C_{2(i2)} & \cdots & 0 & C_{3(iN(i))} & C_{2(iN(i))} \\ -\sum_{m=2}^{N(i)} C_{3(im)} & 0 & -\sum_{m=2}^{N(i)} C_{1(im)} & C_{3(i2)} & 0 & C_{1(i2)} & \cdots & C_{3(iN(i))} & 0 & C_{1(iN(i))} \end{bmatrix} \quad (5.38)$$

where $C_{k(im)}$ ($k = 1, 2, 3$; $m = 2, 3, \dots, N(i)$) are defined as

$$C_{k(im)} = \mu_{(im)} \omega_{(im)} g_{k(im)} V_{(m)}, \quad (5.39)$$

where $g_{k(im)}$ is defined in Eq. (5.2), $V_{(m)}$ is the volume of the node $\mathbf{x}_{(m)}$, $\mu_{(im)}$ and $\omega_{(im)}$ represents the bond status and the weight function, respectively. Based on the constitutive law of classical continuum mechanics, the stress vector of the enriched node $\mathbf{x}_{(i)}$ in discrete form is

$$\{\sigma\}_{(i)}^{er} = \mathbf{D}\mathbf{C}^{(i)}\mathbf{u}^{(i)} = \mathbf{D}\mathbf{C}^{(i)}\mathbf{M}^{(i)}\mathbf{u}_g, \quad (5.40)$$

From Eq. (5.11), for one-point quadrature, we derive the internal force vector of the

enrich node $\mathbf{x}_{(i)}$ in discrete form as follows:

$$\mathbf{L}_{(i)}^{er} = \mathbf{H}^{(i)} \mathbf{u}^{(i)} = \mathbf{H}^{(i)} \mathbf{M}^{(i)} \mathbf{u}_g, \quad (5.41)$$

where $\mathbf{H}$ is defined as

$$\mathbf{H}^{(i)} = \begin{bmatrix} -\sum_{m=2}^{N_{(i)}} \mu_{(im)} \omega_{(im)} \mathbf{G}_{(im)} V_{(m)} & \mu_{(i2)} \omega_{(i2)} \mathbf{G}_{(i2)} V_{(2)} & \cdots & \cdots & \mu_{(iN_{(i)})} \omega_{(iN_{(i)})} \mathbf{G}_{(iN_{(i)})} V_{(N_{(i)})} \end{bmatrix}. \quad (5.42)$$

5.3.2.2 Stiffness matrix of enriched element

Following Eq. (5.18), the virtual inner work of enriched elements is

$$\delta U_e^{er} = \int_{S_e} \delta \mathbf{u}^T \boldsymbol{\sigma} \mathbf{n} dS - \int_{V_e} \delta \mathbf{u}^T \mathbf{L} dV. \quad (5.43)$$

Within the enriched element, we do not employ the Gauss divergence theorem and Gauss integration as we do with the standard element, since discontinuities may exist within the enriched element for which the divergence theorem and Gauss integration are invalid. Instead, we apply the one-point quadrature method, which was employed in many published PD models, and the nonlocal stress (Eq. (5.40)) and nonlocal internal force (Eq. (5.41)) are used.

Based on Eq. (5.41) and the one-point quadrature method, the virtual work of the inner

body force of enriched element is

$$\begin{aligned}
\delta U_{eB}^{er} &= - \int_{V_e} \delta \mathbf{u}^T \mathbf{L} dV \\
&= - \sum_{i=1}^{N_e} \frac{V_e}{N_e} \delta \mathbf{u}_{(i)}^T \mathbf{L}_{(i)}^{er} \\
&= - \sum_{i=1}^{N_e} \frac{V_e}{N_e} \delta \mathbf{u}_g^T \mathbf{M}_{(i)}^T \mathbf{H}^{(i)} \mathbf{M}^{(i)} \mathbf{u}_g \\
&= \delta \mathbf{u}_g^T \left(- \sum_{i=1}^{N_e} \frac{V_e}{N_e} \mathbf{M}_{(i)}^T \mathbf{H}^{(i)} \mathbf{M}^{(i)} \right) \mathbf{u}_g \\
&= \delta \mathbf{u}_g^T \mathbf{K}_{EB}^{er} \mathbf{u}_g,
\end{aligned} \tag{5.44}$$

in which V_e represents the element volume, N_e represents the number of nodes of each element, $\mathbf{K}_{EB}^{er}$ is the stiffness matrix from the interior body force contribution defined as

$$\mathbf{K}_{EB}^{er} = - \sum_{i=1}^{N_e} \frac{V_e}{N_e} \mathbf{M}_{(i)}^T \mathbf{H}^{(i)} \mathbf{M}^{(i)}. \tag{5.45}$$

The interior surface traction of the enriched element can be expressed as

$$\boldsymbol{\sigma} \mathbf{n} = \mathbf{N} \{ \sigma \}. \tag{5.46}$$

For 2-D problems, the normal matrix $\mathbf{N}$ is defined as

$$\mathbf{N} = \begin{bmatrix} n_1 & 0 & n_2 \\ 0 & n_2 & n_1 \end{bmatrix}. \tag{5.47}$$

and for 3-D problems,

$$\mathbf{N} = \begin{bmatrix} n_1 & 0 & 0 & n_2 & 0 & n_3 \\ 0 & n_2 & 0 & n_1 & n_3 & 0 \\ 0 & 0 & n_3 & 0 & n_2 & n_1 \end{bmatrix}. \tag{5.48}$$

The virtual work of the internal surface traction of the enriched element is

$$\begin{aligned}
\delta U_{eS}^{er} &= \int_{S_e} \delta \mathbf{u}^T \boldsymbol{\sigma} \mathbf{n} dS \\
&= \sum_s^{N_s} \sum_i^{N_{sn}} \frac{A_s}{N_{sn}} \delta \mathbf{u}_{(i)}^T \mathbf{N}_s \{\sigma\}_{(i)}^{er} \\
&= \sum_s^{N_s} \sum_i^{N_{sn}} \frac{A_s}{N_{sn}} \delta \mathbf{u}_g^T \mathbf{M}_{(i)}^T \mathbf{N}_s \mathbf{D} \mathbf{C}^{(i)} \mathbf{M}^{(i)} \mathbf{u}_g \\
&= \delta \mathbf{u}_g^T \mathbf{K}_{ES}^{er} \mathbf{u}_g
\end{aligned} \tag{5.49}$$

in which N_s is the number of the surface of the element, N_{sn} is the number of the nodes on the surface s , A_s is the area of the surface s , $\mathbf{N}_s$ is the normal matrix of the surface s as defined in Eq. (5.47) or Eq. (5.48), and $\mathbf{K}_{ES}^{er}$ is the stiffness matrix from surface traction contribution and is defined as

$$\mathbf{K}_{ES}^{er} = \sum_s^{N_s} \sum_i^{N_{sn}} \frac{A_s}{N_{sn}} \mathbf{M}_{(i)}^T \mathbf{N}_s \mathbf{D} \mathbf{C}^{(i)} \mathbf{M}^{(i)}. \tag{5.50}$$

Thus, the total virtual internal work within the enriched element is

$$\delta U_e^{er} = \delta U_{eB}^{er} + \delta U_{eS}^{er} = \delta \mathbf{u}_g^T (\mathbf{K}_{EB}^{er} + \mathbf{K}_{ES}^{er}) \mathbf{u}_g = \delta \mathbf{u}_g^T \mathbf{K}_E^{er} \mathbf{u}_g, \tag{5.51}$$

in which $\mathbf{K}_E^{er}$ is the global element stiffness of the enriched elements defined as

$$\mathbf{K}_E^{er} = \mathbf{K}_{EB}^{er} + \mathbf{K}_{ES}^{er}. \tag{5.52}$$

It is worthy to note that if an element surface is shared by two enriched elements, the interior surface traction has no contribution to the total virtual internal work, since the normal vector is $\mathbf{n}$ on one side, and is $(-\mathbf{n})$ on the other side. Therefore, the virtual work of both will cancel each other.

5.3.3 Governing equations

As presented in Sections 5.3.1 and 5.3.2, the total virtual internal work is

$$\begin{aligned}
\delta U &= \sum_e^{N^{std}} \delta U_e^{std} + \sum_e^{N^{er}} \delta U_e^{er} \\
&= \delta \mathbf{u}_g^T \left(\sum_e^{N^{std}} \mathbf{K}_E^{std} \right) \mathbf{u}_g + \delta \mathbf{u}_g^T \left(\sum_e^{N^{er}} \mathbf{K}_E^{er} \right) \mathbf{u}_g \\
&= \delta \mathbf{u}_g^T \mathbf{K} \mathbf{u}_g
\end{aligned} \tag{5.53}$$

in which N^{std} is the total number of standard element, N^{er} is the total number of enriched elements, and $\mathbf{K}$ is the global stiffness matrix defined as

$$\mathbf{K} = \sum_e^{N^{std}} \mathbf{K}_E^{std} + \sum_e^{N^{er}} \mathbf{K}_E^{er}. \tag{5.54}$$

Furthermore, the virtual work from the inertial term can be transformed as

$$\delta U_I = \int_{V_{tot}} \delta \mathbf{u}^T \rho \ddot{\mathbf{u}} dV = \delta \mathbf{u}_g^T \mathbf{M} \ddot{\mathbf{u}}_g, \tag{5.55}$$

and the virtual work from the external forces $\mathbf{b}$ and $\mathbf{T}$ can be transformed as

$$\delta W = \int_{V_{tot}} \delta \mathbf{u}^T \mathbf{b} dV + \int_{S_{tot}} \delta \mathbf{u}^T \mathbf{T} dS = \delta \mathbf{u}_g^T \mathbf{F}, \tag{5.56}$$

Substituting Eqs. (5.53), (5.55) and (5.56) into Eq. (5.16) leads to the governing equations of the enriched FEM-PD model as follows,

$$\mathbf{M} \ddot{\mathbf{u}}_g + \mathbf{K} \mathbf{u}_g = \mathbf{F}, \tag{5.57}$$

For quasi-static and static problems, Eq. (5.57) is reduced to as

$$\mathbf{K} \mathbf{u}_g = \mathbf{F}. \tag{5.58}$$

In this study, the stiffness matrix $\mathbf{K}$ is assembled and stored in a compressed sparse row format with only storing the non-zero coefficients and their row and column information. The assembling algorithm can be found in an earlier publication by the authors [89].

