MoFEM: An open source, parallel finite element library

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Introduction

`MoFEM` (Mesh-Oriented Finite Element Method) is a C++ library for managing complexities related to the finite element method which is a popular numerical approach for solving partial differential equations (PDEs) arising in various physical problems and engineering applications. `MoFEM` is developed to provide free and open source finite element codes, incorporating modern approximation approaches and data structures, for engineers, students and academics.

The need for solutions to increasingly complex problems demands the control over numerical errors; otherwise, we will be unable to distinguish discretisation artefacts from the real physical phenomena. A brute force approach based on a pure *h-adaptivity*, which relies on the power of parallel computing, leads to a low polynomial convergence rate. Therefore, it is insufficient to have total control over numerical errors. A more sophisticated approach was paved by Ivo Babuska et al. (Babuška and Guo 1992), who showed that if one could increase at the same time the polynomial order and the mesh density, i.e. employ *hp-adaptivity*, the exponential convergence is achievable. This has been seen as the 'Holy Grail' of the finite element method.

However, raising the order of approximation comes with a cost where the algebraic solver time and the matrix assembly time are increased. Unfortunately, there is no universal solution to tackle these two difficulties simultaneously. To reduce the algebraic solver time, one way is to use multi-grid solvers, which can work more efficiently if a hierarchical approximation base is available (Ainsworth and Coyle 2003),(Fuentes et al. 2015). This approach is ideal for elliptic problems such as solid elasticity. However, for hyperbolic problems, e.g. acoustic wave propagation, the efficiency bottleneck could be in the time of the matrix assembly. For that case heterogeneous approximation bases, e.g. Bernstein-Bézier base (Ainsworth, Andriamaro, and Davydov 2011), allowing for a fast numerical integration, could be an optimal solution.

The control of numerical errors is possible if we can estimate the error to

drive the *hp-adaptivity* algorithm. This error estimator needs to be as much efficient as possible, and one possible solution is to use mixed finite element formulations, where error estimators become a part of the formulation, see e.g. (Carstensen 1997). However, the stability of such elements is an issue, which can be addressed by the appropriate use of a combination of H^1, **H-curl**, **H-div** and L^2 spaces. Mixed formulations have other advantages including reduced regularity of approximation, or the resulting sparse system of equations, that can be exploited by problem-tailored solution algorithms. In Fig. 1 we show a convergence study for the mixed formulation for a transport/heat conduction problem.

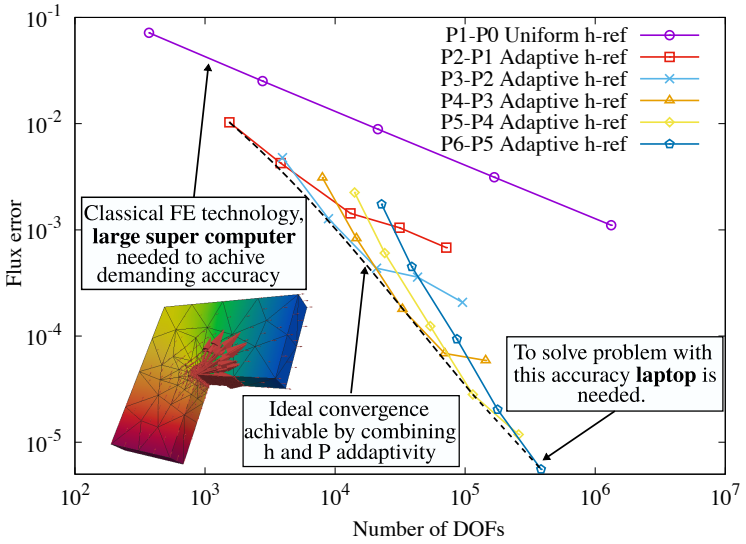

Figure 1: A convergence study of h-adaptivity for the mixed formulation of the stationary transport/heat conduction problem (see inset of the figure for the geometry), with the comparison of different polynomial orders, denoted as 'Pn-Pm', where n is order of approximation for the flux and m is the order for the field values (temperature or density). Note that the flux is approximated by the space **H-div**, while the field values – by the space L^2, see corresponding MoFEM tutorial page for more details.

`MoFEM` is designed to provide all discussed above solutions for *hp-adaptivity*, enabling rapid implementation of the finite element method for solving complex multi-domain, multi-scale and multi-physics engineering problems. Moreover, it releases users from programming complexities related to the bookkeeping of degrees of freedom (DOFs), finite elements, matrix assembly, etc.

