A mixed concurrent multiscale method via CutFEM technology

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SUMMARY

In this paper, we develop a novel unfitted multiscale framework that combines two separate scales represented by only one single computational mesh. Our framework relies on a mixed zooming technique where we zoom at regions of interest to capture micro-scale properties and then mix the micro and macro-scale properties in a transition region. Furthermore, we use homogenization techniques to derive macro model material properties. Our multiscale framework is based on the CutFEM discretization technique where the elements are arbitrarily intersected with two microstructure and zooming surface interfaces. To address the issues with ill-conditioning of the multiscale system matrix due to the arbitrary intersections, we add stabilization terms acting on the jumps of the normal gradient over cut elements faces. We show that our multiscale framework is stable and is capable to reproduce mechanical responses for heterogeneous structures with good accuracy in a mesh-independent manner. The efficiency of our methodology is exemplified by 2D and 3D numerical simulations of linear elasticity problems.

KEY WORDS: concurrent multiscale; CutFEM; unfitted mesh; partition of models, level sets

1 Introduction

Many porous materials in biology and engineering, such as bones and composites, have inherently complex inner structures. For an accurate numerical description of these materials, which own highly oscillatory irregular solution fields because of the complex structures, the finite element method (FEM) requires a discretization that is able to capture the heterogeneities (i.e., pores) within acceptable precision. While resolving the entire structure with extremely high-resolution meshes may result in accurate simulations, the computational costs are also adversely affected and may not be affordable for large structures. One feasible approach for a numerically tractable description of these media is to locally refine the mesh inside the region of interest and coarsen the mesh outside. However, this approach is more applicable when the errors corresponding to the discretization and mechanical behavior in the coarse mesh region remain negligible.\[1][2].
Another common approach is to construct a multiscale system in order to incorporate micro-scale features (such as micropores and inclusions) in macro-scale solution, which can be carried out either over the entire structure or only inside the regions of interest. According to [3], these two techniques are identified as hierarchical and partitioned-domain concurrent multiscale methods, respectively, at which both scale solutions are computed simultaneously. In the hierarchical approach, micro and macro-scale solutions are addressed at the same time and positions, while for the partitioned-domain approach, a particular part of the domain is resolved with micro-scale governing equations and the rest of the medium with macro-scale governing equations. The hierarchical approach, also known as computational homogenization, was proposed in a simplified version based on the effective medium by [4, 5] to homogenize heterogeneities in terms of volume fractions, and then developed with fewer restrictions and for a broad range of problems; such as first and second order computational homogenization methods (see for instance [6, 7, 8]). These approaches rely on the assumption of the existence of scale separation. When this assumption is violated, mainly in critical regions with local defects such as crack tips, damages, and holes, the partitioned domain approaches can be employed instead to alleviate this issue by directly modeling the critical regions with micro-scale governing equations. Partitioned domain approaches can be used to link either same or different mathematical models (in terms of physics and/or scales), such as continuum-to-continuum problems [9, 10], continuum models coupled with molecular dynamic simulations [11, 12, 13, 14] and coupled atomic-to-continuum models [15, 16, 17]. We can use both hierarchical and partitioned-domain methods in a problem simultaneously [18, 19].

There are numerous coupling techniques available in the literature extending the FEM-based monomodels for the partitioned-domain multiscale approaches. The examples of these methods are overlapping domain decomposition methods [20, 21] such as the Arlequin method [22, 23] and non-overlapping domain decomposition methods [24, 25] like the s-method [9] and the mortar method [26], which all rely on superimposing local models with a fine mesh to the lowermost coarse mesh global model. These methods aim at reconstructing a multimesh framework using gluing conditions for the common interface of meshes. The interface conditions are implemented in a framework of coupling operators, such as the Lagrange multiplier approach [27] that is extensively used in the Arlequin method [28, 29] and the Nitsche approach [30, 31] which imposes the interfaces conditions weakly. In contrast to the mentioned coupling techniques that are all intrusive, [25, 32] introduced a non-intrusive strategy for the coupling of global and local models; where the local model does not modify the global model, and all computations are performed with standard FEM. This approach is computationally efficient for large-scale problems with nonlinear phenomena that occur in small portions of the total domain.

From a computational standpoint, classical FEM is not sufficiently flexible for complex and time-dependent geometries, which are prevalent features in micro-scale phenomena. Mesh refinement and regeneration are obvious remedies to preserve the accuracy but these are very costly for large scale problems. In an alternative approach, the CutFEM technique [33, 34, 35] as a generalization of FEM, aims to facilitate the computations of complex and evolving geometries. In this method, the geometry is decoupled from the finite element mesh and the boundary of the computational domain is represented by a level set function or a given surface mesh over a fixed background mesh. The computation and update of the geometry are done in the discretized formulation, reducing the preprocessing computational cost of meshing. Aside from the robust geometry description, the method ensures the stability of its discretization technique by introducing ghost penalty regularization terms in cut elements [36]. The CutFEM technique has been applied for a range of single-scale problems, such as unilateral contact [37], multiphase phenomena [38, 39] and fiber-reinforced composites [40].
It has also been recently developed for modeling multi-component structures using different meshes for each component. In this multimesh framework proposed by [41, 42], the arbitrary intersection and overlapping of different meshes is utilized by enforcing the interface conditions to the actual interface between the meshes and regularizing the intersected elements with the ghost penalty regularization technique.

