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A Partitioned Coupling Framework for Peridynamics and Classical Theory: Analysis and Simulations

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Abstract

We develop and analyze a concurrent framework for coupling peridynamics and the corresponding classical elasticity theory, with applications to the numerical simulations of damage problems. In this framework, the peridynamic model and the elastic model are solved separately and coupled with a partitioned approach. In the region where material failure is expected to initiate, we employ the peridynamic theory. In the rest of the problem domain, the material is modeled by the classical elasticity theory. On the peridynamic-classical theory interface, there is a transition region where the two subdomains overlap. The two solvers communicate by exchanging proper boundary conditions at the peridynamic-classical theory interface, which enables a modular software implementation. We analyze different coupling strategies on a 1D simplified problem and obtain expressions for the optimal reduction factor (convergence rate index). The selection of optimal coupling parameters is verified with numerical experiments, where we demonstrate that the optimal Robin coefficient from 1D simplified problem analysis can be extrapolated to more complicated problems, including cases with damage. Both the analysis and the numerical results suggest that the optimal Robin boundary condition on the classical theory side combined with a Dirichlet boundary condition with Aitken relaxation rule on the peridynamic side would be the most robust choice. Comparing with the commonly employed Dirichlet interface conditions, the optimal Robin boundary condition together with Aitken relaxation accelerates the coupling convergence rate by 10 times. With the developed optimal coupling strategy, we also numerically demonstrate the coupling framework’s asymptotic convergence to the local solution and its capability to capture crack initiation and growth in 2D problems.

Keywords: Peridynamics, Nonlocal models, Coupling method, Mixed boundary conditions, Robin boundary condition

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1. Introduction

Understanding the behavior of materials in extreme loading conditions is critical to advance a variety of applications in science and engineering. Due to operating conditions and performance requirements, stresses and strains can reach values higher than the expected ones. For that reason, understanding material failure, mostly crack formation and propagation, is of great interest. While damage and material failure may result from a combination of chemical and physical processes with origins at the atomistic scale, developing a numerical framework which can capture multiscale phenomena is valuable for studying material failure.

Among the multiscale damage models, the recently developed peridynamic theory [1] has received much attention. In contrast to the classical elasticity, the peridynamic theory is a spatially nonlocal formulation [2] which unifies the modeling of continuum media and discontinuities [1, 3, 4]. Therefore the material damage can be captured autonomously as a natural component of the material deformation [3, 5–10]. In peridynamics, the fundamental assumption is that the interaction between material points vanishes whenever the material points are separated by a distance greater than a certain defined value called the horizon $\delta$. Consider a three-dimensional (3D) peridynamic body subjected to an external body force field $b(x, t)$ and let $u(x, t)$ denote the displacement field. The partial differential equation of the classical theory is replaced by the integro-differential equation [1, 11]

$$\rho(x)\ddot{u}(x, t) = \int_{H_x} (T(Y(x))(x' - x) - T(Y(x'))(x - x'))dV_p + b(x, t), \quad (1.1)$$

where $H_x = \{x'|0 < ||x - x'|| \leq \delta\}$ is a neighborhood of any point $x$ in the undeformed configuration, $Y(x)(\xi)(t) = \xi + u(x + \xi, t) - u(x, t)$ is the deformation state, and $T(Y(x))(\xi)$ is a vector force state function which represents the material response due to deformation. Because it avoids classical notions like the deformation gradient, (1.1) allows less regular solutions, including discontinuous solutions. Therefore, peridynamics can simulate a wide range of complex problems in fracture and damage mechanics.

Moreover, peridynamics has a parallel to molecular dynamics since in both approaches the motion of any point is found by a process of force summation due to interactions with neighboring points [1, 12, 13]. Molecular dynamics provides an approach to understanding the mechanics of materials at the atomistic scale, thus better fidelity in modeling fracture and material failure. However, the time and length scales of molecular dynamics makes these methods computationally very expensive. Peridynamics offers a more computationally efficient choice at larger length and time scales. On the other hand, given sufficient regularity of the boundary data and material properties, the solution from peridynamic theory for small horizon approaches the conventional weak solution of a classical constitutive model [14–19]. To be specific, any elastic constitutive model from the classical theory can be adapted to the peridynamic theory using a nonlocal approximation to the deformation gradient tensor [11, 20, 21].

Although peridynamics provides a model to capture material failure, on the regions where material damage does not occur, the classical theory is completely adequate and also less computationally expensive. Thus, multiscale
coupling strategies are required such that the resultant multiscale solver can support the peridynamic model near the regions where damage occurs as well as the efficient classical model employed for the other parts. In recent years, many strategies have been proposed to couple local-to-nonlocal or two nonlocal models with different nonlocality [22–41]. Just to name a few, examples include the following approaches:

1. Arlequin type domain decomposition, see e.g., [24, 25]. This method obtains a surrogate model by the Arlequin approach which introduces an overlap region in which the two different models are coupled together using Lagrange multipliers.

2. Optimal-control based coupling, see e.g., [26, 29]. In this approach the coupling is formulated as a control problem and the states are the solutions of the nonlocal and local equations, with the objective to minimize their mismatch on the overlap of the nonlocal and local domains under the controls of virtual volume constraints and boundary conditions.

3. Morphing approach as in, e.g., [23, 30, 40]. This method couples nonlocal continuum models to local continuum models in a single unified model by performing coupling through a transition (morphing) affecting only the constitutive parameters, where the definition of the morphing functions relies on energy equivalence.

4. Energy-based blending mechanism, see e.g., [32–34]. In this method a blending region is employed where contributions from different material models are smoothly mixed in the total energy. The resultant framework correctly predicts the total energy of a perfect lattice subjected to uniform strain.

5. Force-based blending mechanism, see e.g., [31, 42]. Similar to the energy-based blending mechanism, this formulation uses blending region, where the forces of the two material models are smoothly blended so as to avoid undesired spurious effects on the boundaries. In contrast to classical blending methods where two or more models are joined together, a coupled nonlocal/local scheme is derived from a single framework in [42]. It is shown that the error can be controlled by the sizes of the nonlocal region and the transition region.

6. Submodeling approach, see e.g., [35–37]. In this approach, one first performs simulation with a classical theory model on the whole computational domain, then employs a peridynamic solver for submodeling. While the classical theory does not monitor the material failure, in the submodeling step peridynamic theory is employed in the region where failure initiation and growth are expected to monitor the damage initiation and propagation.

Other recent formulations of couplings for material models can be found in [38, 39, 41]. Many of the above approaches have developed and utilized methods for coupling peridynamics and the classical theory. However, to the authors’ best knowledge, there is very little work on coupling approaches based on Robin (mixed) boundary conditions. In the classical setting, the Robin type interface condition has been proven to be a very efficient domain decomposition technique for multiphysics coupling problems [43–47]. Therefore, in this paper we develop the Robin interface condition for the peridynamic-classical theory interface, and provide the optimal Robin coefficient through 1D analysis.

To achieve software modularity, in this work we investigate a partitioned approach for coupling peridynamics and the classical theory. We employ different solvers for the peridynamic subdomain and the classical theory subdomain,
respectively. The peridynamics subdomain is discretized with the particle discretization method (via PDLAMMPS [48]) while the classical elastic model is discretized with finite elements, and these two solvers communicate by exchanging proper boundary conditions at the interface. At each time step, iteration is employed to impose continuity at the interface. In this work, we employ the peridynamics subdomain solver as a black box solver, i.e., only the displacement information is available and only Dirichlet boundary condition are applied, while we apply more general boundary conditions to the classical theory subdomain solver. Different mesh sizes and different time step sizes can be employed for these two subdomains, which further enables multiscale coupling in time and space. To investigate the optimal coupling strategy for this partitioned coupling framework, we develop rigorous analysis in simple geometries for predicting the values of the optimal coefficients on the interface boundary conditions. Based on the theoretical analysis, we then demonstrate the performance of this coupling framework and verify the theoretical optimal coefficient with convergence and accuracy verification tests. To investigate the capability of this coupling framework on more complicated scenarios, we also test the flexibility of this method for different application problems. Although the coupling strategies discussed here can be extended to more complicated cases, e.g., time-dependent problems and three-dimensional (3D) problems, in the current paper we focus on two-dimensional (2D) static and quasi-static problems.

The remainder of this paper is organized as follows. In Section 2 we describe the governing equations of peridynamics (see Section 2.1) and classical elasticity (see Section 2.2) theories. The coupling procedure is detailed in Section 2.3 including the transmission of conditions in the peridynamics-classical theory interface and a summary of the iterative procedure for the full partitioned algorithm. In Section 3 we present theoretical analysis of convergence rate for a 1D simplified problem, which is applied later in Section 4 for obtaining the optimal Robin coefficient when we apply the coupling procedures to plane stress problems. The changes on convergence rates by varying overlapping region, mesh size ratios and relaxation parameters are investigated both theoretically and numerically in Section 4.1. Moreover, to demonstrate the accuracy of the framework, in Section 4 we also use the manufactured solutions to show that the numerical solution is faithful to both the nonlocal and local solutions. In Section 5 we apply the coupling framework to further confirm our aforementioned analysis on a problem with damage and also to demonstrate the capability of our solver in modeling the crack initiation and propagation. We end in Section 6 with a brief summary.

2. Mathematical Formulation

In this section, we define the formulation for the displacement field $\mathbf{u}(\mathbf{x})$ in a two-dimensional body occupying the domain $\Omega \subset \mathbb{R}^2$. The domain $\Omega$ is composed of two parts: the peridynamic subdomain $\Omega_p$ where damage might occur and the material is described by a peridynamic model, and the classical theory subdomain $\Omega_c$ occupied by a classical linear elastic model. As shown in the left plot of Figure 1, the peridynamic subdomain is surrounded by the classical theory subdomain, and a transition region $\Omega_{p+c} = \Omega_p \cap \Omega_c$ is introduced on which the peridynamic subdomain and the classical theory subdomain overlap. For the classical theory model, the interface boundary conditions are applied on
a 1D curve, which is marked as \( \Gamma_1 \) in the left plot of Figure 1. For the peridynamic model where a nonlocal operator is involved, its boundary conditions should be applied on a 2D volume \( \Gamma_2 \) (marked by yellow shadow in Figure 1).

Without loss of generality, in \( \Omega_p \) we consider the static prototype microelastic brittle (PMB) peridynamic model which is geometrically nonlinear. In \( \Omega_s \), we employ the linear static elastic model with infinitesimal deformation. Further details of the peridynamic and the classical theory problems will be described in Sections 2.1 and 2.2, respectively.

