

Inexact BDDC methods for the cardiac Bidomain model

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1 Introduction

The cardiac Bidomain model consists in a reaction-diffusion system of PDEs for the intra- and extra-cellular cardiac potentials coupled with a nonlinear system of ODEs accounting for the cellular model of ionic currents. Fully implicit methods in time have been considered in a few studies, see e.g. [16] and references therein. As in most of previous work (see [18] for a review), in this study we consider an Implicit-Explicit operator splitting technique in order to separate the part of the system of PDEs describing diffusion of cardiac potentials from the large and stiff nonlinear system of ODEs accounting for the reaction terms. The resulting space-time discretization of the so-called parabolic-parabolic Bidomain operator leads to a large, sparse, symmetric positive semidefinite linear system which must be solved at each time step of a cardiac beat simulation using a Krylov subspace method. Given a component by component finite element discretization of the cardiac potentials, the coefficient matrix of the linear system to be solved is

$$\widehat{K} = \begin{bmatrix} A_i & 0 \\ 0 & A_e \end{bmatrix} + \frac{\chi}{\delta_t} \begin{bmatrix} M & -M \\ -M & M \end{bmatrix} \quad (1)$$

where δ_t is the value of the time step and χ the membrane capacitance per unit volume; M and $A_{i,e}$ are the mass and stiffness matrices with entries

$$\{M\}_{rs} = \int_{\Omega} \phi_h^r \phi_h^s, \quad \{A_{i,e}\}_{rs} = \int_{\Omega} D_{i,e} \nabla \phi_h^r \cdot \nabla \phi_h^s,$$

where for sake of simplicity the same finite element basis $\{\phi_h^j\}$ is considered for each cardiac potential. Anisotropic conductivity tensors $D_i(x)$ and $D_e(x)$ model propagation of electrical signals with orthotropic anisotropy

$$D_{i,e}(x) = \sum_{j=1}^3 \sigma_j^{i,e}(x) \mathbf{a}_j(x) \mathbf{a}_j(x)^T,$$

with $\sigma_j^{i,e}(x) > 0$ the conductivity coefficient of the intra- and extra-cellular media measured along the orthonormal triplet $\{\mathbf{a}_j(x)\}_{j=1}^3$ describing cardiac fiber rotation [9]. For additional details on the operator splitting technique adopted and the diffusion tensors, see [6].

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Many different preconditioners have been already proposed for the efficient iterative solution of the Bidomain model in its parabolic-parabolic formulation (1). Among them, we mention block Jacobi preconditioners [6], algebraic multigrid [13, 14], multilevel Schwarz preconditioners [11, 15, 12] and balancing Neumann-Neumann methods [19]. An exact BDDC algorithm and a FETI-DP method have been constructed, analyzed and experimentally validated by the Author in [20].

2 Inexact BDDC preconditioner

Following the framework of substructuring algorithms [17], the cardiac domain Ω is decomposed into N non-overlapping open Lipschitz subdomains Ω_j of diameter H_j , forming a coarse conforming finite element partition of Ω and naturally defining the interface, i.e.

$$\overline{\Omega} = \bigcup_{i=j}^N \overline{\Omega}_j, \quad \Gamma = \bigcup_{j \neq k} \partial\Omega_j \cap \partial\Omega_k, \quad \Gamma_j = \partial\Omega_j \cap \Gamma.$$

A triangulation is introduced in each subdomain with matching finite element nodes on the boundaries of adjacent subdomains across the interface. As usual in non-overlapping literature, the finite elements space defined on Ω_j will be denoted by $\mathbf{W}^{(j)}$ and it is further split into its interior (labeled by I) and interface (Γ) parts; the following spaces should then be introduced

$$\mathbf{W}^{(j)} = \mathbf{W}_I^{(j)} \oplus \mathbf{W}_\Gamma^{(j)}, \quad \mathbf{W} = \prod_{j=1}^N \mathbf{W}^{(j)}, \quad \mathbf{W}_I = \prod_{j=1}^N \mathbf{W}_I^{(j)},$$

together with the subspace $\widehat{\mathbf{W}} \subset \mathbf{W}$ of continuous functions. Within the non-overlapping framework, a global matrix is never assembled explicitly; instead a Bidomain linear matrix $K^{(j)}$ is assembled on each subdomain and reordered as

$$\begin{bmatrix} K_{II}^{(j)} & K_{I\Gamma}^{(j)} \\ K_{I\Gamma}^{(j)T} & K_{\Gamma\Gamma}^{(j)} \end{bmatrix}.$$

The unassembled global matrix defined on \mathbf{W} can thus be defined as $K = \text{diag}(K^{(j)})$; similarly, $K_{II} = \text{diag}(K_{II}^{(j)})$.