In this paper, we define the geometry in terms of either analytical distance function or a given surface mesh by projecting them onto a background mesh which is fine in areas of interest and coarse elsewhere. This projection is carried out by CutFEM, and the geometry is approximated by a piecewise linear signed distance function in each background mesh element. However, the combination of fine resolution in areas of interest and very coarse mesh elements elsewhere gives rise to the random appearance of geometrical artifacts in the coarse region, yielding stress singularities. In order to alleviate this issue, we have developed a multiscale approach. Instead of considering the signed distance function description in the coarse mesh domain, we replace it with a homogenized domain. To couple the fine scale region or "zoom region" with the coarse scale region, we develop a smooth mixing approach of the homogenized material and the fine scale region in which we use CutFEM to represent the geometry. Then, we demonstrate the efficiency, robustness and accuracy of the smooth mixing approach between homogenized macro-scale and CutFEM micro-scale region.

In our multiscale framework, the smooth mixing technique is inspired by the Arlequin method. However, in contrary to the Arlequin mixing strategy, we do not cross and glue a high-resolution mesh to the underlying mesh but use a level set function over a single background mesh to define the transition region and then mix the scales in the elements inside. The implicit level-set-based description of geometrical and mixing properties (i.e. macro and micro-scale domains, zooming location and transition region) beside robust CutFEM integration has enabled us to propose a versatile mesh-independent multiscale framework. In this framework, we can modify the geometrical and mixing properties by only changing the level set functions, leading to less computational preprocessing costs in comparison to the previous methods.

The outline of the paper is as follows. In section 2, we present the continuous formulation of the multiscale framework, in strong and weak forms. Then, in section 3, we discretize the formulations using CutFEM and introduce the transition area for mixing purposes. In section 4, we first test the idea of taking the functional description of micro-scale and projecting it onto an adaptive mesh background. Then we corroborate the efficiency of the proposed smooth mixed multiscale framework with 2-D and 3-D elasticity problems. In 2D examples, we study a heterogeneous structure where the micropores are distributed either locally or uniformly. In the 3D case, we simulate a trabecular bone with complex microstructure derived directly from micro-CT image data (also available in [43, 44]).
2 Governing equations of the mixed multiscale problem

In this section, the formulation for the mixed elasticity problem is presented. First, we will introduce definitions and notations related to the domain partitioning of the method and then present the strong and weak formulation for the concurrent multiscale elasticity problem. Eventually, we will discretize the governing equations.

2.1 Domain partitioning

Let \( \Omega \) be the computational domain of a micro-porous heterogeneous medium comprised of a matrix subdomain \( \Omega_1 \) and a pores subdomain \( \Omega_2 \), as illustrated in Figure 1a and

\[
\Omega_i \subset \mathbb{R}^d, \quad i = 1, 2, \quad d = 2, 3, \tag{1}
\]

where the interface between \( \Omega_1 \) and \( \Omega_2 \) is determined by a continuous level set function \( \phi_1 \) defined as follows

\[
\phi_1(x) = \begin{cases} 
> 0 & x \in \Omega_2, \\
= 0 & x \in \Gamma_1, \\
< 0 & x \in \Omega_1.
\end{cases} \tag{2}
\]

The normal vector in \( x \in \Gamma_1 \), pointing from \( \Omega_1 \) to \( \Omega_2 \), is given by

\[
n_1 = \frac{\nabla \phi_1(x)}{\|\nabla \phi_1(x)\|}. \tag{3}
\]

In the previous definition, \( \|x\| \) denotes the Euclidean norm \( \|x\| = \sqrt{x \cdot x} \).

![Figure 1](image-url)

Figure 1: Domain partitioning for the mixed multiscale method, a) micro-porous domain \( \Omega \) partitioned into matrix subdomain \( \Omega_1 \) and pores subdomain \( \Omega_2 \) (\( \Omega = \Omega_1 \cup \Omega_2 \)) with interface \( \Gamma_1 \) and b) partition of the computational domain \( \Omega \) into macro subdomain \( \Omega_M \) and micro subdomain \( \Omega_m \) (\( \Omega = \Omega_M \cup \Omega_m \)). Note that \( \Gamma_1 \) and \( \Gamma_2 \) are closed curves.
Next, we define the micro-scale zoom region $\hat{\Omega}_m$ for our multiscale analysis by a continuous level set function $\phi_2$ given by

$$\phi_2(x) = \begin{cases} 
> 0 & x \in \hat{\Omega}_M, \\
= 0 & x \in \Gamma_2, \\
< 0 & x \in \hat{\Omega}_m,
\end{cases}$$

(4)

whose zero isoline defines the boundary of the zoom. In this stage, the outside of the zoom is considered as macro domain denoted by $\Omega_M$. For an illustration see Figure 1b, with $\hat{\Omega}_m$ shown as the shaded area. Furthermore, the normal vector on the interface $\Gamma_2$ pointing from $\hat{\Omega}_m$ to $\hat{\Omega}_M$ is given by

$$n_2 = \frac{\nabla \phi_2(x)}{||\nabla \phi_2(x)||}.$$  

(5)