![Figure 1: Left: a sketch that illustrates the problem of interest and the domain decomposition: (blue) damaged region simulated by a peridynamic model; (green) undamaged region simulated by classical solid model; (yellow) overlapping region. Right: Notation for the peridynamic model.](image)

In this section, we present the detailed models and discretization methods for the peridynamic and classical theory subdomains, respectively. We also describe a strong partitioned coupling method, which iteratively solves the coupling system with the Robin boundary condition at the peridynamic-classical theory interface. In this section, we assume that the peridynamic subdomain is surrounded by the classical theory subdomain and suitable Dirichlet or Neumann boundary conditions are imposed on the external boundary of the classical theory subdomain. We omit these external boundary conditions in our description. To ensure the continuity on the interface, iterations are employed. In this paper we denote the iteration number by the subscript \( n \).

2.1. Peridynamic model

The peridynamic theory proposed in [1] makes minimal regularity assumptions on the deformation field. Instead of spatial differential operators, integration over differences of the displacement field is used to describe the existing, possibly nonlinear, forces between material points of the solid body. In this work, we consider the static prototype microelastic brittle (PMB) peridynamic model

\[
\int_{\mathcal{H}_\delta} f(\mathbf{u}_p(x'), \mathbf{u}_p(x) - x')dV_{x'} + \mathbf{b}(x) = 0, \quad x \in \Omega_p.
\]

where \( \mathcal{H}_\delta \) is a circular neighborhood of \( x \in \Omega_p \) with radius \( \delta \) known as the peridynamic horizon, \( \mathbf{u}_p \) is the displacement vector field of the peridynamic model, \( \mathbf{b} \) is the prescribed body force density field, and the integral expresses that the...
internal force density at \( \mathbf{x} \) is the summation of forces over all vectors \( \mathbf{x}' - \mathbf{x} \). For two material points with initial positions \( \mathbf{x}' \) and \( \mathbf{x} \), we denote the relative position of them in the initial configuration as \( \xi \) and their relative displacement as \( \eta \):

\[
\xi = \mathbf{x}' - \mathbf{x}, \quad \eta = \mathbf{u}(\mathbf{x}', t) - \mathbf{u}(\mathbf{x}, t).
\]  

As shown in the right plot of Figure 1, \( \xi + \eta \) represents the current relative position vector between the two particles. In the prototype microelastic model, the direct physical interaction between the two particles can then be defined by a pairwise force function:

\[
f(\eta, \xi) = c_{d, \delta} s(\eta, \xi) \frac{\xi + \eta}{\|\xi + \eta\|},
\]

where

\[
s(\eta, \xi) = \frac{\|\xi + \eta\| - \|\xi\|}{\|\xi\|}.
\]

These equations denote the bond stretch which is the relative change of the length of a bond. Here the subscript \( d \) is the dimension of the problem domain and \( \| \cdot \| \) denotes the Euclidean norm. In this material model, the magnitude of the force in a bond varies linearly with its bond stretch, and \( c_{d, \delta}/\|\xi + \eta\| > 0 \) characterizes the stiffness per unit volume squared. Here we note that the prototype microelastic peridynamic model is bond-based, that means, the kernel \( f \) is a pairwise force function whose value is the force vector (per unit volume squared) that the particle \( \mathbf{x}' \) exerts on the particle \( \mathbf{x} \). The bond-based peridynamic model (2.1) has the assumption that each bond connected to \( \mathbf{x} \) responds independently of all the others, which limits the elastic response that can be reproduced by the model. Therefore, in the 3D case the response of a prototype microelastic model corresponds to a fixed Poisson ratio \( \nu = 1/4 \), while in the 2D case the model limits the Poisson ratio to \( \nu = 1/3 \) [49]. Peridynamic models with more general elastic responses can be found in [50] and they are not considered in this paper, although they can be readily substituted into the coupling framework proposed here.

With the fixed Poisson ratio, the coefficient \( c_{d, \delta} \) is determined by the Young’s modulus \( E \) and the horizon \( \delta \). By matching the energy density from (2.1) with the elastic energy density from the classical theory, for the 3D prototype microelastic model one has

\[
\nu = \frac{1}{4}, \quad c_{3, \delta} = \frac{18K}{\pi \delta^3},
\]

and for the 2D prototype microelastic model

\[
\nu = \frac{1}{3}, \quad c_{2, \delta} = \frac{9K}{\pi \delta^3},
\]

Equations (2.3) and (2.4) are frequently represented in terms of the spatial \( y \) and material \( x \) coordinates

\[
f(y' - y, x' - x) = cs \frac{y' - y}{\|y' - y\|}, \quad s = \frac{\|y' - y\| - \|x' - x\|}{\|x' - x\|}.
\]
which corresponds to the plane stress assumption. The bulk modulus $K$ is defined as $K = \frac{E}{3(1-2\nu)}$. In this paper, we employ the 2D prototype microelastic model with parameters in (2.6) for all the theoretical derivations and numerical examples, and we therefore denote the parameter as $c_{2,\delta} = c$ for simplicity.

Damage is incorporated into the peridynamic constitutive model by allowing the bonds of solid interactions to break irreversibly. Here we employ the critical stretch criterion where breakage occurs when a bond is extended beyond some predetermined critical bond deformed length. This criterion can be implemented by multiplying the pairwise force function with a history-dependent scalar boolean function

$$
\mu(\xi, \eta, t) = \begin{cases} 
1 & \text{if } s(\xi, u(x', \tau) - u(x, \tau)) \leq s_0 \forall \tau \leq t, \\
0 & \text{otherwise},
\end{cases}
$$

(2.7)

where $s_0$ is a prescribed critical bond stretch for breakage. Note that the resulting pairwise force function explicitly depends on time $t$. In damage applications, $s_0$ can be related to the energy release rate $G_0$ following [51], i.e.,

$$
s_0 = \sqrt{\frac{10G_0}{\pi c_{3,\delta}^3}}
$$

(2.8)

in the 3D prototype microelastic brittle (PMB) model and

$$
s_0 = \sqrt{\frac{4G_0}{c_{2,\delta}^4}}
$$

(2.9)

in the 2D PMB model [52]. The energy release rate $G_0$ denotes the work required to completely separate the two parts of a body across the fracture surface, (see [32, 50, 53] for further details.

In our coupling framework, the peridynamic problem is solved with a large-scale parallel simulator, PDLAMMPS [49, 54]. Spatially, the variables in PDLAMMPS are discretized in a particle-based approach and therefore has the same computational structure as the molecular dynamics model. For a structured mesh with fixed mesh size $h_p$, the region defining a peridynamic material is discretized into particles forming a simple cubic lattice, where each particle $i$ is associated with some volume fraction $V_i$. Let $\mathcal{H}_i = \{ j : 0 < ||x_i - x_j|| \leq \delta \}$ denote the family of particles for which particle $i$ shares a bond in the reference configuration. With the particle-based approach, the governing equation (2.1) for the PMB model is discretized as follows:

$$
\sum_{j \in \mathcal{H}_i} f(u_p(x_j) - u_p(x_i), x_j - x_i)V_j + b_i = 0, \quad x_i \in \Omega_p.
$$

(2.10)

To solve for the peridynamic displacement $u_p(x_i)$ of (2.10) with PDLAMMPS, we perform an energy minimization of the peridynamic problem by iteratively adjusting particle coordinates until either the change in energy or the $L^2$ norm of the right hand side vector reaches the prescribed tolerance $10^{-15}$. For further details, see [49, 54].
2.2. Classical theory model

Here we consider the linear elastic model which is consistent with the peridynamics model described in Section 2.1. In this paper we assume infinitesimal deformation in the classical theory subdomain, although we note that a hyperelastic model with finite deformations [55] can readily be substituted in. The equation describing the deformation field can be expressed as follows:

\[ \nabla \cdot S(u_i(x)) + b(x) = 0, \quad x \in \Omega, \quad (2.11) \]

where \( S \) and \( b \) are the second Piola-Kirchhoff stress tensor for the specific material and the body load field on the structure, respectively. Considering the geometrically linear elastic model, the stress tensor is given by

\[ S(u_i) = \frac{vE}{2(1 + v)(1 - 2v)} \left[ \text{tr}\left( \left( \frac{\partial u_i}{\partial x} \right)^T \right) + \frac{E}{2(1 + v)} \left( \left( \frac{\partial u_i}{\partial x} \right)^T \right) \right], \quad (2.12) \]

where \( E \) and \( v \) are the Young’s modulus and the Poisson ratio of the material, respectively. In this paper, we consider a fixed Poisson ratio \( v = 1/3 \) which is consistent with the 2D prototype microelastic peridynamic model discussed in Section 2.1.

The linear elastic problem is solved with a finite element code. Spatially, we employ the linear shape functions for

\[ \int_{\Omega} S(u_i) : \nabla v d\Omega + R \int_{\partial \Omega_D} u_i \cdot n d\Omega_D = \int_{\partial \Omega_N} t \cdot v d\Omega_N + \int_{\partial \Omega_R} r \cdot v d\Omega_R + \int_{\Omega} b \cdot v d\Omega, \quad \forall v \in \mathbb{U}_0 \quad (2.13) \]

where the displacement field \( u_i(x) \in \mathbb{U} = \{ w(x) \in [H^1(\Omega)]^2 | w(x) = u_{id}(x) \text{ on } \partial \Omega_D \} \) and \( \mathbb{U}_0 = \{ w(x) \in [H^1(\Omega)]^2 | w(x) = 0 \text{ on } \partial \Omega_D \} \). \( u_{id} \) stands for the normal vector pointing outward from the classical theory subdomain. With linear shape functions \( \phi_p(x) \) for each element, the displacement \( u_i = (u_1, u_2) \) and the test function \( v = (v_1, v_2) \) are expanded as:

\[ (u_i(x)) = \sum_{p=1}^{N_e} (U_j)_{ip} \phi_p(x), \quad v_i(x) = \sum_{p=1}^{N_e} V_{ip} \phi_p(x), \quad i = 1, 2, \quad (2.14) \]

where \( N_e \) is the total number of shape functions for displacement on this element and \( (U_j)_{ip} \), \( V_{ip} \) are the expansion coefficients. Substituting expression (2.14) into the weak form (2.13) and assembling globally, we obtain

\[ KU = F. \quad (2.15) \]
Here $U$ is the global vector of unknown expansion coefficients, $F$ is the global vector of the external loads, and $K$ is the stiffness matrix. For further implementation details, see [55, 57].

