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for the Linear Bidomain Equations

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Bericht 2018/6

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Olaf Steinbach and Huidong Yang

Abstract In this work, we study a Galerkin–Petrov space–time finite element method for a linear system of parabolic–elliptic equations with in general anisotropic conductivity matrices, which may be considered as a simplified version of the nonlinear bidomain equations. The discretization is based on a stable space–time variational formulation employing continuous and piecewise linear finite elements in both spatial and temporal directions simultaneously. We show stability of the space–time formulation on both the continuous and discrete level for such a coupled problem under a rather general condition on the conductivity matrices. We further discuss the construction of a monolithic algebraic multigrid (AMG) method for solving the coupled linear system of algebraic equations globally. Numerical experiments are performed to demonstrate the convergence of the space–time finite element approximations, and the performance of the AMG method with respect to the mesh discretization parameter. Finally, we apply the space–time finite element method to the nonlinear bidomain equations in order to show the applicability of the proposed approach.

1 Introduction

The modelling of the electrical activity of the human heart relies on the Maxwell equations when neglecting the time derivative in Faraday’s law. Hence we may use a scalar potential to describe the electric field, where the potential inside a cell is called intracellular potential, while the potential exterior to a cell is called extracel-

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lular potential. When the cells are at rest, there is a potential difference across the cell membrane which is called the transmembrane potential. Hence, using the continuity equation and Ohm's law, and considering the ionic current exciting the cell, this results in a coupled system of nonlinear parabolic and elliptic partial differential equations, and a system of ordinary differential equations to describe the ionic current via cellular state variables. For a more detailed discussion of the mathematical model we refer to, e.g., [6, 10, 25].

As model problem we consider the simplified linear bidomain equations to find the transmembrane potential u_T and the extracellular potential u_e satisfying the linear parabolic–elliptic system

$$C_m \partial_t u_T(x, t) - \operatorname{div}_x [M_i(x) \nabla_x u_T(x, t)] - \operatorname{div}_x [M_i(x) \nabla_x u_e(x, t)] = s_i(x, t), \quad (1)$$

$$-\operatorname{div}_x [M_i(x) \nabla_x u_T(x, t)] - \operatorname{div}_x [(M_i(x) + M_e(x)) \nabla_x u_e(x, t)] = s_e(x, t) \quad (2)$$

for $(x, t) \in Q := \Omega \times (0, T)$, where $\Omega \subset \mathbb{R}^n$ is assumed to be Lipschitz, $n = 2, 3$, with homogeneous Dirichlet boundary conditions $u_T = 0$ and $u_e = 0$ on the lateral boundary $\Sigma := \partial\Omega \times (0, T)$, and a given initial condition $u_T = 0$ in Ω , $t = 0$. Note that inhomogeneous data can be handled via a standard homogenisation approach by using a suitable extension. Moreover, s_i and s_e are some given current sources, M_i and M_e are, in general anisotropic, conductivity matrices, that are assumed to be symmetric and positive definite, and satisfying

$$\mu (M_i(x)v, v) \leq (M_e(x)v, v) \leq \bar{\mu} (M_i(x)v, v) \quad \text{for all } v \in \mathbb{R}^n \quad (3)$$

uniformly for $x \in \Omega$ for some $0 < \mu \leq \bar{\mu}$. Finally, C_m is the capacitance of the cell membrane.

In this simplified model we have neglected the nonlinear coupling term among the two potentials and the third variable, a vector of cellular state variables, via dropping the nonlinear ionic current term and the related nonlinear system of ordinary differential equations. In [6], a similar linear model problem is considered, with Robin boundary conditions instead of Dirichlet conditions. Admittedly, the bidomain reaction–diffusion system in its simplified form (1)–(2) will be a reasonable starting point towards the construction of robust monolithic algebraic multigrid (AMG) methods for the fully coupled nonlinear bidomain equations. For general concepts of AMG methods, we refer to [1, 2, 20].

As it is well known, most conventional methods for discretizing the nonlinear bidomain equations, i.e. the coupled parabolic–elliptic equations and the system of ordinary differential equations to describe the ionic current, are proper combinations of explicit/implicit time stepping methods and finite element methods with respect to the temporal and spatial directions, respectively; see, e.g., [3, 4, 10, 13, 14, 15, 16, 17, 18, 19, 22, 27].

Recently, a space–time discontinuous Galerkin finite element discretization on arbitrary simplex meshes has been employed to approximate the solution of the bidomain equations and the coupled electro–mechanical system [6, 7]. Such a space–time discontinuous Galerkin scheme has been investigated for the heat equa-

tion in [11, 12], by treating the time as another variable, and adding an upwind with respect to the time derivative.

On the other hand, iterative and parallel solution methods for the bidomain equations have been considerably studied in the past years, that are mainly based on time stepping methods and operator splitting schemes. Related references on the splitting solution methods for the bidomain equations can be found, e.g., in [10, 13, 26].

In [3], the system of ordinary differential equations is solved by a combination of an exact solution of related scalar linear ordinary differential equations, and the explicit Euler method for the remaining equations. The coupled reaction–diffusion part is tackled as an elliptic problem via a NURBS–based isogeometric discretization [5] in space and a semi–implicit scheme in time, i.e., an implicit Euler method for the diffusion term, and an explicit treatment for the nonlinear reaction term. The optimal convergence rate of two–level additive Schwarz preconditioners for the resulting linear system is shown. Earlier results for multilevel Schwarz preconditioners for the bidomain parabolic–parabolic and parabolic–elliptic formulations (both become elliptic problems after temporal discretization) can be found in [14, 15]. A similar operator splitting scheme has been used in [27], where the resulting discrete bidomain elliptic equations at each time step are solved by a balancing Neumann–Neumann preconditioned conjugate gradient method.