### 2.2 Field equations of the multiscale elasticity problem

Let us consider linear elastic behavior for the background domain $\Omega = \hat{\Omega}_M \cup \hat{\Omega}_m$. In our multi-model, we are seeking the deformation field $u : \hat{\Omega}_M \times \hat{\Omega}_m \rightarrow \mathbb{R}^d \times \mathbb{R}^d$ which satisfies

$$\text{div } \sigma_M + f_M = 0 \quad \text{in } \hat{\Omega}_M,$$

$$\text{div } \sigma_m + f_m = 0 \quad \text{in } \hat{\Omega}_m,$$

(6a)

(6b)

where

$$\sigma_M(u) := D_M : \nabla_s u$$

$$\sigma_m(u) := D_m : \nabla_s u$$

(7a)

(7b)

The boundary of the solid is partitioned into $\partial \Omega_u$ and $\partial \Omega_t$ ($\partial \Omega = \partial \Omega_t \cup \partial \Omega_u$), where $\partial \Omega_u$ is the part where the body is clamped and $\partial \Omega_t$ is the part with applied traction $t$ with $\partial \Omega_t \cap \partial \Omega_u = \emptyset$.

In the expressions above, $f_M$ and $f_m$ are volume source terms, $\nabla_s = \frac{1}{2}(\nabla + (\nabla)^T)$ is the symmetric gradient operator, and $D \in (\mathbb{R}^d)^4$ is the fourth order Hooke tensor of isotropic linear elastic material represented as follows:

$$D : \nabla_s = \lambda \text{Tr}(\nabla_s) \mathbb{I} + 2\mu \nabla_s,$$

(8)

where $\text{Tr}$ is the trace operator on a tensor, $\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)}$, $\mu = \frac{E}{2(1+\nu)}$ are the Lamé parameters expressed by the Young’$s$ modules $E$ and the Poisson’s ratio $\nu$.

On the zooming interface, $\Gamma_2$, between micro and macro model, the traction is required to satisfy the following coupling condition

$$\sigma_m \cdot n_2 = -\sigma_M \cdot n_2 \quad \text{on } \Gamma_2.$$  

(9)

Integrating governing equations (6a)-(6b) over the given domains, i.e. macro domain $\hat{\Omega}_M$ and micro zoom domain $\hat{\Omega}_m$, the weak form of the multiscale elasticity problem is given as follows. We seek a displacement field $u : \hat{\Omega}_M \times \hat{\Omega}_m \rightarrow \mathbb{R}^d \times \mathbb{R}^d$, $u \in H^1(\hat{\Omega}_M) \times H^1(\hat{\Omega}_m)$, satisfying

$$\int_{\hat{\Omega}_M} \sigma_M(\nabla_s u) : \nabla_s \delta u \, dx + \int_{\hat{\Omega}_m} \sigma_m(\nabla_s u) : \nabla_s \delta u \, dx = \int_{\hat{\Omega}_M} f_M \cdot \delta u \, dx + \int_{\hat{\Omega}_m} f_m \cdot \delta u \, dx + \int_{\partial \Omega_t} t \cdot \delta u \, dx,$$

(10)
for all test functions $\delta u : \hat{\Omega}_M \times \hat{\Omega}_m \rightarrow \mathbb{R}^d \times \mathbb{R}^d$, $\delta u \in H^1_0(\Omega_M) \times H^1_0(\Omega_m)$ which satisfy the homogeneous Dirichlet boundary condition

$$\delta u = 0 \quad \text{on} \quad \partial \Omega_u.$$ (11)

3 Discretization for mixed multiscale problems

In this section, we introduce a CutFEM-based approximation scheme of the multiscale elasticity problem proposed in section 2 using a novel mixed cut finite element approach. The arbitrary intersection of the porous domain by the sharp zooming interface, $\Gamma_2$, can result in bad conditioning for the assembled system matrix. To alleviate this problem, we introduce a mixing strategy between the macroscale and microscale regions. In this mixed approach, we create an overlap between the two models. We refer to the overlapping domain as "transition domain", as highlighted in Figure 2a in yellow.

For mixing purposes, we extend the macro and micro domains defined in the previous section. First we extend the macro domain by $\Omega_M := \hat{\Omega}_m \cup \Omega_T$. Then we extend the micro domain inside zoom to $\Omega_m := \hat{\Omega}_m \cup \Omega_T$, where $\Omega_T$ is the transition domain. In this framework, $\Omega_M$ and $\Omega_m$ are overlapping in the transition domain. The transition domain is determined by level set function $\phi_2$, signed distance function to $\Gamma_2$, with a width of $2\epsilon$. We define a smooth weight function $\alpha$ for the mixing, as shown in Figure 2a and denote it in terms of $\phi_2$ by

$$\alpha(x) = \begin{cases} 0 & \text{if} \, \phi_2(x) \leq -\epsilon, \\ S & \text{if} \, -\epsilon < \phi_2(x) < \epsilon, \\ 1 & \text{if} \, \phi_2(x) \geq \epsilon. \end{cases}$$ (12)

In the previous expression, $S$ is a smooth function varying from 0 to 1 inside transition zone, and as shown in Figure 2b, $-\epsilon$ and $+\epsilon$ are the lower and upper bounds of $\Omega_T$ inside micro and
macro domains, respectively. Therefore, macro domain weight function $\alpha_M = 1$ in $\Omega_M \setminus \Omega_T$ while the micro domain weight function $\alpha_m = 0$ in $\Omega_m \setminus \Omega_T$ and,

$$\alpha_M + \alpha_m = 1 \text{ in } \Omega_T.$$  (13)

This creates a smooth transition region in which the macro and micro models are mixed.

