

# AN ORDER OPTIMAL SOLVER FOR THE DISCRETIZED BIDOMAIN EQUATIONS

KENT-ANDRE MARDAL, BJØRN FREDRIK NIELSEN,

XING CAI AND ASLAK TVEITO

ABSTRACT. The electrical activity in the heart is governed by the Bidomain equations. In this paper we analyze an order optimal method for the algebraic equations arising from the discretization of this model. Our scheme is defined in terms of block Jacobi or block symmetric Gauss-Seidel preconditioners. Furthermore, each block in these methods is based on standard preconditioners for scalar elliptic or parabolic partial differential equations (PDEs). Such preconditioners can be realized in terms of multigrid or domain decomposition schemes, and are thus readily available by applying “off-the-shelves” software. Finally, our theoretical findings are illuminated by a series of numerical experiments.

## 1. INTRODUCTION

In this work we analyze an order optimal solution algorithm for the Bidomain model. This model describes the electrical activity in the heart. The physiological relevance and background of the model is discussed in the book [1]. The general equations are on the following

form

$$(1.1) \quad \frac{\partial s}{\partial t} = F(t, s, v, x), \quad x \in H,$$

$$(1.2) \quad \frac{\partial v}{\partial t} = \nabla \cdot (M_i \nabla v) + \nabla \cdot (M_i \nabla u_e) - I(v, s), \quad x \in H,$$

$$(1.3) \quad 0 = \nabla \cdot (M_i \nabla v) + \nabla \cdot ((M_i + M_e) \nabla u_e), \quad x \in H.$$

Here,  $H$  denotes the domain occupied by the heart, the unknowns are the transmembrane potential  $v$  and the extracellular potential  $u_e$ . The tensors  $M_i$  and  $M_e$  describe the intra and extra-cellular conductivities of the heart, and  $s$  denotes the state of the heart cells. In addition, suitable boundary and initial conditions must be specified. Equation (1.1) is a system of (nonlinear) ordinary differential equations (ODEs) that model the behavior of a typical heart cell. Many such cell-models exist, see [2] for an overview. The number of ODEs in (1.1) that must be solved at each grid point typically ranges from 1 to 100 depending on the complexity of the involved cell-model. Further details concerning this topic can be found in [3]. Finally, the equations (1.2) and (1.3) are PDEs of elliptic and parabolic type that are coupled.

The electrophysiology of the heart is characterized by steep gradients in space and time. Thus, very fine scaled meshes and short time steps must be applied, see [4] for a discussion. In 3D the number of nodes needed within the heart is typically between 25 and 50 millions. This implies that it is very important to apply order optimal methods. We

introduced such a method for the Bidomain equations in [5], but there we only provided numerical evidence of optimality.

Ideally, we would like to solve the system (1.1)-(1.3) simultaneously using an implicit numerical scheme. Due to the complexity of the ODEs involved, see e.g. [6], a fully implicit approach is not feasible, and it is common to use some sort of operator splitting; see [4] or [7]. A second order scheme (in time) can be formulated as successive solutions of the two subsystems

$$(1.4) \quad \begin{aligned} \frac{\partial s}{\partial t} &= F(t, s, v, x), \\ \frac{\partial v}{\partial t} &= -I(v, s), \end{aligned}$$

and

$$(1.5) \quad \begin{aligned} \frac{\partial v}{\partial t} &= \nabla \cdot (M_i \nabla v) + \nabla \cdot (M_i \nabla u_e), \\ 0 &= \nabla \cdot (M_i \nabla v) + \nabla \cdot ((M_i + M_e) \nabla u_e). \end{aligned}$$

The details of the splitting can be found in [7].

A complete simulator for cardiac electrophysiology consists of solving the systems (1.4)-(1.5) above at each time step. Here, it is quite obvious that solving (1.4) is an order  $N$  process, where  $N$  denotes the number of computational cells within the heart; since (at least) one ODE is to be solved at each cell. The CPU time needed for this process is proportional to  $N$ . The latter system is much harder to solve and non-optimal approaches may lead to very CPU-demanding computations. It is the purpose of this paper to prove that also this system can be

solved in order  $N$  operations - i.e., that this system can be solved in an order optimal manner.

In Section 2 a discrete approximation of the Bidomain equations is introduced, and Section 3 contains a discussion of block preconditioners, as well as our main result. Our analysis and numerical experiments are presented in sections 4 and 5, respectively. Finally, a brief summary of our findings is given in Section 6.

Note that computational results for the schemes discussed in this text have been reported in [3] and [5], but that their general analysis is presented for the first time in this paper. The basic building blocks for our algorithms are order optimal preconditioners designed for scalar elliptic and parabolic PDEs. For these scalar problems, such methods are typically defined in terms of multigrid or domain decomposition algorithms, see e.g. [8], [9], [10], [11] and [12].

Block preconditioners have been studied by many researchers, e.g., for saddle point problems arising from discretized PDEs [13], [14], [15] and [16]. Rather general results for positive definite matrices are also available; see [17], [18] and [19]. However, as far as the authors know, this is the first paper that provides a theoretical discussion of order optimal block preconditioners for the discretized Bidomain equations.

For a more general discussion of numerical methods for the Bidomain equations, we would like to refer to [20].

## 2. THE DISCRETE PROBLEM

In [5] the following set of equations was studied,

$$(2.1) \quad \frac{\partial v}{\partial t} = \nabla \cdot (M_i \nabla v) + \nabla \cdot (M_i \nabla u_e) \quad \text{in } H,$$

$$(2.2) \quad 0 = \nabla \cdot (M_i \nabla v) + \nabla \cdot ((M_i + M_e) \nabla u_e) \quad \text{in } H,$$

which appear as one step in the operator splitting method for solving the coupled system (1.1)-(1.3). As boundary conditions, we may assign homogeneous Dirichlet conditions for both  $v$  and  $u_e$ , i.e.

$$v = 0 \text{ and } u_e = 0, \quad \text{on } \partial H,$$

or homogeneous Neumann conditions, i.e.

$$\mathbf{n} \cdot (M_i \nabla v + M_i \nabla u_e) = 0 \text{ and } \mathbf{n} \cdot (M_i \nabla v + (M_i + M_e) \nabla u_e) = 0 \text{ on } \partial H,$$

where  $\mathbf{n}$  is the outwards directed unit normal vector defined along the boundary of the heart. Note that  $u_e$  is only determined up to a constant in the case of Neumann conditions. In an operator splitting approach, the initial condition for  $v$  is typically defined by the solution of the ODE system (1.4).