In [19], an explicit Euler method has been used to solve the parabolic equation and nonlinear system of ordinary differential equations at each time step, and the remaining elliptic problem is solved by an algebraic multigrid method.

Block factorized preconditioners for the coupled bidomain reaction–diffusion 2×2 system in a semi–implicit time stepping method have been investigated in [17, 18], where an AMG method is used to approximate the blocks.

Very recently, a monolithic scheme has been studied in [6] for the fully coupled nonlinear bidomain equations, that are discretized by using a space–time discontinuous Galerkin finite element scheme in the space–time domain. On each Newton iteration, the linearized system is reduced to the Schur complement equation with respect to the two potential variables. Further, discrete stability conditions for both the linear and nonlinear problems are shown therein, with respect to specially chosen DG–norms.

In this work, we follow a continuous Galerkin–Petrov space–time finite element discretization scheme [23] for approximating the solution of the model problem (1)–(2) in the space–time domain. The resulting linear system of algebraic equations is then solved by a monolithic AMG method.

The remainder of this paper is organized as follows. In Section 2, we present a stable space–time variational formulation of the model problem (1)–(2), and in Section 3 we discuss the related continuous Galerkin–Petrov space–time finite element method. The monolithic algebraic multigrid method for the solution of the coupled linear system of algebraic equations is discussed in Section 4. Some numerical results are provided in Sections 5 and 6 where we also consider the nonlinear system including the ionic current. Finally, some conclusions are drawn in Section 7.

2 Space–time variational formulations

Let us define the function spaces

$$\begin{aligned} X &:= \left\{ v \in L^2(0, T; H_0^1(\Omega)) \cap H^1(0, T; H^{-1}(\Omega)), v(x, 0) = 0 \text{ for } x \in \Omega \right\}, \\ Y &:= L^2(0, T; H_0^1(\Omega)) \end{aligned}$$

to consider the Galerkin–Petrov variational formulation of the Dirichlet boundary value problem (1) and (2) to find $(u_T, u_e) \in X \times Y$ such that

$$a(u_T, u_e; v_T, v_e) = \int_0^T \int_{\Omega} [s_i v_T + s_e v_e] dx dt \quad (4)$$

is satisfied for all $(v_T, v_e) \in Y \times Y$ where the bilinear form is given as

$$\begin{aligned} a(u_T, u_e; v_T, v_e) &:= \int_0^T \int_{\Omega} \left[C_m \partial_t u_T v_T + (M_i \nabla_x u_T, \nabla_x v_T) + (M_i \nabla_x u_e, \nabla_x v_T) \right] dx dt \\ &\quad + \int_0^T \int_{\Omega} \left[(M_i \nabla_x u_T, \nabla_x v_e) + ((M_i + M_e) \nabla_x u_e, \nabla_x v_e) \right] dx dt. \end{aligned}$$

To establish unique solvability of the space–time variational formulation (4) we need to have a related stability estimate for the involved bilinear form. For this we first consider an ellipticity estimate for the spatial part.

Lemma 1. *For $u_T, u_e, v_T, v_e \in Y$ we consider the spatial bilinear form*

$$\begin{aligned} a_S(u_T, u_e; v_T, v_e) &:= \int_0^T \int_{\Omega} \left[(M_i \nabla_x u_T, \nabla_x v_T) + (M_i \nabla_x u_e, \nabla_x v_T) \right] dx dt \quad (5) \\ &\quad + \int_0^T \int_{\Omega} \left[(M_i \nabla_x u_T, \nabla_x v_e) + ((M_i + M_e) \nabla_x u_e, \nabla_x v_e) \right] dx dt \end{aligned}$$

and Assumption (3). Then, for $(v_T, v_e) \in Y \times Y$ there holds the ellipticity estimate

$$a_S(v_T, v_e; v_T, v_e) \geq c_S \|(v_T, v_e)\|_{Y \times Y}^2$$

with the positive constant

$$c_S = 1 + \frac{\mu}{2} - \sqrt{\frac{\mu^2}{4} + 1} > 0,$$

and with respect to the norm

$$\|(v_T, v_e)\|_{Y \times Y}^2 := \int_0^T \int_{\Omega} \left[(M_i \nabla_x v_T, \nabla_x v_T) + (M_i \nabla_x v_e, \nabla_x v_e) \right] dx dt.$$