The exact BDDC preconditioner for matrix \widehat{K} can be formulated as (see [8, 10])

$$M_{BDDC}^{-1} = M_I^{-1} + (I - M_I^{-1} \widehat{K}) M_\Gamma^{-1} (I - \widehat{K} M_I^{-1}),$$

where

$$M_I^{-1} = R_I^T K_{II}^{-1} R_I, \quad M_\Gamma^{-1} = R_D^T (P_{coarse} + P_{local}) R_D,$$

with R_I the restriction operator from $\widehat{\mathbf{W}}$ to \mathbf{W} and R_D the scaled restriction operator from $\widehat{\mathbf{W}}$ to \mathbf{W} built using a suitable partition of unity [20]. The coarse term of the preconditioner can be defined by

$$P_{coarse} = \Psi K_c^{-1} \Psi^T, \quad K_c = \Psi^T K \Psi,$$

with the coarse primal basis function matrix given by the solution of the following minimization problem posed on \mathbf{W}

$$\Psi = \arg \min w^T K w, \text{ s.t. } C w = I,$$

where I is the identity matrix and C is the block diagonal matrix of BDDC constraints which ensures the continuity of coarse basis functions at primal degrees of freedom. The action of the local term of the preconditioner is given by

$$\begin{bmatrix} K & C^T \\ C & 0 \end{bmatrix} \begin{bmatrix} P_{local} g \\ \mu \end{bmatrix} = \begin{bmatrix} g \\ 0 \end{bmatrix}.$$

The application of the BDDC preconditioner requires the solution of the block diagonal Dirichlet and Neumann problems given by the matrices K_{II} and K_{rr} respectively, where K_{rr} is obtained from K by removing the matrix entries related to the subdomain vertices belonging to the coarse primal space [8].

It is well known that the local problems defined by the BDDC preconditioner can be bottlenecks in three dimensions, since direct factorizations require too much time and memory if the number of degrees of freedom in any subdomain is large; also, backward and forward substitution algorithms do not map well on modern architectures and accelerators. A possible solution consists in using multigrid preconditioners as black-box inexact solvers for the local Dirichlet and Neumann problems as proposed by Dohrmann [8]; the approach preserves scalability and quasi-optimality of the exact BDDC method provided a sufficient quality of the inexact solvers.

An approximate BDDC preconditioner can be constructed as follows: let \widehat{K}^\flat be the matrix which is equal to \widehat{K} except for the coupling of the interior degrees of freedom and let K^\sharp be the matrix equal to K except for the blocks related to the Neumann problem of the BDDC preconditioner, i.e.

$$\widehat{K}^\flat = \begin{bmatrix} K_{II}^\flat & K_{I\Gamma} \\ K_{I\Gamma}^T & K_{\Gamma\Gamma} \end{bmatrix}, \quad K^\sharp = \begin{bmatrix} K_{rr}^\sharp & K_{rv} \\ K_{rv}^T & K_{vv} \end{bmatrix}.$$

In practice, matrices K_{II}^\flat and K_{rr}^\sharp are not explicitly known, since they represent an approximation of the exact matrices through the multigrid process.

