On the implementation of a locally modified finite element method for interface problems in deal.II

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Abstract

In this work, we describe a simple finite element approach that is able to resolve weak discontinuities in interface problems accurately. The approach is based on a fixed patch mesh consisting of quadrilaterals, that will stay unchanged independent of the position of the interface. Inside the patches we refine once more, either in eight triangles or in four quadrilaterals, in such a way that the interface is locally resolved. The resulting finite element approach can be considered a fitted finite element approach. In our practical implementation, we do not construct this fitted mesh, however. Instead, the local degrees of freedom are included in a parametric way in the finite element space, or to be more precise in the local mappings between a reference patch and the physical patches. We describe the implementation in the open source C++ finite element library deal.II in detail and present two numerical examples to illustrate the performance of the approach. Finally, detailed studies of the behavior of iterative linear solvers complement this work.

Keywords Locally modified finite elements; fitted finite elements; interface problems; C++; deal.II; implementation

1 Introduction

In this paper, we consider interface problems, where the solution is continuous on a domain \( \Omega \subset \mathbb{R}^2 \), but its normal derivative may have a jump in normal direction over an interior interface. Problems of this kind arise for example in fluid-structure interaction, multiphase flows, multicomponent structures and in many other configurations where multiple physical phenomena interact. All these examples have in common that the interface between the two phases is moving and may be difficult to capture due to small scale features.

If the interface is not resolved by the finite element mesh, the accuracy of the finite element approach might decrease severely, see e.g. [4]. For simple elliptic interface problem with jumping coefficients, it has been shown, that optimal convergence can be recovered by a harmonic averaging of the diffusion constants [37, 36].

For more complex couplings, e.g. fluid-structure interactions, where two entirely different equations interact with each other, the list of possible discretisation techniques that yield optimal order can be split roughly in two groups.

The first class of approaches consists of so-called fitted finite element methods, where the meshes are constructed in such a way that the interface is sufficiently resolved, see [20, 11, 40]. If the interface is moving, curved or has small scale features, the repeated generation of fitted finite element meshes can exceed the feasible effort, however. In non-stationary problems, the projection of previous iterates to the new mesh, brings along further difficulties and sources of error. Further developments are based on local modifications of the finite element mesh, that only alter mesh elements close to the interface [14, 18, 25].

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An alternative approach is based on unfitted finite elements, where the mesh is fixed and does not resolve the interface. Here, proper accuracy is gained by local modifications or enrichment of the finite element basis. Prominent examples for these methods are the extended finite element method (XFEM [13]), the generalised finite element method [14] or the unfitted Nitsche method by [20,27]. Based on the latter works, so-called cut finite elements have been developed, see for instance [15,16,28,19]. All these enrichment methods are well analysed and show the correct order of convergence. One drawback of the enrichment methods is a complicated structure that requires local modifications in the finite element spaces leading to a variation in the connectivity of the system matrix and number of unknowns.

In this article, we use a simple approach that is based on a fixed patch mesh consisting of quadrilaterals and will stay unchanged independent of the position of the interface. Inside the patches we refine once more, either in eight triangles or in four quadrilaterals, in such a way that the interface is locally resolved. In this sense the resulting finite element approach can be considered a fitted finite element approach. This approach has first been proposed in [29]. In our practical implementation, we do however not construct this fitted mesh explicitly. Instead, the local degrees of freedom are included in a parametric way in the finite element space, or to be more precise in the local mappings between a reference patch and the physical patches.

The drawback of this approach is that the condition number of the resulting system matrices might be unbounded, when the interface approaches certain vertices or mesh lines. This problem can however be solved by constructing a scaled hierarchical basis of the finite element space. Using this basis the approach can be viewed as a simple enrichment method as well, where the enrichment consists of the standard Lagrangian basis functions on the fine scale.

The mathematical details, including a complete analysis of the discretisation error and the condition number of the system matrix have already been published in [13,15,19]. Later on, related approaches on triangular patches have been developed by [16,20] and [19]. Furthermore, the approach has been applied by the authors to simulate fluid-structure interaction problems with large deformations in [17,22] and [34] and by Gangl to simulate problems of topology optimisation [28].

The goal of this article is to explain in detail the implementation of the fitted finite element method and to provide a programme code based on the C++ finite element library deal.II [23]. In extension to [29] further details concerning the implementation of the finite element approach, and in particular on the construction of the hierarchical basis are given. Moreover, we study the performance of some iterative solvers, i.e. a simple and preconditioned conjugate gradient method (CG/PCG) to solve the arising linear systems, while ‘only’ a direct solver was used in [20].

The organisation of this article is as follows. In Section 2, a simple elliptic model problem is presented. Next, in Section 3 we introduce the local modifications of the finite element space in the cells that are cut by the interface. In Section 4, the discrete forms and the approximation properties are briefly recapitulated. Then, we introduce the hierarchical finite element space in Section 5. Section 6 consists of two numerical tests, that illustrate the main features and the performance of our approach. Finally, we present algorithmic details and details on the implementation in Section 7.

We conclude in Section 8.

2 Motivation: A simple elliptic model problem

To get started, let us consider a simple Poisson problem in \( \Omega \subset \mathbb{R}^2 \) with a discontinuous coefficient \( \kappa \) across an interface line \( \Gamma \subset \mathbb{R} \). Find \( u : \Omega \rightarrow \mathbb{R} \) such that

\[-\nabla \cdot (\kappa; \nabla u) = f \quad \text{on } \Omega_i, \quad (i = 1, 2), \quad [u] = 0 \quad \text{and } [\kappa \partial_n u] = 0 \quad \text{on } \Gamma, \]

(1)

with constants \( \kappa_i > 0 \) and subject to homogeneous Dirichlet conditions on the exterior boundary \( \partial \Omega \). Here, we denote the subdomains by \( \Omega_i, \quad i = 1, 2 \) and by \( [u] \) the jump of \( u \) across the interface \( \Gamma \). The variational formulation of this interface problem is given by
Definition 2.1 (Continuous variational formulation). Find $u \in H_0^1(\Omega)$ such that

$$a(u, \varphi) := \sum_{i=1}^{2} (\kappa_i \nabla u, \nabla \varphi) = (f, \varphi) \quad \forall \varphi \in H_0^1(\Omega).$$

Figure 1. $L^2$- and $H^1$-error for a standard finite element method using $Q_1$ and $Q_2$ polynomials for the discretisation of the interface problem \[.\] Configuration of the test problem in the right sketch. Further details are given in Section 6.

$$\kappa_1 = 0.1, \kappa_2 = 1$$

3 Locally modified finite elements

In order to define the modified finite elements, let us assume that $\mathcal{T}_{2h}$ is a form and shape-regular triangulation of the domain $\Omega \subset \mathbb{R}^2$ into open quadrilaterals. The discrete domain $\Omega_h$ does not necessarily resolve the partitioning $\Omega = \Omega_1 \cup \Gamma \cup \Omega_2$ and the interface $\Gamma$ can cut the elements $P \in \mathcal{T}_{2h}$.

