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Basava-Raju Akula, Vladislav Yastrebov, Julien Vignollet, Georges Cailletaud

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Domain tying across virtual interfaces: coupling X-FEM with the Mortar method

B.R. Akula[1,2], V.A. Yastrebov[1], J. Vignollet[2], G. Cailletaud[1]

[1] *MINES ParisTech, PSL Research University, Centre des matériaux, CNRS UMR 7633, BP87, 91003 Evry Cedex, France, {basava-raju.akula, vladislav.yastrebov, georges.cailletaud}@mines-paristech.fr*
[2] *Safran Tech, Safran Group, 78772 Magny-les-Hameaux, France {basava-raju.akula, julien.vignollet}@safrangroup.com*

Résumé — In this paper we propose a unified framework of the mortar domain decomposition method and extended finite element method (X-FEM). This framework allows to deal in an efficient manner with two cumbersome aspects of the finite element methods, namely incompatible interface discretizations and internal discontinuities. Features of mortar methods in the context of mesh tying, and of X-FEM in the context of void/inclusion treatment are exploited to formulate the weak coupling along an inclusion's surface and the virtual surface of the host mesh. It has a potential to address a multitude of problems from accurate substructuring to efficient wear simulation in contact problems.
Mots clés — mortar method, extended finite element method, coupling.

1 Introduction

The finite element methods (FEM) is one of the widely used methods to solve mechanical engineering problems. The FEM is extremely flexible and can handle complex geometries, highly non-linear material models, large deformations and multi-physical problems. With the emergence of high performance computing its applicability to larger and more complex problems was only made easier. Among the wide spectrum of engineering applications, the class of problems dealing with interface mechanisms (composites, fracture, contact) is complex both with regard to its mathematical description and the difficulties arising in numerical treatment. Understanding and accurate modeling of these phenomena would contribute significantly to the progress across all fields of mechanical engineering scaling from material microstructure modeling to complex structural problems involving frictional contacts. However, the classical FEM is constrained in handling many problems encountered in interface mechanics. These limitations stem from its inability to independently represent the interface geometry from the underlying discretization. One such constraint imposed by conventional FEM methods is the requirement of conformal meshes along the interfaces. This lays significant restrictions on the possible complexities of geometries that can be handled.

The family of mortar methods has a potential to address these limitations. These are a subclass of domain decomposition methods (DDM), that are tailored for large class of non-conformal spatial interface discretizations [1, 2]. These were originally introduced as DDM for spectral elements [3, 4]. The coupling of different physical models, discretization schemes, or non-matching meshes/discretizations along interior interfaces of the domain can be ensured by mortar methods. The mathematical optimality and applicability of the mortar methods in spectral and finite element frameworks were studied extensively for elliptic problems [4, 3, 5].

The other notable class of problems are those involving discontinuities. The fundamental requirement of the classical FEM is that the mesh has to conform to the geometry and with this it is possible to handle complex geometries comfortably. Since FEM strongly depends on the smoothness of the approximation polynomials, non-smooth behavior like high gradients or singularities in the stress and strain fields, or strong discontinuities in the displacement field as encountered with cracked bodies, pose a computational challenge to attain optimal convergence. However, having conformal geometries across different domains or contacting solids is not always possible or might demand computationally intensive re-meshing and field transfer procedures.

An attractive alternative is the partition of unity based enrichment method (PUM) [6] for disconti-

nuous fields referred to as the extended FEM (X-FEM) in [7]. In X-FEM, special enrichment functions are added to the finite element approximation using the framework of PUM, to account for non-smooth behavior such as high gradients or singularities in the stress and strain fields, or strong discontinuities in the displacement field as in the case of cracked bodies without compromising on the optimal convergence [8].

In an attempt to combine these two requirements of incompatibilities and discontinuities, we propose a unified solution to these problems. As illustrated in Figure 1, we propose to tie the virtual X-FEM boundary Γ_v (discontinuity) introduced on the coarse mesh domain, with the outer boundary Γ_g of the finely meshed inclusion which will be embedded into the X-FEM void of the coarse mesh. The enriched displacement field of the coarse mesh along Γ_v is constrained to be equal to the displacement of the boundary (Γ_g) of the fine mesh via the mortar method. The planned approach for this unified method includes :

— using the level set method (LSM) [9] to describe the contour of the discontinuity,
— using X-FEM Heaviside enrichment (topological) for the nodes of the elements intersected by the discontinuity, [10]
— using the mortar method [11] to tie both the discretized models along the boundary of the finer-mesh patch and the virtual boundary of this patch, which is represented in the parent (coarse) mesh by a level set.

