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 (FEM). FEM is a widely used 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. It was primarily designed to solve crack propagation in nuclear graphite bricks (radiated and oxidised) used in Advanced Gas-cooled reactors (see Fig. 1).

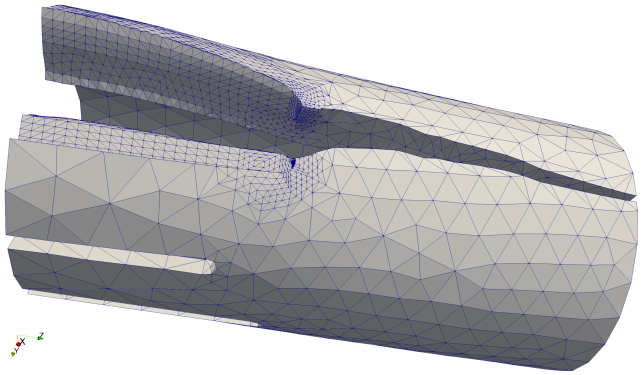

Figure 1: Fracture model of a nuclear graphite brick.

Motivation

The need for solutions to increasingly complex problems demands 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* leads to a low polynomial convergence rate and relies on the machines computing power. Since we want to solve bigger and more complex problems, no matter how big computer we will have, it will be never enough. 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 numerical methods.

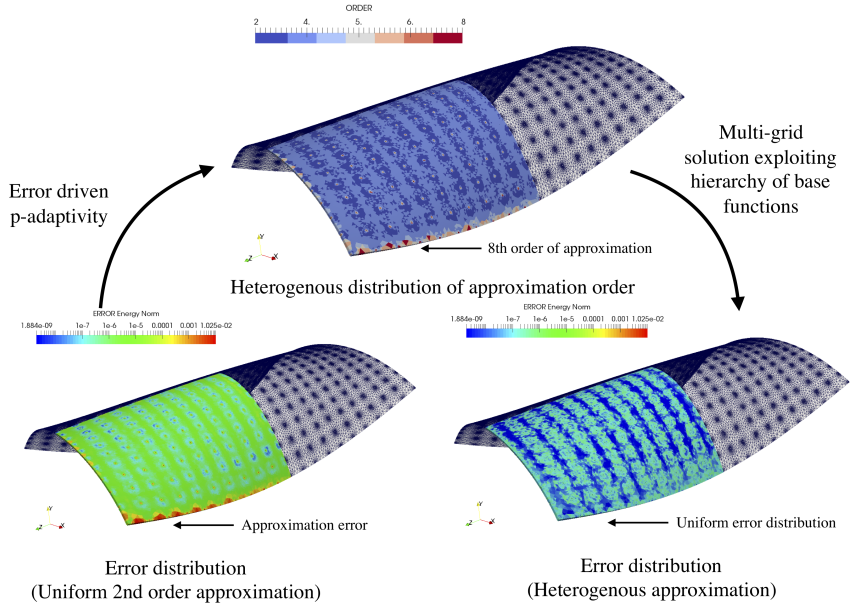

Figure 2: Example of *p-adaptivity* for hierarchical and heterogenous approximation with multi-grid solver applied for solid-shell element.

However, raising the order of approximation comes with a cost; the algebraic solver time and the matrix assembly time are increased. Those two issues can be tackled independently. Use of multi-grid solvers can reduce algebraic solver time exploiting a hierarchical approximation base (Ainsworth and Coyle 2003)(Fuentes et al. 2015), available in `MoFEM`. This approach is ideal for elliptic problems such as solid elasticity, or hyperbolic equations with block solvers. However, for some problems the efficiency bottleneck is assembly time, e.g. acoustic wave

propagation. For that case, different approximation bases, e.g. Bernstein-Bézier base (Ainsworth, Andriamaro, and Davydov 2011), allowing for fast numerical integration, could be an optimal solution. MoFEM is designed to provide tools that users can tackle such efficiency tradeoff and choose the optimal solution for a given problem. Fig. 2 shows *p-adaptivity* on hierarchical approximation base, with multi-grid solver applied to Scordelis-Lo perforated roof problem (Kaczmarczyk, Ullah, and Pearce 2016).