5.4 simulating 2-D quasi-static crack growth

This section presents the simulation model of the quasi-static crack growth for 2-D problems based on EFEM-PD and the linear elastic fracture mechanics (LEFM). The crack propagation criterion is based on the MCTS evaluated from SIFs within the framework of LEFM, where the SIFs are calculated using the I -integral Yau et al. [76], which is derived from the J -integral. The evaluation of SIFs using the I -integral is first discussed in Section 5.4.1. After that, the numerical integration of I -integral is described in Section 5.4.2. Next, the failure criterion is described in Section 5.4.3. Finally, the step-by-step simulation process is presented in Section Section 5.4.4.

5.4.1 Evalution of SIFs

In this work, the SIFs are evaluated based on I -integral which is an extension of J -integral. The concept, first proposed by Yau et al. [76], is reviewed briefly.

Consider two states of a body with crack, that are, the current state (1) denoted by $(u_i^{(1)}, \varepsilon_{ij}^{(1)}, \sigma_{ij}^{(1)})$ and an auxiliary state (2) called by $(u_i^{(2)}, \varepsilon_{ij}^{(2)}, \sigma_{ij}^{(2)})$, the I-integral is defined as

$$I^{(1,2)} = \int_{\Gamma} \left(w^{(1,2)} \mathcal{D}_{1j} - \sigma_{ij}^{(1)} \frac{\partial u_i^{(2)}}{\partial x_1} - \sigma_{ij}^{(2)} \frac{\partial u_i^{(1)}}{\partial x_1} \right) n_j d\Gamma, \quad (5.59)$$

where $\mathcal{D}$ represents the Kronecker delta, n_j represents the normal vector of the integration contour Γ , (x_1, x_2) are local coordinates centered at the crack tip, and $w^{(1,2)}$ is defined as below,

$$w^{(1,2)} = \sigma_{ij}^{(1)} \varepsilon_{ij}^{(2)} = \sigma_{ij}^{(2)} \varepsilon_{ij}^{(1)}. \quad (5.60)$$

Choosing state (2) as the asymptotic fields with $K_I^{(2)} = 1$ and $K_{II}^{(2)} = 0$ leads to the SIF $K_I^{(1)}$

for the current state (1),

$$K_I^{(1)} = \frac{E^*}{2} I^{(1,2)}. \quad (5.61)$$

Similarly, letting the state (2) be the asymptotic fields with $K_I^{(2)} = 0$ and $K_{II}^{(2)} = 1$ leads to the SIF $K_{II}^{(1)}$ for the current state (1) as

$$K_{II}^{(1)} = \frac{E^*}{2} I^{(1,2)}. \quad (5.62)$$

where E^* is defined as

$$E^* = \begin{cases} E, & \text{plane stress,} \\ \frac{E}{1-\nu^2}, & \text{plane strain.} \end{cases} \quad (5.63)$$

5.4.2 Numerical Integration of I -Integral

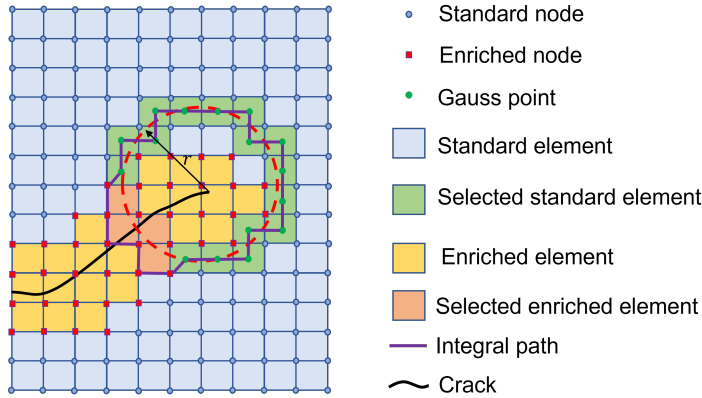


Fig. 5.4: The contour of the I -integral. Elements intersected by the base circle (red dot line) are selected elements. Connecting consecutively all enriched nodes of selected enriched elements (light orange elements) that are outside of the base circle and the Gauss points of selected standard elements (light green element), constructs the integral contour (solid purple lines).

Although it is a common practice to evaluate the J - or I -integral by transforming the contour integral to an equivalent area integral and then using the Gauss integration over the elements of the equivalent area [94], the approach may be invalid for elements cut through with cracks, as Gauss integration requires the integrand to be continuous. To evaluate SIFs, we develop in this section a new numerical method of I -integral over a contour of enriched

nodes and Gauss points of the standard element, based on the rationale that stresses and strains at Gauss points are more accurate than other locations for standard elements. Stresses and strains of enriched nodes can be directly computed based on Eqs. (5.36) and (5.40).

To determine the contour, we define a base circle with radius $r = m_r \Delta_{min}$ centered at the crack tip, as shown in Fig. 5.4, in which m_r is a constant and Δ_{min} is the minimum element size. Next, standard and enriched elements intersected by the circle are designated as selected elements, as illustrated in Fig. 5.4. The integral contour is constructed by connecting consecutively all enriched nodes of selected enriched elements (light orange elements) that are outside of the base circle and the Gauss points of selected standard elements (light green element), as presented by the solid purple lines in Fig. 5.4. With the contour formed by the selected elements, we calculate the interaction integral $I^{(1,2)}$ as

$$I^{(1,2)} = \sum_{p=1}^{N_p} (F_{(p)} + F_{(p+1)}) \frac{l_p}{2}, \quad (5.64)$$

in which l_p is the length between points (p) and $(p+1)$, N_p represents the number of points on the integral contour. Point $(N_p + 1)$ is identical to point (1) , which ensures the closed integral contour. $F_{(p)}$ denotes the integrand at point (p) as:

$$F_{(p)} = \left(w^{(1,2)} \mathcal{D}_{1j} - \sigma_{ij}^{(1)} \frac{\partial u_i^{(2)}}{\partial x_1} - \sigma_{ij}^{(2)} \frac{\partial u_i^{(1)}}{\partial x_1} \right) n_j. \quad (5.65)$$

To evaluate the SIFs by Eqs. (5.61) and (5.62), the displacement, strain, and stress fields $u_i^{(1)}$, $\varepsilon_{ij}^{(1)}$, and $\sigma_{ij}^{(1)}$ of state (1) are calculated from the EFEM-PD model, and $u_i^{(2)}$, $\varepsilon_{ij}^{(2)}$, and $\sigma_{ij}^{(2)}$ of the state (2) are calculated from LEFM formulas with $K_I^{(2)} = 1$, $K_{II}^{(2)} = 0$ or $K_I^{(2)} = 0$, $K_{II}^{(2)} = 1$. Then, the I-integral $I^{(1,2)}$ is calculated by Eq. (5.64).

5.4.3 Crack propagation criterion

To simulate quasi-static crack growth, several conditions must be determined: (1) the onset of growth, (2) the direction of growth, and (3) the amount of growth.

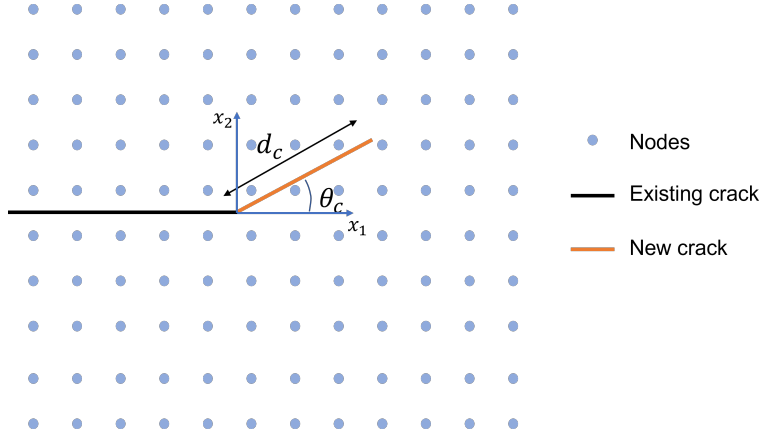


Fig. 5.5: Schematic of crack growth. θ_c is the crack growth direction and d_c is the crack growth amount at each step.