Inexact solvers can be obtained in such a way that K^\flat and K^\sharp will be spectrally equivalent to the exact matrices

$$\begin{aligned} \gamma_1 g^T \widehat{K} g &\leq g^T \widehat{K}^\flat g \leq \gamma_2 g^T \widehat{K} g & \forall g \in \widehat{\mathbf{W}}, & (2) \\ \alpha_1 g^T K g &\leq g^T K^\sharp g \leq \alpha_2 g^T K g & \forall g \in \mathbf{W}. & (3) \end{aligned}$$

where $0 < \gamma_1 \leq \gamma_2$ and $0 < \alpha_1 \leq \alpha_2$ are constants independent on h and $H = \max_j H_j$. A priori estimates for the latter constants are not required for the implementation, but they can be estimated by conjugate gradient iterations. In addition, if the matrix \widehat{K} is singular as for the Bidomain model, matrices K^{\flat} and K^{\sharp} should satisfy the so called null space property

$$\ker(\widehat{K}^{\flat}) = \ker(\widehat{K}), \quad \ker(K^{\sharp}) = \ker(K).$$

Given a candidate preconditioner P_{II}^{-1} for $K_{II}^{\flat-1}$, the following correction was proposed in [8] to satisfy the null space property

$$K_{II}^{\flat-1} = N_I(N_I^T K_{II} N_I)^{-1} N_I^T + E_I^T P_{II}^{-1} E_I, \quad (4)$$

where

$$E_I = I - K_{II} N_I (N_I^T K_{II} N_I)^{-1} N_I^T,$$

with I the identity matrix and N_I the restriction of $\ker(\widehat{K})$ to the interior degrees of freedom. The same argument holds true for the Neumann problem, thus

$$K_{rr}^{\sharp-1} = N_r(N_r^T K_{rr} N_r)^{-1} N_r^T + E_r^T P_{rr}^{-1} E_r, \quad (5)$$

where

$$E_r = I - K_{rr} N_r (N_r^T K_{rr} N_r)^{-1} N_r^T,$$

with P_{rr}^{-1} a candidate preconditioner for $K_{rr}^{\sharp-1}$.

The action of the approximate BDDC preconditioner can then be defined as

$$\widetilde{M}_{BDDC}^{-1} = M_I^{\flat-1} + (I - M_I^{\flat-1} \widehat{K}^{\flat}) M_I^{\sharp-1} (I - \widehat{K}^{\flat} M_I^{\flat-1}),$$

where the superscript \flat (respectively \sharp) denote quantities obtained by replacing the matrix \widehat{K} (resp. K) by K^{\flat} (resp. K^{\sharp}) in the construction of the BDDC operator. In other words,

$$M_I^{\flat-1} = R_I^T K_{II}^{\flat-1} R_I, \quad M_I^{\sharp-1} = R_D^T \left[P_{coarse}^{\sharp} + P_{local}^{\sharp} \right] R_D,$$

with

$$P_{coarse}^{\sharp} = \Psi^{\sharp} K_c^{\sharp-1} \Psi^{\sharp T}, \quad K_c^{\sharp} = \Psi^{\sharp T} K^{\sharp} \Psi^{\sharp},$$

and the block saddle point matrix is modified as

$$\begin{bmatrix} K^{\sharp} & C^T \\ C & 0 \end{bmatrix}.$$

For further details on the inexact approach considered, see [8].

The following theorem holds (see [8] for the proof).

Theorem 1. *The condition number of the approximate BDDC preconditioner can be bounded from above by the condition number of the exact BDDC preconditioner as*

$$\kappa_2(\tilde{M}_{BDDC}^{-1}\hat{K}) \leq C \frac{\alpha_2 \gamma_2^3}{\alpha_1 \gamma_1^3} \kappa_2(M_{BDDC}^{-1}\hat{K}),$$

where γ_1 and γ_2 are given by (2), α_1 and α_2 by (3) and C is a constant independent of the parameters of the spatial discretization h and H and the number of subdomains N . Moreover, if the coarse problem A_c^\sharp is solved inexactly by the action of a preconditioner $A_c^{\sharp\sharp-1}$ satisfying

$$\beta_1 g^T A_c^{\sharp\sharp-1} g \leq g^T A_c^{\sharp\sharp-1} g \leq \beta_2 g^T A_c^{\sharp\sharp-1} g,$$

with $0 < \beta_1 \leq \beta_2$, it will hold

$$\kappa_2(\tilde{M}_{BDDC}^{-1}\hat{K}) \leq C \frac{\max\{1, \beta_2\} \alpha_2 \gamma_2^3}{\min\{1, \beta_1\} \alpha_1 \gamma_1^3} \kappa_2(M_{BDDC}^{-1}\hat{K}).$$

A quasi-optimal bound for the condition number of the exact BDDC method for the Bidomain model in the parabolic-parabolic form has been proved in [20].