The adaptive choice of mesh density and approximation order is driven by the numerical errors. In principle, the numerical error is unknown since we do not know an exact solution. However, a numerical error can be estimated, and an efficient way of that is by embedding error evaluators in FE formulation. This leads to a family of the mixed or mixed-hybrid finite elements that satisfy stability condition using spaces such as H^1, **H-curl**, **H-div** and L^2. MoFEM provides a convenient application programming interface allowing user freely to choose approximation base, e.g. Legrende, Jacobi, independently from approximation space, and type and dimension of the field, e.g. field of symmetric second-order tensors. One can approximate scalar, vectorial fields on scalar base functions, or vectorial and tensorial fields on vectorial bases. The user of MoFEM can freely set approximation order on each entity separately, e.g. edge, face, volume, or define field on the skeleton. Also, MoFEM enables users to construct tensorial field on tensorial bases, e.g. bubble base of zero normal and divergence free base functions, see example of such space in (Gopalakrishnan and Guzmán 2012). The example of five-field mixed formulation (with tensorial bubble base) for large strain elasticity is presented in (Kaczmarczyk, Chalons-Mouriesse, and Pearce 2019), and results are presented in Fig. 3, where MoFEM code declaring spaces is as follows

```
auto add_hdiv_field = [&](
    const std::string field_name, const int order,
                            const int dim) {
 MoFEMFunctionBegin;
 CHKERR mField.add_field(
   field_name, HDIV, AINSWORTH_LEGENDRE_BASE, dim);
 CHKERR mField.add_ents_to_field_by_type(
   meshset, MBTET, field_name);
 CHKERR mField.set_field_order(meshset, MBTET, field_name, order);
 CHKERR mField.set_field_order(meshset, MBTRI, field_name, order);
 MoFEMFunctionReturn(0);
};

auto add_l2_field = [&](
   const std::string field_name, const int order, const int dim) {
 MoFEMFunctionBegin;
 CHKERR mField.add_field(
   field_name, L2, AINSWORTH_LEGENDRE_BASE, dim);
 CHKERR mField.add_ents_to_field_by_type(
```

```
  meshset, MBTET, field_name);
 CHKERR mField.set_field_order(meshset, MBTET, field_name, order);
 MoFEMFunctionReturn(0);
};

// Arguments are field name, field approx. order, and field rank

// Tonsorial field on vectorial base in H-div
CHKERR add_hdiv_field(piolaStress, spaceOrder, 3);
// Tonsorial field on tonsorial base
CHKERR add_bubble_field(bubbleField, spaceOrder + 1, 1);
// Field of symmetric tensor on scalar L2 base
CHKERR add_l2_field(streachTensor, spaceOrder + 1, 6);
// Vectorial fields on scalar L2 base
CHKERR add_l2_field(spatialDisp, spaceOrder - 1, 3);
CHKERR add_l2_field(rotAxis, spaceOrder, 3);
```

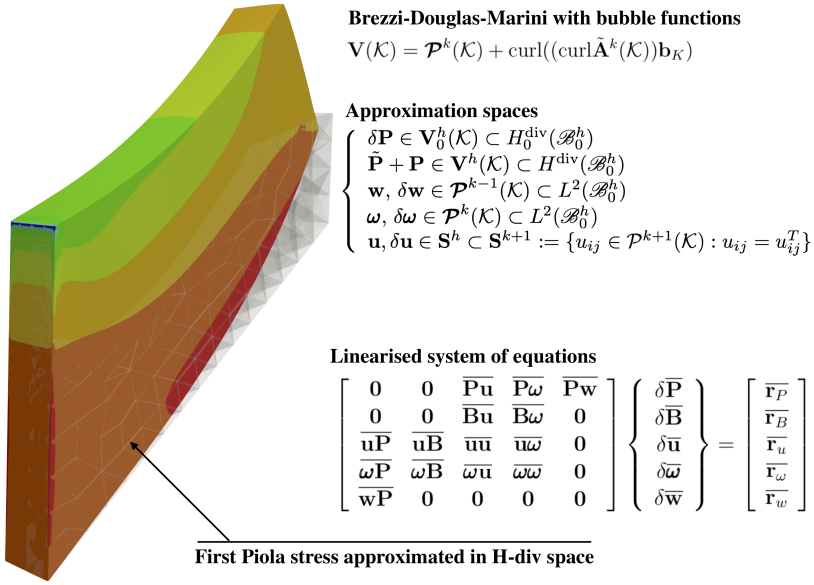

Figure 3: Mixed formulation on five fields for large strain elasticity.

MoFEM is designed to provide all discussed above solutions for *hp-adaptivity*, enabling rapid implementation of the finite element method for solving complex multi-dimension, e.g. solid, shell and beam elements, multi-domain, e.g. one part is solid and another part is fluid, multi-scale, e.g. computer homogenisation with FE^2, and multi-physics, e.g. thermo-elasticity, engineering problems on mixed meshes, e.g. meshes consist of prism and tetrahedron elements. 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. 4. 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. 5 shows different components that are employed in the ecosystem including popular pre- and post-processing software.

