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High-order spectral/*hp* element discretisation for reaction–diffusion problems on surfaces: Application to cardiac electrophysiology ☆

Chris D. Cantwell [a,*], Sergey Yakovlev [b], Robert M. Kirby [b], Nicholas S. Peters [a], Spencer J. Sherwin [c]

[a] National Heart and Lung Institute, Imperial College London, London, UK
[b] School of Computing and Scientific Computing and Imaging (SCI) Institute, Univ. of Utah, Salt Lake City, UT, USA
[c] Department of Aeronautics, Imperial College London, London, UK

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ABSTRACT

We present a numerical discretisation of an embedded two-dimensional manifold using high-order continuous Galerkin spectral/*hp* elements, which provide exponential convergence of the solution with increasing polynomial order, while retaining geometric flexibility in the representation of the domain. Our work is motivated by applications in cardiac electrophysiology where sharp gradients in the solution benefit from the high-order discretisation, while the computational cost of anatomically-realistic models can be significantly reduced through the surface representation and use of high-order methods. We describe and validate our discretisation and provide a demonstration of its application to modelling electrochemical propagation across a human left atrium.

1. Introduction

Partial Differential Equations (PDEs) describe many physical and mathematical processes and are quite often posed on embedded surfaces. PDEs on arbitrary surfaces rarely have analytic solutions and so are solved numerically using, for example, finite difference or finite element techniques. In the case of physical processes, a surface representation of the domain is usually an approximation of the true system and is made for numerical efficiency reasons providing it does not overly degrade the underlying physics. There are many examples of applications where PDEs are solved on surfaces in the literature, including fluid dynamics [1], biology and medicine [2], and computer graphics [3]. In this paper we describe a formulation of high-order spectral/*hp* element methods on curvilinear codimension-one surfaces embedded in three-dimensional space, applied to modelling electrical propagation in the heart.

The standard approach to solving a PDE on an embedded domain using finite element methods is to discretise the surface using a triangulation [4–6], or to parametrise the surface [1]. The latter may be challenging for arbitrary surfaces or require the use of multiple patches. Triangulation may lead to discretisation errors due to poor representation of the

* Corresponding author.
E-mail addresses: c.cantwell@imperial.ac.uk (C.D. Cantwell), sergeyyak@gmail.com (S. Yakovlev), kirby@cs.utah.edu (R.M. Kirby), n.peters@imperial.ac.uk (N.S. Peters), s.sherwin@imperial.ac.uk (S.J. Sherwin).

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surface. It may also be computationally expensive in cases where the surface evolves in time. Finite volume methods have also been considered (for example, [7]), but are not examined further here. Alternative approaches include the level-set [8] or closest point method [9,10]. Level-set methods describe the surface as the zero level-set of a, possibly time-dependent, function $\phi(\boldsymbol{x}, t)$ and extend the PDE from this surface into a higher-dimensional ambient Euclidean space. The extended PDE is solved using finite difference [11,12] or finite element [3,13] techniques. This removes much of the complexity of constructing operators on the manifold, but at the expense of increasing the dimension of the problem and, therefore, the computational cost. Care must also be taken to ensure the extended PDE remains true to the original surface PDE and complications can arise due to the necessity to impose boundary conditions on either side of the surface which may lead to an artificial jump in the solution, degeneracy of the implicit equation and difficulties in ensuring regularity of the solutions [14], although some of these can be addressed [15]. However, these methods allow the surface to move in time, in a relatively computationally efficient manner.

Mathematical formulations for solving PDEs on surfaces using linear finite element methods have been considered previously for a number of applications. One of the most prominent in the literature is the solution of the shallow water equations on the Earth's surface, for example [16], where the local coordinate systems on each element eliminate the singularities inherent when solving in global spherical coordinates. Spectral elements have also been used for the shallow water equations on a sphere by Giraldo [17] and Taylor et al. [18]. They find, for realistic atmospheric problems that these methods achieve comparable accuracy to existing methods, although they anticipate the methods can be more powerful when using local refinement. Their study is also restricted to a parametrised sphere using quadrilaterals. Finally, PDEs on surfaces are important in computer graphics [3] for rendering and texturing on surfaces and visualising flow data from simulations [19]. Fluid flow simulations on surfaces of arbitrary topology have been discussed by Stam [1].