### 3.1 Multiscale finite element space

Here we discretize the weak form (10) of the multiscale model, which locally modifies a global problem by using only one mesh, unlike other similar methods such as the Arlequin method [28] and multimesh CutFEM [42] that superimpose a high resolution mesh onto a coarse background mesh. In our framework, we introduce triangulation $\mathcal{T}$ for the background domain $\Omega$ and then define the corresponding finite element space of continuous linear function as

$$Q_h := \{ w \in C^0(\Omega) : w|_K \in P^1(K), \forall K \in \mathcal{T} \},$$  (14)

where the corresponding mixed multiscale model physical domains, $\Omega_M^h$ and $\Omega_m^h$ are approximated as

$$\Omega_M^h = \{ x \in \Omega | \phi_M^h(x) \geq -\epsilon \}$$  (15)

$$\Omega_m^h = \{ x \in \Omega | \phi_m^h(x) \leq 0 \text{ and } \phi_2^h(x) \leq \epsilon \}$$  (16)

In (15) and (16), $\phi_M^h(x) \in Q_h$ is the linear approximation of the level set function $\phi_1$ and $\phi_m^h(x) \in Q_h$ is the linear approximation of level set function $\phi_2$. By using these level set functions, we define the position of the micro-scale features and pores over a single fixed mesh arbitrarily (in a nonconforming manner). Now we can present the approximate interface $\Gamma_1^h$

$$\Gamma_1^h = \{ x \in \Omega_M^h | \phi_1^h(x) = 0 \}$$  (17)

The pores with arbitrary geometries can have non-zero intersection with either macro or micro domains, where all the elements of $\mathcal{T}$ intersected by $\Gamma_1^h$ will be grouped in set

$$T_1^h := \{ K \in \mathcal{T} : K \cap \Gamma_1^h \neq \emptyset \}$$  (18)

where the corresponding domain is defined as $T_1^h = \bigcup_{K \in T_1^h} K$.

Furthermore, we can approximate the transition domain $\Omega_T^h$ and porous domain $\Omega_p^h$, respectively in

$$\Omega_T^h = \{ x \in \Omega | -\epsilon \leq \phi_2^h(x) \leq \epsilon \}$$  (19)

and

$$\Omega_p^h = \{ x \in \Omega | \phi_1^h(x) \leq 0 \}$$  (20)
3.2 Fictitious domain

First, we define a set of all elements in the background mesh $\mathcal{T}$ which have a non-zero intersection with $\Omega^h_M$ and $\Omega^h_m$

$$\mathcal{T}_h := \{K \in \mathcal{T} : K \cap (\Omega^h_M \cup \Omega^h_m) \neq \emptyset\}$$

(21)

where the domain associated with this set is defined as fictitious domain and is denoted by $\Omega^f := \bigcup_{K \in \mathcal{T}_h} K$

Then to prevent ill-conditioning of the system matrix, we introduce two sets of ghost penalty regularization terms. The first set is used for the intersected elements by $\Gamma^h_1$ in $\Omega^h_m$, and applied to the elements edges (the cut edges are schematically illustrated in Figure 3 with red color). We define penalization edges associated with the intersected elements $\mathcal{T}^h_1$ as,

$$\mathcal{F}_G := \{F = K \cap K' : K \in \mathcal{T}_h \text{ and } K' \in \mathcal{T}_h, F \cap T^h_1 \neq \emptyset\}$$

(22)

The second set of ghost penalty regularization terms are applied for the edge of elements in the transition region $\Omega^f$ that are intersected by $\Gamma^h_1$ or are inside the porous domain. The elements that are in $\Omega^h_p$ and $\Omega^f$ are denoted by . The corresponding edges are shown schematically in Figure 3 with purple color and defined as following,

$$\mathcal{F}_{GT} := \{F = K \cap K' : K \in \mathcal{T}_h \text{ and } K' \in \mathcal{T}_h, F \cap (T^h_1 \cup T^h_2) \neq \emptyset\}$$

(23)

where $T^h_2$ is the domain related to the set of all elements of $\mathcal{T}$ intersected by pores in transition domain defined as $T^h_2 = \bigcup_{K \in T^h_2} K$, and the set $T^h_2$ in previous expression is as following,

$$T^h_2 := \{K \in \mathcal{T} : K \cap (\Omega^h_T \cap \Omega^h_p) \neq \emptyset\}$$

(24)

In this paper, since we use one set of discretization for the multiscale problem, then the displacement field is continuous throughout the whole domain and is approximated by $u_h$ in the following space,

$$U_h := \{u \in C^0(\Omega_T) : u|_K \in P^1(K) \ \forall K \in \mathcal{T}_h\}.$$  

(25)
3.3 Stabilized mixed finite element formulation

The mixed finite element formulation for the proposed multiscale method is the following: find $u_h \in \mathcal{U}_h$, such that

$$(1 - \alpha_h) a_M(u_h, v) + \alpha_h a_m(u_h, v) = (1 - \alpha_h) l_M(v) + \alpha_h l_m(v)$$