2.3. Coupling strategies

In this section we present the procedure of coupling the peridynamic theory and classical continuum mechanics. Here the peridynamic and the classical theory solvers are treated as two independent programs. In [58], a partitioned formulation was proposed for connecting one-dimensional atomistic-to-continuum. We now extend this formulation to the peridynamic-classical elasticity coupling problem in 2D, and employ various types of boundary conditions at the coupling interface. In our framework, the peridynamic and the finite element method solvers are coupled in a partitioned approach, namely, they are linked by exchanging suitable transmission conditions through a wrapper code. Since only the interface conditions are required, this partitioned coupling approach avoids changes in the existing solvers and is capable of coupling two black-box solvers, which is one of our aims while developing this coupling framework.

We solve the coupled problem with an iterative approach. As sketched in Figure 2, at the $n$-th iteration, with the given transmission condition from the peridynamic solver applied on the internal boundary of the overlapping region ($\Gamma_1$) and proper boundary conditions on the rest of $\partial \Omega_s$, we first solve for the displacement field $u^n_s$ from the classical linear elastic model:

$$\nabla \cdot S(u^n_s(x)) + b(x) = 0.$$  \hspace{1cm} (2.16)

In this coupling framework, three types of transmission conditions on the linear elastic model are considered and
compared:

Dirichlet boundary condition: \( u^{n}_{n}(x) = u^{n-1}_{p}(x) \) for all \( x \in \Gamma_1 \).  
(2.17)

Neumann boundary condition: \( S(u^{n}_{n}) \cdot n_{s} = S(u^{n-1}_{p}) \cdot n_{s} \) for all \( x \in \Gamma_1 \).  
(2.18)

Robin boundary condition: \( S(u^{n}_{n}) \cdot n_{s} + Ru^{n}_{n}(x) = S(u^{n-1}_{p}) \cdot n_{s} + Ru^{n-1}_{p}(x) \) for all \( x \in \Gamma_1 \).  
(2.19)

It can be observed that when the coefficient \( R = 0 \) in the Robin boundary condition, the Neumann boundary condition is recovered. On the other hand, when \( R \to \infty \), the Robin boundary condition approaches to the Dirichlet boundary condition. That means, the Robin boundary condition can be seen as a general transmission condition applied on the linear elastic model. Therefore in Sections 3-4 we analyze the Robin boundary condition.

With the displacement field \( u^{n}_{n} \) obtained from the classical theory side, we can then proceed to solve for the displacement field \( u^{n}_{p} \) on the peridynamic subdomain \( \Omega_p \) with the peridynamic solver PDLAMMPS for the equation:

\[
\sum_{j \in H_{i}} f(u^{n}_{n}(x_{j}) - u^{n}_{p}(x_{i}), x_{j} - x_{i}) V_{i} + b_{i} = 0, \quad x_{i} \in \Omega_p.
\]  
(2.20)

Here we treat PDLAMMPS as a black-box solver and only the displacement-type boundary condition can be applied, i.e., on the external boundary of the overlapping region \( \Gamma_2 \), we impose,

\[
u^{n}_{p}(x) = u^{n}_{s}(x), \quad \text{for all} \ x \in \Gamma_2.
\]  
(2.21)

To accelerate the convergence, we perform under-relaxation on the displacement boundary condition (2.21). We update the displacement \( u^{n}_{p} \) on \( \Gamma_2 \) from \( u^{n}_{s} \) and a relaxation parameter \( \tau^{n} \) based on the following rule:

\[
u^{n}_{p}(x) = \tau^{n}u^{n-1}_{p}(x) + (1 - \tau^{n})u^{n}_{s}(x).
\]  
(2.22)

Here \( \tau^{n} \in [0, 1] \) can be a fixed relaxation parameter or it can be updated according to the Aitken rule [59]:

\[
\tau^{n} = \tau^{n-1} + (\tau^{n-1} - 1) \left( \frac{Q_{n} - Q^{n}}{\|Q_{n} - Q^{n}\|^{2}} \right), \quad \text{where} \ Q^{n} = u^{n}_{s} - u^{n-1}_{p}.
\]  
(2.23a)

To get a better control of the convergence rate, we can set the relaxation parameter \( \tau^{n} \) within the range \([\tau_{\text{min}}, \tau_{\text{max}}] \), depending on the specific application [60].

In summary, we solve the peridynamic-classical theory coupling system following an alternating Schwartz method:
1. Set

(Classical Theory) \( u_0^s = 0 \) on \( \Omega_s \), \hspace{1cm} (2.24a)
(Peridynamics) \( u_0^p = 0 \) on \( \Omega_p \). \hspace{1cm} (2.24b)

2. for \( n = 1 : n_{\text{max}} \), do

(a) (Classical Theory) Update the interface condition on \( \Gamma_1 \) with one of the following:
   - Dirichlet boundary condition: \( u_1^s(x) = u_1^{s-1}(x) \) for all \( x \in \Gamma_1 \).
   - Neumann boundary condition: \( S(u_1^s) \cdot n_s = S(u_1^{s-1}) \cdot n_s \) for all \( x \in \Gamma_1 \).
   - Robin boundary condition: \( S(u_1^s) \cdot n_s + R u_1^s(x) = S(u_1^{s-1}) \cdot n_s + R u_1^{s-1}(x) \) for all \( x \in \Gamma_1 \).

(b) (Classical Theory) With the finite element solver, solve for the displacement field \( u_n^s \) from the governing equation (2.16) on the whole classical theory subdomain \( \Omega_s \).

(c) (Classical Theory) Pass the displacement \( u_n^s \) at the interface \( \Gamma_2 \) to the peridynamic solver.

(d) (Peridynamics) Obtain the displacement boundary condition \( u_1^p \) on \( \Gamma_2 \) from the classical theory side.

(e) (Peridynamics) Perform the relaxation (2.22) and obtain the relaxed displacement \( u_1^p \) on \( \Gamma_2 \).

(f) (Peridynamics) With the particle-based peridynamics solver (PDLAMMPS), solve the governing equation (2.10) to get the displacement field \( u_n^p \) on \( \Omega_p \).

(g) (Peridynamics) Pass proper boundary condition at the interface \( \Gamma_1 \) to the finite element solver.

(h) (All) Check convergence of both solvers. If

\[
||u_n^s - u_1^{s-1}||^2_{L^2(\Omega_s)} < \epsilon \quad \text{and} \quad ||u_n^p - u_1^{s-1}||^2_{L^2(\Omega_p)} < \epsilon,
\]

set \( n = n_{\text{max}} \) and update the results as

(Classical Theory) \( u_s = u_n^s \), \hspace{1cm} (2.26a)
(Peridynamics) \( u_p = u_n^p \). \hspace{1cm} (2.26b)

Else, continue to the \((n+1)\)-th iteration.

Remark 1. The peridynamic model considered here converges to the classical theory model with an \( O(\delta^2) \) error as \( \delta \to 0 \). Therefore, when the peridynamic discretization is asymptotically compatible [61, 62], we can expect the solution from the above framework converges to the local solution as the horizon \( \delta \to 0 \) and the finite element mesh size \( h_s \) as well as the peridynamic mesh size \( h_p \) both go to zero. In this paper, we focus on the coupling convergence, especially on reducing the required iterations. To reduce the impact of numerical errors from coupling heterogeneous materials, in applications we assume that the region with possible defects is far enough from the overlapping region. We also consider the convergence to the local solution in the second numerical example (see Section 4.2). As the peridynamic
discretization we use is not asymptotically compatible, we take the limit of the mesh spacing and peridynamic horizon to zero in such a way as to arrive at the correct local limit.

3. Analysis of a Model Problem

![Diagram of a membrane subjected to uniaxial stretch](attachment:image.png)

Figure 3: Domain for the model problem of a membrane subjected to uniaxial stretch.

To provide the stability analysis as well as to investigate the optimal choices of $R$ for accelerating the subiteration convergence, we simplify the coupling problem to a model problem as a membrane under uniaxial stretch in the preferred direction (assumed to be the $x$ direction) and with no body load. As shown in Figure 3, the computational domain

$$\Omega = \{(x, y) \in \mathbb{R} \times [0, L]\}$$

is considered, with the peridynamic subdomain as

$$\Omega_p = \{(x, y) \in [-L_2, L_2] \times [0, L]\}$$

and the classical elastic subdomain as

$$\Omega_e = \{(x, y) \in (-\infty, -L_1] \cup [L_1, \infty) \times [0, L]\}.$$  

Since here we employ an overlapping domain $\Omega_{p+s} = \Omega_p \cap \Omega_e \neq \Phi$, we assume that $L_2 > L_1$, which yields the overlapping domain as follows

$$\Omega_{p+s} = \{(x, y) \in (-L_2, -L_1] \cup [L_1, L_2]) \times [0, L]\}.$$  

Since the stretch along $x$ direction dominates the membrane deformation, here we neglect the displacement in $y$
direction and assume that the displacement is axisymmetric with respect to y axis, i.e.,

\[ u_s(x) = (u_s(x), 0), \quad u_p(x) = (u_p(x), 0), \]

and

\[ u_s(x, y) = -u_s(-x, y), \quad u_p(x, y) = -u_p(-x, y). \]

The upper and lower boundaries of the membrane are subjected to no traction along x direction. Although the classical traction condition is not a well-posed boundary condition for the nonlocal models, we assume that the boundaries are sufficiently far from the damage region and therefore adopt the local traction condition for both \( u_s \) and \( u_p \):

\[ \frac{\partial u_s}{\partial y} \bigg|_{y=0} = \frac{\partial u_s}{\partial y} \bigg|_{y=L} = \frac{\partial u_p}{\partial y} \bigg|_{y=0} = \frac{\partial u_p}{\partial y} \bigg|_{y=L} = 0. \]

For the peridynamic subdomain, we consider a linearized version of the PMB model (2.1). Substituting (2.3) and (2.4) into (2.1) yields

\[ \int_{\mathcal{H}_c} c \left( \frac{||\xi + \eta|| - ||\xi||}{||\xi||} \right) \left( \frac{\xi + \eta}{||\xi + \eta||} \right) \, dV_x = 0. \tag{3.1} \]

