Received: 7 October 2022 | Accepted: 18 November 2022

DOI: 10.1002/pamm.202200151

A Penalty Method for Coupling of Finite-Element and Peridynamic Models

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A classical continuum mechanics model no longer fulfills its basic assumptions, when the deformations are not smooth or discontinuous. Peridynamics (PD) as an integral formulation could better overcome these issues. Therefore, it is better suited to solve fracture problems such as crack initiation, its growth and formation of crack patterns. In PD the magnitudes of internal forces at a material point depend on the collective interaction of all material points within a subdomain called horizon. To take advances from the formulation, typically it is implemented in a mesh-free form. In that case, it is easy to separate interactions between different material points. As consequence, a relatively high resolution is required to describe continuous deformation functions and, consequently computationally expensive. Therefore, the application of mesh-free PD in undamaged regions requires an unnecessary high effort for receiving sufficient accurate results. In contrast, the finite element method (FEM) as a classical continuum mechanics-based approach, is very efficient, if continuous stress distributions can be assumed. Consequently, a computational cost reduction can be achieved, if the PD is applied in the local damaged zone only and the remaining area is modeled and analyzed with the classical FEM. Realization of such an approach requires a sufficient accurate coupling of the PD and the FEM subdomains.

A brief overview about different coupling approaches is given. Then the general approach of an Arlequin based method is presented. Here the coupling is achieved via an overlapping of PD and FEM areas. The coupling equations are developed and realized with help of the Penalty method. The Penalty method is considered as an alternative procedure to the Lagrange multiplier strategy without creating new unknowns, which essentially simplifies the coupled PD-FEM approach. The validity and limits of the proposed technique are demonstrated through analysis, where the choice of the Penalty number is discussed as well as artificial wave oscillations, caused by the coupling area.

1 Introduction

The description of massive complex systems with a large number of components with the damage inside is of great scientific interest. Damage behavior has a non-local character since every real material has a characteristic length of heterogeneity. This means that local theories are not capable to cover such layer of problems, which in turn explains the motivation for using non-local theories.

The peridynamic theory [1], which is an alternative formulation of continuum mechanics, allows to solve fracture problems such as crack propagation and bifurcation, and gives a realistic representation of the crack profile and its propagating velocity [2]. As peridynamics is a non-local theory, it provides a natural setting to model long-range forces with implementation of a striking radius, called horizon δ [1], [3], which is used to define the grad of non-locality.

In state-based formulation [4], the magnitudes of forces inside the bond depend on the collective deformation of all bonds within a spherical region of radius δ. If this deformation of the bond is bigger than a predefined value, it is considered that the bond is broken and cannot be healed [5].

Relatively high resolution is required to describe continuous deformation functions, and calculation methods based on peridynamics are much more expensive. As a result, this requires much more computational cost than any local theory. The boundary conditions are different to model in the peridynamics than in the classical theory. The variational formulation doesn't lead to natural boundary conditions [6], hence the body force must be applied within some region instead of a force on the surface/line [7]. Considering that the boundary conditions are applied within a horizon distance, the softening effect is observed on the material points that are less than one horizon away from the system edges [8]. In addition, non-local theories require the unconventional prescription of non-local boundary conditions, which can be a real challenge, especially for complex models.

In the resent years the topic of coupling local and non-local theories has gained significant attention in order to overcome the above-mentioned problems. A non-local region is supposed to be a part of model in which discontinuities are present or may be generated, and a local region is correspondingly the part, free from discontinuities with conventional boundary and initial conditions.

It was proposed [9] to divide all coupling techniques into two groups: (i) generalized domain decomposition and (ii) atomistic-to-continuum types. The models in generalized domain decomposition group are introduced independently in each sub-domain and interacts with other model parts via special conditions on transition regions. The first example is

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the Optimization-Based Method [10], which treats the coupling conditions as optimization task to minimize the inconsistency between domains. Another representative of this group is the Partitioning procedure by using for example the Schwarz method [11]. The main advantage is that it allows to couple two black box solvers by defining constraints on the common interface. To atomistic-to-continuum coupling techniques belong to the following methods: the energy-based Arlequin [12], [13] and the Quasi non-local [14] procedures, force-based Morphing [15] and Blending [16] approaches and additional Splice methods [17]. In this paper we decided to implement Arlequin based Penalty approach, since energy based methods should have better comparability in comparison to others atomistic-to-continuum group and doesn't slow down as methods in decomposition group.

