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LocModFE: Locally modified finite elements for approximating interface problems in deal.II

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ABSTRACT

We describe the Software package *LocModFE*, which is an implementation of a locally modified finite element method for an accurate solution of interface problems. The code was originally developed in the finite element library Gascoigne 3d and has now been rewritten in the widespread library deal.II. This makes the concept of locally modified finite elements accessible to many users all over the world. Applications range from simple Poisson interface problems over multi-phase flows to complex multi-physics problems, such as fluid–structure interactions. Being based on deal.II, it provides plenty of possibilities for future extensions, e.g., parallel computing, multigrid solvers or mesh adaptivity.

Code metadata

Current code version	v1
Permanent link to code/repository used for this code version	https://github.com/SoftwareImpacts/SIMPAC-2021-21
Permanent link to Reproducible Capsule	https://codeocean.com/capsule/6484880/tree/v1
Legal Code License	GNU LGPL v2.1
Code versioning system used	Git
Software code languages, tools, and services used	C++, deal.II, cmake, gcc
Compilation requirements, operating environments & dependencies	Installation of deal.II (version 8.5.0)
If available Link to developer documentation/manual	https://zenodo.org/record/1457758#.XCYAIp9IkWN
Support email for questions	stefan.frei@uni-konstanz.de

1. Introduction

Interface problems are ubiquitous in nature, science and engineering. Examples range from simple diffusion or wave problems with discontinuous coefficients to fluid–structure interactions or multi-phase flow. These problems have in common that their solution is continuous across an interior interface, its gradient is however discontinuous. An accurate finite element discretisation of such problems must resolve the position of the interface at all times. A simple *fitted* finite element approach that fulfils this requirement is the *locally modified finite element method* introduced in [1].

The method has first been developed in the context of fluid–structure interactions [2,3] and implemented in the finite element library Gascoigne 3d [4], which has a focus on fluid and solid dynamics. Later, the implementation has been ported to the widespread finite element library deal.II [5,6] which covers a large number of numerical discretisations, solvers and interfaces to further software libraries. The realisation in the Software package *LocModFE* is the subject of the present article. Both libraries, Gascoigne 3d and deal.II are written in C++ and in particular deal.II is supported by a large and worldwide community. The mathematical details, including a complete mathematical analysis of the method have been published in [1–3]. The software itself and a brief documentation is available on zenodo [7]. A detailed description of the implementation and functionalities is given in the arXiv documentation [8].

The code (and data) in this article has been certified as Reproducible by Code Ocean: (https://codeocean.com/). More information on the Reproducibility Badge Initiative is available at https://www.elsevier.com/physical-sciences-and-engineering/computer-science/journals.

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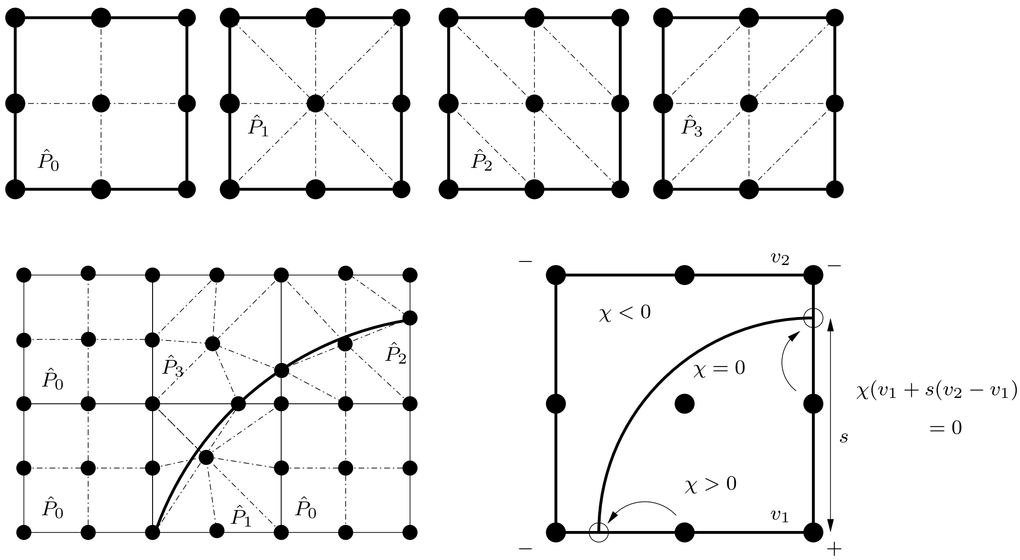

Fig. 1. Visualisation of the *locally modified finite element method*. *Top row:* Four different reference coarse cells (*patches*). *Lower left:* Sample mesh with patches corresponding to all four variants. *Lower right:* Identification of the cut points by means of the level set function χ.