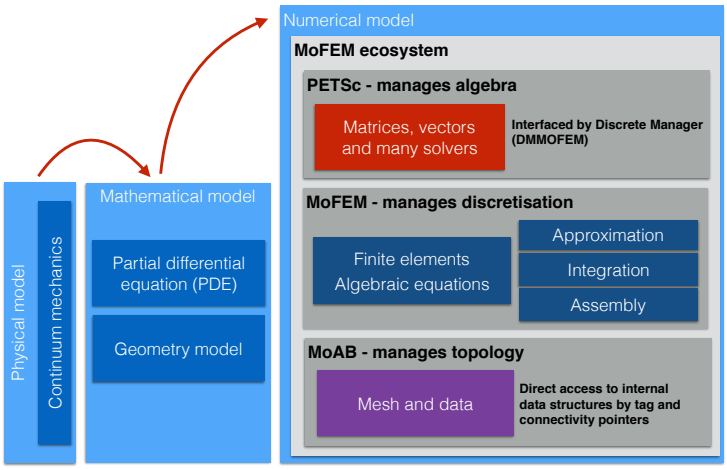

Figure 4: Basic design of `MoFEM`. Adopted from `MoFEM` webpage ("MoFEM Web Page" 2019)).

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.

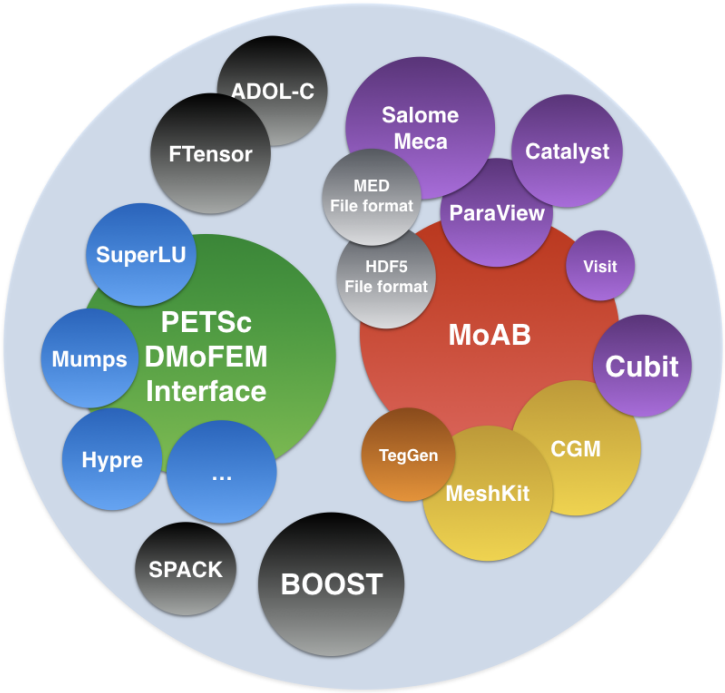

Figure 5: 'Ecosystem' of `MoFEM`. Adopted from `MoFEM` webpage ("MoFEM Web Page" 2019).

`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 modules 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 and 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, 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) 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. 6.

Acknowledgements

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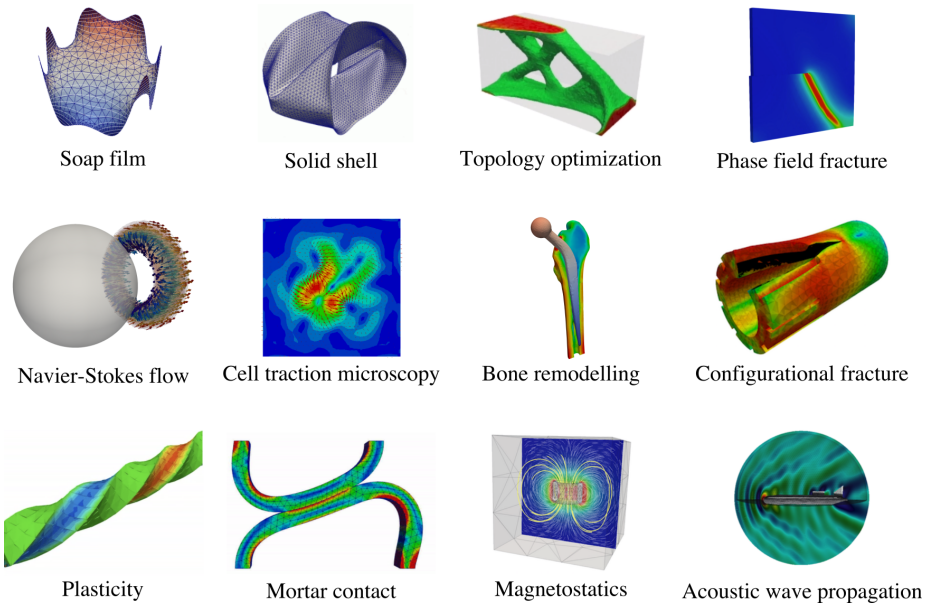

Figure 6: Examples of user modules implemented using `MoFEM`.

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