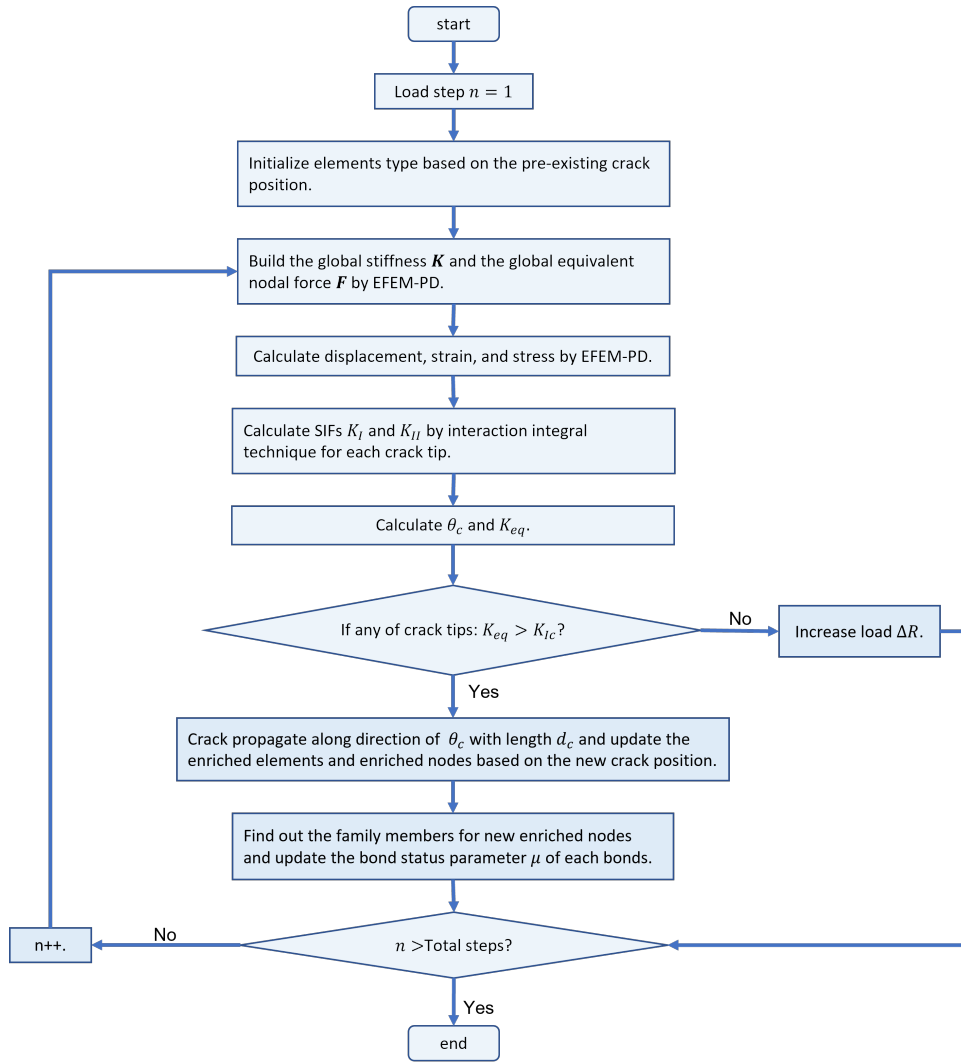


Fig. 5.6: Flowchart of crack propagation simulation.

For mixed-mode loading, various criteria have been developed to determine the first two conditions. In the current work, the MCTS theory [75] is used to determine the onset and the direction of crack growth. For LEFM, the singular asymptotic stresses at the crack tip from LEFM solutions are used in the MCTS criterion to find out the crack growth direction θ_c (Fig. 5.5), which is defined as

$$\theta_c = \begin{cases} 2 \tan^{-1} \left(\frac{K_I}{4K_{II}} - \frac{1}{4} \sqrt{\left(\frac{K_I}{K_{II}} \right)^2 + 8} \right) & \text{for } K_{II} > 0, \\ 2 \tan^{-1} \left(\frac{K_I}{4K_{II}} + \frac{1}{4} \sqrt{\left(\frac{K_I}{K_{II}} \right)^2 + 8} \right) & \text{for } K_{II} < 0, \end{cases} \quad (5.66)$$

For onset of crack growth, the MCTS must reach a critical value, which results in the equivalent SIF as

$$K_{eq} = K_I \cos^3 \frac{\theta_c}{2} - \frac{3}{2} K_{II} \cos \frac{\theta_c}{2} \sin \theta_c. \quad (5.67)$$

with θ_c determined by Eq. (5.66). If $K_{eq} > K_{Ic}$, the crack will grow in the direction of θ_c with an amount of d_c , as shown in Fig. 5.5. In this work, d_c is set to be $\alpha \Delta_{min}$ where Δ_{min} is the minimum element size, and $\alpha \in [0.5, 1.5]$.

5.4.4 Simulation process and flowchart

This section presents the quasi-static crack growth simulation step-by-step to obtain an overall sense of the EFEM-PD model. Fig. 5.6 shows the flowchart of the simulation process.

- Step 1. Initialize all elements as standard elements first. The elements intersecting with the pre-existing crack and their neighboring elements are transformed into enriched elements. A small load is then applied to the material domain, and the nodal force vector $\mathbf{F}$ and the stiffness matrix $\mathbf{K}$ are assembled as described in Section 5.3.
- Step 2. The displacement field is solved by $\mathbf{U} = \mathbf{K}^{-1}$, from which the stress and strain fields are then evaluated. The stresses and strains of the enriched nodes are evaluated by PD Eqs. (5.36) and (5.40), while strains and stresses in the standard elements are obtained based on conventional FEM.

- Step 3. With the fields of displacements, strains, and stresses, the SIFs, K_I and K_{II} are computed from Eqs. (5.61), (5.62), (5.64) and (5.65) for the current crack configuration, and then the θ_c and K_{eq} are evaluated by Eq. (5.66) and Eq. (5.67), respectively.
- Step 4. If $K_{eq} < K_{Ic}$, the crack will propagate along with the direction θ_c by amount d_c . The enriched elements are then updated based on the new crack location. All bonds across the new crack will be treated as broken. The global stiffness K is then updated, which becomes more compliant.

If $K_{eq} > K_{Ic}$, a small load will be added by $\Delta R = \max \left\{ \left(\frac{K_{Ic}}{K_{eq}} - 1 \right) R_n, \Delta R_{max} \right\}$, where R_n is the current loading value, and ΔR_{max} is the pre-defined maximum loading increment.

- Step 5. The simulation goes to the next step.

5.5 Numerical results

To validate the capability of the EFEM-PD model presented in this work, simulations of three 2-D plane stress problems and one 3-D problem of crack propagation are performed and presented in this section. In the first problem, an infinite plate with an inclined stationary crack is subjected to remote uniform traction leading to mixed-mode loading. In the second problem, a diagonal plate with an initial inclined crack is loaded under displacement control, and the crack growth is modeled using a quasi-static simulation approach. In the third problem, a compact tension test specimen with an initial crack in the plane of symmetry is loaded under displacement control. The crack growth is modeled again using the quasi-static approach. In the fourth problem, a 3-D block with a stationary crack is loaded under displacement control. The first, second, and fourth problems have been simulated and reported in an earlier publication using a general method of coupled PD with FEM [86, 89], and they are studied here again using the new EFEM-PD model. The simulations are performed using the PDLSP-FEM solver [95] and results data can be accessed through figshare [96].

In this work, the influence function is specified as

$$\omega(|\boldsymbol{\xi}|) = e^{-\left(\frac{|\boldsymbol{\xi}|}{c\delta(i)}\right)^2}, \quad (5.68)$$

here, c is a constant and is specified as $c = 0.33$ in this work.

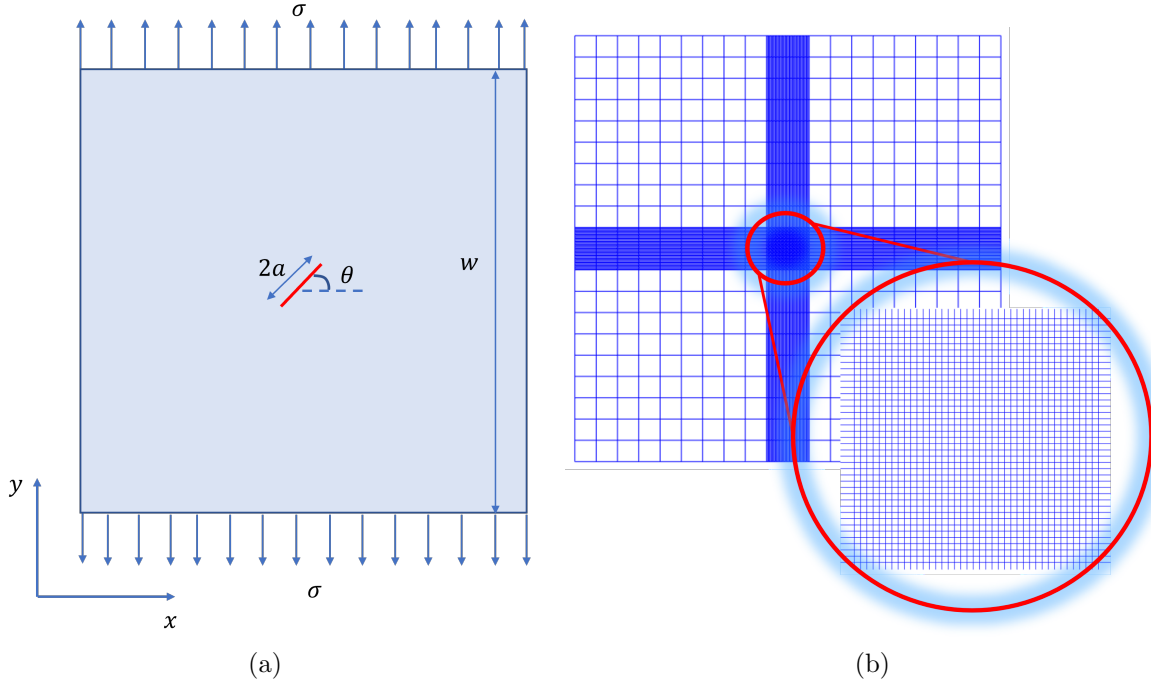


Fig. 5.7: A 2-D infinite plate under mixed-mode loading: (a) Geometry and boundary conditions, (b) Mesh.

5.5.1 A 2-D infinite plate

In this example, we study the SIFs of the 2-D infinite plate to validate the accuracy of the presented EFEM-PD. The effects of enriched elements and the integral path of I -integral are studied. The crack remains stationary, and the primary purpose of this simulation is to investigate the model accuracy and effects of the I -integral contour and the β -enriched element factor.

Fig. 5.7a presents a 2-D square plate with a small crack is subjected to uniform far-field tension $\sigma = 70$ MPa. The plate's material properties are $E = 70$ GPa and $\nu = 0.33$. The

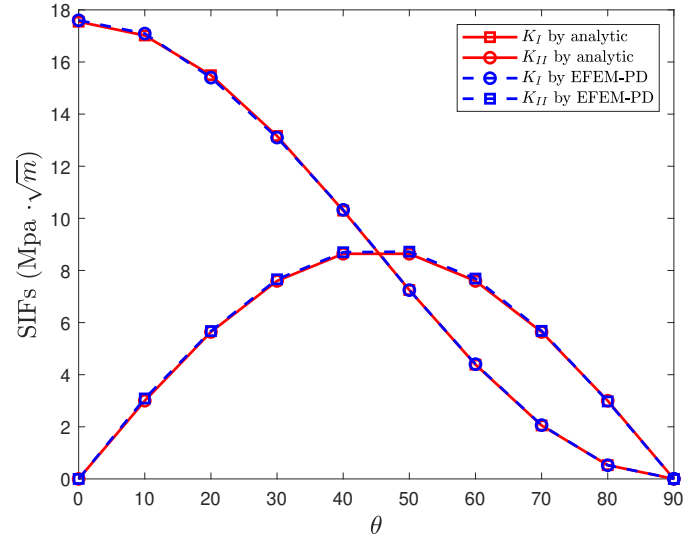


Fig. 5.8: Numerical and analytical evaluation of SIFs at various crack inclined angles θ .