When adopting the infinitesimal deformation assumption, we have \( ||\eta|| \ll ||\xi|| \) and therefore

\[ ||\xi + \eta|| \approx ||\xi|| + \frac{\eta}{||\xi||}, \quad \frac{\xi + \eta}{||\xi + \eta||} \approx \frac{\xi}{||\xi||}. \]

Denoting \( \xi = x' - x = (e_1, e_2) \) and \( \eta = (u_p(x') - u_p(x), 0) \), one can further simplify the above governing equation on the first component:

\[ 0 = \int_{\mathcal{H}_c} c \left( \frac{||\xi + \eta|| - ||\xi||}{||\xi||} \right) \left( \frac{e_1 + u_p(x') - u_p(x)}{||\xi + \eta||} \right) \left( \frac{\xi}{||\xi||} \right) \, dV_x \approx \int_{\mathcal{H}_c} c \left( \frac{\eta \cdot \xi}{||\xi||^2} \right) \left( \frac{e_1}{||\xi||} \right) \, dV_x = \int_{\mathcal{H}_c} c \frac{e_1^2(u_p(x') - u_p(x))}{(e_1^2 + e_2^2)^{3/2}} \, dV_x. \tag{3.2} \]

Note that the resultant model is consistent with the general linearized prototype microelastic model in [50]. In the following analysis, we consider a discretized version of the linear PMB model (3.2) on a uniform mesh with lattice size \( h_p \):

\[ \sum_{\mathcal{H}} c \frac{e_1^2(u_p(x + e_1, y + e_2) - u_p(x, y))}{(e_1^2 + e_2^2)^{3/2}} = 0, \tag{3.3} \]

where \( \mathcal{H} \) denotes the discretized circular neighborhood \( \mathcal{H} = [(e_1, e_2) : i, j \in \mathbb{N} ; \|(e_1, e_2)\| = \|((ih_p, jh_p))\| \leq \delta] \). In the classical theory subdomain, \( \Omega_s \), a corresponding linear elastic model is employed. Using the above assumptions, the
first component of (2.11) can be simplified as follows:

\[
\frac{(1 - \nu)E}{(1 + \nu)(1 - 2\nu)} \frac{\partial^2 u_s}{\partial x^2} + \frac{E}{2(1 + \nu)} \frac{\partial^2 u_s}{\partial y^2} = 0. 
\]

Given the limitation of bond-based peridynamic models, the Poisson ratio is constrained to \(\nu = 1/3\). Substituting \(\nu = 1/3\) into (3.4) gives

\[
\frac{3E}{2} \frac{\partial^2 u_s}{\partial x^2} + \frac{3E}{8} \frac{\partial^2 u_s}{\partial y^2} = 0. 
\]

Therefore, the peridynamic-classical theory coupling system is governed by the following equations

\[
\frac{3E}{2} \frac{\partial^2 u_s}{\partial x^2} + \frac{3E}{8} \frac{\partial^2 u_s}{\partial y^2} = 0, \quad \text{in} \quad \Omega_s, 
\]

\[
\sum_{\mathcal{H}} e_1^2 (u_p(x + e_1, y + e_2) - u_p(x, y)) \frac{1}{(e_1^2 + e_2^2)^{3/2}} = 0, \quad \text{in} \quad \Omega_p, 
\]

(together with the the Robin-type interface boundary condition at \(x = L_1\)

\[
- \frac{3E}{2} \frac{\partial u_p^n}{\partial x} + Ru^n_p = \frac{3E}{2} \frac{\partial u_p^{n-1}}{\partial x} + Ru^n_{p-1}, 
\]

and the relaxed Dirichlet-type interface boundary condition at \(x = L_2\)

\[
u^n_p = \tau^n u_p^{n-1} + (1 - \tau^n) u^n_s. 
\]

Similar to [60], the convergence analysis can be obtained based on the Fourier analysis in the \(y\) direction, which is also the tangential direction to the preferred direction,

\[
u(x, y) = \sum_{\gamma} (\hat{u}_s(x, \gamma)) \cos \left(\frac{\gamma \pi y}{L}\right), \quad u_p(x, y) = \sum_{\gamma} (\hat{u}_p(x, \gamma)) \cos \left(\frac{\gamma \pi y}{L}\right). 
\]

To quantify the convergence rate for displacement at the \(n\)-th iteration for any given frequency \(\gamma\), we define a reduction factor in the frequency space

\[
\rho^n_{\gamma} := \frac{|(\hat{u}^n_p(x, \gamma)) - (\hat{u}_p(x, \gamma))|}{|(\hat{u}^{n-1}_p(x, \gamma)) - (\hat{u}_p(x, \gamma))|}. 
\]

where \((\hat{u}_p)_p(x, \gamma)\) is the Fourier coefficient of the exact displacement solution \(u_p(x, y)\), and \((\hat{u}^n_p)_p(x, \gamma)\) is the Fourier coefficient of the numerical approximation for displacement from the peridynamic model at the \(n\)-th iteration. In this model problem, for convergence analysis we consider the case with vanishing exact displacement solution, i.e., \(u_p(x, y) = 0\). If \(\rho^n_{\gamma}\) is less than 1 for all supported frequencies at every iteration step, the algorithm converges. Moreover, the smaller this reduction factor is, the faster the rate of convergence will be.
We now write out the solution of problem (3.6). In the following we denote

$$\mathcal{H}_1 = \{(e_1, e_2) : i, j \in \mathbb{N}; i \neq 0, j > 0; \| (e_1, e_2) \| = \| (ih_{p}, jh_{p}) \| \leq \delta \},$$

$$\mathcal{H}_2 = \{(e_1, e_2) : i, j \in \mathbb{N}; i \neq 0, j = 0; \| (e_1, e_2) \| = \| (ih_{p}, jh_{p}) \| \leq \delta \},$$

$$\mathcal{H}_3 = \{(e_1, e_2) : i, j \in \mathbb{N}; i > 0, j = 0; \| (e_1, e_2) \| = \| (ih_{p}, jh_{p}) \| \leq \delta \},$$

and

$$\mathcal{H}_4 = \{(e_1, e_2) : i, j \in \mathbb{N}; i > 0, j = 0; \| (e_1, e_2) \| = \| (ih_{p}, jh_{p}) \| \leq \delta \}$$

for simplicity in notation. Substituting the Fourier expansion of $u_{p}^{n}$ into (3.6b), we can see that $(\tilde{u}_{p}^{n})_{y}(x)$ satisfies:

$$0 = e^{2} \left( \sum_{y} \sum_{\mathcal{H}_{1}} e_{1}^{2} \left( (\tilde{u}_{p}^{n})_{y}(x + e_{1}) \cos \left( \frac{\gamma \pi (y + e_{2})}{L} \right) - (\tilde{u}_{p}^{n})_{y}(x) \cos \left( \frac{\gamma \pi y}{L} \right) \right) \right)$$

$$= e^{2} \left( \sum_{y} \sum_{\mathcal{H}_{1}} e_{1}^{2} \left( (\tilde{u}_{p}^{n})_{y}(x + e_{1}) \cos \left( \frac{\gamma \pi y}{L} \right) + \cos \left( \frac{\gamma \pi y - e_{2}}{L} \right) \right) - 2(\tilde{u}_{p}^{n})_{y}(x) \cos \left( \frac{\gamma \pi y}{L} \right) \right)$$

$$+ e^{2} \left( \sum_{y} \sum_{\mathcal{H}_{1}} e_{1} \left( (\tilde{u}_{p}^{n})_{y}(x + e_{1}) \cos \left( \frac{\gamma \pi y}{L} \right) - (\tilde{u}_{p}^{n})_{y}(x) \cos \left( \frac{\gamma \pi y}{L} \right) \right) \right)$$

$$= e^{2} \left( \sum_{y} \cos \left( \frac{\gamma \pi y}{L} \right) \left( \sum_{\mathcal{H}_{1}} e_{1} \left( (\tilde{u}_{p}^{n})_{y}(x + e_{1}) \cos \left( \frac{\gamma \pi y}{L} \right) - (\tilde{u}_{p}^{n})_{y}(x) \right) \right) + \sum_{\mathcal{H}_{1}} e_{1} \left( (\tilde{u}_{p}^{n})_{y}(x + e_{1}) - (\tilde{u}_{p}^{n})_{y}(x) \right) \right).$$

With the axisymmetric property of the model problem, the solution of $(\tilde{u}_{p}^{n})_{y}(x)$ has the general form

$$(\tilde{u}_{p}^{n})_{y}(x) = (\tilde{u}_{p}^{\gamma})_{y} \left( e^{\gamma \pi} - e^{-\gamma \pi} \right),$$

where $\gamma$ is a coefficient to be determined. Substituting (3.12) into (3.11) and divide the equation with the constant
material parameter $c > 0$ on both sides, for each frequency $\gamma$ we have

$$0 = \sum_{\gamma_0} \frac{2e_1^2 (\tilde{u}_p^0)}{e_1^2 + e_2^2} \left( e^{\frac{\gamma}{2}x_1} - e^{\frac{-\gamma}{2}x_1} \right) \cos \left( \frac{\gamma \pi x_2}{L} \right) - \left( e^{\frac{\gamma}{2}x_2} - e^{\frac{-\gamma}{2}x_2} \right) + \sum_{\gamma_0} \frac{(\tilde{u}_p^0)}{e_1} \left( e^{\frac{\gamma}{2}x_1} - e^{\frac{-\gamma}{2}x_1} \right)$$

$$= \sum_{\gamma_0} \frac{2e_1^2 (\tilde{u}_p^0)}{e_1^2 + e_2^2} \left( e^{\frac{\gamma}{2}x_1} - e^{\frac{-\gamma}{2}x_1} + e^{\frac{\gamma}{2}x_2} - e^{\frac{-\gamma}{2}x_2} \right) \cos \left( \frac{\gamma \pi x_2}{L} \right) - 2 \left( e^{\frac{\gamma}{2}x_2} - e^{\frac{-\gamma}{2}x_2} \right)$$

$$+ \sum_{\gamma_0} \frac{1}{e_1} \left( e^{\frac{\gamma}{2}x_2} + e^{\frac{-\gamma}{2}x_2} - 2 \right).$$

Hence at each iteration step $n$, the solution for model problem (3.6b) can be written as

$$u_p(x, y) = \sum_{\gamma} (\tilde{u}_p^\gamma) \cos \left( \frac{\gamma \pi x_2}{L} \right) \left( e^{\frac{\gamma}{2}x_2} - e^{\frac{-\gamma}{2}x_2} \right).$$

where $\gamma$ satisfies

$$\sum_{\gamma_0} \frac{2e_1^2}{e_1^2 + e_2^2} \left( e^{\frac{\gamma}{2}x_2} + e^{\frac{-\gamma}{2}x_2} \right) \cos \left( \frac{\gamma \pi x_2}{L} \right) - 2 + \sum_{\gamma_0} \frac{1}{e_1} \left( e^{\frac{\gamma}{2}x_2} + e^{\frac{-\gamma}{2}x_2} - 2 \right) = 0. \quad (3.15)$$

For each frequency $\gamma$, the corresponding $\gamma$ can be obtained by solving the above equation.