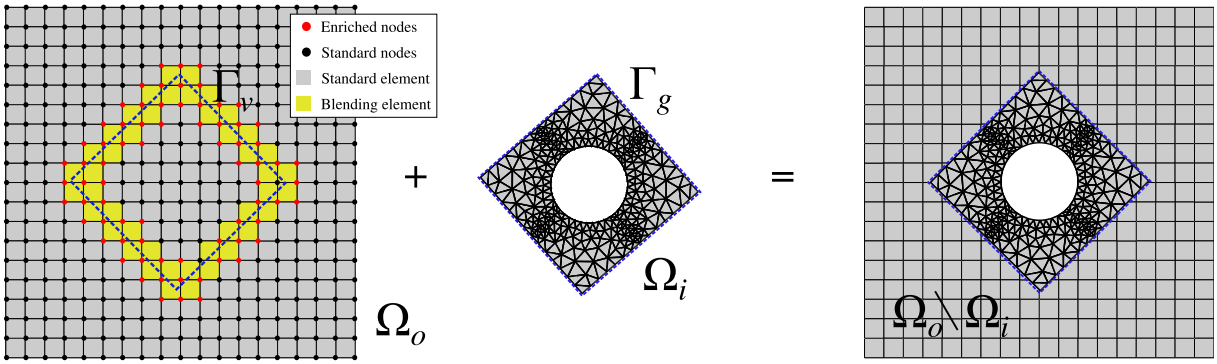


FIGURE 1 – A finely meshed inclusion with border Γ_g is embedded in a coarse mesh and is tied with the corresponding virtual surface Γ_v using the mortar method : (a) coarse host mesh, (b) fine patch to be embedded, (c) the resulting combined mesh.

The X-FEM methods are extensively used in applications such as crack modeling, inclusion and void effects, shock wave front and oxidation front propagation, and other discontinuities (both strong and weak). Coming to the mortar methods they have been the topic of research in a multitude of applications like the non-overlapping domain decomposition methods (DDM), contact, wear etc. There are few works on similar lines where the advantages of these two methods are harnessed in a single application. To name a few we refer to the following works, an exhaustive pointers on the topic can be found in references therein. In [12], the authors try to use the node based bonding between domains with crack. In [13, 14], the authors used the mortar type integration methods to glue a fine mesh surrounding the crack and the coarser mesh domain, where the crack is represented in the X-FEM formulation. But their coupling is limited to existing explicit interfaces, i.e. the inclusion does not cut the elements of the coarse domain but is aligned to the element edges. A dual mortar contact formulation integrated into X-FEM fluid-structure interaction approach is presented in [15]. In [16], the authors have emphasized on a way to impose boundary conditions on the internal boundaries represented by virtual X-FEM interfaces. The proposed method of coupling mortar and X-FEM competes with the volumetric coupling via the Arlequin method [17] close to the overlapping DDM [18], where unlike the conventional non-overlapping DDM the artificial internal boundary condition is provided by its neighboring subdomains. The convergence of the solution on these internal boundaries ensures the convergence of the solution in the entire solution domain.

With the emphasis laid on the interface discretizations, many applications such as substructuring,

arbitrary gluing, mesh construction of complex micro structures, localized mesh refinement near the crack tip, general static and dynamic mesh refinement, and potentially others can be of particular interest with this unified method of the X-FEM and the mortar. However, the applications are not limited only to mesh tying. In analogy to how the mortar method, initially used for tying was extended to contact problems by Belgacem et al. [19], Fischer and Wriggers [20, 21], and Popp et al. [22] the method suggested here can be used to solve contact problems between a virtual surface (represented by the X-FEM) and an explicit surface of the homologue solid [23]. This extension would allow to treat efficiently wear problems without costly remeshing techniques.
The document is structured as follows : In Section 2, we present the core philosophy of the mortar method with respect to the tying problem and the X-FEM with respect to the modeling of voids (closed discontinuity). The equations necessary for FEM framework are given for the unified method in Section 2.3. In Section 3 we show few initial results from the mortar mesh tying problem. In Section 4, we give the concluding remarks on our objective and state the prospective works.