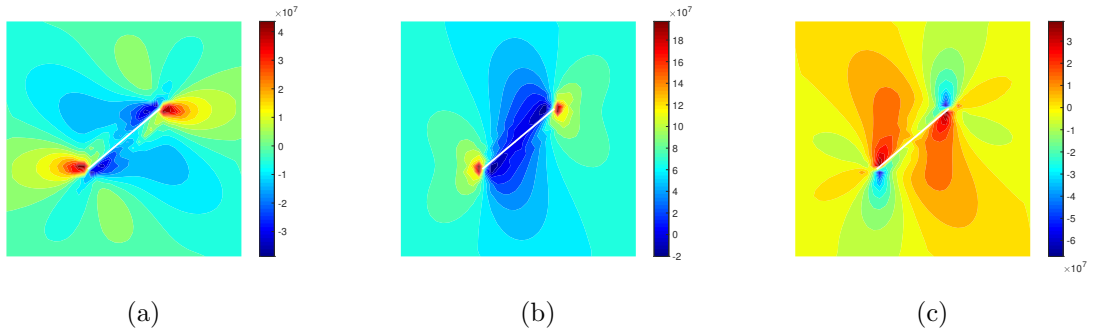


Fig. 5.9: Stress distributions around the crack of the 2-D infinite plate with crack angle $\theta = 40^\circ$: (a) σ_{xx} , (b) σ_{yy} , (c) σ_{xy} .

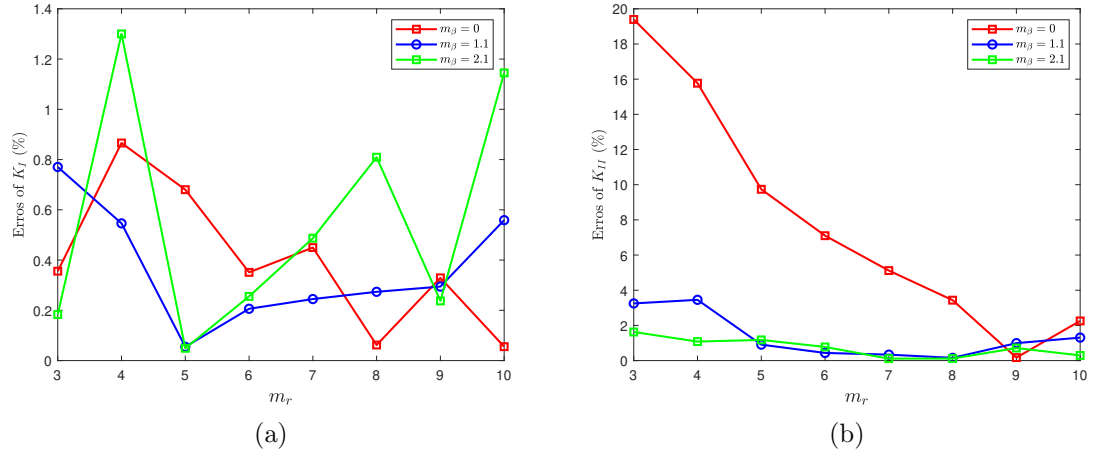


Fig. 5.10: Relative SIFs' error for $\theta = 30^\circ$ at various integration contour and various β -enriched element: (a) K_I , (b) K_{II} .

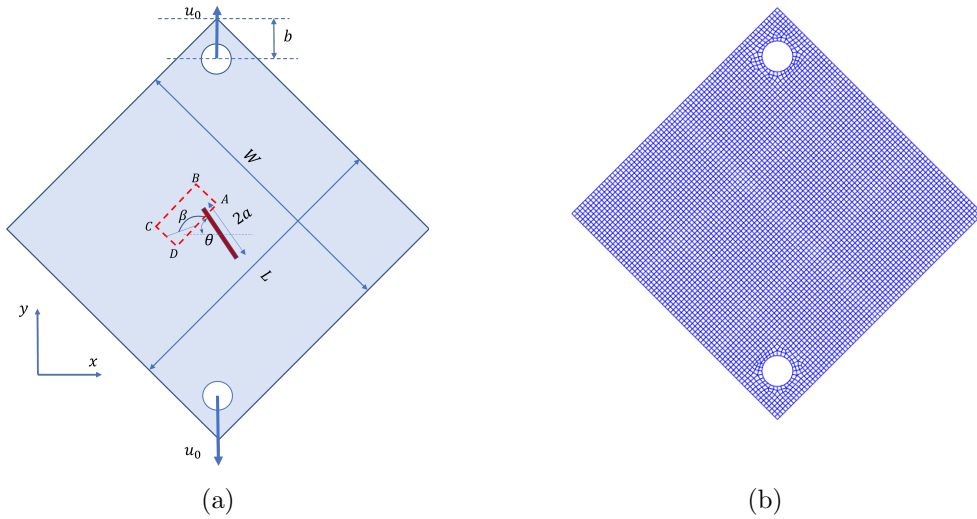


Fig. 5.11: A 2-D diagonal plate with an inclined crack under mixed-mode loading: (a) Geometry and boundary conditions, (b) Meshes.

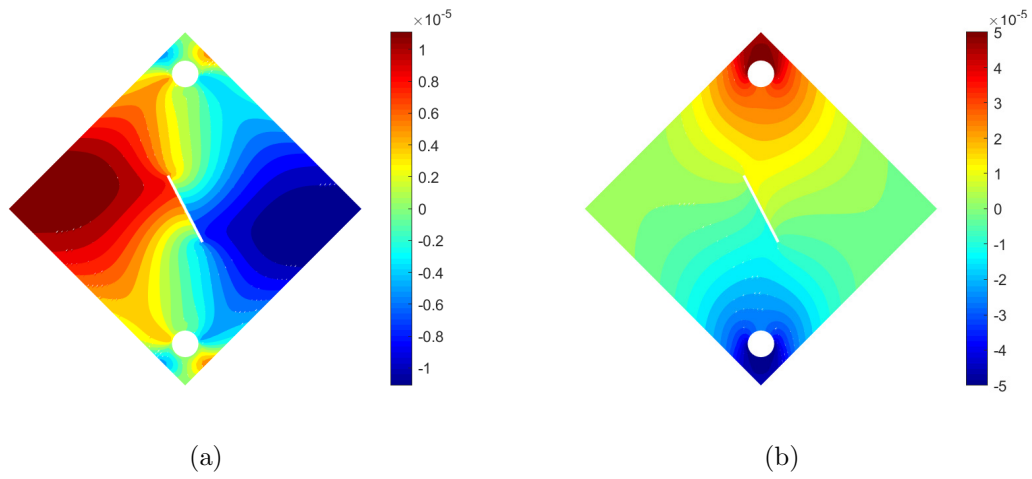


Fig. 5.12: Displacement results diagonal plate by enriched FEM-PD: (a) u_x , (b) u_y .

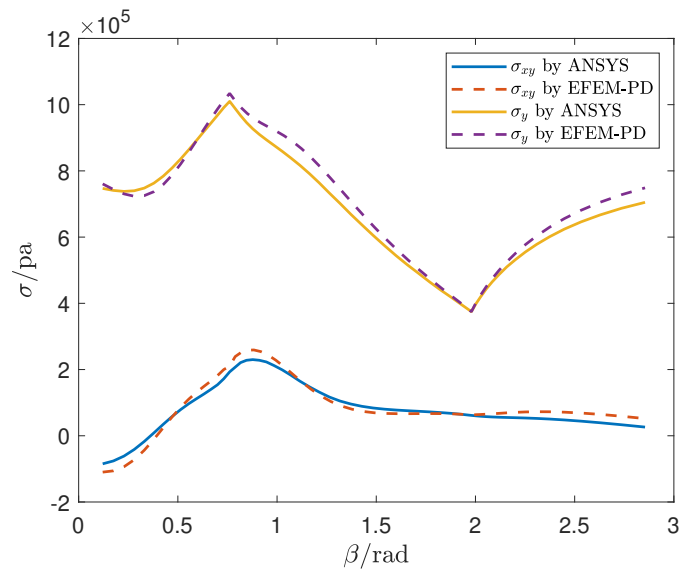


Fig. 5.13: Comparison of FEM (ANSYS) against EFEM-PD for stress results along the path $A - B - C - D$ of the diagonal plate.