(26)

for any $v_h \in \mathcal{U}_h$ satisfying homogeneous Dirichlet boundary conditions. The bilinear form $\alpha_M$ and linear form $l_M$ of the macro model are given by

$$a_M = \int_{\Omega_M} D_M \nabla_s u_h \nabla_s v \, dx,$$

(27)

$$l_M = \int_{\Omega_M} f_M \cdot v \, dx + \int_{\partial \Omega_M} t_d \cdot v.$$

(28)

In the previous problem statement, the regularized bilinear form $a_m$ is defined for the micro scale model as

$$a_m = \int_{\Omega_m} D_m \nabla_s u_h \nabla_s v_h \, dx + \sum_{F \in \mathcal{F}_G} \left( \int_F \frac{\beta h}{E_m} \|[D_m \nabla_s u_h][D_m \nabla_s v_h]\| \, dx \right).$$

(29)

Here, the second term, called ghost-penalty, ensures a uniformly bounded condition number for the system matrix and $\|[\cdot]\|$ denotes the normal jump of quantity $x$ over the facet $F$, and $\beta$ denotes the ghost penalty stabilization parameter that needs to be large enough to guarantee the coerciveness of bilinear form $a_m$ \cite{34, 30} on the fictitious domain. The linear form of the micro scale model is given by

$$l_m = \int_{\Omega_m} f_m \cdot v \, dx$$

(30)
4 Numerical results

In this section, we first test the projection of an analytical signed distance function over an adaptive background mesh using the CutFEM technique. Next, we investigate the performance of the proposed smooth mixing approach in a simplified multiscale problem. Eventually, we adopt a homogenised medium in the coarse domain of the mixed multiscale model and demonstrate the efficacy and robustness for 2D and 3D elasticity problems. In our 2D simulations, we use an analytical signed distance function to define the geometry. In contrast, in our 3D case study, we use a mesh surface derived from micro-CT image data to describe the geometry of a trabecular bone with a complex microstructure. All the numerical results are produced by the CutFEM library [34] developed in FEniCS [45].

4.1 Adaptive CutFEM technique

Let us consider the heterogeneous structure shown in Figure 4 comprised of a matrix and pores which are distributed all over the domain. The matrix domain is defined as \( \Omega_1 = \Omega \setminus \Omega_2 \), where \( \Omega = [0,12] \times [0,10] \) is the rectangular background domain and \( \Omega_2 \) are the pores. We restrict the displacement at the bottom edge and prescribe force \( f = (0,-0.01) \) along the top edge of the domain. We assume the corresponding mechanical properties as following: \( E = 1 \) and \( \nu = 0.3 \).

\[
\mathbf{f} = (0,-0.01)
\]

\[
\begin{align*}
\Gamma_1 & \quad \Omega_1 \\
\Omega_2 &
\end{align*}
\]

\[
\begin{align*}
\sigma_{\text{n}} & \quad = 0 \\
u & \quad = 0 \\
u & \quad = (0,0)
\end{align*}
\]

Figure 4: Schematic presentation of 2D rectangular domain with a quasi-uniform distribution of micro-pores

Here, we define the geometry by a piecewise linear signed distance function over two types of background meshes. As depicted in Figure 5a,b, the first background mesh is uniform and fine everywhere; however, the second background mesh is fine only in regions of interest and coarse elsewhere, and the corresponding adaptive mesh refinement scale is \( s = 1/4 \). The zero level set function \( \Gamma_1^h \) (shown in black lines) represents the pores interfaces intersecting the background meshes arbitrarily. For both mesh configurations, mesh size is defined as \( h = h_x = h_y \) with \( h_{\text{min}} = 0.005 \) and the regularization parameter is set to \( \beta = 0.005 \).

We perform a mechanical compression test and consider the model with uniform fine mesh as a
reference. As shown in Figure 5b, using the signed distance function in the coarse domain leads to the random appearance of geometrical artifacts. The comparison of displacement fields component $u_y$ in Figure 6 shows the response in the fine mesh region of CutFEM is precise; however, in the coarse mesh region, the geometrical artifacts imposes unrealistic additional stiffness. To address this limitation of the CutFEM technique in very coarse meshes, we will employ our mixed multiscale framework in section 4.3, whereby instead of using coarse signed distance function in the coarse domain, we replace it with a homogenised medium.

4.2 Smooth mixing approach adopted for a 2D locally porous medium

Here, we investigate the performance of the proposed smooth mixing approach in a 2D locally porous medium, shown schematically in Figure 7. This structure is a simple case for multiscale modelling, as homogenisation is not essential in the coarse domain due to the local distribution of
We define the rectangular domain as $\Omega = [0,12] \times [0,10]$, comprised of matrix domain $\Omega_1 = \Omega \setminus \Omega_2$ and pores domain $\Omega_2$. We block the displacement at the bottom edge and insert displacement $u = (0, -0.1)$ along the top edge of the domain. Then, we assume the macro and micro scales mechanical properties as following: $E_M = E_m = 1$ and $\nu_M = \nu_m = 0.3$.

We test three structured background meshes consisting of one uniform and two adaptively refined meshes generated independently of the pores and zoom interfaces. We employ linear Langrangian elements, with a uniform background mesh size $h = h_x = h_y$ and the regularization parameter set to $\beta = 0.005$. The corresponding discretisations of the physical domain $\Omega_1$ are shown in Figure 8. The zero level set functions of $\Gamma_1$ (shown in black lines) and $\Gamma_2$ (shown in red lines) represent the micropores and the zooming regions, respectively. The corresponding discretised domains in Figure 8 show the arbitrary intersection of the interfaces with the elements, where the zooming interface determines the middle of the transition region $\Omega_T$ and the mesh is refined inside the zoom.