We assume that the interface $\Gamma$ cuts patches in the following way:

1. Each (open) patch $P \in \mathcal{T}_{2h}$ is either not cut $P \cap \Gamma = \emptyset$ or cut in exactly two points on its boundary: $P \cap \Gamma = \emptyset$ and $\partial P \cap \Gamma = \{x_1^P, x_2^P\}$.

2. If a patch is cut, the two cut-points $x_1^P$ and $x_2^P$ may not be inner points of the same edge.

In principle, these assumptions only rule out two possibilities: a patch may not be cut multiple times and the interface may not enter and leave the patch at the same edge. Both situations can be avoided by refinement of the underlying mesh. If the interface is matched by an edge, the patch is not considered to be cut.
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We define four reference patches \( \hat{P}_1, \ldots, \hat{P}_4 \) on the unit square \((0,1)^2\). These patches are split into 4 quadrilaterals or 8 triangles as illustrated in Figure 2. Moreover, we define 9 nodes \( \hat{x}_1, \ldots, \hat{x}_9 \) in the vertices, edge midpoints and the midpoint of the patches, which will serve as degrees of freedom of the finite element space. Note that the same position of the degrees of freedom can be found always 9. Therefore, the global number of unknowns and the sparsity pattern of the system matrix stays identical, independent of the interface position.

![Figure 2. Left: Triangulation \( \mathcal{T}_{2h} \) of a domain \( \Omega \) that is split into \( \Omega_1 \) and \( \Omega_2 \) with interface \( \Gamma \). The quadrilateral cells in \( \mathcal{T}_{2h} \) are illustrated by the bold lines. Patch \( P \) is cut by \( \Gamma \) at \( x_1^p \) and \( x_2^p \). Right: Subdivision of reference patches \( \hat{P}_0, \hat{P}_1, \hat{P}_2, \hat{P}_3 \) (top left to bottom right) into eight triangles each.](https://example.com/figure2.png)

### 3.1 Construction of the finite element space

We define a mapping \( \hat{T}_p : \hat{P} \rightarrow P \), that is piecewise linear in sub-triangles and piecewise bi-linear in sub-quadrilaterals on \( \hat{P}_i \). This gives us the possibility to map the degrees of freedom \( \hat{x}_1, \ldots, \hat{x}_9 \) to nodes \( x_1^p, \ldots, x_9^p \), in such a way that the interface is resolved in a linear approximation in the physical patch. Denoting by \( \{\hat{\phi}_1, \ldots, \hat{\phi}_9\} \) the standard Lagrange basis of \( \hat{Q} \) or \( \hat{Q}_{\text{mod}} \) with \( \hat{\phi}_i(\hat{x}_j) = \delta_{ij} \), the transformation \( \hat{T}_p \) is given by

\[
\hat{T}_p(\hat{x}) = \sum_{i=1}^{9} x_i^p \hat{\phi}_i(\hat{x}).
\]

Finally, we define the finite element trial space \( V_h \subset H_0^1(\Omega) \) as an iso-parametric space on the triangulation \( \mathcal{T}_{2h} \):

\[
V_h = \left\{ \phi \in C(\hat{\Omega}) \cap H_0^1(\Omega), \phi \circ \hat{T}_p^{-1} \bigg|_P \in \hat{Q}_p \text{ for all patches } P \in \mathcal{T}_{2h} \right\}.
\]

Note that, whatever splitting of the patch is applied, the local number of degrees of freedom is always 9. Therefore, the global number of unknowns and the sparsity pattern of the system matrix stays identical, independent of the interface position.
Figure 3. Different types of cut patches. The subdivision can be anisotropic with \( r, s \in (0, 1) \) arbitrary.

It is important to note, that the functions in \( \tilde{Q} \) and \( \tilde{Q}_{\text{mod}} \) are all piecewise linear on the edges \( \partial P \), such that mixing different element types does not affect the continuity of the global finite element space.

Next, we present the subdivision of interface patches \( P \) into eight triangles.

**Definition 3.1.** We distinguish four different types of interface cuts, see Figure 3:

**Configuration A** The patch is cut in the interior of two opposite edges.

**Configuration B** The patch is cut in the interior of two adjacent edges.

**Configuration C** The patch is cut in the interior of one edge and in one node.

**Configuration D** The patch is cut in two opposite nodes.

Configurations A and B are based on the reference patches \( \hat{P}_2 \) and \( \hat{P}_3 \), configurations C and D use the reference patch \( \hat{P}_1 \), see Figure 2.

By \( e_i \in \mathbb{R}^2 \), \( i = 1, 2, 3, 4 \) we denote the vertices in the interior of edges, by \( m_P \in \mathbb{R}^2 \) the grid point in the interior of the patch. The parameters \( r, s \in (0, 1) \) describe the relative position of the intersection points with the interface on the outer edges.

If an edge is intersected by the interface, we move the corresponding point \( e_i \) on this edge to the point of intersection. The position of \( m_P \) depends on the specific configuration. For configuration A, B and D, we choose \( m_P \) as the intersection of the line connecting \( e_2 \) and \( e_4 \) with the line connecting \( e_1 \) and \( e_3 \). In configuration C, we use the intersection of the line connecting \( e_2 \) and \( e_4 \) with the line connecting \( x_1 \) and \( e_3 \).

As the cut of the elements can be arbitrary with \( r, s \to 0 \) or \( r, s \to 1 \), the triangle’s aspect ratio can be very large. With the described choices for the midpoints \( m_P \) we can guarantee, that the maximum angles in all triangles will be well bounded away from 180°.

**Lemma 3.1** (Maximum angle condition). All interior angles of the triangles shown in Figure 3 are bounded by 144° independent of \( r, s \in (0, 1) \).