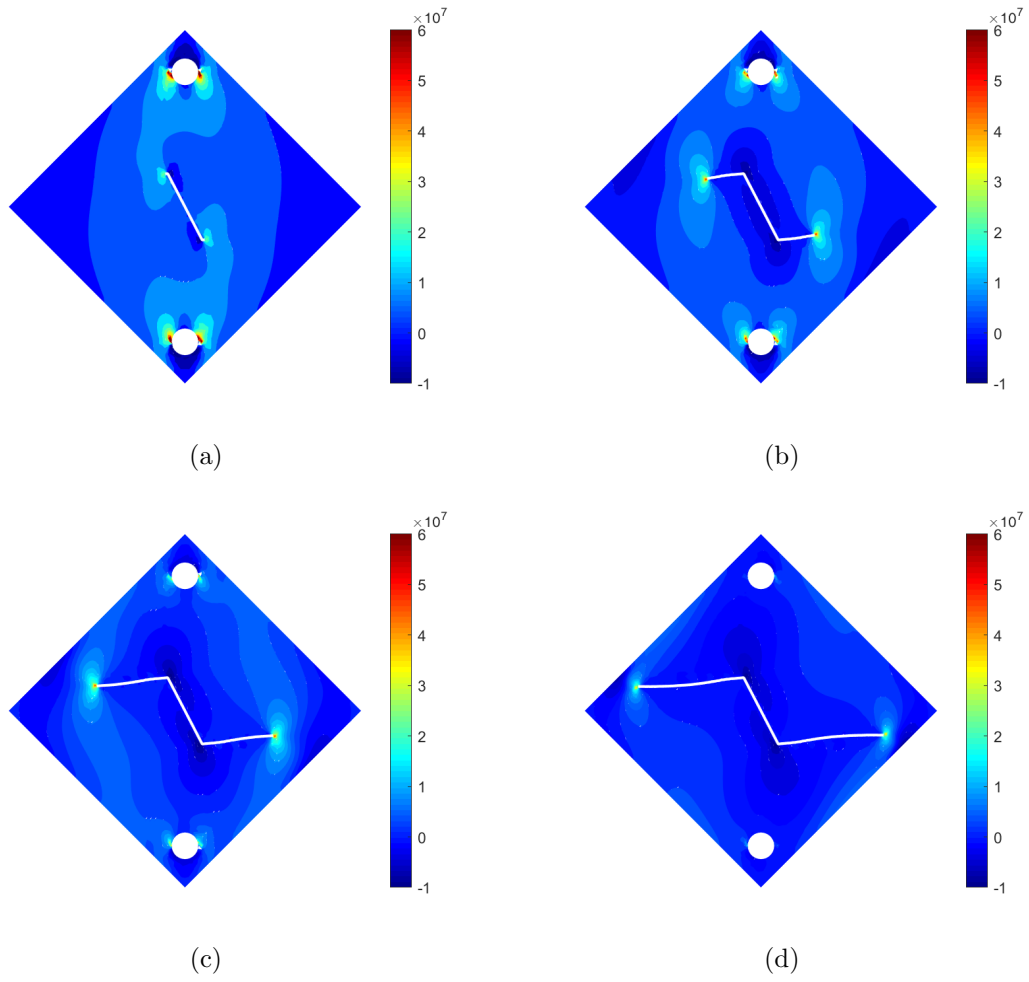


Fig. 5.14: Stress σ_y contour of the 2-D diagonal plate during crack growth.

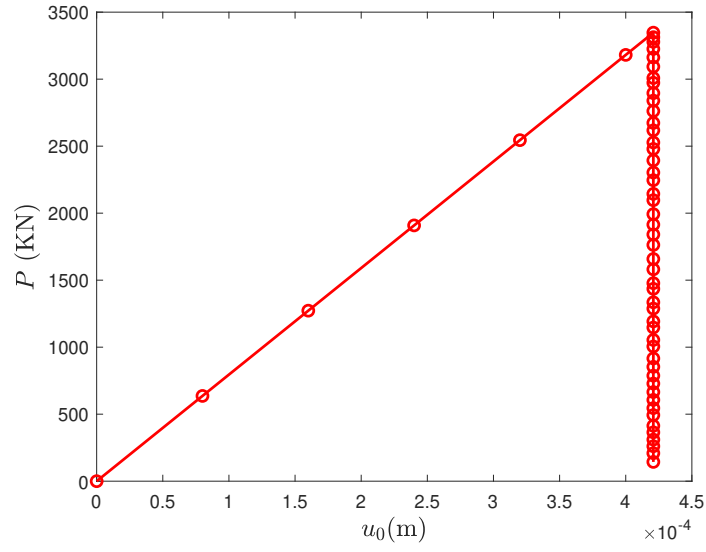


Fig. 5.15: The reaction force of the 2-D diagonal plate during crack growth.

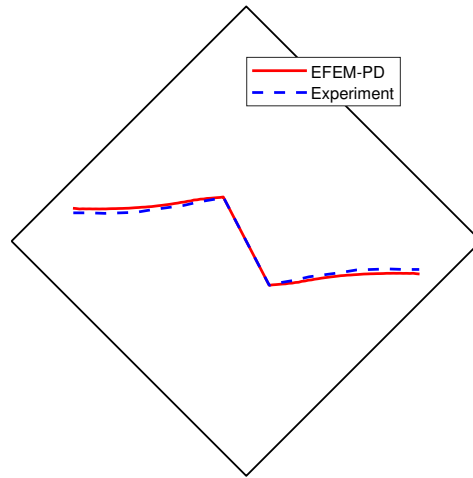


Fig. 5.16: Crack propagation path of the 2-D diagonal plate by EFEM-PD and experiment observation. [1].

plate's dimension is $1 \times 1 \text{ m}^2$, and the initial crack length is specified as $2a = 40 \text{ mm}$. Because of the sufficiently large ratio $W/a = 50$, this plate can be approximately treated as infinity. A small sub-domain of dimension $0.1 \times 0.1 \text{ m}^2$ at the plate center is finely discretized into 1521 elements, and the remaining part is coarsely meshed into 1728 elements (Fig. 5.7b). For this example, the analytical solution of SIFs is defined as

$$\begin{cases} K_I = \sigma \sqrt{\pi a} \cos^2 \beta, \\ K_{II} = \sigma \sqrt{\pi a} \cos \beta \sin \beta. \end{cases} \quad (5.69)$$

In this example, the based circle for the I -integral contour is selected as $r = m_r \Delta_{min}$ where $m_r = 6$ and Δ_{min} is the minimum element size, and the horizon is $\delta_{(i)} = 3\Delta_{(i)}$. The β -enriched elements are defined as $m_\beta = 2.1$.

Fig. 5.8 presents the results of SIFs, K_I and K_{II} at various crack inclined angles θ from theoretical solution and numerical simulation. It is evident that the agreement between numerical and theoretical results is remarkable, and the relative error can be almost neglected. Fig. 5.9 shows the stress distributions around the crack by EFEM-PD with the crack inclined $\theta = 40^\circ$. The result confirms that stresses concentrate at the crack tips.

The effects of integration radius $r = m_r \Delta_{min}$ and the β -enriched element factor m_β on the evaluation of SIFs are also studied for the plate with the crack inclination angle of $\theta = 30^\circ$. The results are presented in Fig. 5.10. Fig. 5.10a shows that, the relative errors of K_I between the theoretical and numerical results remain consistently below 1.4% for various m_β and m_r . Thus, the effect of the m_β -enriched element factor m_β on the evaluation of K_I is practically negligible.

Fig. 5.10b shows the results of K_{II} . For $m_r \leq 8$, the relative errors of K_{II} between the theoretical and numerical results are quite large, with the significant error being up to 19.4% when there are no β -enriched elements ($m_\beta = 0$). In the presence of β -enriched elements, the relative errors of K_{II} are less than 3.25% for $m_\beta = 1.1$, and less than 1.6% for $m_\beta = 2.1$ at different m_r . Overall, the presence of β -enriched elements has a significant beneficial effect on the evaluation of K_{II} and a negligible effect on the evaluation of K_I . With β -enriched

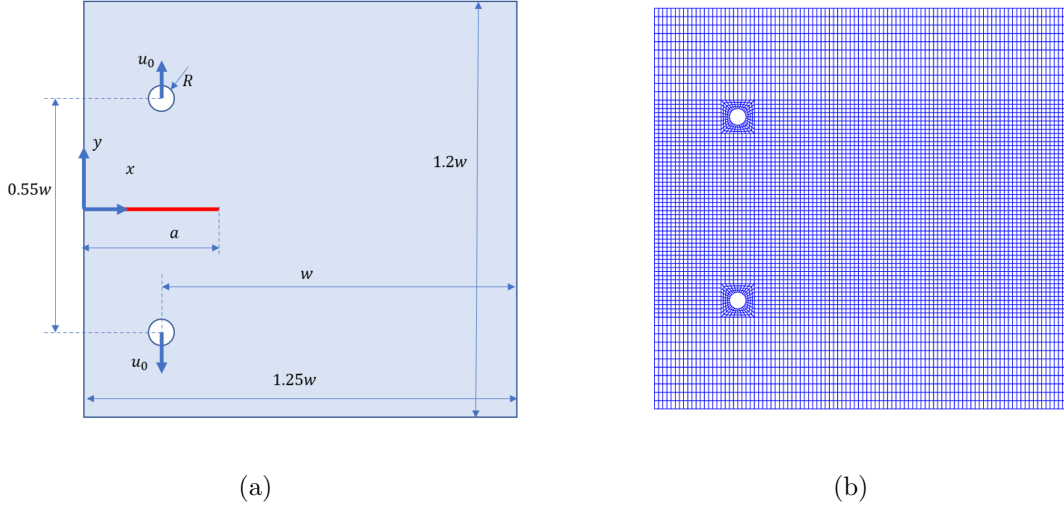


Fig. 5.17: Compact tension test: (a) Geometry and boundary conditions, (b) meshes.

elements, the relative errors of SIFs are almost negligibly minor at different m_r . Thus the evaluation of SIFs by I -integral is path independent.

5.5.2 A 2-D diagonal plate

For the second example, we first conduct a static simulation of the cracked body by both EFEM-PD and FEM (ANSYS) and compare the results to show the accuracy of the proposed EFEM-PD. We then simulate the quasi-static crack propagation using EFEM-PD and compare the simulation results with published experiments.

The problem to be simulated is a diagonal square plate with a pre-existing crack. As presented in Fig. 5.11a, the plate with dimension $150 \times 150 \times 5 \text{ mm}^3$ is under displacement loading u_0 . The crack is inclined with angle $\theta = 62.5^\circ$, and its length is $2a = 45 \text{ mm}$. The loading hole has a radius of 8 mm, and the length between the corner of the plate and the center of the hole is $b = 25 \text{ mm}$. Young's modulus is $E = 2.94 \text{ GPa}$, Poisson ratio $\nu = 0.38$, and fracture toughness is $K_{Ic} = 1.33 \text{ MPa}$. The problem domain is meshed into 5607 elements and 5785 nodes, as presented in Fig. 5.11b. The based circle for the I -integral contour is $r = 6\Delta_{min}$. The horizon is specified as $\delta_{(i)} = 3\Delta_{(i)}$. The β -enriched element factor is set to be $m_\beta = 3$.