In this study, we choose the following smooth weight function to mix the two models inside transition region $\Omega_T$,

$$S = \frac{1}{2}(1 + \sin(\frac{\pi}{2\epsilon} \xi(x))). \tag{31}$$

Figure 9 illustrates how the scalar function $\alpha_h$ is distributed in the discretised physical domain with different mixing lengths. Note that our multiscale mixing approach operates over a single mesh, and its mixing length is defined in a mesh-independent manner. The displacement field component $u_y$ for two smooth mixing lengths $2\epsilon = 0.1,1$ and the finest adaptive mesh with $h_{min} = 0.2$ are shown in Figure 10, d. We choose the standard FEM and unfitted CutFEM as reference models and present the corresponding $u_y$ in Figure 10, a, b. As expected, we find that our CutFEM displacement field converges to the FEM displacement field, verifying our single-scale unfitted method. For the mixed multiscale model, $u_y$ inside the zoom is similar to the corresponding references and exhibits smooth behaviour in the transition domain $\Omega_T$. 

Figure 7: Schematic presentation of 2D rectangular domain with locally distributed pores.
The energy distribution inside $\Omega_T$ is the average of the FEM macro-scale and the CutFEM micro-scale model. Next, we will investigate how the mixing approach via the weight function (31) impacts the stress field in the physical and the fictitious domains. The stress field is given by

$$
\sigma_{\text{mix}}(x) = \begin{cases} 
\sigma_m & \text{in } \Omega_m \setminus \Omega_T, \\
\sigma_M & \text{in } \Omega_M \setminus \Omega_T, \\
\sigma_m \alpha_m + \sigma_M \alpha_M & \text{in } \Omega_T.
\end{cases}
$$

(32)

As shown in Figure 11a,b, the stress component $\sigma_{yy}$ in CutFEM converges to its FEM counterpart. We compute $\sigma_{\text{mix}}$ given in (32) for two smoothing lengths over the physical and fictitious domains in Figure 11c-11f. Our results show that $\sigma_{\text{mix}}$ in $\Omega_T$ is smooth and without oscillations.

To enhance the stability of our multiscale framework, in the micro-scale model, we regularise the elements inside the porous domain in addition to the intersected elements by $\Gamma_h$. Then we compute the condition number of the multiscale system matrix for investigating the stability by using SLEPc [46] which finds the ratio of maximum to the minimum eigenvalue of the system matrix (i.e. $\lambda_{\text{max}} / \lambda_{\text{min}}$). We use a sequence of uniform and adaptive meshes with different mixing lengths and then compare them with the CutFEM reference model. In Figure 12a, we find that the behaviour of our mixed approach with different mixing lengths is well conditioned and similar to
Figure 10: Displacement component $u_y$ contours for different methods: a) FEM, b) CutFEM, c) mixed multiscale model with $2\epsilon = 0.1$, d) mixed multiscale model with $2\epsilon = 1$.

the standard CutFEM approach. The flexibility of the current method for sharp mixing lengths is another convenient factor that distinguishes it from previous superposing methods such as Arlequin. In Figure 10b, we investigate the effects of extended regularisation inside the pores (in addition to the cut elements by the pore interfaces) on the condition number of the multiscale system matrix. As expected, this technique improves the condition number effectively. Also, we find that the corresponding behaviour with respect to the mesh refinement for our mixed approach is proportional to $h^{-2}$ for both cases of regularisation, which is conveniently very close to the results by CutFEM.
Figure 11: Stress component $\sigma_{yy}$ contours, a) FEM model, b) CutFEM model, c) mixed multiscale model physical domain with $2\epsilon = 0.1$, d) mixed multiscale model physical domain with $2\epsilon = 1$, e) mixed multiscale model fictitious domain with $2\epsilon = 0.1$, f) mixed multiscale model fictitious domain with $2\epsilon = 1$. 
Figure 12: The condition number of the system matrix versus mesh size, for different mixing lengths: a) ghost penalty regularization is applied to only cut elements, b) ghost penalty regularization is applied to every element inside porous domain in addition to cut elements. In both cases, the regularization parameter is chosen as $\beta = 0.005$. 
4.3 The mixed multiscale method for a 2D quasi-uniform porous medium

In this section, we consider the quasi-uniform porous domain given in Figure 4 for our mixed multiscale analysis. As discussed in section 4.1, the structures with uniform heterogeneity require homogenisation in the coarse domain to avoid the geometrical artifacts reproducing unrealistic stiffness and stress singularities. Hence, here, we replace the signed distance function in the coarse domain with a homogenised domain and use the smooth mixing approach to couple the fine and coarse-scale domains.