2 Theoretical Background

2.1 Classic Elasticity

The strong form of the boundary value problem [18] can be given as:

$$\rho\ddot{\mathbf{u}} = \nabla \cdot \boldsymbol{\sigma} + \mathbf{b}. \tag{1}$$

The strong form is modified into a weak form of the boundary value problem. For this purpose, the principle of virtual work is performed by multiplication with the test function and the integration over the volume Ω_{CE}:

$$\int_{\Omega_{CE}} \delta\mathbf{u} \cdot \ddot{\mathbf{u}}\rho \, \mathrm{dV} + \int_{\Omega_{CE}} \delta\boldsymbol{\epsilon} : \boldsymbol{\sigma} \, \mathrm{dV} = \int_{\Omega_{CE}} \delta\mathbf{u} \cdot \mathbf{b}\mathrm{dV} + \int_{\partial\Omega_\sigma} \delta\mathbf{u} \cdot \mathbf{t}^* \, \mathrm{dA}. \tag{2}$$

When external forces act on a body, work is being done inside the solid, which causes a deformation. As a result of the work done on the body, it absorbs energy. The first left term in the equation 2 is denoted as virtual work of inertial forces, the second term is the internal virtual work and the right part of the equation is the virtual work of the external forces. The equation is numerically discretized using finite elements, such as continuous variable in the governing equation is approximated using shape functions N^i, and FE equation [19] looks as follows:

$$\mathbf{M}\ddot{\mathbf{u}}(\mathbf{x}, t) + \mathbf{K}\mathbf{u}(\mathbf{x}, t) = \mathbf{f}(t), \tag{3}$$

with mass matrix $\mathbf{M}$, stiffness matrix $\mathbf{K}$ and force vector $\mathbf{f}$, each of them can be calculated for every element:

$$\mathbf{M} = \int_{\Omega_{CE}} \mathbf{N}^T\mathbf{N} \, d\mathrm{V}; \qquad \mathbf{K} = \int_{\Omega_{CE}} \mathbf{B}^T\mathbf{C}\mathbf{B} \, d\mathrm{V}; \qquad \mathbf{f} = \int_{\Omega_{CE}} p\mathbf{N} \, d\mathrm{V};$$

with differential operator $\mathbf{B}$, which connects strain and displacement, distributed load p and Elasticity matrix $\mathbf{C}$. For numerical integration Gauss-Legendre quadrature is used.

2.2 Peridynamic Theory

In this section bond-based peridynamics is reviewed. Remembering, that bond-based peridynamics is a special case of the state-based formulation [4], it is supposed, that it hasn't a significant influence on the coupling strategy.

In the following discussion we identify a few peridynamic terms. Under the extern load each material point $\mathbf{x}$in the body gets the displacement $\mathbf{d}$. The new position of this point in the deformed configuration can be described through $\mathbf{y} = \mathbf{x} + \mathbf{d}$.

Similar to the classic elasticity the resulting equation of motion in peridynamics [20] has the form :

$$\rho\ddot{\mathbf{d}}(\mathbf{x}, t) = \int_{\Omega_{PD}} \mathbf{f}(\mathbf{d}' - \mathbf{d}, \mathbf{x}' - \mathbf{x}, t) dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}, t), \tag{4}$$

with pairwise force function $\mathbf{f}$, whose value is the force that particle $\mathbf{x}'$ exerts on the particle $\mathbf{x}$. H_x is the spherical neighborhood around the particle $\mathbf{x}$ with the radius δ. This radius is also called the horizon and define the grad of non-locality in the model.