2. Software description and purpose

LocModFE solves interface problems in two space dimensions within the finite element library `deal.II`. The method is based on a fixed *unfitted* coarse mesh consisting of quadrilaterals, which is independent of the position of the interface. Inside the coarse cells we refine once by dividing each coarse cell either into eight triangles or four quadrilaterals. This is done in such a way that the interface is locally resolved in at least a linear approximation, see Fig. 1. Due to the fixed coarse grid, the approach is particularly suitable for problems involving moving interfaces.

The implementation is based on a user-defined level-set function χ, which specifies the position of the interface Γ. To be precise, the interface Γ is defined implicitly as the zero-level set of χ ($\chi = 0$), see the bottom right of Fig. 1.

Among others, *LocModFE* provides the following features and functionalities:

- Given a level-set function χ, *LocModFE* moves interior vertices of a finite element mesh to the interface and constructs the necessary topology and geometry information, which is needed to implement a variational finite element formulation. Different equations or parameters can then be set on each side of the interface.
- *LocModFE* provides shape functions and their derivatives, as well as the reference maps $\xi_P : \hat{P} \to P$ from a suitably chosen reference patch $\hat{P} \in \{\hat{P}_0, \dots, \hat{P}_3\}$ (see Fig. 1), for the implementation of finite element formulations in deal.II.
- Accurate Gauss quadrature formulas for integration on the sub-elements are constructed.
- A hierarchical finite element basis can be used to improve the condition number of the system in case of anisotropic cuts.
- Different linear solvers, such as preconditioned conjugate gradients (CG) methods are available within *deal.II* and can be immediately applied to solve the arising linear systems of equations.
- *LocModFE* provides further tools to evaluate norms on the sub-elements, to impose Dirichlet boundary conditions on the modified vertices and to write a *.vtk output for visualisation.

A detailed description of the features and their implementation are given in Section 7 of [8]. A visualisation of a simple Poisson interface problem, which is the first test problem that comes with *LocModFE*, is shown in Fig. 2. For a computational convergence analysis and a comparison between different available solvers in deal.II we refer to [8] (Figure 9 and Table 1, resp.), which confirms the original numerical analysis in [1].

3. Impact

As indicated in the introduction, interface problems are a major research field in applied mathematics, science and engineering. Problems of this kind arise for example for diffusion or wave problems with discontinuous coefficients, in fluid–structure interactions, multiphase flows, multicomponent structures, fracture mechanics, porous media applications and in many other configurations where multiple physical phenomena interact. For recent summaries of such applications, we refer to our own compilations [2,14] including the many references cited therein. A gallery of some application is given in Fig. 3. A further field of application for the *locally modified finite element method* are problems with moving or free boundaries formulated in Eulerian coordinates, such as cancer growth [15], lubricant film dynamics [16] or combustion problems [17].

The method presented in this paper has already been proven to work successfully

- in studies shown by the authors in [1–3,9–11,13,18–22].
- by other research groups [23–27].

Moreover, the methodology has already been applied in complex applications:

- Fluid–structure interactions, including benchmarks [3,13], and FSI with solid contact [11,20,21,27]
- Biomedical applications, such as the simulation of plaque growth [9]
- Topology optimisation and multicomponent structures [24,25].

Moreover, we have used the package successfully within our own education

- within the Bachelor theses [28,29] at the Universities of Heidelberg and Hannover
- in the FEM-C++ finite element course at the Leibniz University Hannover (organised by T. Wick, https://www.ifam.uni-hannover.de/de/wick/lehre/)

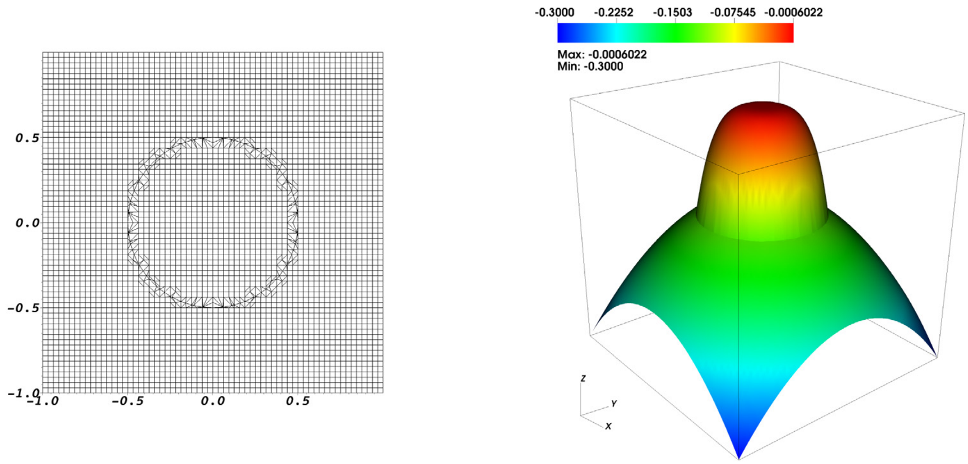

Fig. 2. Results of the first test problem: The cut-mesh (left) and a 3D surface plot of the solution of a Poisson interface problem (right).