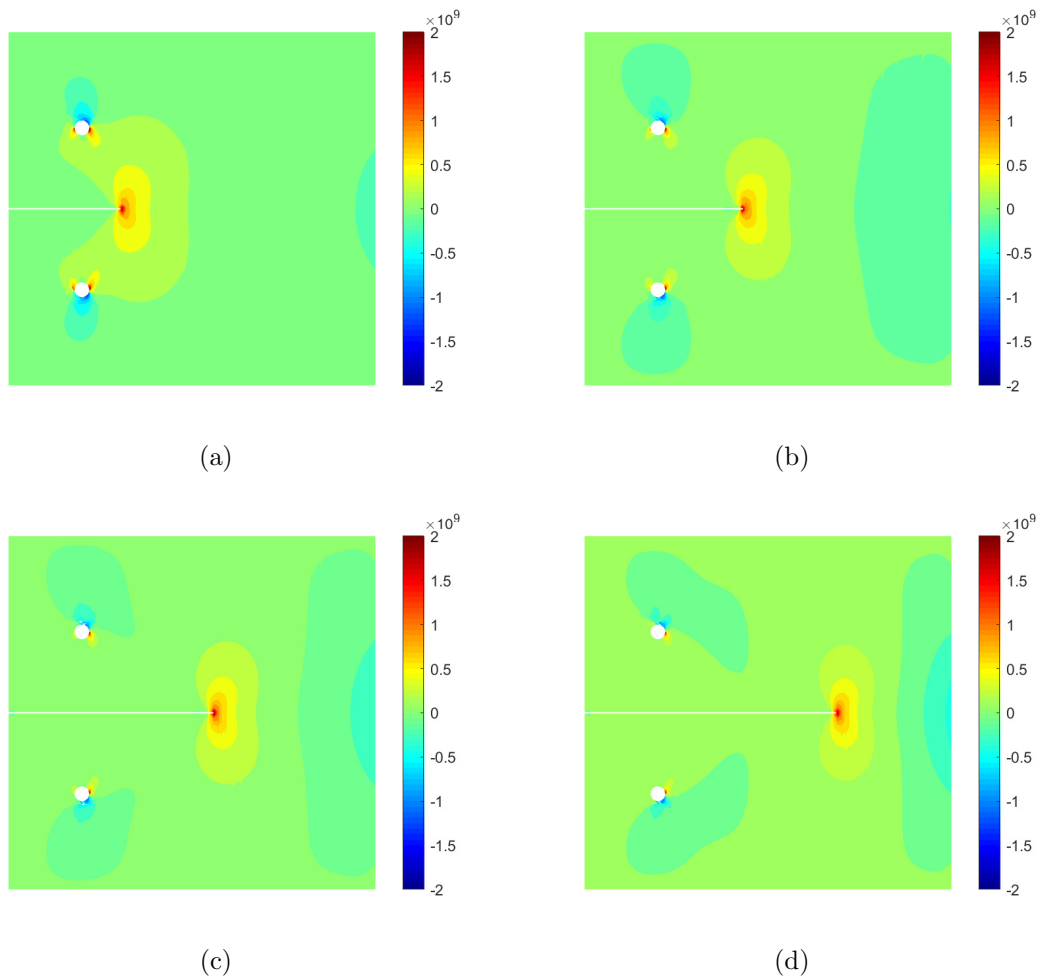


Fig. 5.18: Stress distributions of σ_y of compact tension test: (a) $u_0 = 0.0476$ mm; (b) $u_0 = 0.0670$ mm; (c) $u_0 = 0.0928$ mm; (d) $u_0 = 0.1218$ mm.

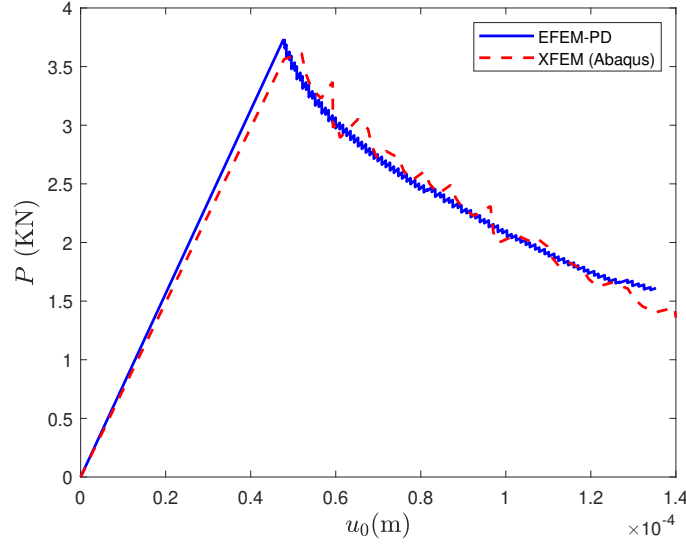


Fig. 5.19: The reaction force the CT specimen under displacement control.

A static stimulation for this problem is first performed with displacement loading $u_0 = 5 \times 10^{-5}$ m. Fig. 5.12 depicts the displacement field of the whole domain obtained by EFEM-PD. The figure reveals apparent displacement discontinuities across the crack. Fig. 5.13 shows the static results of the shear stresses, σ_{xy} and the normal stresses, σ_y by EFEM-PD and FEM (ANSYS) along path $A - B - C - D$ defined in Fig. 5.11a, where the key points' coordinates are A (7.43, 28.6) mm, B (-13.8, 49.9) mm, C (-49.9, 13.8) mm and D (-13.8, 49.9) mm. As shown in Fig. 5.13, the results of these two methods are in good agreement.

After the static simulation comparison, a quasi-static analysis is performed to simulate the crack propagation. The amount of crack growth for each step is set to be $d_c = \Delta_{min}$. Distributions of stress σ_y of the diagonal plate at various stages of crack growth are shown in Fig. 5.14. The figure reveals that the stresses concentrate at the crack tip. Variations of the reaction force at the loading points with crack propagation are shown in Fig. 5.15. The figure shows that the crack starts to grow unstably when displacement loading reaches $u_0 = 0.421$ mm with the reaction force decreasing as the crack grows. The critical reaction force at instability is $P = 3347$ N from the EFEM-PD simulation, whose relative error is 4.85%, comparing to the experimental result of $P_{cr} = 3192$ N [1]. Fig. 5.16 presents the crack

propagation path of the plate from EFEM-PD simulation and the result from experimental observation, and they are in good agreement.

5.5.3 Compact tension test

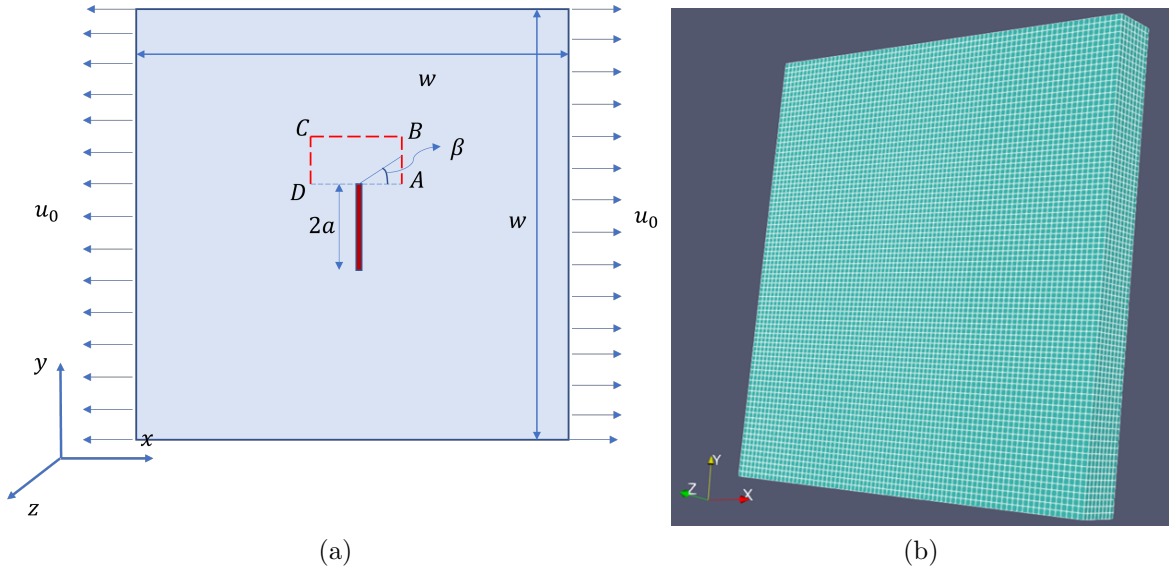


Fig. 5.20: The 3-D block with a pre-existing crack under displacement constraint: (a) Geometry and boundary conditions, (b) Hexahedron meshes.

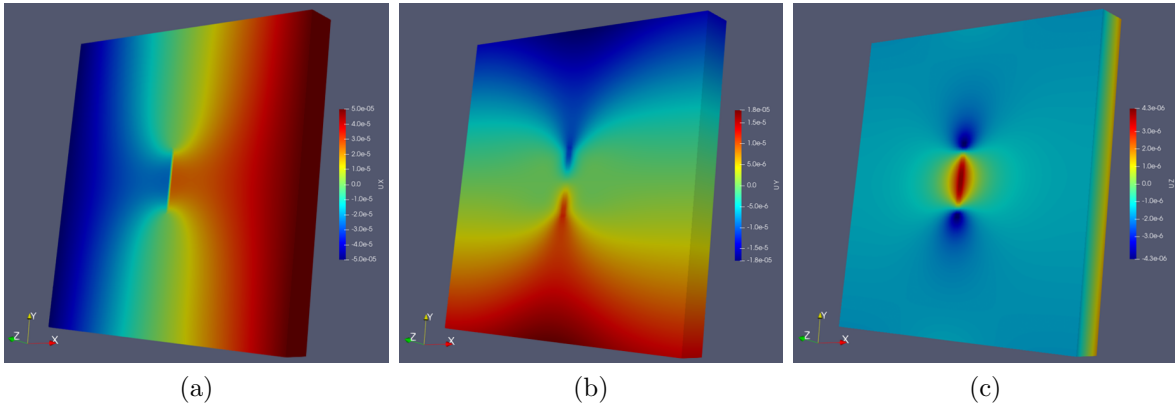


Fig. 5.21: Displacement solutions of the 3-D block with a pre-existing crack by EFEM-PD: (a) u_x , (b) u_y , (c) u_z .