For the microelastic material [1], the pairwise potential is found as:

$$\mathbf{f}(\boldsymbol{\xi}, \boldsymbol{\eta}) = \frac{\partial w(\boldsymbol{\xi}, \boldsymbol{\eta})}{\partial \boldsymbol{\eta}}, \tag{5}$$

where $\boldsymbol{\xi} = \mathbf{x}' - \mathbf{x}$ is called bond and represents the direct physical interaction, which occurs between those particles. In case of simple elastic materials this can be interpreted as a spring. The relative displacement can be found as: $\boldsymbol{\eta} = \mathbf{d}' - \mathbf{d}$. The relative position vector in the current configuration gives $\boldsymbol{\xi} + \boldsymbol{\eta} = \mathbf{y}' - \mathbf{y}$. Also the bond force depends only on the relative bond stretch [4], which can be found from:

$$s = \frac{|\mathbf{y}' - \mathbf{y}| - |\mathbf{x}' - \mathbf{x}|}{|\mathbf{x}' - \mathbf{x}|} = \frac{|\xi + \eta| - |\xi|}{\xi}. \tag{6}$$

For linear elasticity pairwise force, defined through the micro-potential, looks as follows:

$$\mathbf{f}(\boldsymbol{\xi}, \boldsymbol{\eta}) = \frac{c(\boldsymbol{\xi}) s^2 |\boldsymbol{\xi}|}{2}, \tag{7}$$

where c is the micro-modulus. A relative bond stretch function is an indicator of the presence or absence of damage. If the value is larger than the predefined number, the bond between two corresponding particles breaks and the pairwise force vanishes.

3 Formulation of Arlequin Based Penalty Coupling

The main idea of the Arlequin Method [13] is that the total energy of the system is presented as the weighted sum of local and non-local energies. The whole area is divided into three domains: pure classic elasticity (CE) domain, pure peridynamic (PD) domain and overlapping zone, which consists of both theories:

$$H(\mathbf{u}, \dot{\mathbf{u}}, \mathbf{d}, \dot{\mathbf{d}}) = \alpha(\mathbf{x}) H_{CE}(\mathbf{u}, \dot{\mathbf{u}}) + (1 - \alpha(\mathbf{x})) H_{PD}(\mathbf{d}, \dot{\mathbf{d}}). \tag{8}$$

Here $\alpha(\mathbf{x})$ is the weighted function, which can be chosen variously. We have used the following form:

$$\alpha(\mathbf{x}) = \begin{cases} 1 & \forall \mathbf{x} \in \Omega_{CE} \cap \Omega_o, \\ 0 & \forall \mathbf{x} \in \Omega_{PD} \cap \Omega_o, \\ \frac{l_1}{l_1 + l_2} & \forall \mathbf{x} \in \Omega_o, \end{cases} \tag{9}$$

where l_1 and l_2 is the distance to Ω_{CE} and Ω_{PD} boundary, respectively. The total Hamiltonian in CE has the value of total energy of CE system, which can be found as:

$$H_{CE} = W_{CE}^{kin} + W_{CE}^{int} - W_{CE}^{ext}, \tag{10}$$

with $W_{CE}^{kin}, W_{CE}^{int}, W_{CE}^{ext}$ as a kinetic, internal and external energies, respectively. Similarly, it is also possible to write the total Hamiltonian in Peridynamics as:

$$H_{PD} = W_{PD}^{kin} + W_{PD}^{int} - W_{PD}^{ext}. \tag{11}$$

Assume, that the classical elasticity domain is discretized using finite elements with N_{ct} nodes. The peridynamic area is also discretized using the meshfree method [3]. A PD element is represented by particles, connected by bonds. N_{pt} is the total number of particles. The Hamilton's equivalence is used to find the equation of motion for each part of domain. The internal force vector is detected from internal energy:

$$\mathbf{f}_{CE}^{int} = \frac{\partial(\alpha(\mathbf{x}) W_{CE}^{int})}{\partial \mathbf{u}} = \int_{\Omega_{CE}} \alpha(\mathbf{x}) \mathbf{B}^T \boldsymbol{\sigma} \, \mathrm{d}\Omega;$$

$$\mathbf{f}_{PD}^{int} = \frac{\partial((1 - \alpha(\mathbf{x})) W_{PD}^{int})}{\partial \mathbf{d}} = \int_{\Omega_{PD}} (1 - \alpha(\mathbf{x})) \mathbf{f}(\mathbf{d}' - \mathbf{d}, \mathbf{x}' - \mathbf{x}, t) dV_{\mathbf{x}'}. \tag{12}$$

