Nonconformal Finite Element methods applied to the real time design of digital twins of organs

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To solve partial differential equations, among the broad class of methods, the **finite element method** is one of the most commonly used. However, this method faces important limitations when considering **complex geometries**, such as organs, since its use relies on the construction of conforming meshes. To bypass this difficulty, several nonconformal methods have been introduced. In this thesis, we mainly focus on the φ-FEM approach, proposed in [8, 2, 1, 3]. This **unfitted method** relies on the idea of immersing a domain Ω in a Cartesian grid, where Ω and its boundary Γ are defined by a **level-set** function φ such that

$$\Omega = \{\varphi < 0\}, \quad \text{and} \quad \Gamma = \{\varphi = 0\},$$

as represented in Fig. 1 (left). This has the benefit of avoiding the generation of complex meshes in opposition to the classical conforming finite element method (as illustrated in Fig. 1, right). The level-set function is then used to impose the boundary conditions, directly in the variational formulation. Indeed, we use the φ-FEM paradigm, which consists of seeking a new unknown w such that $\varphi w = u$ with u satisfying the considered equation.

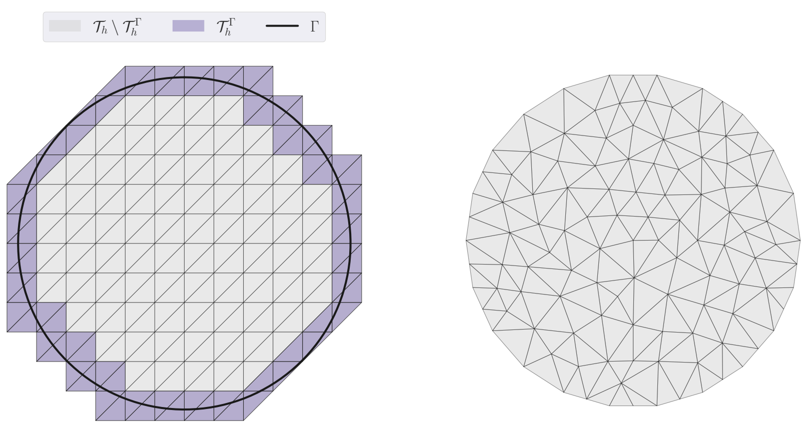

Figure 1: Left: Representation of the considered situation for φ-FEM. Right: example of conforming mesh.

The first chapter of the manuscript is devoted to the introduction, where we expose the scientific context of the thesis, exploring the existing methods in the literature. This review of the literature allows us to justify the choice of the φ-FEM as the main based approach of this work. Then, we introduce more precisely two important aspects of the φ-FEM method that have already been proposed in [8, 2]: a first scheme to solve the Poisson-Dirichlet equation, and a scheme to solve the Poisson-Neumann equation, that are a first approximation of the elastic equations.

The second chapter of the manuscript is devoted to the presentation of multiple φ-FEM schemes to solve different equations. We first present a new φ-FEM formulation to solve the Poisson-Dirichlet equation using a **penalized formulation** [9], that has the advantage of using the φ-FEM paradigm $u = \varphi w$ only in a small number of cells of the mesh (the purple cells in Fig. 1). In this section, we propose a complete theoretical and numerical study of the method to illustrate its convergence and numerical cost on complex geometries, such as illustrated in Fig. 2. The method is coherent, well conditioned, and achieves optimal convergence. This scheme is then combined along with the φ-FEM techniques for the Poisson-Neumann equation, to construct a new scheme capable of solving the mixed Dirichlet/Neumann Poisson equation, for which we propose a numerical study on test cases, varying according to the position of the changes in boundary condition singularities.