In this paper we are interested in defining spectral/*hp* element discretisations of surfaces of arbitrary and complex geometry as are typically found in biomedical applications. Such surfaces are frequently extracted from medical imaging: a global surface parametrisation is infeasible. Instead we tessellate the surface with geometrically high-order curvilinear elements, each defined by a mapping from a planar reference region. The mapping is then incorporated into the differential operators during their construction. The particular application we consider is the simulation of human left atrium electrophysiology. We discard the mechanical aspects of the heart, so do not require the capabilities to model moving surfaces.

1.1. Cardiac electrophysiology

Cardiac conduction occurs due to a complex sequence of ion transport mechanisms between cells. As ions flow from adjacent excited cells and the potential difference across the cell membrane exceeds a threshold level, a complex sequence of ionic currents begins to flow between the intracellular and extracellular spaces creating a prescribed variation of the transmembrane potential known as the action potential. This process begins with a complete and rapid depolarisation of the cell due to the inward sodium current. Other ionic currents gradually restore the polarised state to complete the cycle. The depolarisation of the cell causes contraction and the cumulative effect results in coordinated contraction of the heart muscle with each activation wave. In some cases, due to disease, infarction or age, inhomogeneities in the myocardium result in abnormal activation patterns, known as cardiac arrhythmias, leading to irregular contraction of the heart and poor cardiac throughput. If such dysfunction occurs in the ventricles it is rapidly fatal, causing cessation of effective blood circulation, and is the most common cause of cardiac arrest. When occurring in the atria, it causes symptoms such as tiredness and leaves the person prone to the formation of blood clots in the poorly contracting atrium and puts them at greater risk of stroke.

Identifying those areas of myocardium responsible for the initiation or perpetuation of an arrhythmia is key to successful clinical intervention and therefore accurate and rapid computer simulation of a patient's atrial electrical activity is potentially a highly valuable tool in planning treatment. Significantly improving the performance of cardiac electrophysiology computer simulations is key for them to attain clinical utility. Spectral elements are capable of providing high-resolution solutions, necessary to capture the sharp gradients at the leading edge of the depolarisation wave, with fewer degrees of freedom than linear finite element methods [20]. In addition, these high-order methods can be extended to perform local polynomial refinement where needed during the simulation, such as on those elements in close proximity to the wavefront, without needing to resort to computationally expensive mesh refinement.

Simplifying the geometric model of the atrium is another approach to accelerating simulations. To date most computer simulations of mammalian atria represent the chamber walls as fully three-dimensional substrate, typically from a volume segmentation of magnetic resonance angiography (MRA) images. The wall of the human atrium is typically only 1–3 mm thick, but with a surface area in excess of 50 cm^2. Electrical propagation and arrhythmogenic features are therefore predominantly two-dimensional in nature and can be efficiently modelled as a two-dimensional surface. To illustrate this, we quantify the effect of transmural variability in a 3D tissue slice, described in Fig. 1, when the epicardial and endocardial surfaces have orthogonal fibre directions. Additionally, we compare this to the same geometry using isotropic conductivities, computed as the transmural average of those in the anisotropic case. In each case, the tissue is stimulated from the centre point of the tissue with a current of 50 μA, applied for 2 ms over a spherical region of radius 3 mm. Fig. 2 shows the maximum difference in activation time between the epicardial and endocardial layers for the anisotropic case, as well as a comparison between the endocardial layers of the isotropic and anisotropic cases. For a thickness of 2 mm – the average thickness of the left atrial wall – the maximum difference in local activation time between corresponding points on the