Similarly, the external force vector is obtained as follows:

$$\mathbf{f}_{CE}^{ext} = \frac{\partial(\alpha(\mathbf{x}) W_{CE}^{ext})}{\partial \mathbf{u}} = \int_{\Omega_{CE}} \alpha(\mathbf{x}) \mathbf{N} \rho \mathbf{b} d\Omega + \int_{\partial\Omega_\sigma} \mathbf{N} \mathbf{t}^* \, \mathrm{dA};$$

$$\mathbf{f}_{PD}^{ext} = \frac{\partial((1 - \alpha(\mathbf{x})) W_{PD}^{ext})}{\partial \mathbf{d}} = \mathbf{b} V. \tag{13}$$

Considering all, the equation of motion for the CE case in finite elements and the PD case are obtained as:

$$\alpha_i(\mathbf{x}) \rho \ddot{\mathbf{u}}_i = (\mathbf{f}_{CE}^{ext})_i - (\mathbf{f}_{CE}^{int})_i; \qquad (1 - \alpha_j)(\mathbf{x}) \mathbf{M} \ddot{\mathbf{d}}_j = (\mathbf{f}_{PD}^{ext})_j - (\mathbf{f}_{PD}^{int})_j. \tag{14}$$

To reach the mechanical compatibility between these domains we include constraints in the overlapping zone. Let the equation of constraints in the general case $\mathbf{z}$ consist of displacement-dependent term $\mathbf{Zu}$ and some constant term $\mathbf{z}_0$, as:

$$\mathbf{z}(\mathbf{u}) = \mathbf{z}_0 + \mathbf{Z}\mathbf{u}. \tag{15}$$

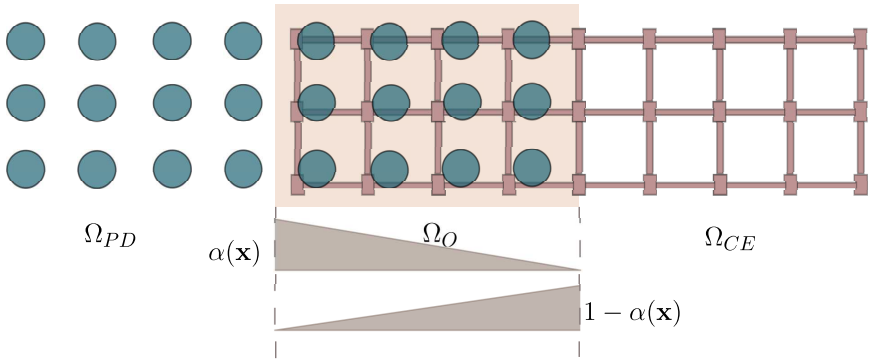

Fig. 1: Arlequin coupling concept with model decomposition

These constraints can be included into the equation of motion using the Penalty Method. For this purpose, the functional Ξ should be constructed, concerning the introduced degrees of freedom. Taking into account constraints, the functional is demanded to reach a minimum value [21].

$$\Xi = \mathcal{L}(\mathbf{x}, \mathbf{u}, t) + \frac{1}{2}\kappa \int_{\Omega_o} \mathbf{z}^T \mathbf{z} d\Omega_o \rightarrow \text{Min}, \tag{16}$$

where $\mathcal{L}(\mathbf{x}, \mathbf{u}, t)$ is Lagrangian of the dynamic system and κ - the penalty number. In simple terms it can be thought, that nodes from local and non-local regions are connected through a spring with "spring constant" κ. As the result, the constraints are approximately fulfilled, and theoretically getting better as the number κ increases. However, the value is numerically limited and the determination of it is a challenging task, which would be discussed later. The integral term in equation (16) is simplified, as the constraints are fulfilled locally, node by node:

$$\Xi = \frac{1}{2}\dot{\mathbf{u}}^T \mathbf{M} \dot{\mathbf{u}} + \frac{1}{2}\mathbf{u}^T \mathbf{K} \mathbf{u} - \mathbf{u}^T \mathbf{f} + \frac{1}{2}(\mathbf{z}_0 + \mathbf{Z}\mathbf{u})^T (\mathbf{z}_0 + \mathbf{Z}\mathbf{u}). \tag{17}$$