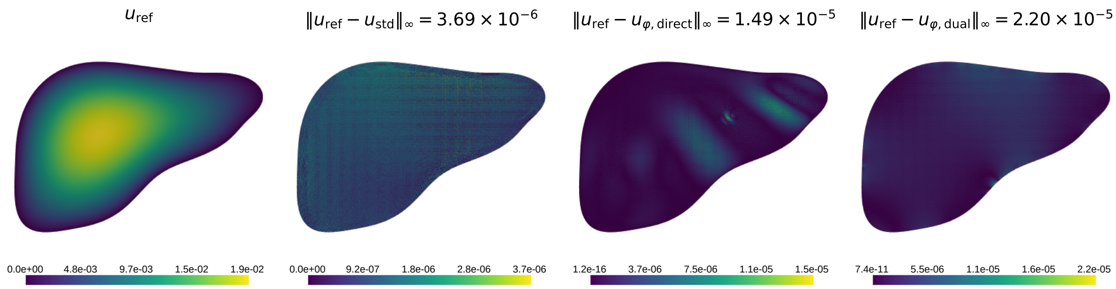

Figure 2: Left: reference solution. Then, from left to right: difference between reference solution and the projection of a classical FEM solution, the classical φ-FEM solution, and the penalized φ-FEM solution.

In a second part, we extend the method to the case of the resolution of the **heat equation** with Dirichlet boundary conditions. The method, proposed in [6], is studied theoretically and numerically, highlighting a theoretical sub-optimal convergence, $\mathcal{O}(h^{k+1/2})$ in $l^\infty(L^2)$ norm, whereas the optimal $\mathcal{O}(h^{k+1})$ convergence is reached in practice.

The last two parts of the chapter propose extensions to the cases of **linear and non-linear elastic problems**, in which we detail several φ-FEM schemes to deal with various situations such as the deformation of a material or the case of interfaces between two materials, for the linear case, or the deflection of a beam for the non-linear case. All these schemes are studied numerically to illustrate their performance compared to a classic conforming finite element method.

In the third chapter of the manuscript, we propose an adaptation of the φ-FEM paradigm to the case of the **finite difference method**, which is faster and easier to implement numerically. We present theoretical and numerical studies of a φ-FD scheme [4] based on the penalized version of φ-FEM, to solve the Poisson-Dirichlet equation, highlighting the advantages and drawbacks of using finite differences against finite elements.

The fourth chapter of the manuscript focuses on combinations between finite element methods and **neural networks**. In particular, we propose a combination between φ-FEM and the Fourier Neural Operator [10], to bypass the issues of the FNO to handle the cases of complex geometries. To do so, since we consider the φ-FEM approach, we encode the geometry using the level-set function φ and use this function as an input to an operator along with the functions defining the problem to solve. The method has been proposed in [5], and applied for example to the case of the deformation of a rectangular plate with variable holes, as depicted in Fig. 3.

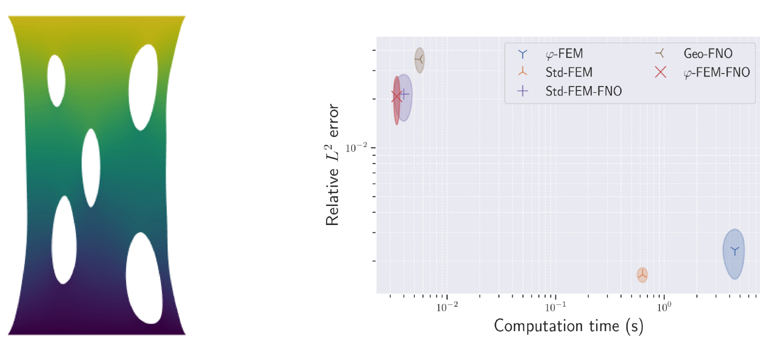

Figure 3: Left: example of deformation. Right: L^2 relative errors with respect to CPU time (s).

The last chapter is divided into three parts. In the first part, we detail numerical aspects of using level-set functions in practice. We first propose a robust way to create precise conforming meshes starting from level-set functions and then propose a starting point to construct level-set functions satisfying the regularity constraints of the φ-FEM method, relying on the optimization of the parameters of Gaussian functions multiplied together to obtain a smooth φ.

The last parts of the chapter consist of presenting two extensions of the φ-FEM method using the **multigrid approach** to reduce the computational cost of the method. In the first part, we only consider the use of φ-FEM, presenting the idea that relies on two main steps: first a coarse step, for which we consider a coarse mesh and apply φ-FEM and then a fine step, where we refine the computational mesh of the coarse step and use an interpolation of the coarse solution as an initial guess for an iterative solve. In the second part, we propose a hybrid method using φ-FEM-FNO for the coarse step. These two methods [7] are studied numerically with **2D and 3D test cases**, highlighting their impacts on the gain both in accuracy and in CPU time.

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