On the other hand, on the classical theory subdomain we can similarly solve (3.6a) analytically and obtain

$$u_p^\gamma(x, y) = \sum_{\gamma} (\tilde{u}_p^\gamma) \cos \left( \frac{\gamma \pi x_2}{L} \right) \left( e^{\frac{\gamma}{2}x_2} - e^{\frac{-\gamma}{2}x_2} \right). \quad (3.16)$$

Therefore, at the $n$–th iteration, the solution of the whole coupled system (3.6) can be written as

$$u_p^n(x, y) = \sum_{\gamma} (\tilde{u}_p^n) \cos \left( \frac{\gamma \pi x_2}{L} \right) \left( e^{\frac{\gamma}{2}x_2} - e^{\frac{-\gamma}{2}x_2} \right). \quad (3.17a)$$

$$u_p^n(x, y) = \sum_{\gamma} (\tilde{u}_p^n) \cos \left( \frac{\gamma \pi x_2}{L} \right) \left( e^{\frac{\gamma}{2}x_2} - e^{\frac{-\gamma}{2}x_2} \right). \quad (3.17b)$$
Substituting the expressions of \( u_p \) and \( u_s \) in (3.17) into the Robin-type interface boundary condition (3.7), we obtain

\[
\sum_y (\tilde{u}_p^n)_y \cos \left( \frac{\gamma y p}{L} \right) \left( \frac{3E \gamma y}{4L} \left( e^{\frac{\gamma y p}{L}} + e^{-\frac{\gamma y p}{L}} \right) + R \left( e^{\frac{\gamma y p}{L}} - e^{-\frac{\gamma y p}{L}} \right) \right) = \sum_y (\tilde{u}_p^{n-1})_y \cos \left( \frac{\gamma y p}{L} \right) \left( \frac{3E \gamma y}{4L} \left( e^{\frac{\gamma y p}{L}} + e^{-\frac{\gamma y p}{L}} \right) + R \left( e^{\frac{\gamma y p}{L}} - e^{-\frac{\gamma y p}{L}} \right) \right).
\]

(3.18)

Therefore

\[
(\tilde{u}_p^n)_y \left( e^{\frac{\gamma y p}{L}} - e^{-\frac{\gamma y p}{L}} \right) = -\frac{3E \gamma y}{4L} \left( e^{\frac{\gamma y p}{L}} + e^{-\frac{\gamma y p}{L}} \right) + R \left( e^{\frac{\gamma y p}{L}} - e^{-\frac{\gamma y p}{L}} \right),
\]

(3.19)

Similarly, at \( x = L_2 \) the relaxed Dirichlet boundary condition (3.8) gives

\[
\sum_y (\tilde{u}_p^n)_y \cos \left( \frac{\gamma y p}{L} \right) \left( e^{\frac{\gamma y p}{L}} - e^{-\frac{\gamma y p}{L}} \right) = \tau^n \sum_y (\tilde{u}_p^{n-1})_y \cos \left( \frac{\gamma y p}{L} \right) \left( e^{\frac{\gamma y p}{L}} - e^{-\frac{\gamma y p}{L}} \right)
+ (1 - \tau^n) \sum_y (\tilde{u}_p^n)_y \cos \left( \frac{\gamma y p}{L} \right) \left( e^{\frac{\gamma y p}{L}} - e^{-\frac{\gamma y p}{L}} \right).
\]

(3.20)

Hence

\[
(\tilde{u}_p^n)_y \left( e^{\frac{\gamma y p}{L}} - e^{-\frac{\gamma y p}{L}} \right) = \tau^n (\tilde{u}_p^{n-1})_y \left( e^{\frac{\gamma y p}{L}} - e^{-\frac{\gamma y p}{L}} \right) + (1 - \tau^n)(\tilde{u}_p^n)_y \left( e^{\frac{\gamma y p}{L}} - e^{-\frac{\gamma y p}{L}} \right)
\]

(3.21)

and

\[
(\tilde{u}_p^n)_y \left( e^{\frac{\gamma y p}{L}} - e^{-\frac{\gamma y p}{L}} \right) = \tau^n (\tilde{u}_p^{n-1})_y \left( e^{\frac{\gamma y p}{L}} - e^{-\frac{\gamma y p}{L}} \right)
+ R \left( e^{\frac{\gamma y p}{L}} - e^{-\frac{\gamma y p}{L}} \right) \left( e^{\frac{\gamma y p}{L}} - e^{-\frac{\gamma y p}{L}} \right).
\]

(3.22)

We then obtain the reduction factor in the frequency space as a function of the Robin coefficient \( R \) and the relaxation parameter \( \tau^n \):

\[
\rho_p^n(R, \tau^n) = \frac{(\tilde{u}_p^n)_y \left( e^{\frac{\gamma y p}{L}} - e^{-\frac{\gamma y p}{L}} \right)}{(\tilde{u}_p^{n-1})_y \left( e^{\frac{\gamma y p}{L}} - e^{-\frac{\gamma y p}{L}} \right)} = \frac{(\tilde{u}_p^n)_y}{(\tilde{u}_p^{n-1})_y}
\]

\[
= \tau^n + (1 - \tau^n) \left( -\frac{3E \gamma y}{4L} \left( e^{\frac{\gamma y p}{L}} + e^{-\frac{\gamma y p}{L}} \right) + R \left( e^{\frac{\gamma y p}{L}} - e^{-\frac{\gamma y p}{L}} \right) \right) \left( e^{\frac{\gamma y p}{L}} - e^{-\frac{\gamma y p}{L}} \right).
\]

(3.23)

When the relaxation parameter \( \tau^n = \tau \) is fixed, \( \rho_p^n(R, \tau^n) \) is actually independent of the iteration step \( n \) although it varies with the parameter \( \tau \).
Remark 2. In this model problem, the interface boundary condition on peridynamic subdomain is imposed on two 1D lines \( \{(x, y) : |x| = L_2\} \), while in numerical simulations the peridynamic boundary conditions should be provided on a 2D area which was shown as \( \Gamma_2 \) in the left plot of Figure 1 due to the nonlocal nature of peridynamic models. However, in applications the 2D area \( \Gamma_2 \) can be considered as a very thin layer whose thickness is typically proportional to the horizon size \( \delta \). Therefore, while applying the above analysis in numerical tests, we have observed that the \( \rho_x^i(R, \tau^a) \) does not vary much when taking \( L_2 \) as either the coordinate of the left border of \( \Gamma_2 \) or the coordinate of the right border of \( \Gamma_2 \). In the following convergence tests and applications, we take \( L_2 \) as the coordinate of the center line in \( \Gamma_2 \), which is highlighted in red in the left plot of Figure 1.

Remark 3. We note that the subdomains in the 1D analysis (as displayed in Figure 3) differ from the ones employed in the 2D simulations (as displayed in Figure 1). Specifically, in the 1D problem the classical theory subdomain is assumed to be of infinite width along the \( x \) axis, while in the 2D problem it is of finite width. Moreover, in the 1D problem we assume that the two subdomains are of the same height, hence there exists no peridynamics-classical theory interface on the top and bottom sides of the peridynamics subdomain. However, in the 2D simulations the peridynamics subdomain is fully surrounded by the classical theory subdomain, and there are four interfaces in total. Such difference would all potentially cause discrepancy between the analysis based on 1D problem and the computation based on 2D settings.

4. Convergence Tests

In this section, we present a series of 2D numerical tests using the peridynamic-classical theory coupling framework with the domain set up as shown in the left plot of Figure 1. In the classical theory region, linear quadrilateral finite element meshes are employed and in the peridynamics region evenly spaced grids with piecewise constant basis functions are employed. With these tests, we aim to provide a validation for our 1D theoretical analysis in Section 3 and to investigate the performance of several coupling strategies. With manufactured solutions, we also confirm that the coupling framework passes the patch test and when taking \( h_p = o(\delta) \) the solution from our coupling framework converges to the local solution asymptotically as \( \delta \to 0 \). In particular, we consider two types of interesting problems with manufactured solutions. In Section 4.1, we study an object subjected to uniaxial tensions applying on the right external boundary. In this problem, the analytical solution for displacement is linear and therefore both the peridynamic problem and the linear elastic problem have the same analytical solution. In Section 4.2, as the second numerical example we demonstrate the performance of the proposed coupling framework on a linear elastic problem with nonlinear analytical solution for displacement, and investigate the asymptotic convergence to the local solution.

4.1. Test I: plate under uniaxial tension

In the following, we consider the classical problem in tensile test: a 2m by 2m thin plate subjected to a uniaxial tension along the \( x \)-axis with \( \sigma = 0.8\, \text{Pa} \) at the right boundary, as shown in the left plot of Figure 4. The problem
domain is \{(x, y) \in [-1,1] \times [-1,1]\}. The boundaries at \(x = -1\) and at \(y = -1\) are supported on their normal directions. This problem has the following manufactured solution for the displacement of the linear elastic subdomain:

\[
\mathbf{u}_s = \begin{pmatrix}
\frac{0.8(1 - \nu)(1 + \nu)}{E} (x + 1) \\
\frac{-0.8\nu(1 + \nu)}{E} (y + 1)
\end{pmatrix}.
\] (4.1)

This solution is also an analytical solution for the peridynamics problem. Therefore, for this problem the peridynamic and classical theory models have consistent analytical solutions. In our tests, we use the following material parameters:

\[E = 10\, \text{Pa}, \quad \nu = 1/3.\] (4.2)

Unless stated otherwise, the numerical tests in this section use uniform tessellations in the classical theory subdomain with element size \(h_s = 0.05\). On the peridynamic subdomain, we employ a finer mesh with element size \(h_p = h_s/k\) where the constant integer \(k \in [2, 6]\), and the horizon size \(\delta\) is proportional to \(h_p\), namely, \(\delta = 3h_p\).

