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The Bulk-Surface Virtual Element Method for Reaction-Diffusion PDEs: Analysis and Applications

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Abstract. Bulk-surface partial differential equations (BS-PDEs) are prevalent in many applications such as cellular, developmental and plant biology as well as in engineering and material sciences. Novel numerical methods for BS-PDEs in three space dimensions (3D) are sparse. In this work, we present a bulk-surface virtual element method (BS-VEM) for bulk-surface reaction-diffusion systems, a form of semilinear parabolic BS-PDEs in 3D. Unlike previous studies in two space dimensions (2D), the 3D bulk is approximated with general polyhedra, whose outer faces constitute a flat polygonal approximation of the surface. For this reason, the method is restricted to the lowest order case where the geometric error is not dominant. The BS-VEM guarantees all the advantages of polyhedral methods such as easy mesh generation and fast matrix assembly on general geometries. Such advantages are much more relevant than in 2D. Despite allowing for general polyhedra, general nonlinear reaction kinetics and general surface curvature, the method only relies on nodal values without needing additional evaluations usually associated with the quadrature of general reaction kinetics. This latter is particularly costly in 3D. The BS-VEM as implemented in this study retains optimal convergence of second order in space.

AMS subject classifications: 35K57, 65M12, 65M15, 65M20, 65M50, 65M60

Key words: Bulk-surface PDEs, bulk-surface reaction-diffusion systems, polyhedral meshes, bulk-surface virtual element method, convergence.

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1 Introduction

Bulk-surface partial differential equations (BS-PDEs) arise from a wide variety of real-life problems. They describe many natural problems including, but are not limited to, the formation of spatial patterning in developmental biology [46], cell polarisation in molecular and cellular biology [18, 26, 33, 45, 50], fluid dynamics [17, 20, 44], the formation of an appressorium by the infection of the fungus *Magnaporthe grisea* causing rice blast [52], spine growth in sea urchins [43], root formation and food uptake in plant biology [5], and so on. Given the complex nature of BS-PDEs, their numerical treatment is generally not trivial, in particular in three space dimensions (3D). Hence, developing novel numerical methods and constructing stable and accurate algorithms to approximate their numerical solutions becomes crucially important, given their rapid applications to areas such as biomedical engineering, fluid dynamics, materials science, biology, cancer biology, image processing, astrophysics and battery modeling, to mention just a few examples.

Given $d \in \mathbb{N}$ denoting the number of space dimensions, a bulk-surface reaction-diffusion system (BS-RDS) comprises of $m \in \mathbb{N}$ reaction-diffusion equations (RDEs) posed in the *bulk* domain $\Omega \subset \mathbb{R}^d$ $(d \geq 2)$ coupled, through either linear or non-linear mixed Robin-type boundary conditions, with $n \in \mathbb{N}$ surface RDEs posed on the manifold $\Gamma := \partial\Omega$. The generalised BS-RDS takes the following form:

$$\begin{cases} \dot{u}_i - d_{u,i}\Delta u_i = q_i(u_1,\cdots,u_m), & \boldsymbol{x} \in \Omega; \\ \dot{v}_j - d_{v,j}\Delta_\Gamma v_j + \sum_{k=1}^{m} \eta_{jk} \nabla u_k \cdot \boldsymbol{\nu} = r_j(u_1,\cdots,u_m,v_1,\cdots,v_n), & \boldsymbol{x} \in \Gamma; \\ \nabla u_i \cdot \boldsymbol{\nu} = s_i(u_1,\cdots,u_m,v_1,\cdots,v_n), & \boldsymbol{x} \in \Gamma, \end{cases} \tag{1.1}$$

for $i = 1,\cdots,m$, $j = 1,\cdots,n$ and $t \in [0,T]$, where $T > 0$ is the final time. In the above, $\dot{u}_i$ and $\dot{v}_j$ denote partial time derivatives. The functions q_i, r_j, s_i are nonlinear reaction kinetics, $d_{u,i}, d_{v,j} > 0$ are the diffusion coefficients and $\eta_{jk} > 0$ are coupling coefficients fulfilling $\sum_{j=1}^{n} \eta_{jk} = d_{u,k}$ for all $k = 1,\cdots,m$, which can be interpreted as a balance law across bulk and surface, see [46]. In (1.1), Δ and Δ_Γ denote the Laplace and Laplace-Beltrami operators respectively, while $\boldsymbol{\nu} : \Gamma \to \mathbb{R}^d$ is the outward unit normal vector field on Γ (see [35] for full definitions). The model comprises several time-dependent BS-PDE models currently existing in the literature, see for example [33, 46, 51]. The BS-VEM builds substantially on the virtual element method (VEM), which in turn, is an extension of the well-known finite element method (FEM) for the numerical approximation of PDEs on flat [8] and 3D domains [49] as well as on surfaces [38].

Several element-based numerical methods have been developed for the spatial discretisation of BS-PDEs; current-state-of-the-art methods existing in the literature include classical finite elements [31, 42, 46, 47], cut finite elements [20], discontinuous Galerkin methods [24], kernel collocation methods [23] and trace finite elements [41]. We seek to contribute to this area by developing the *bulk-surface virtual element method* (BS-VEM)