In our mixed multiscale framework, we construct the homogenised model by using the Modified Mori Tanaka (MMT) approach [47] to reproduce the effects of micropores in the homogenised macro model. Employing the MMT homogenisation approach for $\Omega_m$ with $n$ circular pores of different radii, the effective young modulus will be computed as follows.

$$E^i_M = (1 - \bar{\phi}_i)E^{i-1}_M (\bar{\phi}_i L_i + (1 - \bar{\phi}_i)I)^{-1}, \quad i = 1, ..., n,$$

where $E^i_M$ and $E^{i-1}_M$ are the homogenized young modulus with inclusion of $i^{th}$ and $(i - 1)^{th}$ circular pores, respectively, and $\bar{\phi}_i$ is the instantaneous porosity parameter defined as

$$\bar{\phi}_i = \frac{V^i_v}{V_t},$$

where $V^i_v$ is the void volume with $i$ number of pores and $V_t$ is the total volume. $L_i$ is the Eshelby parameter given for circular inclusions in [48]. To calculate the effective elastic modulus of a domain with $n$ pores, we add the inclusions one by one, and in each step number $i$, we update Equation 33. For more details regarding the MMT approach, see [47].

4.3.1 The mixed multiscale with one arbitrary zoom

Here, we use the mixed multiscale framework with one zoom and compare it with the equivalent adaptive CutFEM approach discussed in section 4.1. The zooming interface is projected over the background mesh and shown with a red line in Figure 13. The material properties and boundary conditions are adopted the same as in the adaptive CutFEM model in section 4.1. To compute the homogenised material properties, we consider the representative volume element (RVE) all over the domain $\Omega_m$. We use Equation 33 for this purpose and then calculate the corresponding effective young modulus as $E_M = 0.78$.

We use two length sizes for the transition region and compute displacement field component $u_y$, as shown in Figure 14. When compared to the full microscale model as a reference, shown in Figure 9, the mixed multiscale results show a tremendous improvement in comparison to the adaptive CutFEM approach. Therefore, using homogenised models in the coarse domains is necessary when the signed distance functions fail to detect the microstructure precisely.
Figure 13: Background mesh with projected pores and zooming interfaces of the mixed multiscale method

Figure 14: Displacement component $u_y$ for, a) mixed multiscale, $2\epsilon = 0.2$ and b2) mixed multiscale, $2\epsilon = 0.8$. 

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4.3.2 The mixed multiscale with two arbitrary zooms

We next investigate the efficiency of our mixed multiscale approach for the same quasi-uniform porous domain (see Figure 4) using two separate zooms. The displacement at the bottom edge is blocked and \( u = (0, -0.1) \) is applied along the top edge of the domain. We consider the following micro-scale material properties: \( E_m = 1 \) and \( \nu_m = 0.3 \), while for the macro scale we derive effective material properties by using homogenization Equation 33. For this simulation, we consider two types of RVEs: the first type inside the zooms and the second type all over the domain, which are computed as \( E_M = 0.58, 0.78 \), respectively.

For this example, we employ the same background meshes used for the locally porous domain (Figure 7) and show the corresponding discretised domain and generated interfaces in Figure 15. The indicator smooth function with three lengths is also computed for the finest adaptive mesh in Figure 16. In Figures 15 and 16, we observe the independency of the microstructure, zooming geometry and mixing length to the computational mesh, which creates a straightforward preprocessing pipeline and saves mesh regeneration costs.

We compute displacement field component \( u_y \) for two smoothing lengths \( 2\epsilon = 0.1, 1 \) and show the corresponding results over the physical and the fictitious domains in Figure 17-c-f. The results prove a high relevance of the multiscale framework in the micro-scale domain to the corresponding reference models (depicted in Figure 17-a,b). In the transition regions, \( u_y \) as a global response is smooth in both mixing lengths, and for the outside of zooms, which is homogenised, the trend is similar to the references.

Next, we inspect the distribution of the mixed stress field for two zooming problems. The results obtained for stress field component \( \sigma_{yy} \) for two smoothing lengths and over physical and fictitious domains are given in Figure 18. The comparison with reference models (see Figure 18) ensure the efficiency of our method in improving the oscillations in cut elements and also the transition area. The ghost penalty regularisation, which extends the solution from the physical domain to the fictitious domain, has slight effects on the solution and improves the oscillations successfully.
Figure 15: Computational mesh for physical domain of 2D model with quasi-uniform distributed pores, a) uniform meshing, b) adaptive meshing type 1, c) adaptive meshing type 2.
Figure 16: Smooth weight function $\alpha$ field over finest adaptive mesh, a) $\epsilon = 0.1$ b) $\epsilon = 0.4$ c) $\epsilon = 1$.

Figure 17: Displacement component $u_y$ field, a) FEM model, b) CutFEM model, c) mixed multiscale model with $\epsilon = 0.1$, d) mixed multiscale model with $\epsilon = 1$. 
Figure 18: stress component $\sigma_{yy}$ contours, a) FEM model, b) CutFEM model, c) mixed multiscale model with $\epsilon = 0.1$, d) mixed multiscale model with $\epsilon = 1$. 
The condition number of the multiscale system matrix with the RVE defined over $\Omega_m$ and for different mesh configurations and smoothing lengths are compared with the counterpart CutFEM micro-scale model in Figure 19. The comparison shows that our multiscale assembled matrix is well-conditioned under various smoothing lengths and mesh sizes and converges proportional to $h^{-2}$ that is similar to the CutFEM convergence. On the other side, for the RVE restricted to $\Omega_m$ (inside two zooms), as shown in Figure 19, the condition number is improved considerably and converges proportional to $h^{-2}$.