4.1.1. Convergence to the manufactured solution

We first demonstrate the convergence of the numerical solution to the manufactured solution by plotting the total \(L^2(\Omega_s) + L^2(\Omega_p)\) errors of displacement as a function of iteration steps. In this test, we employ the classical theory subdomain as

\[\Omega_s = ([-1, -0.6] \times [-1, 1]) \cup ([0.6, 1] \times [-1, 1]) \cup ([-1, 1] \times [-1, -0.6]) \cup ([-1, 1] \times [0.6, 1])\]

with element size \(h_s = 0.05\), and the peridynamic subdomain as

\[\Omega_p = [-0.7625, 0.7625] \times [-0.7625, 0.7625]\]
with mesh size $h_\Omega = 0.025$. The interface $\Gamma_1$ on the classical theory subdomain then locates on the inner boundary of $\Omega_s$, i.e., as $[x] = 0.6, y \in [-0.6, 0.6])$ or $[y] = 0.6, x \in [-0.6, 0.6])$. $\Gamma_2$ consists of a layer with thickness 0.075, i.e.,

$$\Gamma_2 = \{(0.6875, 0.7625) \times [-0.7625, 0.7625] \cup [-0.6875, 0.6875] \times [-0.6, 0.6] \cup [-0.7625, 0.7625] \times [0.6875, 0.7625] \cup [-0.7625, 0.7625] \times [-0.6875, 0.6875] \cup [-0.7625, 0.7625] \times [-0.6, 0.6] \}.$$

Later we are going to refer to this domain setting as the “original” setting. In the right plot of Figure 4, we show the results of displacement errors in logarithmic scale as functions of the iteration number $n$ in linear scale. Different coupling strategies are employed, and the results are shown with different colors. In the legend, the first word (“Dirichlet”, “Neumann” or “Robin”) denotes the boundary condition employed on $\Gamma_1$ and the second word (“Dirichlet or “Aitken”) denotes the strategy on $\Gamma_2$. On $\Gamma_1$, the “Dirichlet”, “Neumann” and “Robin” cases represent the results where the Dirichlet boundary condition (2.17), the Neumann boundary condition (2.18) and the Robin boundary condition (2.19) with the optimal Robin coefficient are employed, respectively. On $\Gamma_2$, the “Dirichlet” case means the original unrelaxed Dirichlet boundary condition (2.21) is employed. On the other hand, the “Aitken” denotes the cases with Aitken relaxation (2.22) applied while imposing the boundary condition on $\Gamma_2$. Here the optimal Robin coefficients are obtained from numerical experiments. For the case without Aitken relaxation on $\Gamma_2$, we have observed that $R = 2E = 20 (Pa)$ gives the best performance, as displayed in the green line, where $E = 10 Pa$ is the material Young’s modulus. When the Aitken relaxation rule is employed, the optimal Robin coefficient is decreased to $R = 0.2E = 2 (Pa)$ and the results are shown in deep green. In the next section, we will further investigate the robust Robin coefficient both analytically and numerically.

From the right plot of Figure 4, we can observe that except for the “Neumann-Dirichlet” case, the computational results from all the cases converge to the analytical solution as the iteration number increases. The cases with the Aitken relaxation rule applied on $\Gamma_2$ converge faster than the cases without relaxation. The Robin boundary condition with optimal coefficient greatly accelerates the iteration convergence for both the cases with and without the Aitken relaxation rule. With a prescribed convergence tolerance $\epsilon = 10^{-9}$, we have the following performance ranking according to the number of required iterations: Optimal Robin-Aitken (16 steps) > Optimal Robin-Dirichlet (35 steps) > Neumann-Aitken (39 steps) > Dirichlet-Aitken (94 steps) > Dirichlet-Dirichlet (161 steps) >> Neumann-Dirichlet (divergent). It can be seen that comparing with the trivial case of exchanging displacement information with the “Dirichlet-Dirichlet” interface conditions, the optimal Robin boundary condition together with Aitken relaxation have greatly improved the coupling efficiency by 10 times. Therefore, employing the Robin boundary condition and obtaining the optimal Robin coefficient are very critical for achieving the best performance.

To check the asymptotic convergence behavior of the coupling conditions, we further investigate the coupling framework in the patch test. Specifically, we keep the horizon size $\delta = 0.1$ fixed and refine the mesh on the peridynamics side, to see if the solution converges to the linear analytical solution (4.1). Here we note that since (4.1) is a linear function, the coupling framework will be accurate if both solvers have piecewise linear functions in their
basis functions. However, in PDLAMMPS the spatial discretization are based on piecewise constant functions, which creates numerical errors in the coupling framework. Therefore, it is critical to check if the solution from the coupling framework converges to the analytical solution as the spatial resolution increases. In this test we employ the classical theory subdomain as in the “original” setting, and take a larger peridynamics subdomain with size $1.625 \times 1.625$. On the peridynamics-classical theory interfaces, the optimal Robin-Dirichlet boundary conditions are employed. Three cases are investigated with parameters summarized in Table 1. Note that in the finite element solver first order polynomials are employed as the basis functions, hence for the classical theory side one can expect the numerical solver to be accurate on linear problems. Therefore, we keep a fixed mesh size $h_s = 0.1$ on the classical theory side and refine the peridynamics mesh size $h_p$ from 0.1 to 0.033. From the $L^2$ errors of displacement shown in Table 1, it can observed that the error converges to 0 as $h_p \rightarrow 0$. Therefore, the coupling framework successfully passes the patch test, since its solution asymptotically converges to the accurate solution on linear problems.

4.1.2. Optimizing the coupling strategy

In this section, we aim to improve the coupling efficiency and reduce the required iteration number by

1. Optimizing the Robin coefficient;
2. Increasing the overlapping domain size;
3. Varying the mesh size ratio $h_s/h_p$;
4. Employing different relaxation parameter $\tau$.

For the linear elastic material model, the stress tensor $S(u) = \frac{\nu E}{2(1 + \nu)(1 - 2\nu)} \left[ \text{tr} \left( \frac{\partial u^e}{\partial x} \right) + \frac{E}{2(1 + \nu)} \left( \frac{\partial u^e}{\partial x} \right)^T \right] \cdot n_s + R u^p(x)$ is proportional to the Young’s modulus $E$. The Robin boundary condition (2.19) can then be written as

$$\frac{\nu E}{2(1 + \nu)(1 - 2\nu)} \left[ \text{tr} \left( \frac{\partial u^{e-1}}{\partial x} \right) + \frac{E}{2(1 + \nu)} \left( \frac{\partial u^{e-1}}{\partial x} \right)^T \right] + \frac{E}{2(1 + \nu)} \left( \frac{\partial u^{e-1}}{\partial x} \right) \cdot n_s + R u^p(x)$$

or, equivalently

$$\frac{\nu E}{2(1 + \nu)(1 - 2\nu)} \left[ \text{tr} \left( \frac{\partial u^{e-1}}{\partial x} \right) + \frac{E}{2(1 + \nu)} \left( \frac{\partial u^{e-1}}{\partial x} \right)^T \right] + \frac{E}{2(1 + \nu)} \left( \frac{\partial u^{e-1}}{\partial x} \right) \cdot n_s + R u^p(x)$$
Therefore, the optimal Robin coefficient should be linearly dependent on $E$. In the following analysis and numerical tests, instead of looking for the optimal Robin coefficient, we investigate the optimal ratio $R/E$, i.e., the optimal ratio of the Robin coefficient to the Young’s modulus.

Optimizing the Robin coefficient: We first investigate the optimal Robin coefficient with the “original” domain setting employed in the last section. To test the applicability of the 1D analysis of Section 3 in 2D simulations, we plot the reduction factors (3.23) as functions of $R/E$ for several frequencies $\gamma$ in the left plot of Figure 5. To emphasize the impact of varying Robin coefficients, here no relaxation is employed when imposing the boundary conditions on $\Gamma_2$, i.e., $\tau^n = 0$. In the analysis, we take $L_1 = 0.6$, $L_2 = 0.725$ and $h_p = 0.025$. From the left plot of Figure 5, we can observe that when $R/E$ is close to 0, the Robin boundary condition gets close to the Neumann boundary condition and the reduction factor $\rho_n^\gamma$ is slightly larger than 1 for all frequencies. Therefore, when applying the Neumann boundary condition on $\Gamma_1$ in this setting, we can expect a divergent behavior of the coupling framework. On the other hand, for $R/E \to \infty$ we have $\rho_n^\gamma < 1$, which indicates that the Dirichlet boundary should be converging. Since the low frequency modes are related to the largest Fourier coefficients and therefore are the most critical ones, we focus on the lowest reduction factor for $\gamma = 1$ to investigate the optimal Robin coefficient. When $R/E \in [2, 3]$, the reduction factor $\rho_1^\gamma$ reaches its minimum, which suggests an optimal $R/E$ around this range. With convergence tolerance $\epsilon = 10^{-9}$, the required iteration numbers with respect to different Robin coefficients are displayed in the right plot of Figure 5. It can be seen that the coupling with Neumann boundary condition is divergent while the case with Dirichlet boundary condition is convergent, which validates the reduction factor analysis of the 1D simplified problem. On the other hand, from the numerical results in the right plot of Figure 5 we can observe that the coupling framework becomes the most efficient when $R/E = 2$, which is slightly smaller but still close to the optimal coefficient predicted by the 1D analysis. Therefore, the reduction factor from the 1D analysis in (3.23) can serve as a guidance for the optimal choice of coupling coefficients in higher-dimensional simulations. In the following we continue using the 1D analysis to investigate different coupling strategies.

Remark 4. In general domain-decomposition problems, typically the low frequency mode is the most unstable one (cf. [60, 63]) which causes the coupling framework to converge slowly or even diverge. Therefore, in cases where high
frequency modes exist, we still take the Robin coefficient so as to suppress the lowest frequency modes, and this Robin coefficient is indeed the optimal one in the nonlinear problem of section 4.2 and in the plate with damage problem of section 5.

Figure 6: Test problem I: plate under uniaxial tension, with varying overlapping region sizes. Left: reduction factor with respect to \( \frac{R}{E} \) for varying frequencies from the 1D analysis. Right: required number of iterations with respect to \( \frac{R}{E} \), for tolerance \( \epsilon = 10^{-9} \).

Optimizing the overlapping domain size: We now further investigate the effect of varying overlapping regions by considering the following three domain settings:

- Setting 1 is the “original” setting employed in Section 4.1.1, which corresponds to \( L_1 = 0.6 \) and \( L_2 = 0.725 \) in the 1D analysis.