The weak form of (2.1)-(2.2), in the case of homogeneous Dirichlet conditions, reads:

$$\text{Find } (v, u_e) \in L^2(0, T; H_0^1) \times L^2(0, T; H_0^1), \text{ with } \partial v / \partial t \in L^2(0, T; H^{-1}),$$

such that  $v(x, 0) = v_0(x)$  and

$$\begin{aligned} \left(\frac{\partial v}{\partial t}, l\right) + (M_i \nabla v, \nabla l) + (M_i \nabla u_e, \nabla l) &= 0, \quad \forall l \in H_0^1 \text{ and } t \in (0, T], \\ (M_i \nabla v, \nabla m) + ((M_i + M_e) \nabla u_e, \nabla m) &= 0, \quad \forall m \in H_0^1 \text{ and } t \in (0, T], \end{aligned}$$

where  $[0, T]$  is the time interval under consideration, and  $v_0$  incorporates the initial condition for the transmembrane potential  $v$ . Here,  $(\cdot, \cdot)$  denotes the  $L_2$  inner product, as well as the duality pairing between  $H_0^1$  and  $H^{-1}$ . Furthermore,  $H^{-1}$  represents the dual space of  $H_0^1$ .

By applying the Crank-Nicolson method we derive the corresponding semi-discrete problem:

For  $n = 1, 2, \dots, \bar{n}$ , find  $v^n$  and  $u_e^n$  in  $H_0^1$  such that

$$\begin{aligned} (v^n - v^{n-1}, l) + \frac{\Delta t}{2}(M_i \nabla v^n, \nabla l) + \frac{\Delta t}{2}(M_i \nabla u_e^n, \nabla l) &= f_1(l), \quad \forall l \in H_0^1, \\ \frac{\Delta t}{2}(M_i \nabla v^n, \nabla m) + \frac{\Delta t}{2}((M_i + M_e) \nabla u_e^n, \nabla m) &= f_2(m), \quad \forall m \in H_0^1, \end{aligned}$$

where we have scaled the last equation with  $\Delta t$  in order to obtain a symmetric system,  $\bar{n}$  denotes the number of time steps and

$$\begin{aligned} v^0 &= v_0, \\ f_1(l) &= -\frac{\Delta t}{2}(M_i \nabla v^{n-1}, \nabla l) - \frac{\Delta t}{2}(M_i \nabla u_e^{n-1}, \nabla l), \\ f_2(m) &= -\frac{\Delta t}{2}(M_i \nabla v^{n-1}, \nabla m) - \frac{\Delta t}{2}((M_i + M_e) \nabla u_e^{n-1}, \nabla m). \end{aligned}$$

This scheme also requires the extracellular potential at time  $t = 0$ , i.e.  $u_e^0$  is needed. This quantity may naturally be defined as the solution

of the following elliptic equation

$$(2.3) \quad ((M_i + M_e)\nabla u_e^0, \nabla m) = -(M_i\nabla v^0, \nabla m), \quad \forall m \in H_0^1,$$

provided that  $v^0 \in H^1$ . If  $v^0$  is less regular, then a different time stepping scheme must be used. Equation (2.3) is obtained by assuming that (2.2) is valid also for  $t = 0$ .

A Finite Element (FE) approximation is derived by seeking  $(v_h^n, u_{e,h}^n)$  in  $V_h \times V_h \subset H_0^1 \times H_0^1$ , for  $n = 1, 2, \dots, \bar{n}$ , and using test functions  $(l_h, m_h)$  in  $V_h \times V_h$ . This gives the following linear system<sup>1</sup>

$$(2.4) \quad \begin{pmatrix} I + \frac{\Delta t}{2}A_i & \frac{\Delta t}{2}A_i \\ \frac{\Delta t}{2}A_i & \frac{\Delta t}{2}A_{i+e} \end{pmatrix} \begin{pmatrix} v_h^n \\ u_{e,h}^n \end{pmatrix} = \begin{pmatrix} b^n \\ c^n \end{pmatrix},$$

where the matrices  $I, A_i, A_{i+e} \in \mathbb{R}^{k \times k}$ ,  $k = \dim(V_h)$ , satisfy

$$(2.5) \quad (I\psi, \phi) = (\psi, \phi), \quad \forall \psi, \phi \in V_h,$$

$$(2.6) \quad (A_i\psi, \phi) = (M_i\nabla\psi, \nabla\phi), \quad \forall \psi, \phi \in V_h,$$

$$(2.7) \quad (A_{i+e}\psi, \phi) = ((M_i + M_e)\nabla\psi, \nabla\phi), \quad \forall \psi, \phi \in V_h.$$

In the following we will drop the superscript  $n$ , as well as the subscript  $h$ , and focus on how to solve (2.4) at each time step  $n$ . Furthermore,

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<sup>1</sup>We introduced  $(v_h^n, u_{e,h}^n)$  to denote approximations of  $(v, u_e)$  at time step  $n$ .

That is,  $v_h^n$  and  $u_{e,h}^n$  are functions in the finite element space  $V_h$ . In (2.4), however,  $v_h^n$  and  $u_{e,h}^n$  represent the vectors associated with these finite element approximations, rather than the functions. Throughout this paper, we will, for the sake of simplicity, allow this sort of mild abuse of notation.

throughout this text  $b^n$  and  $c^n$ , or simply  $b$  and  $c$ , are used to denote generic right-hand sides, and  $u_e$  will be abbreviated  $u$ .

Above, we applied Dirichlet boundary conditions, and (2.1)-(2.2) was discretized by the Crank-Nicolson method. For the sake of simplicity, our analysis will be presented for this problem. However, by using straightforward techniques, the results derived below can be modified to also cover cases involving Neumann boundary conditions and/or implicit Euler schemes.