2 Methodology

2.1 Mortar mesh tying

Let us consider a classical boundary value problem for a domain Ω. We assume that the domain is split into n subdomains $\Omega = \cup\Omega_i$ which are glued across their interfaces Γ_{ij}. The resulting optimization problem should then include displacement-equality constraints imposed on glued boundaries, e.g. they take form $\boldsymbol{g}(\boldsymbol{u}) = \boldsymbol{u}^{ij} - \boldsymbol{u}^{ji} = 0$, where $\boldsymbol{u}^{ij}$ and $\boldsymbol{u}^{ji}$ are the displacements of initially coinciding points of subdomains Ω_i and Ω_j, respectively. These constraints can be incorporated into the system energy functional ($W(\boldsymbol{u})$) using the Lagrange multiplier method forming a Lagrangian :

$$\mathcal{L}(\boldsymbol{u},\lambda) = W(\boldsymbol{u}) + \bigcup_{\forall ij} \int_{\Gamma_{ij}} \boldsymbol{\lambda} \cdot \boldsymbol{g}(\boldsymbol{u})\, d\Gamma_{ij}, \tag{1}$$

where λ are the Lagrange multiplier functions representing interface tractions needed to ensure domain tying. Applying the principle of virtual work, equilibrium is ensured when the total virtual work on the solution path is zero : $\delta W^{ext}(\boldsymbol{u},\delta\boldsymbol{u}) - \delta\mathcal{L}(\boldsymbol{u},\delta\boldsymbol{u},\boldsymbol{\lambda},\delta\boldsymbol{\lambda}) = 0$, where δW^{ext} corresponds to the virtual work of external forces, and $\delta\boldsymbol{u}$, $\delta\boldsymbol{\lambda}$ are test functions chosen from respective functional spaces for primal and dual quantities.

This weak form can be directly used in the discretized finite element framework formulated for an extended vector of unknowns including primal (displacements) and dual (Lagrange multipliers) degrees of freedom : isoparametric elements are used with similar interpolation functions for geometry and displacement on both tied subdomains, whose surfaces will be termed mortar and non-mortar ones (”m“ and ”nm“ indices are used for them, respectively) :

$$\boldsymbol{u}^m(t,\xi,\eta)|_{\Gamma^m_{ij}} = \sum_{k=1}^{n^m} N^m_k(\xi,\eta)\,\mathbf{u}^m_k(t), \quad \boldsymbol{u}^{nm}(t,\zeta,\mu)|_{\Gamma^{nm}_{ij}} = \sum_{l=1}^{n^{nm}} N^{nm}_l(\zeta,\mu)\,\mathbf{u}^{nm}_l(t), \tag{2}$$

where n^m is the total number of nodes on the discretized mortar side Γ^m_{ij} of the interface, and n^{nm} is on the discretized non-mortar side Γ^{nm}_{ij}. The classical isoparametric shape functions N^m_k and N^{nm}_l (which are not necessary similar or of the same order) defined on the parametric space $\{\xi,\eta\}$ and $\{\zeta,\mu\}$ are used. The Lagrange multipliers (defined on the mortar surface) are also interpolated using classical shape functions Φ :

$$\boldsymbol{\lambda}(\xi,\eta,t) = \sum_{i=1}^{n^{lm}} \Phi^m_i(\xi^m,\eta^m)\,\boldsymbol{\lambda}_i(t). \tag{3}$$

Here n^{lm} refers to the number of nodes of the mortar side of the interface that carry additional dual dofs. The virtual work of the equality constrains embedded in the Lagrangian (1) takes the following form :

$$\delta W_g = \int_{\Gamma^m_{ij}} \boldsymbol{\lambda} \cdot \delta g(\boldsymbol{u})\, d\Gamma_{ij} + \int_{\Gamma^m_{ij}} \delta\boldsymbol{\lambda} \cdot \boldsymbol{g}(\boldsymbol{u})\, d\Gamma_{ij} \tag{4}$$

Using Eq. 2, Eq. 3 in Eq. 4 results in the discretized interface virtual work (Eq. 5)

$$\delta W_g = \sum_{i=1}^{n^{lm}} \sum_{k=1}^{n^m} \boldsymbol{\lambda}_i^\intercal \cdot \delta \boldsymbol{u}_k^m \underbrace{\left(\int_{\Gamma_{ij}^m} \Phi_i N_k^m \, dA_0 \right)}_{D_{ik}} - \sum_{j=1}^{n^{lm}} \sum_{l=1}^{n^{nm}} \boldsymbol{\lambda}_j^\intercal \cdot \delta \boldsymbol{u}_l^{nm} \underbrace{\left(\int_{\Gamma_{ij}^m} \Phi_j N_l^{nm} \, dA_0 \right)}_{M_{il}} \tag{5}$$
$$+ \sum_{i=1}^{n^{lm}} \sum_{k=1}^{n^m} \delta \boldsymbol{\lambda}_i^\intercal \cdot \boldsymbol{u}_k^m D_{ik} - \sum_{j=1}^{n^{lm}} \sum_{l=1}^{n^{nm}} \delta \boldsymbol{\lambda}_j^\intercal \cdot \boldsymbol{u}_l^{nm} M_{jl}$$