Proof. Using Assumption (3) we have, for some $\gamma > 0$,

$$\begin{aligned}
a_S(v_T, v_e; v_T, v_e) &= \\
&= \int_0^T \int_{\Omega} \left[(M_i \nabla_x v_T, \nabla_x v_T) + 2(M_i \nabla_x v_e, \nabla_x v_T) + ((M_i + M_e) \nabla_x v_e, \nabla_x v_e) \right] dx dt \\
&\geq \int_0^T \int_{\Omega} \left[(M_i \nabla_x v_T, \nabla_x v_T) + 2(M_i \nabla_x v_e, \nabla_x v_T) + (1 + \mu)(M_i \nabla_x v_e, \nabla_x v_e) \right] dx dt \\
&= \int_0^T \int_{\Omega} \left[\left(1 - \frac{1}{\gamma}\right) (M_i \nabla_x v_T, \nabla_x v_T) + (1 + \mu - \gamma)(M_i \nabla_x v_e, \nabla_x v_e) \right] dx dt \\
&\quad + \int_0^T \int_{\Omega} \left(M_i \nabla_x \left(\frac{1}{\sqrt{\gamma}} v_T + \sqrt{\gamma} v_e \right), \nabla_x \left(\frac{1}{\sqrt{\gamma}} v_T + \sqrt{\gamma} v_e \right) \right) dx dt \\
&\geq (1 + \mu - \gamma^*) \int_0^T \int_{\Omega} \left[(M_i \nabla_x v_T, \nabla_x v_T) + (M_i \nabla_x v_e, \nabla_x v_e) \right] dx dt
\end{aligned}$$

if

$$1 - \frac{1}{\gamma^*} = 1 + \mu - \gamma^*$$

is satisfied, i.e.

$$\gamma^* = \frac{\mu}{2} + \sqrt{\frac{\mu^2}{4} + 1}, \quad c_S = 1 + \mu - \gamma^* = 1 + \frac{\mu}{2} - \sqrt{\frac{\mu^2}{4} + 1} > 0.$$

□

In fact, the bilinear form (5) induces a norm in $Y \times Y$, i.e. for $(v_T, v_e) \in Y \times Y$ we have

$$\|(v_T, v_e)\|_M^2 := a_S(v_T, v_e; v_T, v_e)$$

satisfying

$$c_S \|(v_T, v_e)\|_{Y \times Y}^2 \leq \|(v_T, v_e)\|_M^2 \leq \left(1 + \frac{\bar{\mu}}{2} + \sqrt{\frac{\bar{\mu}^2}{4} + 1} \right) \|(v_T, v_e)\|_{Y \times Y}^2.$$

Hence we can define $(w_T, w_e) \in Y \times Y$ as the unique solution of the variational formulation

$$a_S(w_T, w_e; v_T, v_e) = a(u_T, u_e; v_T, v_e) \quad \text{for all } (v_T, v_e) \in Y \times Y, \quad (6)$$

where $(u_T, u_e) \in X \times Y$ is given. For the latter we introduce the norm

$$\|(u_T, u_e)\|_{X \times Y} := \sup_{0 \neq (v_T, v_e) \in Y \times Y} \frac{a(u_T, u_e; v_T, v_e)}{\|(v_T, v_e)\|_M}, \quad (7)$$

and where we can write the bilinear form, by using integration by parts, as

$$\begin{aligned}
a(u_T, u_e; v_T, v_e) &= \langle C_m \partial_t u_T - \operatorname{div}_x [M_i \nabla_x u_T] - \operatorname{div}_x [M_i \nabla_x u_e], v_T \rangle_Q \\
&\quad + \langle -\operatorname{div}_x [M_i \nabla_x u_T] - \operatorname{div}_x [(M_i + M_e) \nabla_x u_e], v_e \rangle_Q.
\end{aligned}$$

Recall that $\langle \cdot, \cdot \rangle_Q$ denotes the duality pairing as extension of the L^2 inner product in the space time domain. The norm (7) is indeed the adjoint norm of the partial differential operator in (1) and (2) applied to (u_T, u_e) . Although the norm definition (7) already implies a related stability condition, we will present a proof in order to establish the forthcoming relation (9).

Lemma 2. *For all $(u_T, u_e) \in X \times Y$ there holds the stability condition*

$$\|(u_T, u_e)\|_{X \times Y} \leq \sup_{0 \neq (v_T, v_e) \in Y \times Y} \frac{a(u_T, u_e; v_T, v_e)}{\|(v_T, v_e)\|_M}. \quad (8)$$

Proof. For the unique solution $(w_T, w_e) \in Y \times Y$ of the variational problem (6) we first have

$$\begin{aligned} \|(w_T, w_e)\|_M^2 &= a_S(w_T, w_e; w_T, w_e) \\ &= a(u_T, u_e; w_T, w_e) \leq \|(u_T, u_e)\|_{X \times Y} \|(w_T, w_e)\|_M, \end{aligned}$$

i.e.

$$\|(w_T, w_e)\|_M \leq \|(u_T, u_e)\|_{X \times Y}.$$

On the other hand,

$$\begin{aligned} \|(u_T, u_e)\|_{X \times Y} &= \sup_{0 \neq (v_T, v_e) \in Y \times Y} \frac{a(u_T, u_e; v_T, v_e)}{\|(v_T, v_e)\|_M} \\ &= \sup_{0 \neq (v_T, v_e) \in Y \times Y} \frac{a_S(w_T, w_e; v_T, v_e)}{\|(v_T, v_e)\|_M} \leq \|(w_T, w_e)\|_M, \end{aligned}$$

implying

$$\|(w_T, w_e)\|_M = \|(u_T, u_e)\|_{X \times Y}.$$

Hence we conclude

$$\|(u_T, u_e)\|_{X \times Y}^2 = \|(w_T, w_e)\|_M^2 = a_S(w_T, w_e; w_T, w_e) = a(u_T, u_e; w_T, w_e), \quad (9)$$