- Setting 2 serves as a large overlapping domain setting, where \( \Omega_s \) is the same as in the “original” setting, and the peridynamic subdomain is expanded to

\[
\Omega_p = [-0.8625, 0.8625] \times [-0.8625, 0.8625], \quad h_p = 0.025.
\]

The interface \( \Gamma_1 \) on the classical theory subdomain is kept the same while \( \Gamma_2 \) becomes

\[
\Gamma_2 = \left([-0.8625, -0.7875] \times [-0.8625, 0.8625]\right) \cup \left([0.7875, 0.8625] \times [-0.8625, 0.8625]\right)
\]
\[
\cup \left([-0.8625, 0.8625] \times [-0.8625, -0.7875]\right) \cup \left([-0.8625, 0.8625] \times [0.7875, 0.8625]\right).
\]

This setting corresponds to \( L_1 = 0.6 \) and \( L_2 = 0.825 \).

- Setting 3 also has large overlapping domain, where \( \Omega_p \) and \( \Gamma_2 \) are the same as in the “original” setting, and \( \Omega_s \) is changed to

\[
\Omega_s = \left([-1, -0.5] \times [-1, 1]\right) \cup \left([0.5, 1] \times [-1, 1]\right) \cup \left([-1, 1] \times [-1, -0.5]\right) \cup \left([-1, 1] \times [0.5, 1]\right).
\]

The interface \( \Gamma_1 \) on the classical theory subdomain becomes \( |x| = 0.5, \ y \in [-0.5, 0.5] \) \cup \( |y| = 0.5, \ x \in [-0.5, 0.5] \). This setting corresponds to \( L_1 = 0.5 \) and \( L_2 = 0.725 \) in the 1D analysis.
Here we note that although settings 2 and 3 have different overlapping regions, their overlapping region sizes are both 0.2625 which is larger than the overlapping region size of setting 1.

For each of the coupling domain settings, we plot the reduction factor for \( \gamma = 1 \) and \( \gamma = 10 \) as functions of \( R/E \) in the left plot of Figure 6. It can be observed that the reduction factor decreases for larger overlapping regions, especially when \( \gamma \) is larger than 1. Therefore, faster convergence is expected when the overlapping region gets larger. The reduction factors from settings 2 and 3 are almost equivalent, while in setting 3 the optimal \( R/E \) is slightly larger.

In the right plot of Figure 6, we display the required iteration numbers as functions of \( R/E \) for each of the three settings. Here the iteration convergence tolerance is \( \epsilon = 10^{-9} \). For all three settings, the optimal \( R/E \) does not vary much, which is different from the observation of the 1D analysis. For a fixed value of \( R/E \), we can see that the settings 2 and 3 have faster convergence. Therefore, increasing the overlapping region accelerates the iteration convergence, and this observation is consistent with the conclusion from other nonlocal-local coupling frameworks [25, 42]. On the other hand, while comparing the iteration numbers for settings 2 and 3, in the right plot of Figure 6 we can see that these two cases have almost the same performances. We can then conclude that while a larger overlapping region size has a positive impact on the coupling efficiency, the location of this region does not matter much, which also validates the observation of the 1D analysis in the left plot of Figure 6.

![Figure 7: Test problem I: plate under uniaxial tension, with varying mesh size ratios. Left: reduction factor with respect to \( R/E \) for varying frequencies from the 1D analysis. Right: required number of iterations with respect to \( R/E \), for tolerance \( \epsilon = 10^{-9} \).](image)

**Varying the mesh size ratio** \( h_s/h_p \): To illustrate the effect of varying mesh size ratios, we now show the reduction factors from the 1D analysis and the required iteration numbers from 2D simulations, for a fixed finite element mesh size \( h_s = 0.05 \) and varying peridynamic mesh sizes \( h_p \). In the left plot of Figure 7, we show the reduction factors as functions of \( R/E \) for \( \gamma = 1 \) and \( \gamma = 10 \). Except for the peridynamics mesh size \( h_p \), here all the other parameters are the same as in the “original” setting. In the first case, we employ the “original” setting, i.e., \( h_p = h_s/2 \). In the second and the third cases we decrease \( h_p \). Specifically, in the second case we have \( h_p = h_s/4 \) and in the third case \( h_p = h_s/6 \). From the 1D analysis, it can be observed that varying the mesh size ratio does not change the reduction factors, and this observation is verified by the numerical tests displayed in the right plot of Figure 7. It was shown that the required iteration numbers for all three cases are almost equivalent. Therefore, both the 1D analysis and the numerical results indicate that the coupling convergence rate is independent of the mesh size ratio.
Figure 8: Test problem I: plate under uniaxial tension, with varying relaxation parameters in (2.22). Left: reduction factor with respect to $R/E$ for varying frequencies from the 1D analysis. Right: required number of iterations with respect to $R/E$, for tolerance $\epsilon = 10^{-9}$.

Varying the relaxation parameter $\tau^n$: In the previous discussions, we have been focusing on the cases that the Dirichlet boundary condition (2.21) without relaxation is applied on the peridynamics solver. In all cases the coupling framework is unstable when employing the Neumann boundary condition on $\Gamma_1$. The optimal Robin coefficient is around $R/E = 2$, which is also the lowest value of $R/E$ making the coupling framework stable. We now investigate the effect of applying the relaxed boundary condition (2.22) on $\Gamma_2$. With the “original” domain setting employed, the reduction factors of the 1D analysis are provided in the left plot of Figure 8. In this test, we employ 3 cases: the Robin-Dirichlet case where the unrelaxed boundary condition (2.21) is employed on $\Gamma_2$, the Robin-relaxed Dirichlet case where the boundary condition (2.22) is employed on $\Gamma_2$ with a fixed relaxation parameter $\tau^n = 0.5$ and the Robin-relaxed Dirichlet case with an increased relaxation parameter $\tau^n = 0.9$. From the left plot of Figure 8, it can be observed that for both frequencies increasing the relaxation parameter helps decreasing the reduction factor when $R/E$ is small. That means, when the Robin boundary condition is close to the Neumann side, the relaxation parameter helps stabilizing the coupling procedure and accelerating the convergence. On the other hand, when $R/E$ is large, the increased relaxation parameter gives a larger reduction factor, which indicates a slower convergence. When comparing the optimal $R/E$ where the reduction factor reaches the minimum, it can be observed that for both $\gamma = 1$ and $\gamma = 10$, when increasing the relaxation parameter the function nadir shifts to the right. Therefore, when employing a larger relaxation parameter, we can expect to observe a smaller optimal Robin coefficient $R/E$. In the right plot of Figure 8, we show the required number of iterations as functions of $R/E$ for the above three cases, together with the Robin-Aitken relaxation case where the relaxation parameter is updated via the Aitken rule (2.23a). One can see that when the relaxation parameter reaches 0.9, the coupling algorithm is stable with Neumann boundary condition on $\Gamma_1$, meanwhile, it takes longer for the coupling algorithm with Dirichlet boundary condition on $\Gamma_1$ to converge. These findings have validated the observations from 1D analysis: increasing the relaxation parameter helps stabilizing the Neumann-relaxed Dirichlet case, but it slows down the convergence in the Dirichlet-relaxed Dirichlet case. On the
other hand, as observed in the 1D analysis, when the relaxation parameter increases, the optimal Robin coefficient tends to decrease. However, comparing with the analysis prediction, the actual simulation shows a larger decrease in the optimal coefficient. When $\tau^a = 0.5$, the optimal $R/E$ has been shifted to 0.5; when $\tau^a = 0.9$, the Neumann boundary condition gives the best performance, which is equivalent to $R/E = 0$. Therefore, the optimal Robin coefficient from 1D analysis seems too conservative when the relaxation rule is employed on $\Gamma_2$. This discrepancy may be due to the differences on the subdomain settings as noted in remark 3, or caused by the complexity of 2D problems. Among all cases, it can be observed that the case with Robin-Aitken relaxation boundary condition has the best performance, with the optimal $R/E \approx 0.2$. Overall we can conclude that when the relaxation parameter increases, the performance from Neumann boundary condition improves, and a smaller Robin coefficient is desired. For choosing a proper relaxation parameter, the Aitken formulation (2.23a) is a very robust choice.

4.2. Test II: problem with nonlinear solution

We take here a problem with nonlinear analytic solution when considering linear elastic model on the whole domain, and study the asymptotic convergence behavior of the local-nonlocal coupling framework. In this problem, we take the material properties as $E = 10 \text{Pa}$, $\nu = 1/3$. The displacements on the faces $x = \pm 1$ and $y = \pm 1$ are known

$$u_x = \begin{cases} 
0.05(x^2 - 4y^2) \\
0.05(4x^2 - y^2)
\end{cases}.$$ (4.3)

When considering the classical theory on the whole domain, the displacement field is given by (4.3). Note that in this problem (4.3) is not an analytical solution for the peridynamic model. Employing the “original” domain setting, the simulation results of our coupling framework are displayed in Figure 9. In this section, we first study the convergence of the numerical results to the local solution (4.3) in Section 4.2.1. Secondly, since the solution in this problem is nonlinear and therefore differs from the 1D stretching problem, it motivates us to investigate the efficiency performance
of the coupling framework and check if the 1D analysis and the experiences in the linear problem (see Section 4.1) can be applied here.

4.2.1. Convergence to local solution

Similar to a peridynamic model, two types of numerical convergence can be introduced for a local-nonlocal coupling framework: the $\delta$-convergence in which the horizon size goes to zero, and the $m$-convergence where the horizon size is fixed and the mesh is refined. Since the $m$-convergence was verified via the patch test in section 4.1.1, we now investigate the $\delta$-convergence in this section. In the coupling framework, the peridynamic model is consistent with the linear elastic model, in the sense that the peridynamic model converges to the linear elastic model as $O(\delta^2)$. Therefore, a key desirable property for the coupling framework is that it should be faithful to the classical theory in the case that the displacement has sufficient regularity. That means, in the limit as $h_s$, $\delta$ and $h_p$ simultaneously approach zero, the solution of the current framework should recover the solution of the linear elastic model. In the following we will then investigate the convergence to the local solution when $\delta \ll 1$. Specifically, we firstly keep a fixed element size $h_s$ to investigate the convergence of solution in the peridynamics subdomain with different interface conditions (as shown in Table 2), and secondly demonstrate the order of convergence in $\delta$ with $h_p$, $h_s \ll \delta$ (as shown in Table 3).