### 3. PRECONDITIONERS

As we will show below, equation (2.4) defines a symmetric and positive definite (SPD) linear system. For SPD matrices, the Preconditioned Conjugate-Gradient method (PCG) is the standard method, provided that a suitable SPD preconditioner can be constructed - see [9] for further details.

Two SPD matrices  $\mathcal{B}^{-1}$ ,  $\mathcal{A} \in \mathbb{R}^{p \times p}$ , where  $p$  represents some positive integer, are spectrally equivalent, denoted by  $\mathcal{B}^{-1} \sim \mathcal{A}$ , if

$$(3.1) \quad c_0(\mathcal{B}^{-1}w, w) \leq (\mathcal{A}w, w) \leq c_1(\mathcal{B}^{-1}w, w), \quad \forall w \in \mathbb{R}^p,$$

or equivalently

$$(3.2) \quad c_1^{-1}(\mathcal{B}w, w) \leq (\mathcal{A}^{-1}w, w) \leq c_0^{-1}(\mathcal{B}w, w), \quad \forall w \in \mathbb{R}^p,$$



where  $c_0$  and  $c_1$  must be independent of the discretization parameters<sup>2</sup>  $h$  and  $\Delta t$ . It is well known that if  $\mathcal{B}^{-1} \sim \mathcal{A}$ , then the condition number of the preconditioned operator  $\mathcal{BA}$  satisfies

$$(3.3) \quad \kappa = \kappa(\mathcal{BA}) \leq \frac{c_1}{c_0}.$$

Furthermore, the maximum number of PCG-iterations needed to reach a given convergence criterion is proportional to  $\sqrt{\kappa}$ , cf. e.g. [21]. The solution process is thus order optimal, provided that the storage and evaluation of  $\mathcal{B}$  is similar to that of  $\mathcal{A}$ , i.e.  $\mathcal{O}(N)$  where  $N$  is the number of unknowns.

The system (2.4) can be written on the form

$$(3.4) \quad \mathcal{A} \begin{pmatrix} v \\ u \end{pmatrix} = \begin{pmatrix} A & B \\ B & C \end{pmatrix} \begin{pmatrix} v \\ u \end{pmatrix} = \begin{pmatrix} b \\ c \end{pmatrix},$$

where

$$(3.5) \quad A = I + \frac{\Delta t}{2} A_i,$$

$$(3.6) \quad B = \frac{\Delta t}{2} A_i,$$

$$(3.7) \quad C = \frac{\Delta t}{2} A_{i+e},$$

$$v = v_h^n,$$

$$u = u_{e,h}^n.$$

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<sup>2</sup>We are considering families of matrices  $\mathcal{A}_{h,\Delta t}$  and  $\mathcal{B}_{h,\Delta t}^{-1}$ , and the constants  $c_0$  and  $c_1$  must be independent of both  $h$  and  $\Delta t$ .

Throughout this paper we will assume that the conductivity tensors  $M_i$  and  $M_e$  are symmetric, uniformly positive definite and bounded, i.e. we assume that the matrix entries of  $M_i$  and  $M_e$  are  $L^\infty$  functions and that there exist positive constants  $m_0^i, m_1^i, m_0^e$  and  $m_1^e$  such that

$$(3.8) \quad 0 < m_0^i(\nabla u, \nabla u) \leq (M_i \nabla u, \nabla u) \leq m_1^i(\nabla u, \nabla u), \quad \forall u \in H_0^1,$$

$$(3.9) \quad 0 < m_0^e(\nabla u, \nabla u) \leq (M_e \nabla u, \nabla u) \leq m_1^e(\nabla u, \nabla u), \quad \forall u \in H_0^1.$$

Therefore, the matrices  $A$ ,  $B$  and  $C$  are symmetric and positive definite. For all these submatrices, efficient preconditioners can be constructed in terms of multigrid or domain decomposition algorithms. As we will see below, the use of block structured preconditioners enables us to reuse these “off-the-shelves” preconditioners in a straightforward manner.

We will investigate the efficiency of the following two block preconditioners applied to (3.4).

- Block Jacobi:

$$(3.10) \quad \mathcal{B}_J^{-1} = \begin{pmatrix} A & 0 \\ 0 & C \end{pmatrix}.$$

- Symmetric block Gauss-Seidel:

$$(3.11) \quad \mathcal{B}_{SGS}^{-1} = \begin{pmatrix} A & 0 \\ B & C \end{pmatrix} \begin{pmatrix} A^{-1} & 0 \\ 0 & C^{-1} \end{pmatrix} \begin{pmatrix} A & B \\ 0 & C \end{pmatrix}.$$

Our goal is to prove that  $\mathcal{B}_J^{-1}$  and  $\mathcal{B}_{SGS}^{-1}$  are spectrally equivalent to  $\mathcal{A}$ , i.e. to show that

$$\mathcal{B}_J^{-1} \sim \mathcal{A} \text{ and } \mathcal{B}_{SGS}^{-1} \sim \mathcal{A}.$$

We will refer to the preconditioners  $\mathcal{B}_J$  and  $\mathcal{B}_{SGS}$  in (3.10)-(3.11) as exact preconditioners ( $\mathcal{B}_J$  and  $\mathcal{B}_{SGS}$  are defined in terms of the exact inverses of  $A$  and  $C$ ). These preconditioners are of course not interesting to use in practice. However, as will explained below, it is easy to construct approximations  $\widehat{\mathcal{B}}_J \approx \mathcal{B}_J$  and  $\widehat{\mathcal{B}}_{SGS} \approx \mathcal{B}_{SGS}$  that are spectrally equivalent to  $\mathcal{B}_J$  and  $\mathcal{B}_{SGS}$ . Furthermore, spectral equivalence is associative in the sense that, if  $\mathcal{A}^{-1} \sim \mathcal{B}$  and  $\mathcal{B} \sim \widehat{\mathcal{B}}$ , then  $\mathcal{A}^{-1} \sim \widehat{\mathcal{B}}$ . Therefore, these approximate preconditioners will be spectrally equivalent to  $\mathcal{A}^{-1}$ , provided that  $\mathcal{A}^{-1} \sim \mathcal{B}_J$  and  $\mathcal{A}^{-1} \sim \mathcal{B}_{SGS}$ .