and therefore

$$\|(u_T, u_e)\|_{X \times Y} = \frac{a(u_T, u_e; w_T, w_e)}{\|(w_T, w_e)\|_M} \leq \sup_{0 \neq (v_T, v_e) \in Y \times Y} \frac{a(u_T, u_e; v_T, v_e)}{\|(v_T, v_e)\|_M}$$

follows. □

Since the norm (7) is defined as adjoint norm of the partial differential operator applied on (u_T, u_e) we may ask for equivalent norms which are probably simpler to handle. Hence we introduce the space

$$\begin{aligned} \mathbb{Y}_0 := \left\{ (v_T, v_e) \in Y \times Y : \right. \\ \left. \langle M_i \nabla_x v_T, \nabla_x \phi_e \rangle_{L^2(Q)} + \langle (M_i + M_e) \nabla_x v_e, \nabla_x \phi_e \rangle_{L^2(Q)} = 0 \forall \phi_e \in Y \right\} \end{aligned}$$

and the norm

$$\|C_m \partial_t u_T\|_{Y'} := \sup_{0 \neq (v_T, v_e) \in \mathbb{Y}_0} \frac{\langle C_m \partial_t u_T, v_T \rangle_Q}{\|(v_T, v_e)\|_M}. \quad (10)$$

Corollary 1. For $(u_T, u_e) \in X \times Y$ there holds the stability condition

$$\frac{1}{\sqrt{2}} \left[\|(u_T, u_e)\|_M^2 + \|C_m \partial_t u_T\|_{Y'}^2 \right]^{1/2} \leq \sup_{0 \neq (v_T, v_e) \in Y \times Y} \frac{a(u_T, u_e; v_T, v_e)}{\|(v_T, v_e)\|_M}. \quad (11)$$

Proof. We start to consider, by using (9),

$$\begin{aligned} \|(u_T, u_e)\|_{X \times Y}^2 &= a(u_T, u_e; w_T, w_e) \\ &= a(u_T, u_e; u_T, u_e) + a(u_T, u_e; w_T - u_T, w_e - u_e) \\ &= \langle C_m \partial_t u_T, u_T \rangle_{L^2(Q)} + a_S(u_T, u_e; u_T, u_e) + a_S(w_T, w_e; w_T - u_T, w_e - u_e) \\ &\geq a_S(u_T, u_e; u_T, u_e) + a_S(w_T, w_e; w_T - u_T, w_e - u_e) \\ &= a_S(u_T, u_e; u_T, u_e) + a_S(w_T - u_T, w_e - u_e; w_T - u_T, w_e - u_e) \\ &\quad + a_S(u_T, u_e; w_T - u_T, w_e - u_e) \\ &\geq \|(u_T, u_e)\|_M^2 + \|(w_T - u_T, w_e - u_e)\|_M^2 - \|(u_T, u_e)\|_M \|(w_T - u_T, w_e - u_e)\|_M \\ &\geq \frac{1}{2} \left[\|(u_T, u_e)\|_M^2 + \|(w_T - u_T, w_e - u_e)\|_M^2 \right]. \end{aligned}$$

It remains to compute

$$\begin{aligned} \|(w_T - u_T, w_e - u_e)\|_M^2 &= a_S(w_T - u_T, w_e - u_e; w_T - u_T, w_e - u_e) \\ &= a_S(w_T, w_e; w_T - u_T, w_e - u_e) - a_S(u_T, u_e; w_T - u_T, w_e - u_e) \\ &= a(u_T, u_e; w_T - u_T, w_e - u_e) - a_S(u_T, u_e; w_T - u_T, w_e - u_e) \\ &= \langle C_m \partial_t u_T, w_T - u_T \rangle_Q \\ &= \langle C_m \partial_t u_T, z_T \rangle_Q, \end{aligned}$$

where $(z_T, z_e) := (w_T - u_T, w_e - u_e) \in Y \times Y$ is the unique solution of the variational problem

$$a_S(z_T, z_e; v_T, v_e) = \langle C_m \partial_t u_T, v_T \rangle_Q \quad \text{for all } (v_T, v_e) \in Y \times Y, \quad (12)$$

i.e.

$$\begin{aligned} \int_0^T \int_\Omega \left[(M_i \nabla_x z_T, \nabla_x v_T) + (M_i \nabla_x z_e, \nabla_x v_T) \right] dx dt &= \int_0^T \int_\Omega C_m \partial_t u_T v_T dx dt, \\ \int_0^T \int_\Omega \left[(M_i \nabla_x z_T, \nabla_x v_e) + ((M_i + M_e) \nabla_x z_e, \nabla_x v_e) \right] dx dt &= 0. \end{aligned}$$

Hence we conclude

$$\|(z_T, z_e)\|_M^2 = a_S(z_T, z_e; z_T, z_e) = \langle C_m \partial_t u_T, z_T \rangle_Q,$$

i.e.

$$\|(z_T, z_e)\|_M = \frac{\langle C_m \partial_t u_T, z_T \rangle_Q}{\|(z_T, z_e)\|_M} \leq \sup_{0 \neq (v_T, v_e) \in \mathbb{Y}_0} \frac{\langle C_m \partial_t u_T, v_T \rangle_Q}{\|(v_T, v_e)\|_M} =: \|C_m \partial_t u_T\|_{Y'}.$$