The respective reference patches \( \hat{P}_0, \ldots, \hat{P}_3 \) (see Figure 2) are chosen based on the following criteria: First, it is mandatory that a maximum angle can be guaranteed. Second, it is beneficial for practical purposes to keep the maximum angle as small as possible on the one hand and on the other hand to conserve the symmetry in the discretisation, in the case of a symmetric problem. From these considerations, we choose type \( \hat{P}_2 \) if \( r + s > 1 \) and \( \hat{P}_3 \) if \( r + s < 1 \) for configuration A in our implementation. For an example, consider the left patch in Figure 3, where \( \hat{P}_3 \) has been chosen, as \( r + s > 1 \). Note that the symmetry criterion would not be fulfilled, if we would choose always either \( \hat{P}_2 \) or \( \hat{P}_3 \), independent of \( r \) and \( s \). In configuration B, we choose \( \hat{P}_3 \), when the cut separates the lower left or the upper right vertex from the rest of the patch and \( \hat{P}_2 \), when only the lower right or the upper left vertex lie on one side of the interface.
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Figure 4. Left: Patch elements and interface $\Gamma$ that goes through two patches. Right: Sub-triangulation and splitting of the mesh into subdomains $\Omega^1_h$ and $\Omega^2_h$. The interface $\Gamma_h$ is a linear approximation of the interface $\Gamma$ shown on the left-hand side.

4 Discrete variational formulation and approximation properties

In the previous sections, we tacitly assumed that the interface can be resolved in a geometric exact way. In the case of a curved interface, a linear approximation by mesh lines is constructed.

With the help of the discrete approximation of the interface, we introduce a second splitting of the domain $\Omega$ into the discrete subdomains

$$\Omega = \Omega^1_h \cup \Omega^2_h,$$

such that all cells of the sub-triangulation are either completely included in $\Omega^1_h$ or in $\Omega^2_h$, see Figure 4.

Using these definitions, we define a discrete bilinear form $a_h(\cdot, \cdot)$. For the elliptic model problem, this form is given by

$$a_h(u_h, \phi_h) := (\kappa_h \nabla u_h, \nabla \phi_h)_{\Omega_h},$$

where

$$\kappa_h = \begin{cases} 
\kappa_1 & \text{in } \Omega^1_h, \\
\kappa_2 & \text{in } \Omega^2_h. 
\end{cases}$$

Note that $\kappa_h$ differs from $\kappa$ in a small layer between the continuous interface $\Gamma$ and the discrete interface $\Gamma_h$.

Definition 4.1 (Discrete variational formulation). The discrete problem is to find $u_h \in V_h$ such that

$$a_h(u_h, \phi_h) = (f, \phi_h)_{\Omega_h} \quad \forall \phi_h \in V_h.$$

The maximum angle conditions of Lemma 3.1 is sufficient to ensure that the Lagrangian interpolation operators $I_h : H^2(T) \cap C(\bar{T}) \to V_h$ are of optimal order for smooth functions $v \in H^2(T) \cap C(\bar{T})$ on an element $T$, i.e.

$$\|\nabla^k (v - I_h v)\|_T \leq c h_{T,\text{max}}^{2-k} \|\nabla^2 v\|_T, \quad k = 0, 1$$

(5)

where $c > 0$ is a constant and $h_{T,\text{max}}$ is the maximum diameter of a triangle $T \in P$ (see e.g. [1]). If the interface $\Gamma$ is curved, the solution $u$ to (1) is however non-smooth across the interface. Here, we have to argument using smooth extensions of $u|_{\Omega_i}, i = 1, 2$ to the other sub-domain and the smallness of the region

$$S_h = (\Omega_1 \cap \Omega^2_h) \cup (\Omega_2 \cap \Omega^1_h)$$

around the interface.

The following result has been shown for the elliptic interface problem (1):

6
Theorem 4.1 (A priori estimate). Let $\Omega \subset \mathbb{R}^2$ be a domain with convex polygonal boundary, split into $\Omega = \Omega_1 \cup \Gamma \cup \Omega_2$, where $\Gamma$ is a smooth interface with $C^2$-parametrisation. We assume that $\Gamma$ divides $\Omega$ in such a way that the solution $u \in H^1_0(\Omega)$ satisfies the stability estimate

$$u \in H^1_0(\Omega) \cap H^2(\Omega_1 \cup \Omega_2), \quad \|u\|_{H^2(\Omega_1 \cup \Omega_2)} \leq c_s \|f\|.$$  

For the corresponding modified finite element solution $u_h \in V_h$, it holds that

$$\|\nabla (u - u_h)\|_{\Omega} \leq Ch_p \|f\|, \quad \|u - u_h\|_{\Omega} \leq Ch_p^2 \|f\|.$$  

Proof. For the proof, we refer to [34] or [18].

5 Hierarchical basis functions

The drawback of the previously described simple approach is that the condition number of the system matrix is unbounded for certain anisotropies ($r, s \to 0$). This is an unresolved issue in many of the presently used enriched finite element methods for interface problems. We refer to [30] or [3] for two of the few positive results in the case of extended finite elements of low-order. In our case, this can be circumvented by using a scaled hierarchical finite element basis, that will yield system matrices $A_h$ that satisfy the optimal bound $\text{cond}_2(A_h) = O(h_p^{-2})$ for elliptic problems, with a constant that does not depend on the position of the interface $\Gamma$ relative to the mesh elements. A detailed proof of this result has been given in [20].
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![Image of diagrams](image.png)

Figure 7. Configuration of the hierarchical basis functions $V_b$ for the different patch types. In each sketch, we consider the case $r \to 0$ or $s \to 0$ or both.

We split the finite element space $V_h$ in a hierarchical manner

$$V_h = V_{2h} + V_b,$$

where $N := \dim(V_h) = \dim(V_{2h}) + \dim(V_b) =: N_{2h} + N_b$.

The space $V_{2h}$ is the standard space of piecewise bilinear or linear functions on the patches $P \in \mathcal{T}_{2h}$ equipped with the usual nodal Lagrange basis $V_{2h} = \text{span}\{\phi_{2h}^1, \ldots, \phi_{2h}^{N_{2h}}\}$. Patches cut by the interface are split into two large triangles.