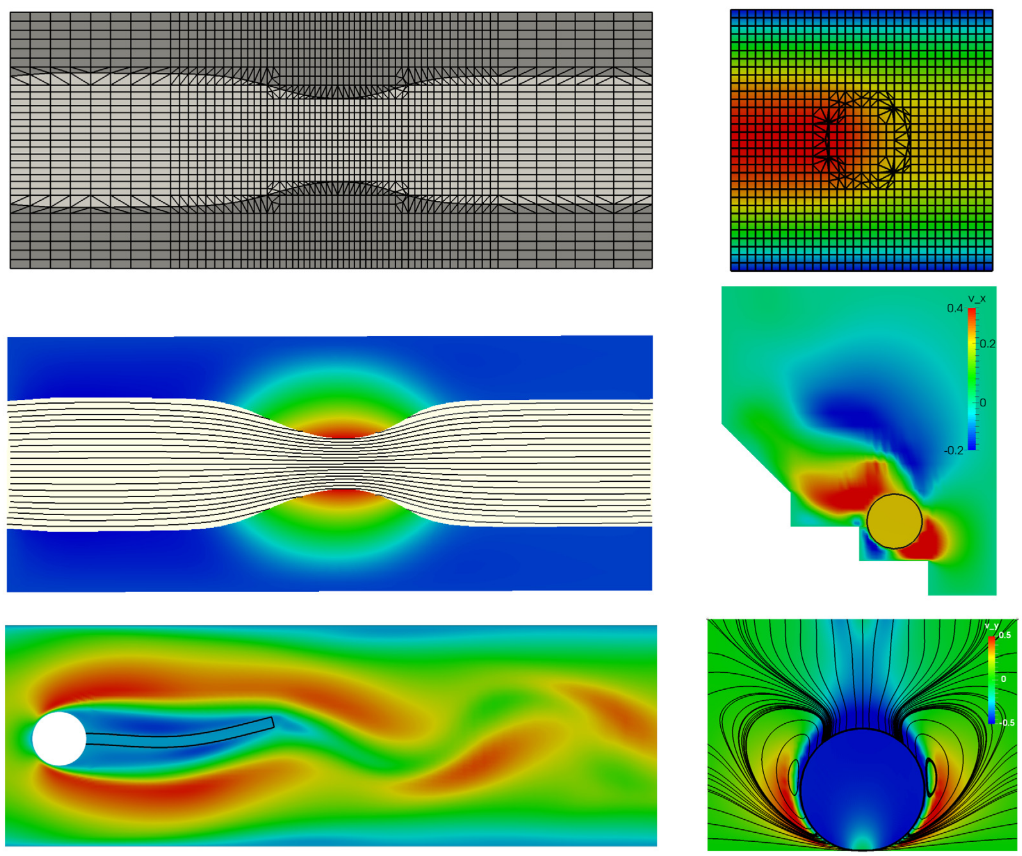

Fig. 3. Gallery of some results obtained with the locally modified finite element method. *Top left and center left:* Modified finite element discretisation for plaque growth [9]. *Top right:* Solid ball transported by a fluid flow [10]. *Center right:* Ball bouncing down some stairs [11]. *Bottom left:* FSI3 benchmark [11,12]. *Bottom right:* FSI-contact problem [11,13].

We note that most of these publications are based on the original implementation in Gascoigne 3d, which was written in 2013 and led to the first publication [1] in 2014. The implementation *LocModFE* in deal.II is in large parts identical or very similar to the prior, and appeared first in 2018, see [8]. The first publications with results obtained in *LocModFE* are [27] and [29].

Current research with *LocModFE* focuses on the extension to higher-order discretisation [22], including a second-order representation of the interface, as well as inf–sup stable finite element approaches for interface problems in fluid dynamics.

The implementation of the *locally modified finite element method* in the widespread open source finite element library `deal.II` enables users all over the world to use this approach. Moreover, numerous tools at hand in deal.II such as parallel computing with MPI, local mesh adaptivity, pre-implemented linear iterative solvers up to multigrid can be employed with relatively small effort. To the knowledge of the authors this is the first publicly available source code for interface problems based on `deal.II`.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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