On the other hand,

$$\begin{aligned} \|C_m \partial_t u_T\|_{Y'} &= \sup_{0 \neq (v_T, v_e) \in \mathbb{Y}_0} \frac{\langle C_m \partial_t u_T, v_T \rangle_Q}{\|(v_T, v_e)\|_M} \\ &= \sup_{0 \neq (v_T, v_e) \in \mathbb{Y}_0} \frac{a_S(z_T, z_e; v_T, v_e)}{\|(v_T, v_e)\|_M} \leq \|(z_T, z_e)\|_M \end{aligned}$$

implies

$$\|C_m \partial_t u_T\|_{Y'} = \|(z_T, z_e)\|_M,$$

where $(z_T, z_e) \in Y \times Y$ solves the variational problem (12), i.e. the norm (10) is induced by the Schur complement operator of the system (12) when eliminating z_e from the second equation. \square

Remark 1. Instead of the parabolic–elliptic system (1) and (2) we may also consider the related Schur complement system when eliminating the extracellular potential u_e . This results in a parabolic evolution equation with the bounded and elliptic Schur complement operator, and applying arguments as for the standard heat equation, see, e.g., [23], we would conclude a similar stability estimate as given in (11).

3 A Galerkin–Petrov space–time finite element method

We decompose the space–time cylinder $Q = \Omega \times (0, T) \subset \mathbb{R}^{n+1}$ into simplicial finite elements q_ℓ , i.e. $Q_h = \cup_{\ell=1}^N \bar{q}_\ell$. For simplicity, we assume that Ω is polygonal or polyhedral, i.e., $\bar{Q} = Q_h$. The finite element spaces are given by $X_h = S_h^1(Q_h) \cap X$ and $Y_h = X_h$ with $S_h^1(Q_h) = \text{span}\{\varphi_i\}_{i=1}^M$ being the span of piecewise linear and continuous basis functions φ_i .

The conforming discrete Galerkin–Petrov variational formulation of (4) is to find $(u_{T,h}, u_{e,h}) \in X_h \times Y_h \subset X \times Y$ such that

$$a(u_{T,h}, u_{e,h}; v_{T,h}, v_{e,h}) = \int_0^T \int_\Omega [s_i v_{T,h} + s_e v_{e,h}] dx dt \quad (13)$$

is satisfied for all $(v_{T,h}, v_{e,h}) \in Y_h \times Y_h$, where we assume $X_h \subset Y_h$. Analogously as in [23, Theorem 3.1] we can show a discrete inf–sup condition which ensures unique solvability of (13). Related to the variational formulation (12) we define an approximate solution $(z_{T,h}, z_{e,h}) \in Y_h \times Y_h$ of the variational problem

$$a_S(z_{T,h}, z_{e,h}; v_{T,h}, v_{e,h}) = \langle C_m \partial_t u_{T,h}, v_{T,h} \rangle_Q \quad \text{for all } (v_{T,h}, v_{e,h}) \in Y_h \times Y_h, \quad (14)$$

and as in (10) we define the discrete norm

$$\|C_m \partial_t u_{T,h}\|_{Y',h} = \|(z_{T,h}, z_{e,h})\|_M \leq \|(z_T, z_e)\|_M = \|C_m \partial_t u_{T,h}\|_{Y'}.$$

Now we are in a position to prove, as in [23, Theorem 3.1], a discrete stability condition for the bilinear form $a(\cdot, \cdot; \cdot, \cdot)$.

Theorem 1. *Assume $X_h \subset X$, $Y_h \subset Y$, and $X_h \subset Y_h$. Then there holds the discrete stability condition*

$$\begin{aligned} & \frac{1}{2\sqrt{2}} \left[\|(u_{T,h}, u_{e,h})\|_M^2 + \|C_m \partial_t u_{T,h}\|_{Y',h}^2 \right]^{1/2} \\ & \leq \sup_{0 \neq (v_{T,h}, v_{e,h}) \in Y_h \times Y_h} \frac{a(u_{T,h}, u_{e,h}; v_{T,h}, v_{e,h})}{\|(v_{T,h}, v_{e,h})\|_M} \quad \text{for all } (u_{T,h}, u_{e,h}) \in X_h \times Y_h. \end{aligned} \quad (15)$$

Proof. For $(u_{T,h}, u_{e,h}) \in X_h \times Y_h$ let $(z_{T,h}, z_{e,h}) \in Y_h \times Y_h$ be the unique solution of the variational problem (14). We then consider

$$\begin{aligned} a(u_{T,h}, u_{e,h}; u_{T,h} + z_{T,h}, u_{e,h} + z_{e,h}) &= \langle C_m \partial_t u_{T,h}, u_{T,h} \rangle_Q + a_S(u_{T,h}, u_{e,h}; u_{T,h}, u_{e,h}) \\ & \quad + \langle C_m \partial_t u_{T,h}, z_{T,h} \rangle_Q + a_S(u_{T,h}, u_{e,h}; z_{T,h}, z_{e,h}) \\ & \geq a_S(u_{T,h}, u_{e,h}; u_{T,h}, u_{e,h}) + a_S(z_{T,h}, z_{e,h}; z_{T,h}, z_{e,h}) + a_S(u_{T,h}, u_{e,h}; z_{T,h}, z_{e,h}) \\ & \geq \|(u_{T,h}, u_{e,h})\|_M^2 + \|(z_{T,h}, z_{e,h})\|_M^2 - \|(u_{T,h}, u_{e,h})\|_M \|(z_{T,h}, z_{e,h})\|_M \\ & \geq \frac{1}{2} \left[\|(u_{T,h}, u_{e,h})\|_M^2 + \|(z_{T,h}, z_{e,h})\|_M^2 \right] \\ & \geq \frac{1}{2} \left[\|(u_{T,h}, u_{e,h})\|_M^2 + \|C_m \partial_t u_{T,h}\|_{Y',h}^2 \right]. \end{aligned}$$