In order to minimize the functional Ξ, the partial derivative should be calculated:

$$\begin{aligned} &\frac{\partial \Xi}{\partial \mathbf{u}} = 0, \quad \rightarrow \quad \mathbf{M}\ddot{\mathbf{u}} + (\mathbf{K} + \mathbf{K}_z)\mathbf{u} = \mathbf{f} - \mathbf{f}_z; \\ &\mathbf{K}_z = \kappa \mathbf{Z}^T \mathbf{Z}; \\ &\mathbf{f}_z = \kappa \mathbf{Z}^T \mathbf{z}_0, \end{aligned} \tag{18}$$

Assume the displacement constraints in the overlapping zone between local and non-local domains are described as:

$$\mathbf{z} = \mathbf{d} - \mathbf{u} = \mathbf{d} - \sum_{\Omega_o} \mathbf{N}(\xi)\mathbf{u}^e \tag{19}$$

than the coupling matrix results in:

$$\mathbf{K}_z \begin{bmatrix} \mathbf{d} \\ \mathbf{u} \end{bmatrix} = \kappa \begin{bmatrix} \mathbf{I} & \mathbf{N}_d \\ \mathbf{N}_d^T & \mathbf{N}_d^T \mathbf{N}_d \end{bmatrix} \begin{bmatrix} \mathbf{d} \\ \mathbf{u} \end{bmatrix}$$

4 Results and Discussion

To test the coupling strategy we use a 1D example, the task configuration is proposed in Fig. 2. The truss is fixed one side and has the initial stretch on the time start point. After the stretch is removed, the truss experiences free vibrations. The material and numerical parameters are: $E = 1 \cdot 10^9$ Pa, $\nu = 0.25$, $\rho = 7800$ kg/m^2, $L = 1$ m, the spatial discretization for both models differs depending on the chosen size of the overlapping region, but the total number of nodes/particles for both domains is fixed to $N_{tot} = 80$.

It was also considered to include the Rayleigh damping model to reduce some higher order oscillations. It is also to emphasize, that these oscillations also appear in FE case, so the small damping would decrease the miscalculation of high-frequency modes. Classical Rayleigh damping is a viscous damping which is proportional to a linear combination of mass and stiffness:

$$\mathbf{D} = \alpha \mathbf{M} + \beta \mathbf{K},$$

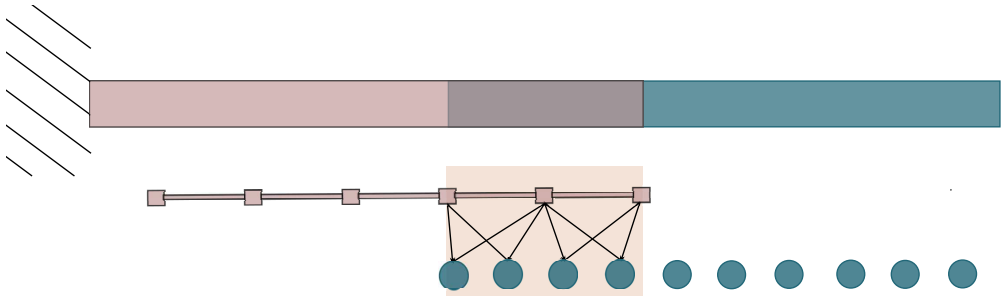

Fig. 2: 1D truss under prescribed strain, fixed on one side

where each numerical constant was chosen with the value: $\alpha = 0.1,\ \beta = 3.210^{-6}$.

The upper left graph in Fig. 3 shows the displacement of the last node of the truss if the same example is calculated with pure FEM, PD theories and their coupled version. The results have a good agreement, but a slight delay can be noticed after each half-period of the oscillation, which the coupled model transfers from the peridynamic model. FE and PD models don't have an equal ratio. This is expected, because PD model converges to CE, when $\delta \to 0$ and $N_{pt} \to \infty$. The bottom left graph in Fig. 3 gives the information about the displacement of the point, located in the middle of the truss in the overlapping zone. This result is compared to the solution of the same problem in FEM and PD, as it is shown early. The Penalty number study is also provided and it shows, that the solution reaches the required accuracy after selection $\kappa = 10^9$, which depends on the value of Young's modulus of the truss.