The space $V_b = V_h \setminus V_{2h}$ collects all functions, that are needed to enrich $V_{2h}$ to $V_h$. These functions are defined piecewise on the sub-elements in the remaining 5 degrees of freedom, see Figure 5 for an example of the splitting and Figure 6 for an illustration of the local basis functions. These basis functions are denoted by $V_b = \text{span}\{\phi_b^1, \ldots, \phi_b^{N_b}\}$. The finite element space $V_{2h}$ on the other hand is fully isotropic and standard analysis holds. Functions in $V_{2h}$ do not resolve the interface, while the basis functions $\phi_b^i \in V_b$ will depend on the interface location if $\Gamma \subset \text{supp} \phi_b^i$.

In order to define the hierarchical ansatz space, we have to modify some of the basic triangles in the cases A, B and C, see Figure 7. In contrast to Section 3, the midpoint can be moved along one of the diagonal lines only, such that the space $V_{2h}$ can be defined as space of piecewise linear functions on two large triangles. Note that in order to guarantee a maximum angle condition in the cases A.1 and C.1 in Figure 7, we must also move the outer node $x_2$ belonging to the space $V_b$, due to the additional constraint on the position of $m_P$.

### Scaling of the basis functions

Moreover, in order to ensure the optimal bound for the condition number, we have to normalise the Lagrangian basis functions on the fine scale $\phi_b^i, i = 1, \ldots, N_b$, by setting

$$\tilde{\phi}_b^i := \frac{\phi_b^i}{\|\nabla \phi_b^i\|},$$

such that it holds that

$$C^{-1} \leq \|\nabla \tilde{\phi}_b^i\| \leq C, \quad i = 1, \ldots, N_b.$$  (6)
In a practical implementation, one can use the basis $\phi_i, i = 1, \ldots, N$ to assemble the system matrix $A_h$ and apply a simple row- and column-wise scaling with the diagonal elements

$$a_{ij} = (\nabla \phi_j, \nabla \phi_i), \quad \hat{a}_{ij} := \frac{a_{ij}}{\sqrt{a_{ii}a_{jj}}}.$$  

Alternatively, a simple preconditioning of the linear system can be applied multiplying with the diagonal of the system matrix from left and right

$$Ax = b \quad \iff \quad D^{-\frac{1}{2}}AD^{-\frac{1}{2}}\hat{x} = D^{-\frac{1}{2}}b, \quad \hat{x} = D^{\frac{1}{2}}x,$$

where $D = \text{diag}(a_{ii})$.

### 6 Numerical examples

We now present two numerical examples that include all different types of interface cuts (configurations A to D) and arbitrary anisotropies.

#### 6.1 Example 1: Performance under mesh refinement

This first example has already been considered to discuss the interface approximation in Section 3, see Figure 1 for a sketch of the configuration. The unit square $\Omega = (-1, 1)^2$ is split into a ball $\Omega_1 = B_R(x_m)$ with radius $R = 0.5$, midpoint $x_m = (0, 0)$, and $\Omega_2 = \Omega \setminus \Omega_1$. As diffusion parameters we choose $\kappa_1 = 0.1$ and $\kappa_2 = 1$. We use the analytical solution

$$u(x) = \begin{cases} -2\kappa_2 \|x - x_m\|^4, & x \in \Omega_2, \\ -\kappa_1 \|x - x_m\|^2 + \frac{1}{3} \kappa_1 - \frac{1}{8} \kappa_2, & x \in \Omega_1, \end{cases}$$

to define the right-hand side $f_i := -\kappa_i \Delta u$ in $\Omega_i$ and the Dirichlet boundary data. A sketch of the solution is given on the right side of Figure 8.

On the coarsest mesh with 16 patch elements, we have four patches of type D. After some steps of global refinement this simple example includes the configurations A to C with different anisotropies.
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\[ O(h^2) \]
\[ O(h) \]
\[ \| \nabla (u - u_h) \| \]
\[ \| u - u_h \| \]
modified finite elements
mesh size \( h \)
0.001 0.01 0.1 1
1e-05 0.0001 0.01 1

Figure 9. Example 1: \( H^1 \)- and \( L^2 \)-errors under mesh refinement.

In Figure 9, we plot the \( H^1 \)- and \( L^2 \)-norm errors obtained on several levels of global mesh refinement. According to Theorem 4.1, we observe linear convergence in the \( H^1 \)-norm and quadratic convergence in the \( L^2 \)-norm. For comparison, Figure 1 shows the corresponding results using standard non-fitting finite elements.

As we have shown numerically computed condition numbers for this and the following example already in [20], we provide here computational evidence that the arising linear systems can be solved with iterative methods as the conjugate gradient (CG) instead. We incorporate the scaling of the basis functions by means of a diagonal preconditioner, as discussed in Section 5. In order to analyse the effect of the scaling, we compare the performance of the diagonally preconditioned CG method (dPCG) with a standard CG scheme without preconditioning. Moreover, we also show the performance of a CG scheme with SSOR relaxation as preconditioner (SSOR-PCG, without a scaling of the basis functions). For the latter we choose the relaxation parameter \( \omega = 1.2 \), see e.g., [32]. The (absolute) tolerance for the global residual is chosen as \( 10^{-12} \).

The iteration numbers for the non-hierarchical finite element basis introduced in Section 3 (nh) and the hierarchical (h) variant described in Section 5 in combination with the three CG methods are shown in Table 1 on different mesh levels, where each finer mesh is constructed from the coarser one by global mesh refinement.

Theoretically the number of iterations needed to reach a certain tolerance in the CG method should scale with the square root of the condition number \( \Theta(\sqrt{\kappa}) \) (see e.g., [10, 35]), i.e. for the scaled hierarchical approach with a condition number of order \( \kappa = \Theta(h_m^{-2}) \), we can expect that the number of iterations grows asymptotically with \( \Theta(h_m^{-1}) \). This behaviour can be observed quite clearly for the preconditioned CG methods in Table 1. The SSOR preconditioning seems to work even better than the diagonal preconditioning. In this example, the expected convergence of the linear solver can be obtained without using the hierarchical basis functions. The use of the hierarchical basis leads however to an advantage in terms of the absolute numbers of iterations.