On the other hand we have

$$\begin{aligned} \|(u_{T,h} + z_{T,h}, u_{e,h} + z_{e,h})\|_M^2 &\leq \left(\|(u_{T,h}, u_{e,h})\|_M + \|(z_{T,h}, z_{e,h})\|_M \right)^2 \\ &\leq 2 \left(\|(u_{T,h}, u_{e,h})\|_M^2 + \|(z_{T,h}, z_{e,h})\|_M^2 \right) \\ &= 2 \left(\|(u_{T,h}, u_{e,h})\|_M^2 + \|C_m \partial_t u_{T,h}\|_{Y',h}^2 \right), \end{aligned}$$

and therefore

$$\begin{aligned} & a(u_{T,h}, u_{e,h}; u_{T,h} + z_{T,h}, u_{e,h} + z_{e,h}) \\ & \geq \frac{1}{2\sqrt{2}} \left[\|(u_{T,h}, u_{e,h})\|_M^2 + \|C_m \partial_t u_{T,h}\|_{Y',h}^2 \right]^{1/2} \|(u_{T,h} + z_{T,h}, u_{e,h} + z_{e,h})\|_M. \end{aligned}$$

follows which implies the assertion. \square

The discrete stability condition (15) implies unique solvability of the Galerkin–Petrov finite element formulation (13). As in [23, Theorem 3.2] we then conclude Cea’s lemma,

$$\begin{aligned} & \left[\| (u_T - u_{T,h}, u_e - u_{e,h}) \|_M^2 + \| C_m \partial_t (u_T - u_{T,h}) \|_{Y',h}^2 \right]^{1/2} \\ & \leq \inf_{(v_{T,h}, v_{e,h}) \in X_h \times Y_h} \left[\| (u_T - v_{T,h}, u_e - v_{e,h}) \|_M^2 + \| C_m \partial_t (u_T - v_{T,h}) \|_{Y'}^2 \right]^{1/2}, \end{aligned}$$

and as in [23, Theorem 3.3] we can prove the following convergence result.

Theorem 2. *Let $(u_T, u_e) \in X \times Y$ and $(u_{T,h}, u_{e,h}) \in X_h \times Y_h$ be the unique solutions of the variational formulations (4) and (13), respectively. Let $Y_h = X_h = S_h^1(Q_h) \cap X$. Assume $(u_{T,h}, u_{e,h}) \in H^2(Q) \times H^2(Q)$. Then there holds the energy error estimate*

$$\|u_T - u_{T,h}\|_{L^2(0,T;H_0^1(\Omega))} + \|u_e - u_{e,h}\|_{L^2(0,T;H_0^1(\Omega))} \leq ch \left[|u_T|_{H^2(Q)} + |u_e|_{H^2(Q)} \right]. \quad (16)$$

From the definition of the bilinear form

$$a(u_T, u_e; v_T, v_e) = \langle C_m \partial_t u_T, v_T \rangle_Q + a_S(u_T, u_e; v_T, v_e)$$

we conclude, by using Lemma 1,

$$\begin{aligned} a(v_{T,h}, v_{e,h}; v_{T,h}, v_{e,h}) &= \langle C_m \partial_t v_{T,h}, v_{T,h} \rangle_Q + a_S(v_{T,h}, v_{e,h}; v_{T,h}, v_{e,h}) \\ &\geq \frac{1}{2} C_m \|u_{T,h}(T)\|_{L^2(\Omega)}^2 + \|(v_{T,h}, v_{e,h})\|_M^2 > 0, \end{aligned}$$

i.e. the stiffness matrix of the space time finite element variational formulation (4) is positive definite which is desirable for algebraic multigrid methods [1, 2, 20].

4 A monolithic algebraic multigrid method

The coupled system of linear equations arises from the variational formulation (13),

$$Ax = b. \quad (17)$$

Here x denotes the vector of coefficients of the finite element approximations for the transmembrane potential u_T and the extracellular potential u_e . In fact, we use a pointwise ordering of unknowns, which means at each node, we have two potential degrees of freedom. This approach has been utilized in the AMG methods for solving fluid and elasticity problems in some monolithic fluid–structure interaction solvers [9].

For coarsening, we use a simple matrix graph based AMG coarsening strategy [8] to generate the hierarchical matrices on coarse levels, see the algorithm in [24, Section 3.2.1] This coarsening strategy usually leads to a very low operator and grid complexity, approximately 1.2 and 1.1, respectively, in our numerical experiments. Here, grid complexity denotes the total number of degrees of freedom on all levels divided by the number of degrees of freedom on the finest level; operator complexity

is the total number of nonzero entries in all matrices on all levels, divided by the number of nonzero entries on the finest level matrix. We refer to [2] for more details. More sophisticated AMG coarsening strategies for the space–time finite element discretization of parabolic equations are reported in [24], that may be considered for such a coupled system in the near future, and help to improve the AMG convergence rate. In addition, we need to have a proper smoother for such a coupled system. For the current being, we employ blockwise ILU [21] as a smoother for such a nonsymmetric system.