Design

Modern finite element software is an 'ecosystem' managing various complexities related to mesh and topology, sparse algebra and approximation, integration and dense tensor algebra at the integration point level. `MoFEM` has not developed and will not develop all these capabilities from scratch. Instead, `MoFEM` integrates advanced scientific computing tools for sparse algebra from PETSc (Portable, Extensible Toolkit for Scientific Computation) (Balay et al. 2015), components for handling mesh and topology from MOAB (Mesh-Oriented Database) (Tautges et al. 2004) and data structures from Boost libraries ("Boost Web Page" 2019). An illustration of how these packages are utilised in `MoFEM` is shown in Fig. 2. Finally, `MoFEM` core library is developed to manage complexities directly related to the finite element method. Therefore, each part of this ecosystem has its own design objectives and appropriate programming tools from a spectrum of solutions can be selected. Resilience of `MoFEM` ecosystem is ensured since the underpinning components have sustainable fundings, dynamic and established groups of developers and significant user base. Fig. 3 shows different components that are employed in the ecosystem including popular pre- and post processing software.

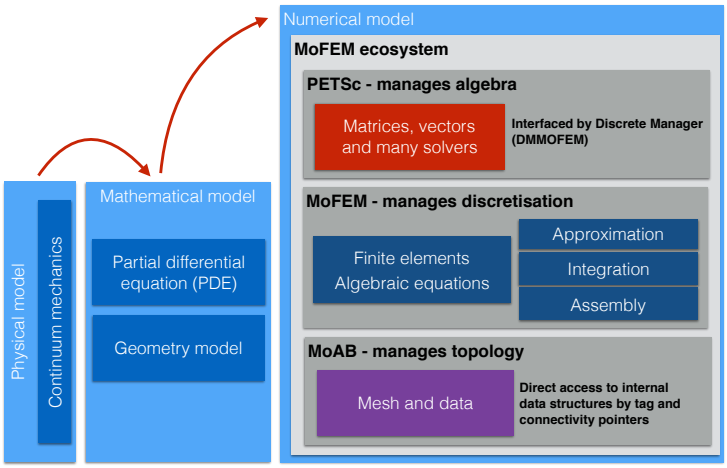

Figure 2: Basic design of `MoFEM` (Adopted from `MoFEM` webpage ("MoFEM Web Page" 2019)).

Traditional finite element codes are element-centric meaning the type of an element defines the approximation space and base. Therefore, they are not able to fully exploit the potential of emerging approximation methods. On the contrary, the design of data structures for approximation of field variables in

MoFEM is independent of the specific finite element, e.g. Lagrangian, Nedelec, Rivart-Thomas, since finite element is constructed by a set of lower dimension entities on which the approximation fields are defined. Consequently, different approximation spaces (H^1, **H-curl**, **H-div**, L^2) can be arbitrarily mixed in a finite element to create new capabilities for solving complex problems efficiently.

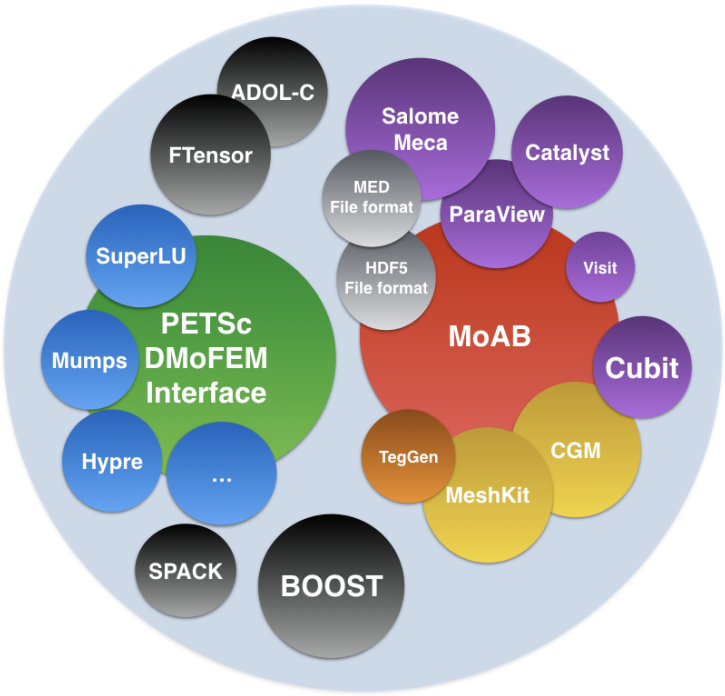

Figure 3: 'Ecosystem' of MoFEM (Adopted from MoFEM webpage ("MoFEM Web Page" 2019)).