For the standard CG method without preconditioning, we observe that the number of iterations grows faster than \( \Theta(h_m^{-1}) \) for both the hierarchical and the non-hierarchical approach. This has to be expected, as the condition number might be unbounded for certain anisotropies. The observation that the iteration numbers for the scaled non-hierarchical approach seem bounded by \( \Theta(h_m^{-1}) \) in this example, might be due to the fact that not all kind of anisotropies are present and that the anisotropies that are present do not necessarily get worse on the finer grids. To study the performance of our approach considering all kinds of anisotropies (see Figure 7), we will next move the circular interface gradually by small fractions of patch cells in vertical direction.
Table 1. Iteration numbers of the linear solvers on different mesh levels for hierarchical (h) and non-hierarchical (nh) versions and the standard CG method compared to a diagonally preconditioned (dPCG) and a SSOR-preconditioned CG (SSOR-PCG) approach.

| Level | #Patches | CG(nh) | dPCG(nh) | SSOR-PCG(nh) | CG(h) | dPCG(h) | SSOR-PCG(h) |
|-------|----------|--------|----------|--------------|-------|---------|------------|
| 0     | 16       | 10     | 10       | 15           | 10    | 10      | 15         |
| 1     | 64       | 43     | 29       | 32           | 64    | 39      | 25         |
| 2     | 256      | 114    | 60       | 56           | 126   | 61      | 32         |
| 3     | 1024     | 253    | 124      | 97           | 197   | 95      | 47         |
| 4     | 4096     | 561    | 238      | 175          | 351   | 167     | 81         |
| 5     | 16384    | 1436   | 484      | 335          | 881   | 322     | 150        |
| 6     | 65536    | 3518   | 967      | 634          | 2053  | 622     | 293        |

6.2 Example 2: Performance for different anisotropies

To include all kind of anisotropies, we fix the refinement level to the fourth level of the previous example (4096 patch cells) and move the circular interface gradually in vertical direction. Precisely, we move the position of the midpoint by

\[
x_m = \left(0, \frac{k}{N} h_p \right)
\]

for \( k = 0, \ldots, N - 1 \), where \( N = 1000 \). Note that for \( k = N \), the interface would have been moved by exactly one patch cell, i.e. exactly the same cuts as for \( k = 0 \) would appear. The problem and parameters are exactly the same as in the previous example (note that the exact solution and the data defined above depend on \( x_m \)).

The meshes for \( k = 0 \) and \( k = 990 \) are shown in Figure 10. Moreover, in order to illustrate the anisotropic sub-cells, a zoom-in of the cut-meshes for \( k = 0, 10, 50 \) and \( 990 \) is displayed in larger in Figure 11. For \( k = 0 \), we find very anisotropic cells in two patches of type C in the patches in the centre; for \( k = 10 \) in four patches of type B; for \( k = 50 \) in two patches of type B in the middle and two patches of type A on the left and right; for \( k = 990 \) very anisotropic cells of type A are present.

In Table 2, we show some properties of the triangulation \( T_h \) consisting of the sub-cells for the four different configurations shown in Figure 11. The most anisotropic cells can be found for \( k = 10 \).
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Figure 11. Example 2: Zoom-in at $k = 0$ (top left), $k = 10$ (top right), $k = 50$ (bottom left) and $k = 990$ (bottom right).

and $k = 990$, where both the largest aspect ratio

$$\max_{k \in \mathbb{N}} \frac{|e_{K,\text{max}}|}{|e_{K,\text{min}}|}$$

of an element and the ratio between the largest and the smallest element's size are of order $10^5$. Note that due to the symmetry of the problem and the discretisation, the values for $k = 10$ and $k = 990$ are identical. The element with the largest aspect ratio can be found on the very left of the circle (and due to symmetry also on the very right, see Figure 10 on the right), where the patch line connecting the vertices $x_1 = (-0.5, 0.03125)$ and $x_2 = (-0.46875, 0.03125)$ is cut by the interface at $x_s \approx (-0.4999999, 0.03125)$.

In order to study the dependence of the iteration numbers on the position of the interface, we plot the number of linear iterations for the three different CG methods and the non-hierarchical and hierarchical basis in Figure 12 over the increment $k$. For both the non-hierarchical and the hierarchical approach, we observe that the iteration numbers decrease by at least a factor of 2 for the diagonal preconditioning and at least by a factor of 4 for the SSOR preconditioning compared to the standard CG method.

For the non-hierarchical approach, the iteration numbers depend considerably on the position
| \( k \) | \( K_{\text{max}} \) | \( K_{\text{min}} \) | \( K_{\text{max}} / K_{\text{min}} \) | \( |e_{\text{max}}| \) | \( |e_{\text{min}}| \) | \( \text{max}_{\, K} |e_{\text{K}, \text{max}}| / |e_{\text{K}, \text{min}}| \) |
|-----|----------------|----------------|----------------|----------------|----------------|----------------|
| 0   | \( 2.44 \cdot 10^{-4} \) | \( 3.82 \cdot 10^{-6} \) | \( 6.39 \cdot 10^{4} \) | \( 3.45 \cdot 10^{-2} \) | \( 4.89 \cdot 10^{-4} \) | \( 3.20 \cdot 10^{4} \) |
| 10  | \( 2.50 \cdot 10^{-4} \) | \( 7.63 \cdot 10^{-10} \) | \( 3.28 \cdot 10^{5} \) | \( 3.45 \cdot 10^{-2} \) | \( 9.77 \cdot 10^{-8} \) | \( 1.60 \cdot 10^{5} \) |
| 50  | \( 2.52 \cdot 10^{-4} \) | \( 1.91 \cdot 10^{-8} \) | \( 1.32 \cdot 10^{4} \) | \( 3.45 \cdot 10^{-2} \) | \( 2.44 \cdot 10^{-6} \) | \( 6.40 \cdot 10^{3} \) |
| 990 | \( 2.50 \cdot 10^{-4} \) | \( 7.63 \cdot 10^{-10} \) | \( 3.28 \cdot 10^{5} \) | \( 3.45 \cdot 10^{-2} \) | \( 9.77 \cdot 10^{-8} \) | \( 1.60 \cdot 10^{5} \) |

Table 2. Properties of the triangulations \( \mathcal{T}_h \) consisting of the sub-cells for the four different configurations shown in Figure 11. In columns 2 to 4, we show the area of the largest and the smallest element \( |K_{\text{max}}| \) and \( |K_{\text{min}}| \) and their ratio; in columns 5 and 6 the largest and smallest edge \( |e_{\text{max}}| \) and \( |e_{\text{min}}| \). Finally, in column 7 the biggest aspect ratio of all elements is shown.