5 Numerical results

In the following numerical example we set $\Omega = (0, 1)^2$ and $T = 1$, i.e., the computational domain is a unit cube, $\mathcal{Q} = (0, 1)^3$. For studying the estimated order of convergence (eoc), we consider the exact solution

$$\begin{aligned} u_T(x, t) &= x_1(1 - x_1)x_2(1 - x_2)t(1 - t), \\ u_e(x, t) &= \sin(\pi x_1) \sin(\pi x_2) \sin(\pi t). \end{aligned}$$

We run simulations on 6 mesh refinement levels with tetrahedral elements. On the coarsest level, there are 250 degrees of freedom (#Dofs). The mesh on the next level is obtained by subdividing each tetrahedron on the previously coarser level into 8 smaller tetrahedra. On the finest level, there are 4,293,378 degrees of freedom.

The conductivity matrices are given by

$$M_i = \begin{bmatrix} 0.25 & 0.15 \\ 0.15 & 0.25 \end{bmatrix}, \quad M_e = \begin{bmatrix} 4.95 & 0.05 \\ 0.05 & 4.95 \end{bmatrix},$$

which are diagonally dominant and therefore positive definite. To check assumption (3) we compute $\mu = 12.5$ and $\bar{\mu} = 49$.

The estimated order of convergence (eoc) in $L^2(0, T; H_0^1(\Omega))$ – and $L^2(\mathcal{Q})$ –norms are shown in Table 1 and Table 2 for u_T and u_e , respectively. In the numerical results we observe an almost linear convergence rate in the $L^2(0, T; H_0^1(\Omega))$ –norm as predicted by the theory. Further, we see a second order convergence rate in the $L^2(\mathcal{Q})$ –norm for u_T , and a bit less for u_e .

For the AMG solver, we set the relative residual norm 10^{-11} as a stopping criterion. In the smoothing steps, we apply Richardson iterations to the blockwise ILU preconditioned system. For the current being, we set the relative residual error 0.08 as a stopping criterion for the Richardson iterations in order to achieve multigrid convergence. This requires different smoothing steps on different mesh levels. Future work will concentrate on finding more robust smoothers for such coupled systems. In Table 3, we show the number of AMG iterations (#It), the computational time in seconds (s), the operator complexity (Opt Comp), and the grid complexity (Grid Opt). As observed, we obtain a reasonable AMG performance in terms of AMG

Table 1 Estimated order of convergence (eoc) of $\|u_T - u_{T,h}\|_{L^2(0,T;H_0^1(\Omega))}$ and $\|u_T - u_{T,h}\|_{L^2(Q)}$

#Dofs	$\ u_T - u_{T,h}\ _{L^2(0,T;H_0^1(\Omega))}$	eoc	$\ u_T - u_{T,h}\ _{L^2(Q)}$	eoc
250	1.01e-1	—	1.96e-2	—
1,458	4.76e-2	1.09	8.15e-3	1.26
9,826	1.78e-2	1.42	2.29e-3	1.83
71,874	7.93e-3	1.16	5.65e-4	2.02
549,250	4.15e-3	0.93	1.40e-4	2.02
4,293,378	2.22e-3	0.90	3.60e-5	1.95

Table 2 Estimated order of convergence (eoc) of $\|u_e - u_{e,h}\|_{L^2(0,T;H_0^1(\Omega))}$ and $\|u_e - u_{e,h}\|_{L^2(Q)}$

#Dofs	$\ u_e - u_{e,h}\ _{L^2(0,T;H_0^1(\Omega))}$	eoc	$\ u_e - u_{e,h}\ _{L^2(Q)}$	eoc
250	7.35e-1	—	1.02e-1	—
1,458	4.10e-1	0.84	3.69e-2	1.47
9,826	2.10e-1	0.96	1.14e-2	1.69
71,874	1.06e-1	1.00	3.60e-3	1.67
549,250	5.27e-2	1.00	1.83e-3	1.60
4,293,378	2.64e-2	1.00	4.02e-4	1.56

iterations. Although the operator/grid complexity is low, the computational time is rather high due to the costly ILU smoother and various smoothing steps. This requires further investigations.

Table 3 AMG performance

#Dofs	#It	Time (s)	Opt Comp	Grid Comp
250	4	0.003 s	1.33	1.22
1,458	5	0.025 s	1.24	1.21
9,826	6	0.8 s	1.19	1.18
71,874	7	18 s	1.17	1.16
549,250	12	497 s	1.16	1.15
4,293,378	18	14343 s	1.15	1.15

6 An extension to the nonlinear model

In this section, we extend the space–time finite element method for the linear model to the fully nonlinear bidomain equations: Find the transmembrane potential u_T , the extracellular potential u_e , and the cellular state variable v , satisfying the system of the nonlinear bidomain equations

$$C_m \partial_t u_T(x, t) + I(u_T(x, t), \mathbf{v}(x, t))$$

$$-\operatorname{div}_x[M_i(x)\nabla_x u_T(x, t)] - \operatorname{div}_x[M_i(x)\nabla_x u_e(x, t)] = s_i(x, t), \quad (18)$$

$$-\operatorname{div}_x[M_i(x)\nabla_x(x, t)] - \operatorname{div}_x[(M_i(x) + M_e(x))\nabla_x u_e(x, t)] = s_e(x, t), \quad (19)$$

$$\partial_t \mathbf{v}(x, t) + H(u_T(x, t), \mathbf{v}(x, t)) = s_v(x, t) \quad (20)$$

