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The bulk-surface finite element method for reaction–diffusion systems on stationary volumes

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ABSTRACT

In this work we present the bulk-surface finite element method (BSFEM) for solving coupled systems of bulk-surface reaction–diffusion equations (BSRDEs) on stationary volumes. Such systems of coupled bulk-surface partial differential equations arise naturally in biological applications and fluid dynamics, for example, in modelling of cellular dynamics in cell motility and transport and diffusion of surfactants in two phase flows. In this proposed framework, we define the surface triangulation as a collection of the faces of the elements of the bulk triangulation whose vertices lie on the surface. This implies that the surface triangulation is the trace of the bulk triangulation. As a result, we construct two finite element spaces for the interior and surface respectively. To discretise in space we use piecewise bilinear elements and the implicit second order fractional-step θ scheme is employed to discretise in time. Furthermore, we use the Newton method to treat the nonlinearities. The BSFEM applied to a coupled system of BSRDEs reveals interesting patterning behaviour. For a set of appropriate model parameter values, the surface reaction–diffusion system is not able to generate patterns everywhere in the bulk except for a small region close to the surface while the bulk reaction–diffusion system is able to induce patterning almost everywhere. Numerical experiments are presented to reveal such patterning processes associated with reaction–diffusion theory.

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1. Introduction

Many problems in science and engineering are modelled mathematically by systems of partial differential equations (PDEs). Some of these problems involve coupling surface and interior (bulk) dynamics resulting in coupled systems of bulk-surface PDEs. Such systems arise naturally in many fluid dynamics applications and biological processes. In developmental biology, for example, it is essential the emergence and maintenance of polarised states in the form of heterogeneous distributions of chemical substances (proteins and lipids). Examples of such processes include (but are not limited to) the formation of buds in yeast cells and cell polarisation in biological cells due to responses to external signals through the outer cell membrane [26,27]. In the context of reaction–diffusion processes, such symmetry breaking arises when a uniform steady state, stable in the absence of diffusion, is driven unstable when diffusion is present thereby giving rise to the formation of spatially inhomogeneous solutions in a process now well-known as the Turing diffusion-driven instability [29]. Classical Turing theory requires that one of the chemical species, typically the *inhibitor*, diffuses much faster than the other, the *activator* resulting in what is known as *long-range inhibition, short-range activation* [10,16].

Recently, there has been a surge in studies on models that couple bulk dynamics to surface dynamics. For example, Rätz and Röger [27] study symmetry breaking in a bulk-surface reaction–diffusion model for signalling networks. In this work, a single diffusion partial differential equation (the heat equation) is formulated inside the bulk of a cell, while on the cell-surface, a system of two membrane reaction–diffusion equations is formulated. The bulk and cell-surface membrane are coupled through a Robin-type boundary condition and a flux term for the membrane system [27]. Elliott and Ranner [8] study a finite element approach to a sample elliptic problem: a single elliptic partial differential equation is posed in the bulk and another is posed on the surface. These are then coupled through Robin-type boundary conditions. Burman et al. [4] recently developed cut finite element methods for coupled bulk-surface problems. In this article, single time-independent elliptic parabolic equations are coupled in the bulk and surface through non-zero flux boundary conditions. A trace finite element method has recently been proposed to study a class of coupled bulk-interface transport problems posed on evolving volumes and surfaces [12]. Again, coupling of the bulk and surface dynamics is through non-zero boundary conditions. Novak et al. [24] present an algorithm for solving a diffusion equation on a curved surface coupled

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to a diffusion model in the volume. Checkkin et al. [6] study bulk-mediated diffusion on planar surfaces. Again, diffusion models are posed in the bulk and on the surface coupling them through boundary conditions. In the area of tissue engineering and regenerative medicine, electrospun membrane are useful in applications such as filtration systems and sensors for chemical detection. Understanding of the fibres' surface, bulk and architectural properties is crucial to the successful development of integrative technology. Nisbet et al. [23] present detailed review on surface and bulk characterisation of electrospun membranes of porous and fibrous polymer materials. To explain the long-range proton translocation along biological membranes, Medvedev and Stuchebrukhov [22] propose a model that takes into account the coupled bulk-diffusion that accompanies the migration of protons on the surface.

In most of the work above, either elliptic or diffusion models in the bulk have been coupled to surface-elliptic or surface-diffusion or surface-reaction–diffusion models posed on the surface through Robin-type boundary conditions [6,8,22–24,26,27]. Here, our focus is to couple systems of reaction–diffusion equations posed both in the bulk and on the surface, setting a mathematical and computational framework to study more complex interactions such as those observed in cell biology, tissue engineering and regenerative medicine, developmental biology and biopharmaceutical [6,8,22–24,26,27].