Evaluation of the interface mortar integrals $[D]$ and $[M]$ involves first the determination of the integration domain by projecting the glued surface elements on an auxiliary plane and their clipping, and second, triangulation of the resulting polygon for Gauss integration (details can be found in [11, 22]). The coupling achieved with mortar method is through weak satisfaction of the equality constraints, which is much more accurate than the conventional strong node-wise coupling like in the node-to-segment method [24].

2.2 X-FEM for void modeling

The model presented in Figure. 1(a) involves a strong discontinuity (Γ_v) encompassing a square void. Across this virtual interface, the displacement field has a jump. To take this jump into account, the nodes of blending elements (elements intersected by the discontinuity) are enriched by multiplying the classical shape function of the node by a Heaviside function. The effective support size of these elements for integration is reduced to its volume fraction [25]. For the elements which lie entirely within the void, their dofs are removed from the global system. Here we use a Heaviside function defined for a level set function ϕ as

$$H(\boldsymbol{X}) = \begin{cases} 1, & \phi(\boldsymbol{X}) > 0 \\ 0, & \phi(\boldsymbol{X}) < 0 \end{cases}. \tag{6}$$

Within every blending element, the interface Γ_v, defined by the zero level-set function $\phi(\xi,\eta) = 0$, can be redefined as : $\xi = \xi_v(\eta)$. The shape function of the enriched element then become $N_i(\boldsymbol{X}) = H(\boldsymbol{X}) N_i(\boldsymbol{X})$. These enriched blending elements bring in the change in the volume on which the total system potential is integrated. The blending elements are remeshed to integrate the virtual energy integrals only in the effective support zones (see Figure. 2). The displacement on the surface Γ_v within every blending element is given by classical interpolation function :

$$\tilde{\boldsymbol{u}}(\xi,\eta,t)|_{\Gamma_v} = \sum_i N_i(\xi_v(\eta),\eta)\boldsymbol{u}_i(t).$$

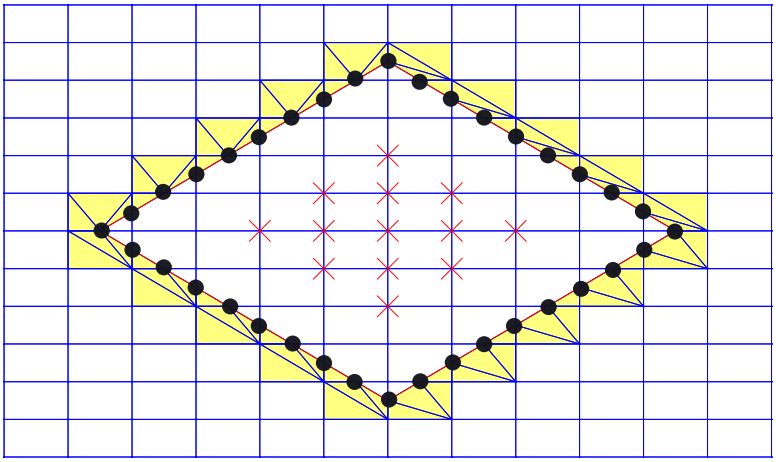


FIGURE 2 – Triangulation of the blending element area which lies out the void defined by the level set function ϕ. The boundary Γ_v intersects the element edges (black points). The dofs of nodes marked x are removed from the global system.