Recall that the operators  $\mathcal{B}_J$  and  $\mathcal{B}_{SGS}$  are defined in terms of the matrices  $A$ ,  $B$  and  $C$ , cf. (3.10) and (3.11). Furthermore,  $A$ ,  $B$  and  $C$  coincide with matrices that arise in connection with FEM discretization procedures of scalar elliptic and parabolic PDEs. For such scalar operators, as mentioned earlier, efficient approximate preconditioners can be constructed by multigrid or domain decomposition methods<sup>3</sup>,

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<sup>3</sup>The coefficients  $M_i$  and  $M_e$  in (2.1)-(2.2) are "well-behaved"; they are symmetric, uniformly positive definite and contain no large jumps. Multigrid and domain decomposition algorithms handle such small variations very well.

see e.g. [8], [9], [10], [11] and [12]. Consequently, approximate preconditioners  $\widehat{\mathcal{B}}_J$  and  $\widehat{\mathcal{B}}_{SGS}$ , that are spectrally equivalent to  $\mathcal{B}_J$  and  $\mathcal{B}_{SGS}$ , are readily available.

Let us now focus on the properties of the operators  $\mathcal{B}_J$  and  $\mathcal{B}_{SGS}$ . Our main result, which we will prove in Section 4, can be formulated as follows:

**Theorem 3.1.** *The preconditioners  $\mathcal{B}_J$  and  $\mathcal{B}_{SGS}$ , defined in (3.10) and (3.11), are spectrally equivalent to the matrix  $\mathcal{A}^{-1}$  in (3.4)-(3.7).*

This means that the PCG method, applying either<sup>4</sup>  $\mathcal{B}_J$  or  $\mathcal{B}_{SGS}$  as preconditioner, defines an order optimal algorithm for the discrete Bidomain equations (2.4).

#### 4. THEORETICAL CONSIDERATIONS

In this section we will, for the sake of generality, start by formulating the algebraic properties that lead to efficient block preconditioners for abstract linear systems on the form

$$(4.1) \quad \mathcal{A} \begin{pmatrix} v \\ u \end{pmatrix} = \begin{pmatrix} b \\ c \end{pmatrix},$$

where

$$(4.2) \quad \mathcal{A} = \begin{pmatrix} A & B \\ B & C \end{pmatrix}.$$

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<sup>4</sup>In practise, we would of course apply approximations  $\widehat{\mathcal{B}}_J \approx \mathcal{B}_J$  or  $\widehat{\mathcal{B}}_{SGS} \approx \mathcal{B}_{SGS}$ .

Thereafter these properties are considered for the system generated by applying the Crank-Nicolson scheme to the Bidomain equations (2.1)-(2.2), i.e. to the system arising by defining the submatrices  $A$ ,  $B$  and  $C$  according to formulas (3.5), (3.6) and (3.7).

Block preconditioners for positive definite matrices are also considered in [17], [18], and [19]. Our derivation of the result for the block symmetric Gauss-Seidel preconditioner in the abstract setting, presented below, is similar to the theory discussed in [17]. However, we end up with suitable bounds expressed in terms of different constants. Our constants, as shown in Section 4.2, are easy to estimate for the discretized Bidomain equations.

**4.1. Results in an abstract setting.** First, we consider the block Jacobi preconditioner  $\mathcal{B}_J$  in (3.10). Recall the definition (3.1) of spectral equivalence. For the matrices (4.2) and (3.10) this means that there must exist constants  $c_0$  and  $c_1$ , independent of  $\Delta t$  and  $h$ , such that

$$(4.3) \quad \begin{aligned} c_0((Av, v) + (Cu, u)) &\leq \\ (Av, v) + 2(Bv, u) + (Cu, u) &\leq \\ c_1((Av, v) + (Cu, u)), \quad \forall v, u \in \mathbb{R}^k \end{aligned}$$

provided that  $B$  is symmetric. Here,  $k$  represents the dimension of the finite element space  $V_h$ .

Assume that

$$(4.4) \quad 2|(Bv, u)| \leq \alpha((Av, v) + (Cu, u)), \quad \forall v, u \in \mathbb{R}^k,$$

where  $0 < \alpha < 1$  is a constant. Please note that this property is closely linked to the coercivity of (4.1) and it turns out to play an important role in our analysis. One might also consider (4.4) to be a sort of "diagonal dominance property" for this block system. We will prove that the linear system associated with the discrete bidomain equations satisfy (4.4) in Section 4.2. The upper bound of (4.3) follows from (4.4):

$$\begin{aligned} (Av, v) + 2(Bv, u) + (Cu, u) & \\ & \leq (Av, v) + 2|(Bv, u)| + (Cu, u) \\ & \leq (1 + \alpha)((Av, v) + (Cu, u)), \quad \forall v, u \in \mathbb{R}^k. \end{aligned}$$

The lower bound of (4.3) also holds:

$$\begin{aligned} (Av, v) + 2(Bv, u) + (Cu, u) & \\ & \geq (Av, v) - 2|(Bv, u)| + (Cu, u) \\ & \geq (1 - \alpha)((Av, v) + (Cu, u)), \quad \forall v, u \in \mathbb{R}^k. \end{aligned}$$

In other words,  $\mathcal{B}_J^{-1} \sim \mathcal{A}$  and  $\kappa(\mathcal{B}_J \mathcal{A}) \leq \frac{1+\alpha}{1-\alpha}$ .