![Figure 12](image-url)  
**Figure 12.** Example 2: Number of linear iterations needed for the different CG methods to decrease the residual below a tolerance of \( 10^{-12} \) plotted over the increment \( k \), where for \( k = 1000 \) the circular interface has been moved by exactly one patch cell. **Left:** Non-hierarchical finite element basis. **Right:** Hierarchical basis.

of the interface, even after preconditioning. Using the diagonal preconditioning the iteration number varies between 239 and 585 iterations, for the SSOR preconditioning between 129 and 260 iterations are needed. These numbers get worse, when the fineness \( N \) is increased. In this example it becomes clear that the non-hierarchical approach shows a condition number issue, even when preconditioning techniques are used.

For the hierarchical approach the iteration numbers seem to be bounded independently of the position of the interface for both preconditioning variants. The diagonally preconditioned CG method needs between 163 and 188 linear iterations, the SSOR preconditioned CG method between 62 and 81 iterations. Again the SSOR preconditioned CG method is superior to the simple diagonal preconditioning, although our analysis for the condition number is based on the scaling of the hierarchical basis \( 6 \), which is only ensured for the diagonal preconditioning.

## 7 Implementation

Our implementation is based on deal.II, version 8.5.0. A short guide on the installation and compilation is given in the file `README.txt`.

We start this section by giving an overview of the basic structure of the source code in Section 7.1. Then, we describe the implementation of the level set function in Section 7.2. In Section 7.3, we give an overview on the additional steps needed compared to a standard finite element code and how they are implemented in the class `LocModFE`. Finally, we show in Section 7.4 how these are incorporated in a standard finite element program.
7.1 Structure of the code

The source code can be split into three parts, which can be found in the files `locmodfe.h` and `locmodfe.cc`, `step-modfe.cc` and `problem.h`. The following lines are copied from the preamble of the file `README.txt`:

```
* The source code includes the following files and classes:
* 1) locmodfe.h: Contain all functions that are specific to the locally modified FE method
   a) class LocModFEValues: Extends the FEValues class in deal.II, where
   the local basis functions on the reference patches are evaluated
   b) class LocModFE: Key class of the locally modified finite element method
* 2) step-modfe.cc:
   a) class ParameterReader: Read in parameters from a separate parameter file
   b) class InterfaceProblem: local user file similar to many deal.II tutorial steps, which controls the general workflow of the code, for example the solution algorithm, assembly of system matrix and right-hand side and output
   c) int main()
* 3) problem.h: Problem-specific definition of geometry, boundary conditions and analytical solution
   a) class LevelSet: Implicit definition of interface and sub-domains
   b) classDirichletBoundaryConditions: Definition of the Dirichlet data
   c) class ManufacturedSolution : Analytical solution for error estimation
```

`locmodfe.h` and `locmodfe.cc`

The files `locmodfe.h` and `locmodfe.cc` contain all functions that are specific for the locally modified finite element discretisation. The class `LocModFEValues` extends the `FEValues` class in `deal.II`. In this class the values of the basis functions and their gradients (in `deal.II` “shape functions”) as well as the derivatives of the map \( \tilde{T}_P \) are evaluated in quadrature points on the reference patch, depending on the reference patch type (\( \tilde{P}_0, \ldots, \tilde{P}_3 \)) and the boolean parameter \_hierarchical, which specifies if a hierarchical basis is to be used.

In the class `LocModFE`, we check if patches are cut and in which sub-domains they are (function `set_material_ids`), define the type of the cut (configurations \( \mathrm{A}, \ldots, \mathrm{D} \)), the reference patch type (\( \tilde{P}_0, \ldots, \tilde{P}_3 \)) and the local mappings \( \tilde{T}_P \) (function `init_FEM`). Moreover, we initialise the respective quadrature formulas depending on the reference patches (function `compute_quadrature`, more details on the quadrature will be given below), provide functions to compute norm errors (function `integrate_difference_norms`), to set Dirichlet boundary values in cut patches (function `interpolate_boundary_values`) and to visualise the solution (function `plot_vtk`).

`step-modfe.cc`

In the file `step-modfe.cc`, we find the `main()` function and the classes `ParameterReader` and `InterfaceProblem`. The class `ParameterReader` is used to read in parameters from a parameter file, as in many `deal.II` tutorial steps. The class `InterfaceProblem` can also be found similarly in many of the local user files in the tutorial steps. It contains for example the loops of the Newton iteration as well as functions to assemble the right-hand side and the system matrix. They differ from other `deal.II` steps only, when specific functions from the `LocModFE` class need to be used. The main modifications that are required for the locally modified finite element method will be explained in detail in the next section.
Finally, the file `problem.h` contains three classes, where the geometry, the Dirichlet boundary data and the analytical solution for the specific example to be solved are specified.

### 7.2 The Level set function

In order to assign an element type to a patch, let us assume, that the interface is represented as zero-contour of a Level-Set function $\chi(x)$. In our examples, the function $\chi(x) = \|x - x_m\|^2 - 0.25, x_m = (0,y_{\text{offset}})$ is specified by the following expressions in the class `LevelSet` in the file `problem.h`:

```cpp
1 template <int dim> class LevelSet
2 {
3      // Compute value of the LevelSet function in a point p
4      double dist(const Point<dim> p) const
5      {
6          return p(0)*p(0) + (p(1)-yoffset)*(p(1)-yoffset) -0.5*0.5;
7      }
8
9      // Derivatives for Newton's method to find cut position
10     double dist_x(const Point<dim> p) const
11     {
12         return 2.0*p(0);
13     }
14
15     double dist_y(const Point<dim> p) const
16     {
17         return 2.0*(p(1)-yoffset);
18     }
19
20     //Determine domain affiliation of a point p
21     int domain(const Point<dim> p) const
22     {
23         double di = dist(p);
24         if (di>0) return 1;
25         else return -1;
26     }
27     ...}
28
dist(...), $\chi$ in a point p. Moreover, we provide the derivatives $\text{dist}_x(...)$ and $\text{dist}_y(...)$, which will be needed by a Newton method to find the position, at which the interface cuts an exterior edge (see Point 3 below). By means of the function `int domain(...)`, we obtain the index of the sub-domain, in which $p$ lies.

### 7.3 Implementation of the class `LocModFE`

Before we describe the additional steps needed for the locally modified finite element approach in detail, let us note that a patch is affected by the interface if $\chi$ shows different signs in two of the four outer vertices. In the same way, we identify the edges cut by the interface. Let $v_1$ and $v_2$ be the two outer nodes of an edge with $\chi(v_1) > 0 > \chi(v_2)$, see Figure 13. The exact coordinate where the interface line crosses an edge, can be found by a simple Newton method to find the zero $s_0$ of

$$f(s) = \chi(v_1 + s(v_2 - v_1)) = 0.$$

The following steps are executed in each patch $P \in \mathcal{T}_{2h}$ before the system matrix and right-hand side are assembled. Note that all these operations are local operations on the patch level:
Implementation of a locally modified finite element method

Step 1 and 2 (implemented in `set_material_ids`)

We will provide some code snippets to illustrate how these steps are implemented in the class `LocModFE`. Step 1 and 2 are implemented in the function `void set_material_ids`:

```cpp
template <int dim>
void LocModFE<dim>::set_material_ids (const DoFHandler<dim> &dof_handler,
                                      const Triangulation<dim> &triangulation)
{
    ...
    unsigned int subdom1_counter;
```
for (unsigned int cell_counter = 0; cell!=endc; ++cell, cell_counter++)
{
    subdom1_counter = 0;
    for (unsigned int v=0; v<GeometryInfo<dim>::vertices_per_cell; ++v)
    {
        //First determine the sub-domain of the four outer vertices
        double chi_local = chi.domain(cell->vertex(v));
        node_colors[cell->vertex_index(v)] = chi_local;
        if (chi_local > 0) subdom1_counter ++;
    }
    //Based on the colors of the vertices, specify a color for the patches
    // (0 stands for an interface patch)
    if (subdom1_counter == 4)
        cell_colors[cell_counter] = 1;
    else if (subdom1_counter == 0)
        cell_colors[cell_counter] = -1;
    else
        cell_colors[cell_counter] = 0;
}

First, we set in line 16 the node_color for each of the four outer vertices of the patch, based on the value of the Level set function \( \chi \) (step 1). Moreover, we count the number of outer vertices of the patch lying in sub-domain 1 (line 18) by means of the counter subdom1_counter. If the result is 0 or 4, the patch lies completely in one sub-domain and the node_color of the four vertices (-1 or 1) is set as cell_color for the patch; otherwise we set the cell_color to 0, which corresponds to an interface patch (line 28).

### Step 3 to 5 (implemented in init_FEM)

The steps 3-5 can be found in the function

```cpp
void init_FEM(const typename DoFHandler<dim>::active_cell_iterator &cell,
               unsigned int cell_counter, FullMatrix<double> &M,
               const unsigned int dofs_per_cell, unsigned int &femtype_int,
               std::vector<double> &LocalDiscChi, std::vector<int> &NodesAtInterface);
```

As the implementation of this function is quite lengthy, let us only discuss its outputs: The resulting reference patch type (step 4) is written to the variable femtype_int. As shown in (3), the map \( \hat{T}_P \) can be parametrised by the coordinates of the nine vertices \( x^P_i, i = 1, \ldots, 9 \) in the physical patch \( P \). These are memorised in the \( 2 \times 9 \)-matrix \( M \). Moreover, we would like to mention the vector LocalDiscChi, which contains the nine values of the Level set function \( \chi(x^P_i) \) in the vertices. These parametrise a discrete level set function \( \chi_h \), that will be used in the computations, see the following paragraph.

### Step 6 (implemented in compute_quadrature)

For the choice of the quadrature formula depending on the reference patch type (step 6), we use the function

```cpp
Quadrature<dim> compute_quadrature (int femtype);
```

The four different quadrature formulas that can be chosen are defined in the function

```cpp
void initialize_quadrature();
```
Implementation of a locally modified finite element method

that has to be called once in the beginning of the program (for example within the function \texttt{run}, see Section 7.4). The integration points are chosen as the four Gauss points of the Gaussian integration formula of order one in each of the sub-quadrilaterals and as the three Gauss points of the corresponding Gaussian integration formula in each of the sub-triangles. This results in a total of 16 integration points in regular patches and of 24 integration points in interface patches.

7.4 Using the functions of the class \texttt{LocModFE} in a standard finite element program

In order to access the functions of the class \texttt{LocModFE} we have added the object

\begin{verbatim}
LocModFE<dim> lmfe;
\end{verbatim}

as a member to the user class \texttt{InterfaceProblem}.

The run method

As in almost all deal.II tutorial steps, the workflow of the code is controlled by the function \texttt{void run()} of the user class \texttt{InterfaceProblem}. We show this function here for test case 2, skipping some lines with ’...’ that contain only output to the console (\texttt{std::cout}):

\begin{verbatim}
template <int dim>
void InterfaceProblem<dim>::run ()
{
 set_runtime_parameters();
 setup_system();
 lmfe.initialize_quadrature();

 // Memorize initial solution
 Vector<double> initial_solution = solution;
 std::cout << std::endl;

 if (test_case == 1)
 {
 ... 
 }
 else if (test_case == 2)
 {
 for (unsigned int i=0; i < N_testcase2; ++i)
 { 
  // Move y-position of circle at each step
  _yoffset = (double)i / (double)N_testcase2 * min_cell_vertex_distance;
  lmfe.LevelSetFunction()->set_y_offset (_yoffset);

  // Reset material_ids based on the new interface location
  lmfe.set_material_ids (dof_handler, triangulation);

  std::cout << ...

  // Solve system with Newton solver
  newton_iteration ();

  // Compute functional values (error norms)
  compute_functional_values (false);

  ... 

  // Write solutions as *.vtk file
  lmfe.plot_vtk (dof_handler,fe,solution,i);
  }
 } 

 // end test_case 2
}
\end{verbatim}
void initialize_quadrature() and level set function

The first function of the class LocModFE that is used, is void initialize_quadrature() in line 6, which initialises the four quadrature formulas for the four reference patch types $\hat{P}_0, ..., \hat{P}_3$, that can be accessed by means of lmfe.compute_quadrature(int femtype) later on. In the lines 21 and 22, the vertical position of the circular interface is updated by means of the y-coordinate ($y_{offset}$) of the midpoint $x_m$ of the circle and then passed to the level set function of the class LocModFE. Remember that in this test case the interface is moved gradually upwards.

void set_material_ids(...) and newton_iteration()

Next, the function void set_material_ids(...) is called in line 25, which sets the colours for vertices and patches as explained above. All the computations are then done within the function newton_iteration() in line 30. The source code of this function itself contains no content that is specific to the locally modified finite element method. In fact the Newton solver is mostly copy and paste from [39]. The only modified functions that are called within newton_iteration() are the assembly of the system matrix and right-hand side, which will be discussed below and the function set_initial_bc, which has to be modified in interface patches by calling lmfe.interpolate_boundary_values(...). After the Newton iteration, functional values are computed in the function compute_functional_values(...) that uses the modified function lmfe.integrate_difference_norms(...). Finally, the results are written to a vtk file by lmfe.plot_vtk in line 37, together with a mesh consisting of the sub-cells of the patches.

assemble_system_matrix()

Within the function newton_iteration, the functions assemble_system_matrix() and assemble_system_rhs() are called. We show here the prior exemplarily, the modifications in the assembly of the right-hand side are analogous:

```cpp
template <int dim>
void InterfaceProblem<dim>::assemble_system_matrix ()
{
    ... 

    LocModFEValues<dim>* fe_values;

    // We initialize one LocModFEValue object for patch type 0 and one for patch types 1 to 3, due to the different number of integration points
    Quadrature<dim> quad0 = lmfe.compute_quadrature(0);
    LocModFEValues<dim> fe_values0 (fe, quad0, 
        _hierarchical, update_values | update_quadrature_points | 
        update_JxW_values | update_gradients);

    Quadrature<dim> quad1 = lmfe.compute_quadrature(1);
    LocModFEValues<dim> fe_values1 (fe, quad1, 
        _hierarchical, update_values | update_quadrature_points | 
        update_JxW_values | update_gradients);
```

After some variable definitions that we have skipped here in line 4, we initialise a pointer LocModFEValues<dim>* fe_values(...). Depending on the patch type, this pointer will be set for each patch in the following loop to one of the objects LocModFEValues<dim> fe_values0(...) (patch type $\hat{P}_0$) or LocModFEValues<dim> fe_values1 (patch type $\hat{P}_1, ..., \hat{P}_3$) defined in the lines 11 and 16. We initialise these two objects before the loop over all patches for efficiency reasons. Two different objects are needed as the local number of quadrature points is different for patch type $\hat{P}_0$ compared to the interface patch types.

Next, we start the loop over all patches, in which the local contribution to the global system matrix is computed. Before we can compute the local basis functions and their gradients, we have
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to call the function \texttt{init\_FEM(...)} that sets the patch type (\texttt{femtype}), the local mapping \(T_p(M)\) and the discrete level set function \(\chi_h(\text{LocalDiscChi})\), see line 25. Then, the quadrature formula that corresponds to the patch type is set in line 27 and one of the two objects of type \texttt{LocModFEValues}, that were initialised above, is chosen. The quadrature formula, as well as the patch type and the local mapping \(T_p\) are then passed to this object in line 34. Now, we are ready to compute the local basis functions, their gradients and the derivatives of the mapping \(T_p\), that are needed to compute the entries of the system matrix. This is done by \texttt{fe\_values->reinit(J)} in line 38:

```cpp
for (unsigned int cell_counter = 0; cell!=endc; ++cell,++cell_counter)
{
    local_matrix=0;
    //Set patch type (femtype), map T_P (M), local level set function (LocalDiscChi)
    //and list of nodes at the interface
    lmfe.init_FEM (cell,cell_counter,M,dofs_per_cell,femtype, LocalDiscChi, NodesAtInterface);
    Quadrature<dim> quadrature_formula = lmfe.compute_quadrature(femtype);
    const unsigned int n_q_points = quadrature_formula.size();
    //Choose one of the initialized objects for LocModFEValues
    if (femtype==0) fe_values = &fe_values0;
    else fe_values = &fe_values1;
    fe_values->SetFemtypeAndQuadrature(quadrature_formula, femtype, M);
    std::vector<double> J(n_q_points);
    //Now the shape functions on the reference patch are initialized
    fe_values->reinit(J);
}
```

Next, we have a loop over the quadrature points and over the local degrees of freedom as usual in a finite element program. In order to compute the diffusion coefficient \(\kappa\) (viscosity), we use the discrete level set function \(\chi_h\). The value of \(\chi_h\) in the quadrature point \(q\) is extracted from the vector \texttt{LocalDiscChi} by the function \texttt{lmfe.ComputeLocalDiscChi(...)} in line 50. Note that it is important to use this discrete level set function for the assembly of matrix and right-hand side, as otherwise \(\kappa\) would jump within a sub-element and the program would not be robust with respect to high-contrast coefficients. The remaining lines are standard and very similar to many other \texttt{deal.II} tutorial steps (e.g., \texttt{deal.II-step-22}):
Finally, we remark that besides the described function calls no further modifications are necessary in comparison to any other standard FEM code or deal.II tutorial program.

8 Conclusion and outlook

In this paper, we have explained the implementation of the locally fitted finite element method first proposed in [20] in detail. The underlying framework is based on the open-source finite element library deal.II [2]. Moreover, we have illustrated the performance of the method by means of two numerical tests. We have shown that iterative methods such as the CG method can be used to solve the arising linear systems of equations and analysed the performance of the linear iterative solvers with respect to mesh refinement and different anisotropies.

The method can be applied to simulate the Stokes or Navier-Stokes equations with equal-order elements and pressure stabilisations. The only difficulty lies in the treatment of the anisotropic cells within the stabilisation terms. A solution for the Continuous Interior Penalty (CIP) stabilisation has been proposed by [18], [19].

In order to obtain higher-order accuracy, the interface has to be resolved with higher order. This can be achieved by using maps $\tilde{T}_p$ of higher polynomial degrees. We would like to remark, however, that this might lead to additional difficulties concerning the degeneration of the sub-elements within the patches. A promising alternative is the use of so-called “boundary value correction” techniques at the interface, see [13].

Moreover, the locally modified FEM method has a natural extension to three space dimensions. The mathematical, numerical, and algorithmic requirements are currently ongoing work. Another desirable feature is the parallelisation of the approach. Here, we do not assume major difficulties since the programming structure is similar to step-42 of the deal.II tutorial programs. As all the additions compared to a standard deal.II code are local on the patch level, this should in principle be possible without further difficulties.

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