Figure 19: Condition numbers for CutFEM model and mixed multiscale method for different smoothing lengths and mesh configurations and with, a) homogenization RVE all over domain, b) homogenisation RVE inside the zooms. In all models, the regularization parameter is chosen as $\beta = 0.005$. 


4.4 3D mixed multiscale modelling of trabecular bone

This numerical example illustrates the efficacy of the proposed mixed multiscale framework in 3D simulations. We use a 3D bone sample with a trabecular microstructure which is transferred directly from a micro-CT medical image. The corresponding 3D reconstructed micro-CT image is presented in Figure 20a. We use the 3D reconstructed image to compute a surface mesh (STL mesh data) which will be converted into a level set function. For more information on the digital pipeline that we have used to convert STL mesh data into a level set function, see [40]. According to our proposed zooming technique, we select the zoom region and implement the mixing scheme to the bone as shown in Figure 20b with red and black lines representing schematically the surfaces of zooming and upper/lower bounds of mixing regions, respectively. The bone microstructure is defined by the zero level set function \( \Gamma_h^1 \) and the corresponding surface meshing and the CutFEM cell subtesselation are depicted in Figures 21a and 21b, respectively.

![Figure 20: 3D trabecular bone with zooming: (a) Micro-CT image 3D reconstruction, (b) CutFEM interfaces.](image)

In this example, we employ the MMT homogenisation approach in order to compute the macro-scale effective material properties. The mixing approach is implemented using the level-set-based indicator function \( \alpha \), presented for two smoothing lengths shown in Figure 31. For the homogenisation, we obtain the volume fractions of trabecular bone from [43], where the bone volume fraction is reported as \( B_v = 0.192 \). Assuming the micro-scale properties as \( E_m = 1 \) and \( \nu_m = 0.3 \), we derive the homogenised properties as following: \( E_M = 0.15 \) and \( \nu_M = 0.3 \).

We perform the compression test for a full micro-scale FEM (as reference) and the mixed multiscale method with an arbitrary location of zooming region and show their displacement field component \( u_y \) in Figure 23. For the mixed multiscale approach, the 3D simulations are carried out for two different smoothing lengths (\( 2\epsilon = 0.01, 0.1 \)) to study the mixing technique’s stability for both sharp and wide transitions regions. The comparison between full microscale and multiscale results shows that our level-set-based multiscale method can also be applied for 3D complex problems successfully, in a mesh independent manner, and the mixing technique is stable for both types of
To further investigate the accuracy of numerical results, we show the variation of stress component $\sigma_{yy}$ for two smoothing lengths in Figure 24. The results show that the response inside the zoom is consistent with the corresponding FEM reference model, and the behaviour is promising in terms of stability and accuracy.

We also study the condition number of the 3D mixed multiscale system matrix for three smoothing lengths. The results in Figure 25 show that the well conditioning of the mixed multiscale system
matrix is promising for the 3D problems with complex geometries. Moreover, the condition numbers stay stable with respect to the size of smoothing length.
Figure 23: 3D and 2D representations of FEM and mixed multiscale displacement field $u_y$, a) 3D FEM reference model, b) $2\varepsilon = 0.1$, c) $2\varepsilon = 0.01$, d) $2\varepsilon = 0.1$ and e) $2\varepsilon = 0.01$. 

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Figure 24: Stress component $\sigma_{yy}$: a) FEM with $h = 0.036$, b) mixed multiscale model-A with $h_{\text{min}} = 0.036$, $\epsilon = 0.01$ and only cut elements regularized, and c) mixed multiscale model-B with $h_{\text{min}} = 0.036$ $\epsilon = 0.01$, cut and porous elements are regularized.

Figure 25: Condition numbers for mixed multiscale models with various mesh sizes and smoothing lengths.
5 CONCLUSIONS

A framework was proposed to construct an unfitted concurrent multiscale model for heterogeneous structures. In our multiscale framework, we developed a mixing approach over a single background mesh to couple micro and macro-scale models. Therefore, unlike the conventional domain decomposition methods where an interface condition is required between macro and micro-scale models, the interface constraint is not needed anymore.

We demonstrated the validity of our mixed multiscale framework by modelling the elasticity problem in 2D and 3D cases. In the 2D case, we first tested the idea of a functional description of the whole heterogeneous structure by projecting it onto a background mesh which is fine in areas of interest and coarse outside. This projection of the functional description onto a background mesh was done successfully by CutFEM, in which the geometry was approximated by a piecewise linear signed distance function in each background mesh element. We showed that the accuracy of results in the fine regions is good; however, the very coarse mesh cells outside of the regions of interest gives rise to the random appearance of geometrical artifacts in the coarse region, yielding stress singularities. Next, we tested the same problem within the mixed multiscale framework where an equivalent homogenized domain was adopted in the coarse region. The results showed that employing the multiscale approach could improve the results in the coarse domain tremendously. Eventually, we extended the application of our multiscale framework for 3D elasticity problems. Here, we employed a given surface mesh of trabecular bone to define the microscale geometry. The results obtained showed a good agreement with the corresponding reference model in terms of global and local responses, where the corresponding multiscale system matrix remained well-conditioned under different sizes of mixing. The numerical results in 2D and 3D simulations demonstrated the accuracy and robustness of our unfitted multiscale framework in modelling highly heterogeneous structures where the geometry and zoom location could be detected automatically and in a stable manner, and the numerical efforts were successfully concentrated inside the interested regions.

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