In this example, the quasi-static crack propagation in a compact tension (CT) specimen is simulated. The results are compared with those obtained using the method of XFEM

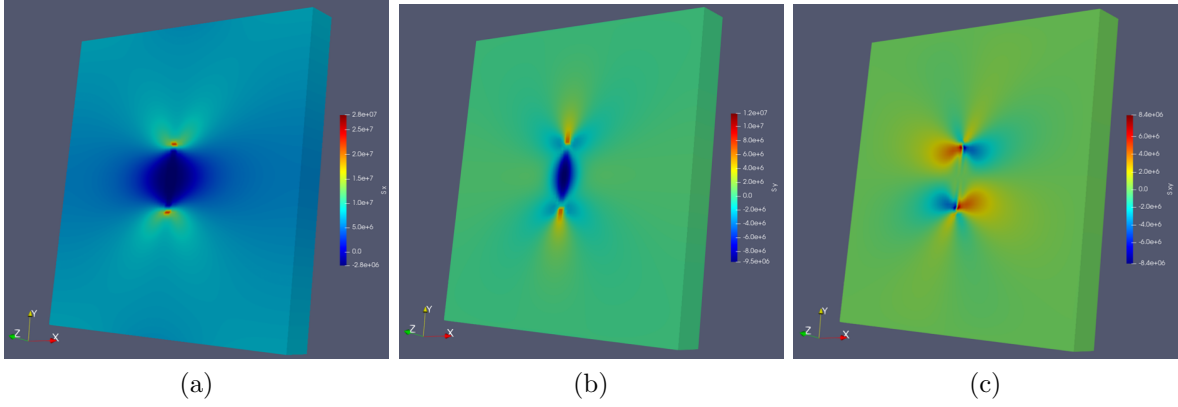


Fig. 5.22: Stress solutions of the 3-D block a with pre-existing crack by EFEM-PD: (a) σ_x , (b) σ_y , (c) σ_{xy}

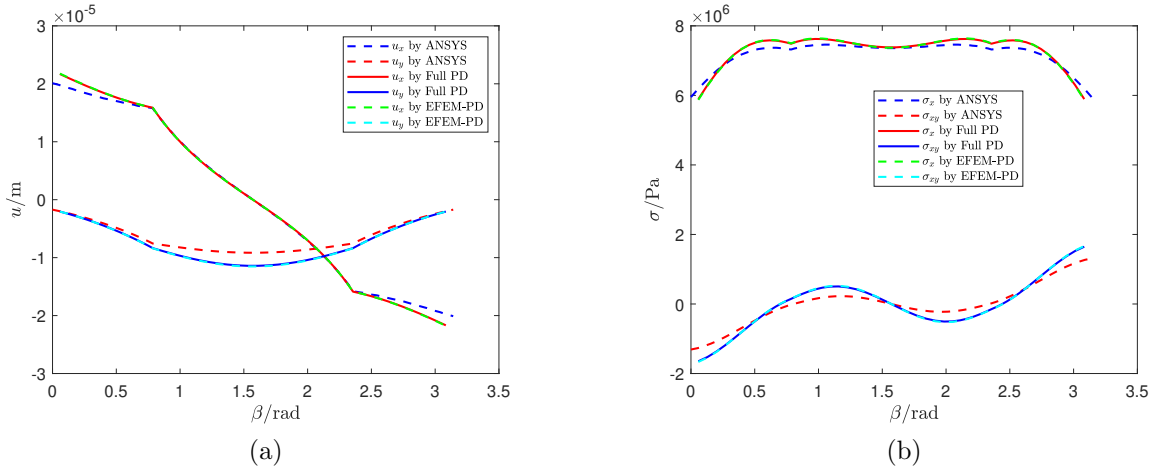


Fig. 5.23: Comparison of FEM (ANSYS) against EFEM-PD for displacement and stress results along with the path $A - B - C - D$ of the 3-D block: (a) Displacements Comparison; (b) Stresses comparison.

from ABAQUS.

The compact tension (CT) specimen is subjected to displacement loading u_0 , as depicted in Fig. 5.17a. The plate's dimension is specified as $w = 50$ mm with thickness $B = 1$ mm. The initial length of the crack is $a = 15$ mm. The material properties of the plate are specified as $E = 214$ GPa, $\nu = 0.27$, and $K_{Ic} = 64.2$ MPa $\sqrt{\text{m}}$. The plate is meshed into 7834 nodes and 7628 elements, as shown in Fig. 5.17b. The amount of crack growth is defined as $d_c = \Delta_{min}$, where Δ_{min} is the minimum element size. The horizon is $\delta_{(i)} = 3\Delta_{(i)}$, and the I -integral contour is defined as $r = 6\Delta_{min}$. The β -enriched elements are defined by $m_\beta = 3$.

Fig. 5.18 depicts the crack growth along with stress contours of σ_y of the plate at various simulation steps. It reveals that the crack grows horizontally as expected and confirms the stresses concentrating at the crack tip with the neat-tip stress fields, consistent with analytical solutions from LEFM. For comparison, the problem is also solved by XFEM with the virtual crack closure technique using ABAQUS. The variations of reaction forces with prescribed displacement u_0 of the CT test obtained from EFEM-PD and XFEM are plotted in Fig. 5.19. The figure shows a good agreement between the two methods.

5.5.4 A 3-D block

Because of the nonlocal nature of nodal interactions, PD simulations are typically much more computationally intensive than FEM simulations for similar problems, especially for 3-D cases. In this section, simulations of a 3-D body with a stationary crack using EFEM-PD, full PD in which PDLSE equations enrich the entire elements, and FEM (using ANSYS) models are conducted and reported. The 3-D block is loaded under displacement control. The purpose of these simulations is to compare the model accuracy and efficiency.

This 3-D example is much more computationally intensive than other previous 2-D examples. The EFEM-PD and full PD simulations are parallel run on four cores of the *Moles* computing nodes of the high-performance cluster *Beocat* at *Kansas State University* by message passing interface.

Fig. 5.20a shows the model geometry with a pre-existing crack subjected to displacement

loading $u_0 = 5 \times 10^{-5}$ m. The dimensions of the block are thickness $B = 0.1$ m and width $w = 1$ m. The crack length is $2a = 0.2$ m. The whole domain is constructed by 52976 hexahedron elements and 61074 nodes, as shown in Fig. 5.20b. The horizon is specified as $\delta_{(i)} = 3\Delta_{(i)}$. β -enriched elements are defined by $m_\beta = 2.1$.

Table 5.1: Wall time to assemble the global stiffness matrix and solve for displacement solutions, and the memory usages to store the global stiffness matrix, of the 3-D block with a pre-existing crack.

m_δ	Wall time (s)		Memory usage (MB)	
	Enriched FEM-PD	Full PD	Enriched FEM-PD	Full PD
3	13.5	63.7	200.4	700.6
4	18.6	169.3	218.5	1576.8
5	25.6	410.5	247.1	2940.9

Fig. 5.21 shows the u_x , u_y , and u_z displacement fields, and Fig. 5.22 shows the σ_x , σ_y and σ_{xy} stress fields of the 3-D block from EFEM-PD. As revealed in these figures, stresses concentrate at the crack tips. Fig. 5.23 compares the displacements u_x and u_y and the stresses σ_{xy} and σ_x , from EFEM-PD, full PD, and FEM (ANSYS), along path A-B-C-D as marked in Fig. 5.20a, in which the key points' coordinates are A (0.15, 0.1, 0) m, B (0.15, 0.25, 0) m, C (-0.15, 0.25, 0) m, and D (-0.15, 0.1, 0) m. The comparison shows that the results from the full PD and results from EFEM-PD are in excellent agreement and are practically indistinguishable. It is observed that for the horizontal segment $B - C$, results of u_x from EFEM-PD and full PD model are close to those from ANSYS, while for the vertical segments $A - B$ and $C - D$, results of u_x from EFEM-PD and full PD model are slightly larger than those from ANSYS. Nevertheless, for the horizontal segment $B - C$, results of u_y from EFEM-PD and full PD model are slightly larger than those from ANSYS, while for the vertical segments $A - B$ and $C - D$, results of u_y from EFEM-PD and full PD model are very close to those from ANSYS. It is evident that for both stresses and displacements, the results by all three methods are in good agreement.

To demonstrate the improved computational efficiency of the presented EFEM-PD, the wall time to assemble the global stiffness matrix and solve displacement solutions on four computing cores is tracked, and the memory usages store the global stiffness matrix for each

core is monitored. As shown in Table 5.1, the wall time for EFEM-PD is 13.5-25.6 s for various horizon size $\delta_{(i)} = m_\delta \Delta_{(i)}$ ($m_\delta = 3, 4, 5$), while the full PD model requires 63.7-410.5 s, which is 4.7-16.0 times that of the EFEM-PD model. The memory usage of EFEM-PD is 200.4-247.1 MB, while the full PD model requires 700.6-2940.9 MB, which is 3.5-11.9 times that of the EFEM-PD model. Therefore, in general, the EFEM-PD dramatically improves the computational cost in CPU run time and memory usage compared to the full PD model.