**Lemma 4.1.** *Let  $\mathcal{A}$  and  $\mathcal{B}_J$  be the block matrices defined in (4.2) and (3.10), respectively. If the submatrices  $A$  and  $C$  are invertible,  $B$  is*

symmetric and (4.4) holds, then  $\mathcal{B}_J^{-1} \sim \mathcal{A}$  and the spectral condition number of the preconditioned operator  $\mathcal{B}_J \mathcal{A}$  satisfies

$$\kappa(\mathcal{B}_J \mathcal{A}) \leq \frac{1 + \alpha}{1 - \alpha}.$$

Let us now turn our attention to the symmetric block Gauss-Seidel preconditioner  $\mathcal{B}_{SGS}$  defined in (3.11). In this case, assuming that  $B^T = B$ , the condition (3.1) for spectral equivalence between  $\mathcal{A}$  and  $\mathcal{B}_{SGS}^{-1}$  reads:

(4.5)

$$\begin{aligned} c_0((Av, v) + 2(Bv, u) + (Cu, u) + (BA^{-1}Bu, u)) &\leq \\ (Av, v) + 2(Bv, u) + (Cu, u) &\leq \\ c_1((Av, v) + 2(Bv, u) + (Cu, u) + (BA^{-1}Bu, u)), \quad \forall v, u \in \mathbb{R}^k. \end{aligned}$$

Here, and in the following,  $c_0$  and  $c_1$  are used to denote generic constants (that are independent of the discretization parameters  $h$  and  $\Delta t$ ). Assume that (4.4) is satisfied and that

$$(4.6) \quad 0 \leq (BA^{-1}Bu, u) \leq \beta(Cu, u), \quad \forall u \in \mathbb{R}^k,$$

where  $\beta > 0$  is a constant independent of both  $\Delta t$  and  $h$ .

If (4.6) holds, then

$$\begin{aligned} (Av, v) + 2(Bv, u) + (Cu, u) + (BA^{-1}Bu, u) \\ (4.7) \quad \leq (Av, v) + 2(Bv, u) + (1 + \beta)(Cu, u), \quad \forall v, u \in \mathbb{R}^k. \end{aligned}$$

In addition, since  $\alpha \in (0, 1)$ , assumption (4.4) implies that

$$\begin{aligned} 0 &\leq \alpha(Av, v) + 2(Bv, u) + \alpha(Cu, u) \\ &\leq (Av, v) + 2(Bv, u) + \alpha(Cu, u), \end{aligned}$$

and consequently

$$0 \leq \frac{\beta}{1-\alpha} [(Av, v) + 2(Bv, u) + \alpha(Cu, u)].$$

Adding the right hand side of this inequality to the right hand side of (4.7) yields

$$\begin{aligned} (Av, v) &+ 2(Bv, u) + (Cu, u) + (BA^{-1}Bu, u) \\ &\leq \left(1 + \frac{\beta}{1-\alpha}\right) (Av, v) + 2 \left(1 + \frac{\beta}{1-\alpha}\right) (Bv, u) \\ &\quad + \left(1 + \beta + \frac{\beta\alpha}{1-\alpha}\right) (Cu, u), \quad \forall v, u \in \mathbb{R}^k, \end{aligned}$$

or

$$\begin{aligned} (Av, v) &+ 2(Bv, u) + (Cu, u) + (BA^{-1}Bu, u) \\ &\leq \frac{1-\alpha+\beta}{1-\alpha} [(Av, v) + 2(Bv, u) + (Cu, u)], \quad \forall v, u \in \mathbb{R}^k. \end{aligned}$$

This shows that the lower bound of (4.5) holds with

$$c_0 = \frac{1-\alpha}{1-\alpha+\beta}.$$

The upper bound of (4.5) follows directly from (4.6):

$$\begin{aligned} &(Av, v) + 2(Bv, u) + (Cu, u) + (BA^{-1}Bu, u) \\ &\geq (Av, v) + 2(Bv, u) + (Cu, u) \quad \forall v, u \in \mathbb{R}^k. \end{aligned}$$



In other words,  $\mathcal{B}_{SGS}^{-1} \sim \mathcal{A}$  and  $\kappa(\mathcal{B}_{SGS}\mathcal{A}) \leq \frac{1-\alpha+\beta}{1-\alpha}$ , see (3.3).

**Lemma 4.2.** *Let  $\mathcal{A}$  and  $\mathcal{B}_{SGS}$  be the block matrices defined in (4.2) and (3.11), respectively, and assume that the submatrices  $A$  and  $C$  of  $\mathcal{A}$  are invertible. If (4.4) and (4.6) hold and  $B$  is symmetric, then  $\mathcal{B}_{SGS}^{-1} \sim \mathcal{A}$  and the spectral condition number of the preconditioned operator  $\mathcal{B}_{SGS}\mathcal{A}$  satisfies*

$$\kappa(\mathcal{B}_{SGS}\mathcal{A}) \leq \frac{1-\alpha+\beta}{1-\alpha}.$$

**On Assumption (4.6).** Above we established Lemma 4.2 by assuming that inequalities (4.4) and (4.6) hold. We have already mentioned that (4.4) is closely linked to the coercivity of (4.1). Let us now have a closer look at the latter assumption, i.e. at (4.6). It turns out that this inequality can be established by showing that  $A \sim B$  and  $B \sim C$ . More precisely, if  $A \sim B$  and  $B \sim C$  then  $BA^{-1}B \sim C$ , which in turn implies that (4.6) must hold. The details are as follows: The following inequalities

$$(4.8) \quad c_0(Bu, u) \leq (BA^{-1}Bu, u) \leq c_1(Bu, u), \quad \forall u \in \mathbb{R}^k,$$

and

$$(4.9) \quad \frac{1}{c_1}(Bu, u) \leq (Au, u) \leq \frac{1}{c_0}(Bu, u), \quad \forall u \in \mathbb{R}^k,$$

are equivalent cf. e.g. [22]. Furthermore, by combining (4.8) with

$$(4.10) \quad d_0(Cu, u) \leq (Bu, u) \leq d_1(Cu, u), \quad \forall u \in \mathbb{R}^k,$$

we find that

$$(4.11) \quad c_0 d_0(Cu, u) \leq (BA^{-1}Bu, u) \leq c_1 d_1(Cu, u), \quad \forall u \in \mathbb{R}^k.$$

That is, if  $A \sim B$  and  $B \sim C$  then  $BA^{-1}B \sim C$ . In particular

$$(4.12) \quad 0 \leq (BA^{-1}Bu, u) \leq c_1 d_1(Cu, u), \quad \forall u \in \mathbb{R}^k,$$

provided that  $C$  is positive semidefinite. Finally, we note that only the constants  $c_1$  and  $d_1$  in this argument need to be independent of the  $h$  and  $\Delta t$  in order for (4.12), and consequently (4.6), to hold. Note that  $\beta = c_1 d_1$  in (4.6).