The coupled system of bulk-surface reaction–diffusion equations (BSRDEs) may be numerically solved using various discretisation schemes and techniques. We choose to employ the bulk finite element method [9] to numerically solve the bulk-reaction–diffusion system while the surface finite element method [7] is employed to compute numerical solutions corresponding to the surface-reaction–diffusion system. The key idea of the finite element method is that two finite element spaces are constructed, the bulk and surface finite element spaces, by taking a set of all continuous piecewise polynomial functions on each bulk simplex or boundary face element [8]. The bulk and surface reaction–diffusion systems are coupled through Robin-type boundary conditions. The coupled bulk-surface finite element algorithm is implemented in **deal.II** [1].

Other plausible numerical methods for solving such systems include (but are not limited to) finite volume methods [5], particle methods using level set descriptions of the surface [11,14] and closest-point methods [18,19].

Our article is therefore structured as follows. In Section 2 we present the coupled bulk-surface reaction–diffusion system on stationary volumes with appropriate boundary conditions coupling the bulk and surface partial differential equations. Within this section, we give some specific examples of the applications of the coupled system of PDEs. The bulk-surface finite element framework is presented in Section 3. Here we describe how the two finite element spaces are constructed to enable us to carry out the spatial discretisation of the model system. We also detail how the bulk and surface triangulations are carried out. To discretise in time, we use the fractional-step θ method coupled with the Newton method to treat nonlinearities arising from the nonlinear reactions. Numerical experiments are presented in Section 4 where we discuss how bulk dynamics influence patterning on the surface and vice versa. We conclude and discuss the implications of our studies in Section 5 as well as setting foundations for future research.

2. Coupled system of bulk-surface reaction–diffusion equations (BSRDEs) on stationary volumes

In this section we present our model system which comprises a system of coupled bulk-surface reaction–diffusion equations (BSRDEs) posed in a three-dimensional volume as well as on its surface. We impose boundary conditions on the system of reaction–diffusion equations in the interior of the volume that couple internal dynamics to surface dynamics. Since we are interested in closed surfaces (whose boundary is empty) then the system of reaction–diffusion system on the surface is devoid of boundary conditions.

2.1. Notation

Let Γ be a closed, compact and smooth hypersurface without boundary in $\mathbb{R}^{N+1}$ enclosing a convex volume Ω. Let $\boldsymbol{n}$ denote the unit outer normal to Γ, and let U be any open subset of $\mathbb{R}^{N+1}$ containing Γ, then for any function u which is differentiable in U, we define the tangential gradient on Γ by

$$\nabla_\Gamma u = \nabla u - (\nabla u \cdot \boldsymbol{n})\boldsymbol{n},$$

where $\cdot$ denotes the dot product and ∇ denotes the gradient in $\mathbb{R}^{N+1}$. The tangential gradient is the projection of the gradient onto

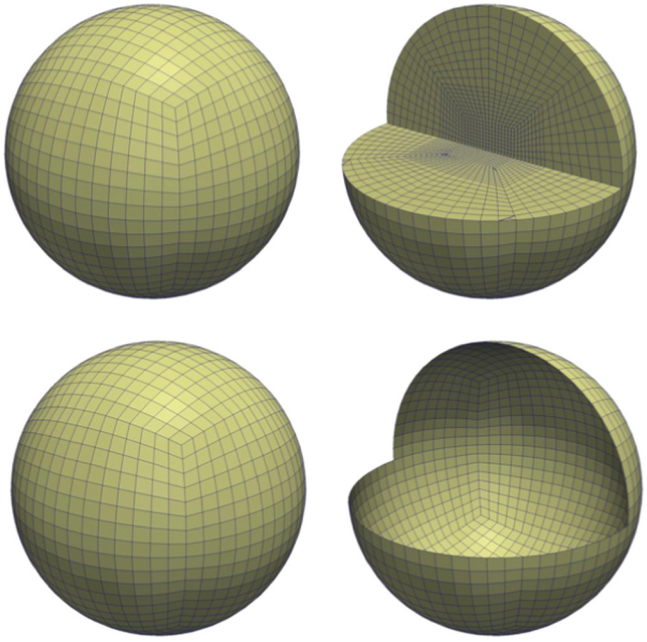

Fig. 1. An example illustrating how the surface triangulation (bottom row) is naturally induced by the volume or bulk (top row) triangulation. Part of the domain has been cut away and shown on the right to reveal some internal mesh structure [21].

Table 1
Parameter values for the coupled system of bulk-surface reaction–diffusion equations (2.1)–(2.6).

a	b	d	α_1	α_2	β_1	β_2	κ_1	κ_2
0.1	0.9	100	5/12	5	5/12	0	0	5

Table 2
Model parameter values used in simulations for Figs. 2–9.

Figure	d_Ω	d_Γ
2	1.0	1.0
3	1.0	10.0
5	1.0	20.0
6	10.0	1.0
7	10.0	10.0
8	20.0	10.0
9	20.0	20.0

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