In the first test, we employ the domain decomposition as in the “original” setting in Section 4.1.1 with fixed element size $h_s = 0.05$ and $h_p, \delta \to 0$. We systematically vary the horizon size $\delta$ from 0.075 to 0.03333 while decreasing the corresponding $h_p$ from 0.025 to 0.00625. Three meshes are considered in the peridynamic subdomain: the first case is the same as in the “original” setting where we have $h_p = 0.025$ and $\delta = 3h_p = 0.075$, in the second case $h_p = 0.0125$.

| Case No. | $\delta$ | $h_p$ | $h_s$ | Boundary Conditions | $|\text{error}|_{L^2(\Omega_s)}$ | $|\text{error}|_{L^2(\Omega_p)}$ |
|----------|----------|-------|-------|----------------------|-------------------------------|-------------------------------|
| 1        | 0.075    | 0.025 | 0.05  | Neumann-Dirichlet    | 8.925385 $\times 10^{-3}$    | 2.151058 $\times 10^{-2}$    |
| 2        | 0.05     | 0.0125| 0.05  | Neumann-Dirichlet    | 8.565629 $\times 10^{-3}$    | 2.078626 $\times 10^{-2}$    |
| 3        | 0.0333   | 0.00625| 0.05  | Neumann-Dirichlet    | 8.063529 $\times 10^{-3}$    | 1.882105 $\times 10^{-2}$    |

Table 2: Test II problem with nonlinear solution: parameters and $L^2$ errors to the local solution, with $h_s$, $h_p \ll \delta$.
and $\delta = 4h_p = 0.05$, and in the third case $h_p = 0.00625$ while $\delta = 16h_p/3 = 0.03333$. We can see that from case 1 to case 3 $\delta \to 0$ and $h_p = O(\delta)$. Neumann-Dirichlet, optimal Robin-Dirichlet and Dirichlet-Dirichlet coupling conditions are employed for all cases. Table 2 gives the parameters and the $L^2$ errors with respect to the local solution (4.3) for each case. From the results, we observe that generally the Neumann-Dirichlet coupling condition gives the numerical results closest to the local solution, while the Dirichlet-Dirichlet coupling condition is the least accurate. While comparing the errors between different cases, we can see that from case 1 to case 3, the $L^2$ errors decrease gradually. However, the order of convergence is much worse than $O(\delta^2)$, which is the convergence rate from the peridynamic model to the linear elastic model. Such a slow convergence is caused by the fact that the peridynamic solver based on piecewise constant discretization methods is generally not asymptotically compatible [62], i.e., the numerical solution converges to the solution of the corresponding classical theory only if $h_p = o(\delta)$ as $\delta \to 0$. Therefore, the numerical error from PDLAMMPS contaminates the coupling solution and leads to slow $\delta$-convergence. To investigate the $\delta$-convergence from coupling, in the second test we keep $h_p, h_s \ll \delta$ so the numerical errors from discretization methods are negligible. In this test we keep $\Omega_s$ as in the “original” setting and set $\Omega_p = [0.8125, 0.8125] \times [0.8125, 0.8125]$ with $h_s = 1/40$ and $h_p = 1/80$. 6 cases are employed where we gradually decrease $\delta$ from 0.1875 (marked as case 4) to 0.15625 (marked as case 9). The optimal Robin-Dirichlet coupling conditions are applied for all cases. In Table 3 we summarize the parameters and the $L^2$ errors with respect to the local solution. It can be observed that as $\delta$ decreases, the $L^2$ error of displacement decreases with an averaged rate of order 1.8. Therefore, when $\delta$ decreases, the coupled framework converges to the local operator for all coupling conditions with a rate close to $O(\delta^2)$.

### 4.2.2. Optimizing the Robin coefficient

![Figure 10: Required number of iterations with respect to $R/E$ for tolerance $\epsilon = 10^{-10}$ in test problem II: a nonlinear problem.](image)

We now take the nonlinear problem and study the optimal interface condition. Figure 10 gives the required number of iterations for reaching $\epsilon = 10^{-10}$, as a function of $R/E$. Two cases are investigated: the blue line shows the results with Robin boundary condition on $\Gamma_1$ and the unrelaxed Dirichlet boundary condition (2.21) on $\Gamma_2$, while the red line represents the results with the Aitken relaxation rule employed when updating the boundary condition on $\Gamma_2$. Here the subdomains are with the same setting as in the “original” case in Section 4.1.1. Without the relaxation rule the coupling algorithm has the best performance when $R/E = 2$, which is consistent with the 1D analysis on this setting (as shown in the right plot of Figure 5) although the 1D assumption in Section 3 does not hold here. When the Aitken
relaxation rule is applied, the optimal performance is achieved when \( R/E = 0.2 \), which is also consistent with the observations on the linear problem in Test I (see Figure 8). Similar as in the linear problem, we observe that the case with the Aitken relaxation rule outperforms the case without relaxation. Among all cases, the coupling framework with the optimal Robin boundary condition and the Aitken relaxation rule converges the fastest. Therefore, although this test problem is nonlinear, the observations regarding its optimal coupling strategy are very close to the conclusions based on the linear problem in Section 4.1. That means, the ID analysis can still serve as a guidance for the optimal Robin coefficient, especially in the case when the relaxation rule is not applied. When the relaxation rule is applied, a small Robin coefficient is preferred.

5. Application: Brittle Fracture in a Plate Loaded in Tension

Having demonstrated the asymptotic convergence and the optimal coupling strategy, we now apply our approach to a practical damage problem as illustrated in Figure 11. Here we consider a plate with a hole which is loaded in tension by traction \( \sigma \) on both the left and the right external boundaries. To model the bond breaking procedure, we employ the dynamic runs instead of the energy minimization in the peridynamic solver PDLAMMPS. In this problem, the traction load is assumed to be slowly increasing from \( \sigma = 12.20 MPa \) to \( \sigma = 17.56 MPa \). The damage progression can then be modeled as a quasi-static problem by applying the traction load in an incremental way: at each step we increase the traction load by \( \Delta \sigma = 0.244 MPa \) and solve this new static problem with damage until the coupling framework converges. In order to circumvent premature failure due to high local displacement gradients, damage is allowed in a subregion of size \( 0.5 m \times 0.5 m \) inside the peridynamic domain, as delimited by the dashed red line in Figure 11. The “original” setting is employed in all simulations in this section, where we employ the finite element mesh with mesh size \( h_s = 0.05 \) in the classical theory subdomain and the peridynamic subdomain has grid size \( h_p = 0.025 \) and horizon.
size $\delta = 3h_p = 0.075$. In the simulations, we take the following material properties:

$$E = 72.0\,\text{GPa}, \quad \nu = \frac{1}{3}, \quad \text{and} \quad G_0 = 270.0\,\text{J/m}^2.$$ 

In Figure 12-13, we show the numerical simulation results. From the top to the bottom rows we provide the
Figure 13: Simulation of a plate with a hole loaded with increasing tension: results of stresses. From top to bottom, the traction load is incrementally increasing as: $\sigma = 12.44\,\text{MPa}$, $\sigma = 12.93\,\text{MPa}$, $\sigma = 13.41\,\text{MPa}$, $\sigma = 14.63\,\text{MPa}$ and $\sigma = 17.56\,\text{MPa}$. 
displacement profiles, the resulting damage patterns and the stress profiles at five quasi-static steps which corresponds to different incremental traction loads: step 1 with traction load $\sigma = 12.44\,\text{MPa}$, step 3 with $\sigma = 12.93\,\text{MPa}$, step 5 with $\sigma = 13.41\,\text{MPa}$, step 10 with $\sigma = 14.63\,\text{MPa}$ and step 22 with $\sigma = 17.56\,\text{MPa}$. We can see that as the traction load increases, the cracks initiate at the hole near high deformation areas and then propagate towards the edges of the damage region. We note that the damage patterns are straight lines from the hole towards the edge of the domain, which is consistent with the results in [64].

We also investigate if the optimal Robin coefficient analysis can be applied to this problem. In Figure 14, we present the averaged required number of iterations at each incremental load step, as functions of $R/E$. Here the convergence tolerance is set as $\epsilon = 10^{-11}$. Both the case with unrelaxed Dirichlet boundary condition on $\Gamma_2$ (plotted in blue) and the cases with the Aitken relaxation rule on $\Gamma_2$ (plotted in red) are investigated. It can be observed that with the same domain settings applied, although the actual required numbers vary the trends of changes in iteration numbers in Figure 14 are very close to the results from the previous two test problems (see Figures 6 and 10). We still have the optimal $R/E \approx 2$ in the unrelaxed Dirichlet boundary condition case, and the optimal $R/E \approx 0.2$ in the case with the Aitken relaxation rule. Therefore, in this complicated damage scenario, the optimal Robin boundary condition on the classical theory side together with the relaxed Dirichlet boundary condition on the peridynamic side is again the most robust choice, and the 1D analysis helps in predicting the optimal Robin coefficient.

6. Summary and future work

In this work, we have developed an implicit coupling method with the partitioned approach to couple the peridynamics and the corresponding classical theory. A particle-based discretization is used in the peridynamics domain, and a first order finite element method is employed for the classical theory domain. In this coupling framework, the two solvers communicate by exchanging interface conditions, which enables a modular software implementation where the solvers can be treated as black boxes. We also present new theoretical analysis for simple geometries that provides optimal values for accelerating the coupling efficiency. Different coupling boundary conditions are investigated, and both the numerical and analytical results suggest that the best performance is achieved when employing the Robin boundary condition at the classical theory side and the Aitken relaxation rule at the peridynamics side. Comparing
with the popular Dirichlet-Dirichlet boundary condition, this robust boundary condition improves the coupling convergence by a factor of 10, and overall we have the following sequence on the boundary conditions according to their performance: Optimal Robin-Aitken > Optimal Robin-Dirichlet > Neumann-Aitken > Dirichlet-Aitken > Dirichlet-Dirichlet >> Neumann-Dirichlet (divergent). We have also investigated the impact of other factors on the coupling convergence, and found that to achieve faster convergence, a larger overlapping domain is preferred, while the mesh size ratio has less impact.

An additional research direction suggested by this work is to improve the accuracy of this framework. One of the natural choice would be to couple the novel meshfree quadrature rule for peridynamics in [65] with the high-order finite method solver for classical theory in [55]. We may also investigate the performance of this framework on dynamic problems, which will be of interest for simulating time-involved damage problems.

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