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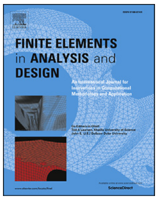

An object-oriented framework for multiphysics problems combining different approximation spaces

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ABSTRACT

An object-oriented framework is developed to implement discrete models in a monolithic solution of coupled systems of partial differential equations by combining different kinds of finite element approximation spaces chosen for each field. In this sense, we aim at contributing to applications of what is currently classified as “multiphysics simulation”, by composing numerical techniques where each physical phenomenon or scale component is approximated by its most appropriate numerical scheme. The integration of the methods is discussed, in a systematic and generic manner, based on an existing object oriented finite element computational framework, allowing any of the usual kinds of affine and/or curved element geometry (point, segment, triangle, quadrilateral, tetrahedral, hexahedral, prismatic or pyramidal). They can be used in several finite element formulations that require continuous, discontinuous, **H**(div)-conforming functions, or interactions with lower dimensional approximations, which typically occurs in hybrid methods or reduced models. Furthermore, to improve accuracy and/or efficiency, when necessary and/or allowed by the adopted mathematical formulation, different levels of mesh refinements can be adopted for each field, with different refinement configurations (h, p, hp, and directional refinements), as long as the meshes are nested. The generality and flexibility of the proposed framework is verified against a particular set of two dimensional test problems modeled by different formulations - Darcy’s problem coupled with tracer transport, fluid flow coupled with geomechanical interaction, multiscale hybrid formulation for linear elasticity, and a hybrid mixed formulation for discrete fracture networks. The main implementation ideas can also be applied to three dimensional problems, as well as to other kinds of approximation space combinations.

1. Introduction

Numerical simulations have been extensively explored during the last half century and they are now generally accepted as an essential tool in the understanding of physical phenomena. Furthermore, motivated by the persistent growth of computational capacity and greater aspirations in Science and Engineering, new challenges that require innovative techniques have been common. For instance, the treatment of complex problems, which are characterized by the interaction between sub-systems that differ in nature of associated differential equations and/or by its time scale or characteristic length, have received increasing attention by the scientific community. An approach that tries to simulate such models in a single framework often leads to very stringent restraints in terms of spatial and temporal resolution, and consequently, to high computational costs. Moreover, these approaches can cause problems of poor numerical conditioning, and therefore, affect the convergence of the scheme. Similar issues occur when approximating multiscale problems, as it is generally impossible to treat the different scales in a unique framework at the same time.

These facts motivate the development and applications of what is currently named as “multiphysics simulation”, by composing numerical techniques, with each physical phenomenon or scale component being approximated by its most appropriate numerical scheme in a coherent framework, as described in Ref. [1], where different contexts of interest are emphasized. Some recent papers concerning the design, implementation and application of object-orientation in finite element analysis

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for multiphysics problems have been published in Refs. [2–9].

The purpose of this article is to describe how the combination of different space configurations, given by finite element approximation to represent state variables of different nature, can be implemented simultaneously. The object-oriented approach results in a general purpose framework in which arbitrary types/number of approximation spaces can be combined to obtain highly efficient approximations. The developments have been incorporated from an existing standard computational framework based on Finite Element (FE) method (called NeoPZ [10]), creating a new class structure [11], but we expect that they can be useful to update other FE codes with similar organization of class structure.

As it can be applied to multiple-coupled physical situations, the new implemented capabilities are referred as being of multiphysics character. For code verification purposes, the following two-dimensional coupled problems are solved, and the results are analyzed in terms of expected accuracy orders:

- A single phase tracer transport is considered in porous media where the fluid has two components, whose motions are accounted by different flow models, namely, tracer advection and Darcy's flow. The purpose of this implementation is to illustrate the combination of three approximation spaces types in two-dimensional cases: discontinuous approximations in a context of finite volume for the advection equation, a mixed finite element formulation for Darcy's problem to obtain fluid velocity, and pressure in the porous media by using space approximations in $\mathbf{H}(\mathrm{div})$ and L^2, respectively. This example is also included to show that, when enabled by the variational formulation of the problem, and required to improve accuracy and/or efficiency, different mesh refinements can be adopted for the involved variables to promote space configuration from multiphysics approximation (see Section 4.1).
- In a poroelastic problem, the fluid flow through a porous medium, and the deformation of the solid matrix are coupled [12]. A test case with the exact solution is chosen, as presented in Ref. [13], to verify three approximation spaces combined in the same implementation: in $(H^1)^2$ for the solid displacement, and in $\mathbf{H}(\mathrm{div})$ and L^2 for the fluid flux and pressure, respectively (see Section 4.2).
- A multiscale hybrid method for linear elasticity requires different approximations spaces for the involved variables: the body displacement u is piecewise defined within macro elements, where $\mathbf{H}^1$-conforming approximations are used at two different scale levels, and the Lagrange multipliers are defined on the mesh skeleton formed by the macro-element sides that require piecewise polynomial approximations, without continuity constraint [14]. Note that these approximation spaces are associated with several regions of different dimensions (see Section 4.3). The relaxed displacement continuity over the mesh skeleton allows the localization of the displacement computations, the global system to be solved being expressed only in terms of the multiplier and a coarse piecewise rigid body approximation over the macro elements.
- A discrete fracture network is composed of porous media with some fractures inside it, having different permeability patterns [15,16]. Mixed finite element formulations are applied to model the fluid flow inside both domains: the fracture domain and the porous medium (one and two dimensional environments, respectively). Hybridization is applied to combine both fluid flows, and to consider fracture intersections. Thus, the multiphysics simulation of this problem combines $\mathbf{H}(\mathrm{div})$-conforming and L^2 approximations for the fluid flux and pressure inside the two-dimensional porous medium and in the one-dimensional fracture manifold; and multipliers are piecewised defined on one and zero dimensional skeletons (see Section 4.4).

The code capabilities developed and documented for these four illustrative coupled problems consider interactions between different approximation spaces despite its unique geometric reference framework (the single phase tracer transport in porous media or the poroelastic problem), or between different geometric frameworks with matching interface meshes, as is the case of hybrids methods (e.g, discrete fracture network, and MHM for elasticity).

Section 2 is dedicated to provide a brief overview on the specific NeoPZ FE code structure, its original form, whose class structures are classified by independent modules, offering the basic functionalities for the implementation of diverse finite element schemes. For the current multiphysics version, new classes and methods needed to be introduced to guide the interaction between different approximation spaces in the simulation. Furthermore, considering there are situations in which the mesh associated with a certain state variable lies on a coarser mesh compared to other variables without causing instability, thus great advantage can be gained by combining meshes at different levels of refinement. In this direction, the described multiphysics class structure enables us to choose different mesh refinement levels for each variable when necessary and allowed by the associated formulation. This upgraded NeoPZ multiphysics version is treated in Section 3. Some details concerning the specific modules affected by the multiphysics structure are included in Appendix A.

Previously, before the incorporation of its current multiphysics capability, NeoPZ has been applied to formulations of coupled systems based on classes *ad hoc* designed for each case of combined configuration of approximation spaces, involving a unique mesh refinement for all variables, and also requiring *ad hoc* post processing tools. Currently, using the proposed data structure, numerical coupled system of equations that demand the combination of different kinds of approximation spaces can be coherently integrated in a systematic and generic manner. The implementation of a mixed formulation for the Poisson problems presented in recent articles [19–22] has been facilitated by combining two different approximation spaces: discontinuous approximations in L^2 for the potential variable, and $\mathbf{H}(\mathrm{div})$-conforming vector shape functions for flux resolution. As demonstrated in these studies, the main implementation ideas can be applied to two and three dimensional problems using a variety of element geometries for meshes, including curved elements with *hp*-adaptivity, or on manifolds.

The generality and flexibility of the multiphysic NeoPZ framework has also been demonstrated in unconventional simulations combining special purpose approximation spaces with the traditional ones. For instance, the study [17] considers a hydraulic fracture simulation, involving the interaction of a three dimensional elastic structure with the fluid flow inside the planar fracture. For structure displacement, approximation spaces spanned by elastic *snapshots* are adopted. The *snapshot* functions are computed offline as the responses to piecewise constant pressures on fracture walls forming a reduced basis approach. To model the 3D geomechanical state of stress and their effect on bi-phasic flow through 3D porous media, a reduced basis method for the geomechanical deformation in conjunction with a sequential solver (fixed-stress split) approach has also been adopted by Ref. [18]. In that approximation, over each finite element, a volumetric expansion to constant pressures is applied, providing a series of global elastic solutions. Thus, the deformation is computed as a linear combination of the precomputed global elastic responses.

It is important to mention that some commercial software have been adapted for multiphysics simulations, such as ADINA Multiphysics,[1] ANSYS Multiphysics,[2] and COMSOL Multiphysics.[3] These software packages mainly rely on the transfer of finite element/volume results between simulations. Then, these optimized solution transfers characterize coupled physics: thermal stress, electromechanical interaction, fluid structure coupling, fluid flow with heat transport and chemical reactions, electromagnetic fluids, electromagnetically induced heating,

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[1] http://www.adina.com/multiphysics.shtml.

[2] http://www.ansys.com/Products/Simulation+Technology/Multiphysics.

[3] https://br.comsol.com/comsol-multiphysics.