5.6 Conclusions

In this work, we have developed a framework of the Enriched Finite Element Method by Peridynamics (EFEM-PD) for modeling discontinuities analogous to the concept of enriched element of XFEM. In EFEM-PD, the Finite Element Method (FEM) is coupled with Peridynamics (PD) with adaptivity to minimize the PD region to maximize the computational efficiency. With the framework of EFEM-PD, the elements intersecting with the crack line and their neighboring elements are enriched by the PDLSP model that is capable of modeling the progression of bond breakages and cracks growth. The remaining elements are governed by conventional FEM. The global stiffness matrix and governing equations of the whole problem domain in 2-D and 3-D are derived. A numerical procedure for the I -integral to calculate SIFs for 2-D problems is proposed and implemented. Crack propagation is modeled using quasi-static with the criterion of maximum hoop tension stress. New contributions of this work include FEM enriched with PD with adaptivity for minimizing the PD region and the application of EFEM-PD to quasi-static crack propagation analysis.

Several numerical examples are conducted to verify the efficacy of the proposed EFEM-PD. The remarks of numerical simulations are as below.

1. One 2-D infinite plate under mixed-mode loading is analyzed, and its SIFs are calculated. Comparing the SIFs between analytical and numerical solutions reveals excellent accuracy of the presented EFEM-PD.
2. Studying the evaluation of SIFs reveals that I -integral is path independent, and β -

enriched elements have a significant beneficial effect on evaluations of SIFs.

3. Static simulation of a diagonal plate is performed, and the static solutions are in excellent agreement with ANSYS results.
4. EFEM-PD also simulates the quasi-static crack propagation of the 2-D diagonal plate under displacement control, and the crack path and peak loading are in close agreement with experiment observation.
5. Simulations of a compact tension test by EFEM-PD and XFEM (ABAQUS) are performed, and the reaction forces from both methods are in good agreement.
6. The static solutions of a 3-D block with pre-existing crack are obtained by EFEM-PD, full PD, and FEM (ANSYS), and the comparison reveals that the results from the three methods are in very good agreement.
7. The performance evaluation of the 3-D example shows that EFEM-PD saves up to 16.0 times in terms of computing time and up to 11.9 times in terms of memory usage against the pure PD model.

Chapter 6

Final conclusions

The research presented in this dissertation focuses on advancing the theory and formulation of Peridynamics and applying Peridynamics in the deformation and failure analysis of solids. New contributions from the current work include the following:

1. RNOSBPD: A new Revised Non-Ordinary State-Based Peridynamics (RNOSBPD) is proposed and formulated. RNOSBPD is proved to recover the original NOSBPD for spherical interaction domains and is valid for interaction domains of arbitrary shapes. It eliminates the need for volume and surface correction used in most published PD models and makes coupling with FEM easy, efficient, and accurate.
2. Quasi-static crack simulation by PDLSM-FEM: Peridynamics based on Least Square Minimization coupled with FEM (PDLSM-FEM) is developed. A quasi-static method is pioneered for simulating crack propagation using PDLSM-FEM. A new numerical method is proposed and used in the crack propagation simulation to evaluate the stress intensity factors based on the I-integral.
3. 3D PDLSM-FEM model with an implicit solution by Message Passing Interface: 3D PD simulations are computationally intensive. Our work is the first to develop a 3D PDLSM-FEM model to assemble the global stiffness matrix in a Compressed Sparse Row (CSR) format based on Message Passing Interface (MPI), and to solve the sys-

tem equations implicitly using parallel computing by a Parallel Direct Sparse Solver (PDSS), also based on MPI.

4. Enriching FEM by PD: Applying DP to regions without discontinuities is inefficient computationally. The current work is the first to explore the adaptive use of DP locally, only for elements surrounding discontinuities. This dramatically increases the computational efficiency and accuracy of PD models.

Peridynamics theory in its earliest form [4, 8] was derived by equating the classical strain energy at a point to that of PD with a complete spherical interaction domain which results in PD numerical implementation requiring a surface correction and a volume correction procedure to improve accuracy. To remove these two drawbacks, this work presents a revised non-ordinary state-based peridynamics (RNOSBPD) based on the concept of the numerical differential operator proposed by Madenci et al. [58]. Based on this numerical differential operator, Madenci et al. [58] presented an explicit PD least square minimization (PDLSPM) and proved that the PDLSPM recovers NOSBPD by a particular example. In this study, the presented RNOSBPD is proved theoretically to recover NOSBPD. By the advantage of the numerical differential operator, the RNOSBPD works for arbitrary interaction domains and does not require surface correction and volume correction.

Compared with the finite element method (FEM), PD is computationally expensive. Thus, coupling PD with FEM is an appealing choice for taking advantage of these two methods. This study presents a new approach based on the weighted residual method (WRM) for coupling RNOSBPD with the finite element method (FEM). Within the coupled RNOSBPD and Finite Element Method (RNOSBPD-FEM) framework, the problem domain is divided into a PD domain and a FEM domain, and both domains are discretized into uniform or non-uniform elements. This coupling method is straightforward, and special techniques, such as overlapping regions, interface elements, or fictitious nodes that have been employed in the literature for coupling PD with FEM are not needed. Since RNOSBPD-FEM is derived based on WRM and the whole domain is discretized into finite elements, it can be easily introduced into commercial finite element codes, and the formulation can be converted con-

veniently between RNOSBPD, FEM, and RNOSBPD-FEM. Four static applications concerning deformations and stresses are performed, and the results show that the proposed RNOSBPD-FEM has excellent accuracy and efficiency.

In general, PD is computationally expensive due to many non-local interactions, much-refined mesh, and PD-based codes written in terms of dynamic equilibrium even for static problems. Typically, the explicit dynamic relaxation method is commonly preferred for static problems because it does not require large-matrix operations. However, Coupled PD with FEM makes it is possible to employ the implicit method to solve fracture problems. Compared to the explicit method, the implicit method of coupled PD with FEM does not need many iterations for a solution and is more efficient for static problems. Therefore, this study applies the coupling framework based on WRM to derive the governing equations of the PDLSM-FEM and applies the PDLSM-FEM to simulate 2D quasi-static crack propagation. To simulate the 2D quasi-static crack growth, we propose and implement an innovative method for handling peridynamic bond breakage and crack growth. The failure criterion of this method is based on the maximum circumferential tensile stress. The crack growth direction θ_c is determined by maximizing the circumferential tensile stress concerning the orientation, and crack propagation is triggered when the equivalent SIF K_{eq} of mixed-mode loading reaches the critical value of material fracture toughness K_{Ic} . The interaction integral of J -integral is employed to compute the stress intensity factors. The criterion removes the limitation on pure mode II or mode III dominant fracture analysis of commonly used critical stretch and energy density criteria. As the J -integral is path independent, the proposed method is much more reliable and accurate than using near-tip stresses directly from the PD model, which are sensitive to mesh refinement and less accurate. One 2D infinite plate with an inclined central crack under far-field tension is performed to calculate its displacement, stress, strain fields, and SIFs. The comparison of the SIFs between numerical and analytical solutions shows good accuracy of the proposed method. Crack propagation in a disk-shaped plate and a diagonal plate under displacement loading are also simulated. The results show that the proposed method models the crack growth efficiently and satisfactorily.

After successfully applying PDLSM-FEM to study discontinuity analysis of 2D struc-

tures, this study extends the coupled PDLSM-FEM to 3D problems, in which the PD domain and FEM domain are connected based on the Gauss integration method. Since storing a full global stiffness matrix is impractical, we present an algorithm to assemble the global stiffness matrix in a compressed sparse row (CSR) format by the message passing interface (MPI) technique. Within the CSR format, only non-zero coefficients of the stiffness matrix and their row and column indices are stored rather than the full matrix. The system equations are solved by a parallel direct sparse solver (PDSS), also developed based on the MPI technique. Three static examples are performed to demonstrate the capability of this proposed 3D PDLSM-FEM. For the first example, the magnitude of the relative errors of the displacement results of each node is up to machine precision, when compared to the analytical results. The performance evaluation of the first example shows the MPI technique improves the computational efficiency generally, and the maximum number of computer cores is suggested as 16. The performance evaluation also demonstrates that the proposed PDLSM-FEM significantly improves the computational efficiency, up to 96 times faster than the pure PDLSM, and significantly saves memory usage, up to 43 times less than the pure PDLSM. For the second and third examples, the displacements and stresses are obtained by PDLSM-FEM, and comparison with results using ANSYS demonstrates the proposed PDLSM-FEM has good accuracy.

To improve the computational efficiency of PD further, this study proposes an Enriched Finite Element Method using Peridynamics (EFEM-PD), following a similar concept of element enrichment in Extended FEM (XFEM). In EFEM-PD, the FEM model is enriched adaptively with PD equations in regions containing cracks. An adaptive algorithm is implemented with the dual goals of meshing regions with cracks using PD equations while minimizing PD interactions to maximize computational efficiency. With the framework of EFEM-PD, only elements intersecting with the crack and the neighboring elements are enriched by the PD least-squares minimization (PDLSM) formulation, which is suitable for modeling the failure of structures. The remaining elements are conventional FEM elements. Based on the weighted residual method, we derive the element stiffness matrix and governing equations of the whole domain in 2-D and 3-D. The numerical integration of interaction

integral is proposed and implemented to evaluate the stress intensity factors (SIFs) used for failure prediction. Several numerical examples are conducted to verify the efficacy of the proposed EFEM-PD. One 2-D infinite plate under mixed-mode loading is analyzed, and its SIFs are calculated. Comparing the SIFs between analytical and numerical solutions reveals excellent accuracy of the presented EFEM-PD. Static simulation of a diagonal plate is performed, and the static solutions are in excellent agreement with ANSYS results. The quasi-static crack propagation simulation of the 2-D diagonal plate shows that the crack path and peak loading are in close agreement with experiment observation. Simulations of a compact tension test by EFEM-PD and XFEM (ABAQUS) are performed, and the reaction forces from both methods are in good agreement. The static solutions of a 3-D block with pre-existing crack are obtained by EFEM-PD, pure PD, and FEM (ANSYS), and the comparison reveals that the results from the three methods are in excellent agreement. The performance evaluation of the 3-D example shows that EFEM-PD saves up to 16.0 times in terms of computing time and up to 11.9 times in terms of memory usage against the pure PD model.

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