for $(x, t) \in Q$, with Dirichlet boundary conditions $u_T = g_T$, $u_e = g_e$ on the lateral boundary $\Sigma := \partial\Omega \times (0, T)$, and given initial conditions $u_T = u_0$, $\mathbf{v} = \mathbf{v}_0$ in Ω , $t = 0$. Here, we use the FitzHugh–Nagumo (FHN) model

$$I(u_T(x, t), \mathbf{v}(x, t)) = c_1 u_T(x, t)(u_T(x, t) - u_{th})(u_T(x, t) - 1) + c_2 \mathbf{v}(x, t), \quad (21)$$

$$H(u_T(x, t), \mathbf{v}(x, t)) = b(d\mathbf{v}(x, t), u_T(x, t)) \quad (22)$$

with given positive constants c_1 , c_2 , u_{th} , b , and d .

In this example, the conductivity matrices are given by

$$M_i = \begin{bmatrix} 0.75 & 0.15 \\ 0.15 & 0.75 \end{bmatrix}, \quad M_e = \begin{bmatrix} 1.25 & 0.30 \\ 0.30 & 1.25 \end{bmatrix},$$

and the constants are $c_1 = 0.175$, $c_2 = 0.03$, $u_{th} = 0.12$, $b = d = 10$. We use the exact solutions

$$u_T(x, t) = x_1(1 - x_1)x_2(1 - x_2)t(1 - t),$$

$$u_e(x, t) = \sin(\pi x_1) \sin(\pi x_2) \sin(\pi t),$$

$$\mathbf{v}(x, t) = \cos(\pi x_1) \cos(\pi x_2) \cos(\pi t).$$

The estimated order of convergence (eoc) in $L^2(0, T; H_0^1(\Omega))$ - and $L_2(Q)$ -norms are shown in Table 4, Table 5, and Table 6 for u_T , u_e and \mathbf{v} , respectively. As in the numerical example for the linear case, we see a linear convergence rate in the $L^2(0, T; H_0^1(\Omega))$ -norm. Further, we observe a quadratic convergence rate in the $L_2(Q)$ -norm for V_{lm} , and a bit less for u_e .

Table 4 Estimated order of convergence (eoc) of $\|u_T - u_{T,h}\|_{L^2(0,T;H_0^1(\Omega))}$ and $\|u_T - u_{T,h}\|_{L_2(Q)}$

#Dofs	$\ u_T - u_{T,h}\ _{L_2(0,T;H_0^1(\Omega))}$	eoc	$\ u_T - u_{T,h}\ _{L_2(Q)}$	eoc
375	1.53e−2	—	9.60e−4	—
2,187	8.22e−3	0.90	2.90e−4	1.72
1,4739	3.99e−3	1.04	9.55e−5	1.60
107,811	1.96e−3	1.03	2.60e−5	1.87
823,875	9.74e−4	1.00	6.90e−6	1.91

Table 5 Estimated order of convergence (eoc) of $\|u_e - u_{e,h}\|_{L^2(0,T;H_0^1(\Omega))}$ and $\|u_e - u_{e,h}\|_{L^2(Q)}$

#Dofs	$\ u_e - u_{e,h}\ _{L^2(0,T;H_0^1(\Omega))}$	eoc	$\ u_e - u_{e,h}\ _{L^2(Q)}$	eoc
375	7.37e-1	–	1.08e-1	–
2,187	4.11e-1	0.84	3.98e-2	1.44
1,4739	2.11e-1	0.96	1.23e-2	1.69
107,811	1.06e-1	1.00	3.83e-3	1.68
823,875	5.28e-2	1.00	1.25e-3	1.61

Table 6 Estimated order of convergence (eoc) of $\|v - v_{e,h}\|_{L^2(0,T;H_0^1(\Omega))}$ and $\|v - v_{e,h}\|_{L^2(Q)}$

#Dofs	$\ v - v_{e,h}\ _{L^2(0,T;H_0^1(\Omega))}$	eoc	$\ v - v_{e,h}\ _{L^2(Q)}$	eoc
375	9.74e-1	–	3.90e-2	–
2,187	4.61e-1	1.08	8.79e-3	2.15
1,4739	2.22e-1	1.05	2.08e-3	2.08
107,811	1.10e-1	1.02	5.08e-4	2.03
823,875	5.48e-2	1.00	1.28e-4	1.99

7 Conclusions

In this contribution we have applied a continuous Galerkin–Petrov space–time finite element method [23] to a linear system of parabolic–elliptic equations, which may be considered as a simplified model towards the fully coupled nonlinear bidomain equations. It requires further development in order to apply such a space–time finite method to the full model which includes the nonlinearity and the cellular state variables. Then, for an accurate resolution of the wave type potentials the use of adaptive refined finite element meshes in the space–time domain seems to be mandatory, and motivates the proposed approach.

Under a rather general condition on the conductivities we have shown the stability of the space–time finite element method for the model problem. The linear order of convergence for both potential variables with respect to the spatial energy norm has been confirmed by numerical results.

A monolithic AMG method has been utilized to solve the coupled system of algebraic equations up to about 4.3 million degrees of freedom, which on the one hand, already shows quite nice performance with respect to the AMG iterations, and on the other hand, demands further exploration on finding more robust and efficient smoothers.

Acknowledgements This work has been supported by the Austrian Science Fund (FWF) under the Grant SFB Mathematical Optimization and Applications in Biomedical Sciences.

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