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Very high order finite volume methods for cardiac electrophysiology

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ABSTRACT

Numerical simulation of the propagation of electrical signals in the heart is a very demanding application. In fact, very fine meshes and small time steps are currently required to capture the phenomena. In this paper, we propose and explore a very high-order scheme specifically designed for this application. Its numerical properties are detailed and the different choices on both the scheme's definition and implementation are discussed and justified. Numerical results show the importance of considering very high-order schemes, even for classical tests such as the propagation of planar or spiral waves.

1. Introduction

There is currently a growing interest for scientific computing methods applied to medical sciences, since they provide quantitative data on biophysical processes. We are specifically interested in accurate numerical simulations of the propagation of action potentials (AP) in the cardiac muscle [1,2]. In practice this propagation provides the synchronization of the contraction of the cardiac cells, which in turn provides an optimal cardiac function. Dysfunctions of this propagation cause a series of major heart diseases. At the ventricular level, tachycardia or fibrillation are responsible for half the 1.9 millions deaths (∼5200/day) attributed to a syndrome called sudden cardiac death [3]. At the atrial level, fibrillation is the most common arrhythmia and a cause of increasing health care costs in western countries [4,5].

The multiplication of biological or medical studies that rely on simulations prompts for a better understanding of the cardiac simulators. As observed in [2,6], and underlined hereafter, providing reliable numerical approximations is challenging.

The propagation of the cardiac AP in an insulated cardiac tissue may be modeled by the reaction–diffusion equation (monodomain model) [7]

$$A_m\left(C_m \partial_t V + J_{ion}\right) = \operatorname{div}\left(\sigma \nabla V\right), \tag{1}$$

coupled to a set of ordinary differential equations that describes the evolution of J_{ion} (see below). This equation states a balance of current per unit volume, in μA cm^{-3}. The main unknown is the difference of potential V between the intra and extracellular parts of the cells, in mV. The current is expressed by unit of surface of membrane, J_{ion} in μA cm^{-2}, and the

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membrane capacitance C_m is measured per unit of surface, in $\mu F\,cm^{-2}$. The model is obtained by homogenization [8], so that σ is an equivalent macroscopic electrical conductivity matrix in $mS\,cm^{-1}$, and A_m is a scaling factor, specifically the surface of membrane per unit of volume of the macroscopic tissue, in cm^{-1}. The time and space dimensions are expressed in ms and cm.

The current J_{ion} is due to ion exchanges through the cell membrane. These ion exchange processes are given by ionic models, which make use of a set of m state variables $w(t, x) \in \mathbb{R}^m$. A normalized total current $I_{ion}(V, w) = J_{ion}/C_m$ in $A\,F^{-1}$, instead of J_{ion} is used to gather the contribution of individual ionic currents. With this notation, and after dividing Eq. (1) by A_m and C_m, we find the scaled monodomain system of equations, that also gathers the ionic model:

$$\partial_t V + I_{ion}(V, w) = \operatorname{div}\big(D\nabla V\big), \tag{2}$$

$$\partial_t w = G(V, w), \tag{3}$$

where V is the transmembrane voltage in mV, $I_{ion}(V, w)$ is the normalized ionic current in $A\,F^{-1}$, and $D = \sigma/A_m C_m$ is the normalized diffusion tensor in $cm^2\,m\,s^{-1}$. Eq. (3) is the system of m nonlinear ordinary differential equations called the ionic model, and specified through the function $G(V, w)$. Here, we will use more or less complex and stiff models G (see Section 5).

The equivalent diffusion tensor reflects the microstructure of the cardiac tissue and may be an anisotropic function of space, $D = D(x)$.

The geometry of the cardiac domain is complex, and up to hundreds of individual variables may participate in the biophysical processes at each point of the tissue. The currently used methods rely most often on unstructured grid discretizations, and result in very large systems of equations, that may be solved thousands of times over the course of a simulation. In this article, we propose to investigate the interest of high-order finite volume discretizations (up to sixth order of accuracy) in this context. Such methods provide several advantages over the classical methods as explained below.

More specifically, there is quite a large amount of works that make use of numerical models for this system of equation for applied means. The most commonly used solvers in applied studies are: CARP [9], Propag [7], and Chaste [10]. CARP and Chaste rely on first order finite element methods, and time-stepping strategies derived from the idea of Rush and Larsen [11], sometimes extended to second order in time. Propag is a finite difference code based on the numerical scheme of Saleheen and Ng [12]. In addition, there exists a common agreement on the spatial and temporal resolution that would be needed for simulation of real cardiac tissues (see the introduction of [13]). The spatial resolution is usually chosen in the range of 200–500 μm, and the time-step in the range of 10–20 μs (see [7,9,14–16] for instance).

Various adaptive strategies have been proposed in [17–21]. While some improvement has been reported in all cases, the error itself is not studied in these articles. In addition, these methods are not easily compatible with parallel computing environment, and demand to complete a difficult technological gap if they are to be used routinely.

A few other studies concentrate on higher-order techniques in space or time. Some detailed one-dimensional and two-dimensional simulations are given in [6], and complementary discussion can be found in [22]. Several difficulties are listed in [6]: nonlinear ionic models include discontinuous functions, the velocity of the AP wave is over or under-estimated with the usual approaches, there are technical issues related to parallel computing and the mass matrix of high order finite element methods. Finally, the spatial and temporal resolution currently used clearly do not allow to reach a satisfactory accuracy of the numerical solutions. This is especially true if realistic ionic models and ratio A_m ($\simeq$1000–2000 cm^{-1}) become necessary.

In this study, we focus on high-order finite volumes methods in space combined with high-order strong stability preserving (SSP) Runge and Kutta methods [23]. We derive a high-order finite volume adapted to the problem based on the work of S. Clain et al. [24,25]. The method provides a numerical solution based on one unknown per mesh element (triangle or tetrahedron, called a cell), through the reconstruction of polynomials of arbitrary order. The reconstructions are based on a least square approximation technique and rely on the definition of a neighboring stencil for each cell or interface between cells, and the choice of some suitable quadrature formulas. The resulting discretization has a diagonal mass-matrix, and a sparse stiffness matrix. As a matter of fact, such techniques allow very easy implementation of very high order schemes. As an example, we implemented up to a sixth order scheme for this study. The actual implementation is matrix free, and partially multi-threaded by using the OpenMP library. Together with high-order, matrix free methods prompt for explicit time-stepping techniques, for a simpler implementation, and because low spatial and temporal resolution may be sufficient for accurate simulations. Moreover the second barrier of Dahlquist implies that implicit schemes of order >2 anyway have a time-step constraint. As compared to Rush and Larsen approaches, there is not any linear system to be solved with explicit methods.

The proposed SSP RK methods allow to preserve admissible states of the variables. This may be useful for cardiac ionic models, which ionic concentrations have to remain positive, and gating-variables have to remain within physical bounds (usually between 0 and 1). Anyway, for realistic ionic models, namely the Beeler–Reuter [26] and TNNP [27] models, we had to impose some limitations on the polynomial reconstructions in order to guarantee the positivity of the ionic concentrations. These limitations, as well as the discontinuity in the models actually impair the overall accuracy of the method, as in [6], see Section 2.

We investigated the numerical accuracy of the methods for two-dimensional simulations of

- simple planar waves, for which we looked at the propagation failure problem, and the convergence of the velocity;
- spiral waves, for which we compared the qualitative resolution of the solution (number of turns depending on the numerical method).

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