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A hybrid finite volume – finite element method for bulk–surface coupled problems

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ABSTRACT

The paper develops a hybrid method for solving a system of advection–diffusion equations in a bulk domain coupled to advection–diffusion equations on an embedded surface. A monotone nonlinear finite volume method for equations posed in the bulk is combined with a trace finite element method for equations posed on the surface. In our approach, the surface is not fitted by the mesh and is allowed to cut through the background mesh in an arbitrary way. Moreover, a triangulation of the surface into regular shaped elements is not required. The background mesh is an octree grid with cubic cells. As an example of an application, we consider the modeling of contaminant transport in fractured porous media. One standard model leads to a coupled system of advection–diffusion equations in a bulk (matrix) and along a surface (fracture). A series of numerical experiments with both steady and unsteady problems and different embedded geometries illustrate the numerical properties of the hybrid approach. The method demonstrates great flexibility in handling curvilinear or branching lower dimensional embedded structures.

1. Introduction

Systems of coupled bulk–surface partial differential equations arise in many engineering and natural science applications. Examples include multiphase fluid dynamics with soluble or insoluble surfactants [25], dynamics of biomembranes [7], crystal growth [29], signaling in biological networks [46], and transport of solute in fractured porous media [1]. In these and other applications, partial differential equations defined in a volume domain are coupled to another PDEs posed on a surface. The surface may be embedded in the bulk or belong to a boundary of the volume domain.

Recently, there has been a growing interest in developing methods for the numerical treatment of bulk–surface coupled PDEs. Different approaches can be distinguished depending on how the surface is recovered and equations are treated. If a tessellation of the volume into tetrahedra is available that fits the surface, then it is natural to introduce finite element spaces in the volume and on the induced triangulation of the surface. The resulting *fitted* bulk–surface finite element method was studied for the stationary bulk–surface advection–diffusion equations [18], for non-linear reaction–diffusion systems modeling biological pattern formation [36,37], for the equations of the two-phase flow with surfactants [5,4], Darcy and transport–diffusion equations in fractured porous media [1].

Unfitted finite element methods allow the surface to cut through the background tetrahedral mesh. In the class of finite element methods also known as cutFEM, Nitsche-XFEM or TraceFEM, standard background finite element spaces are em-

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ployed, while the integration is performed over cut domains and over the embedded surface [8,44]. Additional stabilization terms are often added to ensure the robustness of the method with respect to small cut elements. The advantages of the unfitted approach are the efficiency in handling implicitly defined surfaces, complex geometries, and the flexibility in dealing with evolving domains. In the context of bulk–surface coupled problems, cut finite element methods were recently applied to treat stationary bulk–surface advection–diffusion equations [24], coupled bulk–surface problems on time-dependent domains [26], coupled elasticity problems [9]. The hybrid method developed in this paper belongs to the general class of unfitted methods and resembles the TraceFEM in how the surface PDE is treated.

The methods discussed above treat surfaces and interfaces sharply, i.e. as lower-dimensional manifolds. In the present paper we also consider sharp interfaces. For the application of phase-field or other diffuse-interface approaches for coupled bulk–surface PDEs see, for example, [10,33,51].

If the finite element method is a discretization of choice for the bulk problem, then it is natural to consider a finite element method for surface PDE as well. However, depending on application, desired conservation properties, available software or personal experience, other discretizations such as finite volume or finite difference methods can be preferred for the PDE posed in the volume. One possibility to reuse the same mesh for the surface PDE is to consider a diffuse-interface approach. Alternatively, instead of smearing the interface, one may extend the PDE off the surface to a narrow band containing the surface in such a way that the restriction of the extended PDE solution back to the (sharp) surface solves the original equation on this surface. Further a conventional discretization is built for the resulting volume PDE in the narrow band [6,43]. The methods based on such extensions, however, increase the number of the active degrees of freedom for the discrete surface problem, may lead to degenerated PDE, need numerical boundary conditions and require smooth surfaces with no geometrical singularities.

The present paper develops a numerical method based on the sharp-interface representation, which uses a finite volume method to discretize the bulk PDE. Our goal is (i) to allow the surface to overlap with the background mesh in an arbitrary way, (ii) to avoid building regular surface triangulation, (iii) to avoid any extension of the surface PDE to the bulk domain. To accomplish these goals, we combine the monotone (i.e. satisfying the discrete maximum principle) finite volume method on general meshes [35,11] with the trace finite element method on octree meshes from [12]. In the octree TraceFEM one considers the bulk finite element space of piecewise trilinear globally continuous functions and further uses the restrictions (traces) of these functions to the surface. These traces are further used in a variational formulation of the surface PDE. Effectively, this results in the integration of the standard polynomial functions over the (reconstructed) surface. Only degrees of freedom from the cubic cells cut by the surface are active for the surface problem. Surface parametrization is not required, no surface mesh is built, no PDE extension off the surface is needed. We shall see that the resulting hybrid FV–FE method is very robust with respect to the position of surfaces against the background mesh and is well suited for handling non-smooth surfaces and surfaces given implicitly.

One application of interest is the numerical simulation of the contaminant transport and diffusion in fractured porous media. In this application, transport and diffusion along fractures are often modeled by PDEs posed on a set of piecewise-smooth surfaces, see, e.g., [1,22,39,52]; see also [1,2,38,20] for a similar dimension reduction approach in simulation of flow in fractured porous media. Monotone (satisfying the DMP) finite volume methods on general meshes is the appealing tool for the solution of equations for solute concentration in the porous matrix, see, e.g., [11,17,23,28,30,35,49] (further references can be found in [16,21]). However, a straightforward application of this technique to model transport and diffusion along a fracture would require fitting the mesh or triangulating the surface. For a large and complex net of fractures cutting through the porous matrix this is a difficult task [14], and an efficient method avoids mesh fitting and surface triangulations. Recently, extended finite element method approximations have been extensively studied in transport and flow problems in fractured porous media, see the review [19] and references therein. In XFEM, one also avoids fitting of the background mesh to a fracture, but a separate mesh is still required to represent the fracture. Besides the use of FV for the matrix problem, the approach in the present paper differs from those found in existing XFEM literature in the way the surface problem is discretized.

While the present technique can be applied for tetrahedral or more general polyhedral tessellations of the bulk domain, we consider octree grid with cubic cells here. This choice is not *ad hoc*. Indeed, the Cartesian structure and built-in hierarchy of octree grids makes mesh adaptation, reconstruction and data access fast and easy. For these reasons, octree meshes became a common tool in computational mechanics and several octree-based solvers are available in the open source scientific computing software, [3,45]. However, an octree grid provides at most the first order (staircase) approximation of a general geometry. Allowing the surface to cut through the octree grid in an arbitrary way overcomes this issue, but challenges us with the problem of building efficient bulk–surface discretizations. This paper demonstrates that the hybrid TraceFEM – non-linear FV method complements the advantages of using octree grids by delivering more accurate treatment of the surface PDE problem.

The remainder of the paper is organized as follows. In section 2 we recall the system of differential equations, boundary and interface conditions, which models the coupled bulk–interface (or "matrix–fracture" in the context of flows in porous media) advection–diffusion problem. Section 3 gives the details of the hybrid discretization. After laying out the main ideas behind the method, we discuss the non-linear monotone FV method for the bulk and the TraceFEM for the surface equations, and further we introduce the required coupling. Section 4 presents the results of several numerical experiments with steady analytical solutions on smooth and piecewise smooth branching surface. We also show the results of numerical simulation of the propagating front of solute concentration through fractured porous media.