**4.2. Results for the discretized Bidomain equations.** We will now use the general conditions stated above to prove Theorem 3.1. From the assumed properties of the intra and extra -cellular conductivities  $M_i$  and  $M_e$ , we know that there exist positive constants  $m_0^i$ ,  $m_1^i$ ,  $m_0^e$  and  $m_1^e$  such that (3.8) and (3.9) hold. That is, the operators  $L_i u = \nabla \cdot (M_i \nabla u)$  and  $L_e u = \nabla \cdot (M_e \nabla u)$  are uniformly elliptic. We will use these properties to prove Theorem 3.1.

**Proof of  $\mathcal{B}_J^{-1} \sim \mathcal{A}$ .** Consider the system (3.4)-(3.7), arising at every time step in connection with the discretization procedure of the Bidomain equations (2.1)-(2.2) described in Section 2. In this framework, the matrices  $I$ ,  $A_i$  and  $A_{i+e}$  satisfy (2.5)-(2.7).

Since the intra-cellular conductivity  $M_i$  is a symmetric tensor, it follows that the matrix  $B$ , defined in (3.6), is symmetric - see also

(2.6). Consequently, according to Lemma 4.1, it is sufficient to verify condition (4.4) in order to prove that  $\mathcal{B}_J^{-1} \sim \mathcal{A}$ , where  $\mathcal{B}_J$  denotes the Jacobi preconditioner given in (3.10).

More concretely, we have to show that there exists a constant  $\alpha$ , independent of  $h$  and  $\Delta t$ , such that (4.4) is satisfied. For the system (3.4), this condition reads,

$$(4.13) \quad \Delta t |(M_i \nabla v, \nabla u)| \leq \alpha \left( (v, v) + \frac{\Delta t}{2} (M_i \nabla v, \nabla v) + \frac{\Delta t}{2} ((M_i + M_e) \nabla u, \nabla u) \right)$$

for all  $u, v \in H_0^1$ . In order to prove that there is a constant  $\alpha$ ,  $0 < \alpha < 1$ , such that (4.13) holds, we start by observing that, for any  $\epsilon > 0$ , we have

$$0 \leq \left( M_i (\epsilon \nabla v - \frac{1}{\epsilon} \nabla u), \epsilon \nabla v - \frac{1}{\epsilon} \nabla u \right), \quad \forall u, v \in H_0^1,$$

and

$$0 \leq \left( M_i (\epsilon \nabla v + \frac{1}{\epsilon} \nabla u), \epsilon \nabla v + \frac{1}{\epsilon} \nabla u \right), \quad \forall u, v \in H_0^1,$$

from which we conclude that

$$2 |(M_i \nabla v, \nabla u)| \leq \epsilon^2 (M_i \nabla v, \nabla v) + \frac{1}{\epsilon^2} (M_i \nabla u, \nabla u), \quad \forall u, v \in H_0^1.$$

Consequently

$$(4.14) \quad \Delta t |(M_i \nabla v, \nabla u)| \leq \epsilon^2 \left( (v, v) + \frac{\Delta t}{2} (M_i \nabla v, \nabla v) + \frac{1}{\epsilon^4} \frac{\Delta t}{2} (M_i \nabla u, \nabla u) \right)$$

for all  $u, v \in H_0^1$ . Note that (3.8) and (3.9) imply that

$$(M_i \nabla u, \nabla u) \leq \frac{m_1^i}{m_0^e} (M_e \nabla u, \nabla u), \quad \forall u \in H_0^1$$

and thus

$$\begin{aligned} (M_i \nabla u, \nabla u) &= \frac{m_1^i}{m_1^i + m_0^e} (M_i \nabla u, \nabla u) + \frac{m_0^e}{m_1^i + m_0^e} (M_i \nabla u, \nabla u) \\ &\leq \frac{m_1^i}{m_1^i + m_0^e} (M_i \nabla u, \nabla u) + \frac{m_1^i}{m_1^i + m_0^e} (M_e \nabla u, \nabla u) \\ &= \frac{m_1^i}{m_1^i + m_0^e} ((M_i + M_e) \nabla u, \nabla u), \quad \forall u \in H_0^1. \end{aligned}$$

By choosing

$$\epsilon^2 = \left( \frac{m_1^i}{m_1^i + m_0^e} \right)^{1/2}$$

it follows from (4.14) that

$$\begin{aligned} \Delta t |(M_i \nabla v, \nabla u)| &\leq \left( \frac{m_1^i}{m_1^i + m_0^e} \right)^{1/2} \left( (v, v) + \frac{\Delta t}{2} (M_i \nabla v, \nabla v) \right. \\ &\quad \left. + \frac{\Delta t}{2} ((M_i + M_e) \nabla u, \nabla u) \right) \end{aligned}$$

for all  $u, v \in H_0^1$ , which is (4.13) with

$$\alpha = \left( \frac{m_1^i}{m_1^i + m_0^e} \right)^{1/2} \in (0, 1).$$

Obviously, this  $\alpha$  is independent of  $h$ .

The assumption (4.4) needed in Lemma 4.1 thus holds, and we conclude that  $\mathcal{B}_J^{-1} \sim \mathcal{A}$ .

**Proof of  $\mathcal{B}_{SGS}^{-1} \sim \mathcal{A}$ .** Recall the definition (3.11) of the Gauss-Seidel preconditioner  $\mathcal{B}_{SGS}$ . As explained above, the matrix  $B$ , defined in (3.6) is symmetric, and the submatrices  $A$ ,  $B$  and  $C$  in (3.5)-(3.7) satisfy the condition (4.4). Thus, according to Lemma 4.2, it only remains to verify that inequality (4.6) holds in order to show that  $\mathcal{B}_{SGS}^{-1} \sim \mathcal{A}$  for the discretized Bidomain equations.

As explained in the discussion of inequalities (4.8)-(4.12), (4.6) is valid if  $A \sim B$ ,  $B \sim C$  and  $C$  is positive semidefinite. Recall the definition (3.7) of  $C$ , where  $A_{i+e}$  is given in (2.7). Thus, by applying the properties (3.8) and (3.9) of  $M_i$  and  $M_e$  and standard techniques, we indeed conclude that  $C$  is positive definite. Let us therefore focus on the task of establishing inequalities (4.9) and (4.10) for the matrices  $A$ ,  $B$  and  $C$  defined in (3.5)-(3.7).