The parameter which has a decisive meaning for accuracy is a determination of the overlapping region's size. The mesh density remains unchanged, but the width of Ω_o in terms of dx. The bottom left graph presents, that an increase of size Ω_o leads to certain deviations from the reference PD solution. Since each PD particle in the overlapping region has a so-called connection to FE nodes through "springs" with spring stiffness κ, we assume, that when the wave reaches the overlapping region, each PD particle from Ω_o receives an additional oscillation, as it is connected not only to its neighbors by a spring but also additionally to FE nodes.

5 Outlook

The Arlequin Based Penalty Coupling model was developed and successfully implemented numerically. A delay in the displacement of the coupling model concerning FEM and PD, which increases slightly every half-period, was noticed. The Penalty number study and investigation of the optimal size of overlapping area are also provided. In the future work the numerical treatment of this delay will be considered. Wave propagation analysis under impulse load will be also appropriate

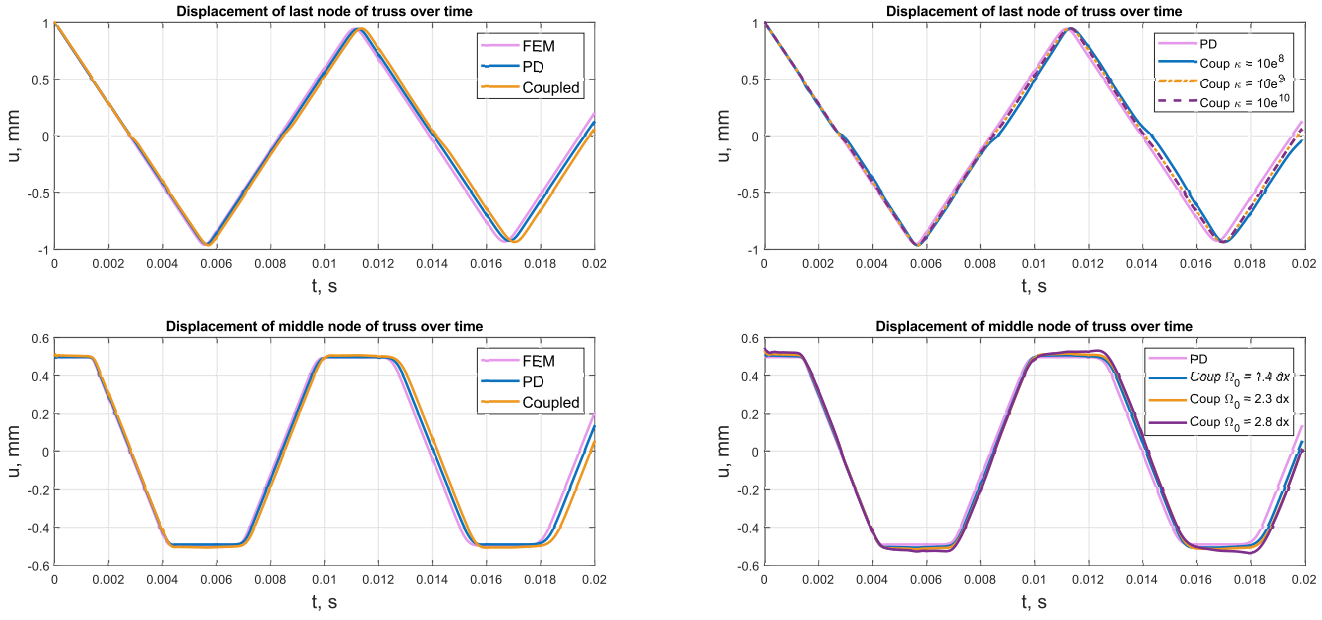

Fig. 3: Displacement of the last point (top) and middle point (bottom) of the truss over time, calculated by different theories with variation of numerical parameters

to evaluate spurious wave reflections at the interface. The study of weighted parameter α as a nonlinear function will also be considered. Introducing damage models in combination with the proposed coupling method will provide the information about the reduction of computational time.

Acknowledgements The project is funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under the Project GA480/16-1 (No 456427423) This financial support is gratefully acknowledged Open access funding enabled and organized by Projekt DEAL.

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