2.3 Mortar coupling along level set

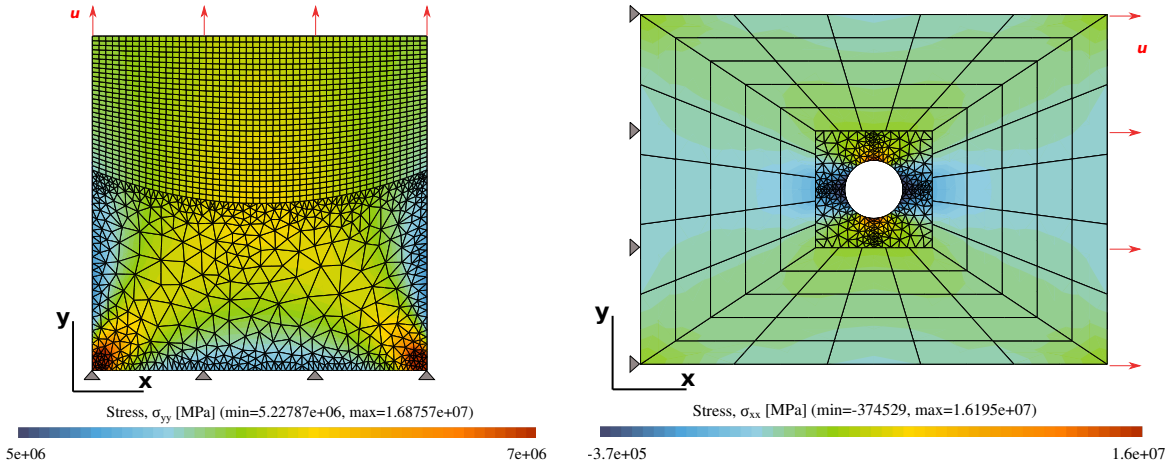
The mortar and the X-FEM methods can be combined to ensure weak mortar-type coupling along virtual interface Γ_v and the inclusion surface Γ_g. The enriched blending elements, the standard elements of the coarsely discretized domain Ω_o the elements from discretized inclusion domain Ω_i along with the new mortar-interface elements are to be incorporated into the virtual work formulation of the global system [see Figure. 1(c)] :

$$\underbrace{\int_{\Omega_o \setminus \Omega_i} \tilde{\boldsymbol{\sigma}} : \delta\tilde{\boldsymbol{\varepsilon}}\, d\Omega_o}_{\delta W_o^{int}} + \underbrace{\int_{\Omega_i} \boldsymbol{\sigma} : \delta\boldsymbol{\varepsilon}\, d\Omega_i}_{\delta W_i^{int}} + \underbrace{\int_{\Gamma_g} \delta\left[\boldsymbol{\lambda} \cdot \boldsymbol{g}(\tilde{\boldsymbol{u}}, \boldsymbol{u})\right] d\Gamma}_{\delta W_{oi}^{tie}} = \underbrace{\int_{\Gamma_o^f} \boldsymbol{t}_0 \cdot \delta\tilde{\boldsymbol{u}}\, d\Gamma + \int_{\Gamma_i^f} \boldsymbol{t}_i \cdot \delta\boldsymbol{u}\, d\Gamma}_{\delta W^{ext}}, \tag{7}$$

where the tilde notation is used for the coarser host mesh quantities. Note that the volume forces are omitted for simplicity. The displacement test functions for both domains are chosen from appropriate functional spaces and have to satisfy Dirichlet boundary conditions. The contribution δW_o^{int} is evaluated only outside the inclusion domain by performing additional triangulation [10] as shown in Figure. 2. Of special interest is the virtual work contribution from the tied interface boundaries Γ_v and Γ_g. Typical to the mortar terminology we classify the virtual boundary Γ_v as the non-mortar side and the inclusion boundary Γ_g as the mortar side, where the mortar integrals are evaluated as in Eq. (5), where the number of non-mortar nodes n^{nm} are typically the intersection points of the element edges of the blending elements and Γ_v. The intersections are not conventional FEM nodes, and so the interpolated values of the element displacement field $\tilde{u}$ of Ω_o is constrained to be integrally equal to the displacement on Γ_g. The mortar algorithms of projections, clipping and triangulation are all done with these intersections and the faces of Γ_g.

3 Examples

In Figure. 3, the mortar methods are used to tie the two domains along the non-matching curved interface. The equality constraints are enforced to a high degree precision which is reflected in a smooth normal stress profiles σ_{yy} and σ_{xx} across the curved (Figure. 3(a)) and flat interfaces (Figure. 3(b)) respectively.



(a) (b)

FIGURE 3 – Mortar method is used for mesh tying along the non-matching (a) curved and (b) flat interfaces.

4 Conclusions and perspectives

The proposed method makes the FEM flexible in its ability to treat efficiently two distinct and fully non-conformal domains, i.e. incompatibilities both at the interface and within the bulk of elements. It

encompasses the intricacies of a diverse and well established fields of the non-overlapping domain decomposition methods and X-FEM, working together to simplify and provide a good alternative solution compared to the conventional ones (node-wise coupling and/or remeshing). The spectrum of applications is wide and includes mesh tying and substructuring and a generic framework for frictional contact including the wear model handled by X-FEM.

The next step is the extension of the implementation to three-dimensional problems. In perspective the method will be taken forward into the realm of parallel computing, thus enabling to solve large and complex problems in a flexible and accurate way.

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