For the matrices defined in (3.5)-(3.7) and (2.5)-(2.7), the condition (4.9) can be written on the form:

$$(4.15) \quad \begin{aligned} \frac{1}{c_1} \frac{\Delta t}{2} (M_i \nabla u, \nabla u) &\leq (u, u) + \frac{\Delta t}{2} (M_i \nabla u, \nabla u) \\ &\leq \frac{1}{c_0} \frac{\Delta t}{2} (M_i \nabla u, \nabla u), \quad \forall u \in H_0^1. \end{aligned}$$

The lower bound obviously holds for  $c_1 = 1$ , and the upper bound follows from Poincaré's inequality and (3.8),

$$(u, u) \leq C(\nabla u, \nabla u) \leq \frac{C}{m_0^i} (M_i \nabla u, \nabla u) \leq \frac{C}{m_0^i \frac{\Delta t}{2}} \frac{\Delta t}{2} (M_i \nabla u, \nabla u), \quad \forall u \in H_0^1,$$

where the constant  $C$  only depends on the domain  $H$  (where  $H$  denotes the domain occupied by the heart). Consequently, the upper bound in (4.15) holds.

Next, we turn our attention towards condition (4.10). In the present situation, this inequality may be written on the form

$$(4.16) \quad \begin{aligned} d_0((M_i + M_e)\nabla u, \nabla u) &\leq (M_i\nabla u, \nabla u) \\ &\leq d_1((M_i + M_e)\nabla u, \nabla u), \quad \forall u \in H_0^1, \end{aligned}$$

cf. (3.6)-(3.7) and (2.6)-(2.7). From (3.8) and (3.9) it follows that

$$\begin{aligned} ((M_i + M_e)\nabla u, \nabla u) &= (M_i\nabla u, \nabla u) + (M_e\nabla u, \nabla u) \\ &\leq (M_i\nabla u, \nabla u) + m_1^e(\nabla u, \nabla u) \\ &\leq (M_i\nabla u, \nabla u) + \frac{m_1^e}{m_0^i}(M_i\nabla u, \nabla u) \\ &= \left(1 + \frac{m_1^e}{m_0^i}\right)(M_i\nabla u, \nabla u), \quad \forall u \in H_0^1, \end{aligned}$$

and we conclude that the lower bound in (4.16) is fulfilled. The upper bound is true for  $d_1 = 1$ .

From these considerations, it thus follows that inequalities (4.9) and (4.10) hold with  $c_1 = d_1 = 1$ . Note that  $c_0$  depends on  $\Delta t$ . However, as explained in the derivation of (4.12), (4.6) will follow from (4.9) and (4.10) even if  $c_0 = c_0(\Delta t)$ . More specifically, (4.6) holds with  $\beta = c_1 d_1 = 1$ .

The submatrices appearing in the discretized Bidomain equations (3.4) thus satisfy all the assumptions needed in Lemma 4.2, and therefore  $\mathcal{B}_{SGS}^{-1} \sim \mathcal{A}$ . This completes the proof of Theorem 3.1.

## 5. NUMERICAL EXPERIMENTS

For all the experiments to be reported in Tables 5.1 and 5.2, we have partitioned the unit square into bilinear elements and used the standard Galerkin FE method in space and the Crank-Nicolson scheme in time. The 2D conductivity tensors used in these experiments are as follows:

$$(5.1) \quad M_i = \begin{pmatrix} 3.0 & 0 \\ 0 & 0.3 \end{pmatrix} \text{ and } M_e = \begin{pmatrix} 2.0 & 0 \\ 0 & 1.3 \end{pmatrix}.$$

We will first focus on the condition numbers of the linear systems, intending to shed some light onto the consequences of Theorem 3.1. Moreover, cases involving approximate preconditioners  $\widehat{\mathcal{B}}_J \approx \mathcal{B}_J$  and  $\widehat{\mathcal{B}}_{SGS} \approx \mathcal{B}_{SGS}$ , as briefly discussed in Section 3, and Neumann boundary conditions will also be studied.

Table 5.1 shows the condition numbers of the preconditioned operators  $\mathcal{B}_J \mathcal{A}$  and  $\mathcal{B}_{SGS} \mathcal{A}$  for various values of the discretization parameters  $\Delta t$  and  $h$ . These results are clearly in accordance with Theorem 3.1, i.e., the condition numbers are bounded independently of both  $h$  and  $\Delta t$ . Note that these numbers were generated with homogeneous Dirichlet boundary conditions.

Prec	$\mathcal{B}_J\mathcal{A}$					$\mathcal{B}_{SGS}\mathcal{A}$				
$h \setminus \Delta t$	$2^0$	$2^{-1}$	$2^{-2}$	$2^{-3}$	$2^{-4}$	$2^0$	$2^{-1}$	$2^{-2}$	$2^{-3}$	$2^{-4}$
$2^{-1}$	5.9	5.4	4.8	4.0	3.2	2.1	2.0	1.8	1.6	1.4
$2^{-2}$	7.9	7.9	7.7	7.4	6.9	2.8	2.7	2.7	2.6	2.5
$2^{-3}$	8.2	8.2	8.2	8.1	8.0	2.9	2.8	2.8	2.8	2.8
$2^{-4}$	8.3	8.3	8.3	8.2	8.2	2.9	2.9	2.9	2.9	2.9
$2^{-5}$	8.3	8.3	8.3	8.3	8.3	2.9	2.9	2.9	2.9	2.9

TABLE 5.1. Condition numbers obtained with the exact preconditioners  $\mathcal{B}_J$  and  $\mathcal{B}_{SGS}$ .