MoFEM data structures enable easy enrichment of approximation fields and modification of base functions, for example, in case of resolving singularity at the crack front. Applying this technology, it is effortless to construct transition elements between domains with different problem formulation and physics, e.g. from two-field mixed formulation to single-field formulation, or elements with anisotropic approximation order, e.g. with arbitrary high order on surface and arbitrary low order through thickness of solid shells). This approach also sets the benchmark in terms of how finite element codes are implemented, introducing a concept of user-defined data operators acting on fields that are associated with entities (vertices, edges, faces and volumes) rather on the finite element directly. Such an approach simplifies code writing, testing and validation, making the code resilient to bugs.

Furthermore, MoFEM core library provides functionality for developing user mod-

ules where applications for particular problems can be implemented. This toolkit-like structure allows for independent development of modules with different repositories, owners and licences, being suitable for both open-access academic research and private industrial sensitive projects.

`MoFEM` is licensed under the [GNU Lesser General Public License] (https://www.gnu.org/licenses/lgpl.html), can be deployed and developed using the package manager Spack, see MoFEM installation instructions for more details.

Examples

`MoFEM` was initially created with the financial support of the Royal Academy of Engineering and EDF Energy to solve the problem of crack propagation in the nuclear graphite (Kaczmarczyk, Nezhad, and Pearce 2014),(Kaczmarczyk, Ullah, and Pearce 2017). Over time, the domain of applications expanded to include computational homogenisation (DURACOMP EPSRC Project EP/K026925/1), (Ullah et al. 2019, @zhou2017stochastic),(Ullah et al. 2017) bone remodelling and fracture (Kelvin Smith Scholarship), modelling of the gel rheology and acoustics problems. Moreover, `MoFEM` includes an extensive library of example applications such as soap film, solid shell, topology optimisation, phase field fracture, Navier-Stokes flow, cell traction microscopy, bone remodelling, configurational fracture, plasticity, mortar contact, magnetostatics and acoustic wave propagation as shown in Fig. 4.

Acknowledgements

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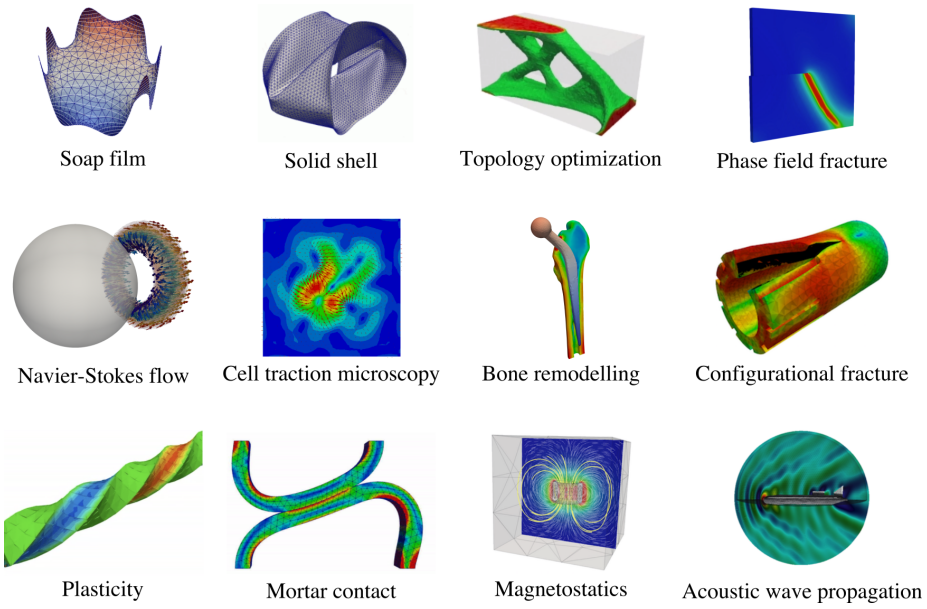

Figure 4: Examples of user modules implemented using `MoFEM`.

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