In Table 5.2 we investigate this issue further. More precisely, the multigrid preconditioner  $\widehat{\mathcal{B}}_J$  was applied instead of the exact preconditioner  $\mathcal{B}_J$ . Furthermore, homogeneous Neumann boundary conditions were used. The multigrid preconditioner consisted of a V-cycle with one pre- and post-smoothing sweep with the symmetric Gauss-Seidel method. As a coarse grid solver, we applied 30 Gauss-Seidel sweeps. (The Neumann boundary conditions make the submatrix  $C$  singular, it can thus not be inverted exactly.) The coarsest grid was defined in terms of a  $2 \times 2$  partition of the unit square, and the grid hierarchy was constructed by applying a successive  $2 \times 2$  refinement procedure. The condition numbers were estimated as a by-product of the CG method; see Chapter 6 of [23]. The CG solver was stopped when the Euclidean norm of the relative residual was less than  $10^{-18}$ .



Again, we observe that the condition numbers are bounded independently of both  $h$  and  $\Delta t$ . Therefore, at least in this case, also  $\widehat{\mathcal{B}}_J$  provides an order optimal preconditioner for the discretized Bidomain equations.

$h \setminus \Delta t$	$2^0$	$2^{-1}$	$2^{-2}$	$2^{-3}$	$2^{-4}$	$2^{-5}$	$2^{-6}$	$2^{-7}$
$2^{-1}$	7.7	7.5	7.1	6.5	5.7	4.6	3.6	2.7
$2^{-2}$	8.1	8.0	7.9	7.6	7.2	6.6	5.7	4.6
$2^{-3}$	8.3	8.2	8.1	8.0	7.8	7.6	7.2	6.6
$2^{-4}$	8.5	8.4	8.3	8.2	8.1	8.0	7.8	7.6
$2^{-5}$	8.5	8.5	8.4	8.4	8.3	8.2	8.1	8.0
$2^{-6}$	8.5	8.5	8.5	8.4	8.4	8.3	8.2	8.2
$2^{-7}$	8.5	8.5	8.5	8.5	8.5	8.4	8.4	8.3
$2^{-8}$	8.5	8.5	8.5	8.5	8.5	8.5	8.4	8.4

TABLE 5.2. Condition numbers obtained with the multi-grid preconditioner  $\widehat{\mathcal{B}}_J$ , i.e. the condition number of  $\widehat{\mathcal{B}}_J \mathcal{A}$  for various values of  $h$  and  $\Delta t$ .

As a set of more challenging cases, we studied the performance of the PCG solver, using the approximate block Jacobi preconditioner  $\widehat{\mathcal{B}}_J$ , for a series of electro-cardiac simulations. In these experiments, a realistic 3D heart domain was discretized by four consecutively refined unstructured meshes, which contained between 11,306 and 4,942,624 mesh points, and a fixed time step  $\Delta t = 0.125$  was applied. Linear

tetrahedral elements were used in the standard Galerkin method, and the conductivity tensors  $M_i$  and  $M_e$  were dependent on the spatial position. That is, the conductivities incorporate the fibrous structure of the heart, see also [3, Chapters 2 and 6]. All the experiments were carried out in the case of homogeneous Neumann boundary conditions.

Four numerical experiments were performed on the four consecutively refined meshes. For approximately inverting the submatrices  $A$  and  $C$ , which are needed in the approximate preconditioner  $\widehat{\mathcal{B}}_J$ , one multigrid V-cycle was used to treat each of the two submatrices. The grid hierarchy associated with each numerical experiment consisted of the chosen mesh and its preceding coarser meshes. That is, the smallest experiment used only one grid level, whereas the largest experiment applied all four levels. On the coarsest grid level, which had 11,306 mesh points, 10 SSOR iterations were used as a coarse grid solver. On the finer levels, two SSOR sweeps were applied as both pre- and post-smoothers. The PCG solver was stopped whenever the Euclidean norm of the relative residual was less than  $10^{-4}$ .

Table 5.3 contains the results obtained in these 3D experiments. The average number of PCG iterations, reported in the table, is based on ten time steps. All of the simulations were performed on a 600 MHz R14000 processor. In particular, we observe that the fraction CPU/ $N$ , where  $N$  denotes the number of mesh points, does not grow as  $N$

$N$	Average Iterations	Average CPU	CPU/ $N$
11,306	12.7	4.85	4.2906e-04
82,768	12.4	20.64	2.4937e-04
632,432	12.4	369.06	5.8356e-04
4,942,624	13.3	2394.33	4.8443e-04

TABLE 5.3. The results obtained in a series of realistic 3D experiments; the average numbers of PCG iterations needed (using the approximate block Jacobi preconditioner  $\widehat{\mathcal{B}}_J$ ) and the CPU usage (measured in seconds) per time step. In this table,  $N$  denotes the number of mesh points in the domain  $H$  occupied by the heart.

increases. This is in accordance with Theorem 3.1, i.e.  $\widehat{\mathcal{B}}_J$  defines an order optimal preconditioner for the discretized Bidomain equations.

For further information about electro-cardiac experiments, including several case studies, we would like to refer to [3].

## 6. SUMMARY

The purpose of this paper has been to analyze block Jacobi and block Gauss-Seidel preconditioners for the discretized Bidomain equations. We have studied this problem as it typically appears in an operator splitting approach for simulating the electrical activity in the human heart. Due to the presence of steep gradients in the involved potentials, this model must be solved on very fine meshes. The number of

unknowns used in this kind of computations, therefore tend to be very large, typically between 25 and 50 million unknowns in 3D.

Our main result, Theorem 3.1, shows that the preconditioned conjugate gradient method defines an order optimal method for solving the discretized Bidomain equations, provided that either the block Jacobi or the block Gauss-Seidel preconditioner is used. Consequently, the CPU time needed by these algorithms will only grow linearly with the number of unknowns used in the computations - leading to very efficient methods. Finally, our theoretical findings were illuminated through a series of numerical experiments, including examples involving realistic geometries and model data.

This paper also contains some rather general results regarding Jacobi and Gauss-Seidel preconditioners for  $2 \times 2$  block systems of linear equations. More precisely, for symmetric and positive definite problems, we have derived suitable conditions that lead to order optimal conjugate gradient schemes for systems of this kind.

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SIMULA RESEARCH LABORATORY, P.O. BOX 134, 1325 LYSAKER, NORWAY.

EMAIL: kent-and@simula.no, bjornn@simula.no, xingca@simula.no, aslak@simula.no