Theorem 2. *Let the BDDC coarse primal space be spanned by the vertex nodal finite element functions and the edge cut-off functions. Then, for the three-dimensional Bidomain model, it will hold*

$$\kappa_2(M_{BDDC}^{-1}\hat{K}) \leq C(1 + \log(H/h))^2,$$

with $H = \max_j H_j$ and C a constant independent of h , H , N and possible jumps in conductivity coefficients $\sigma_k^{(i,e)}$ of the Bidomain operator aligned with Γ .

3 Numerical results

In this Section parallel numerical experiments are presented for a parallelepipedal domain Ω subdivided into $N = N_x \times N_y \times N_z$ subdomains. Each Ω_j is discretized by low-order Q^1 finite elements, i.e. conforming hexaedral shape-regular isoparametric tri-linear finite elements of characteristic diameter h . The linear system (1) is solved by the preconditioned conjugate gradient (PCG) algorithm with a zero initial guess and stopping criterion $\|r_k\|_2 / \|r_0\|_2 \leq 10^{-6}$, where r_k is the preconditioned residual at the k th iterate. The right-hand side is always random and uniformly distributed. Extreme eigenvalues of the preconditioned operators, denoted by λ_m and λ_M in the following, are estimated using the well-known recursive formula for Lanczos iterations; the experimental condition number is computed as $\kappa_2 = \lambda_M / \lambda_m$.

The parallel code used to obtain the numerical results has been developed in Fortran and C; the Message Passing Interface (MPI) library has been used for paral-

lization, assigning one subdomain to one MPI process. The BDDC preconditioner has been developed using the Portable Extensible Toolkit for Scientific Computation [5] (PETSc) and it is available for download within the development version of the library (see <https://bitbucket.org/petsc/petsc>). Whenever the BDDC algorithm is exactly applied, local problems are solved using the Unsymmetric Multifrontal sparse LU factorization package [7] (UMFPACK), while the algebraic multigrid (AMG) method boomerAMG provided by the HYPRE library [3] is used as a black-box solver within the inexact BDDC algorithm. The interested reader is referred to [13, 14] where the AMG method has been successfully applied to the serial and parallel solution of the Bidomain linear system. The BDDC coarse problem is solved in parallel either with the MULTifrontal Massively Parallel sparse direct Solver [4] (MUMPS) or inexactly with the parallel boomerAMG method. For all test cases considered, the coarse space is spanned by subdomain vertices and edge averages for both cardiac potentials; unless otherwise stated, the conductivity coefficients used are reported in [6]. One $V_{1,1}$ -cycle with Gauss-Seidel smoothing is always used for the AMG method in order to preserve symmetry of the resulting operator.

Table 1 contains results of a quasi-optimality test obtained on the x86_64 Linux cluster Matrix of CASPUR [1], where each core is equipped with 2GB memory. In this test case, Ω is divided in $3 \times 3 \times 3$ subdomains, $h=1E-2$, $\delta_i=1E-2$ and increasing values of H are considered; thus, the volume of Ω increases as H/h increases. Inexact solvers are used for both sets of local problems whereas the coarse problem is solved exactly with a parallel factorization. AMG based local solvers does not make the performances of the BDDC deteriorate with respect to H/h and they allow us to manage larger local problems, since the memory requirements for a multigrid preconditioner are linear in the local size. Quasi-optimality is thus preserved by the inexact BDDC algorithm for the Bidomain model.

Table 1 Comparison between exact and inexact BDDC method for different values of H/h . For each run, extreme eigenvalues, condition number and number of iterations are shown. Test case with $h=1E-2$ and $3 \times 3 \times 3$ subdomains.

$\frac{H}{h}$	$M_{BDDC}^{-1} \widehat{K}$				$\widetilde{M}_{BDDC}^{-1} \widehat{K}$			
	λ_m	λ_M	κ_2	it	λ_m	λ_M	κ_2	it
5	1.00	1.45	1.45	6	0.88	1.42	1.61	7
10	1.00	2.28	1.28	9	0.88	2.14	2.45	10
15	1.00	2.98	2.98	11	0.87	2.66	3.06	11
20	1.00	3.49	3.49	13	0.87	3.17	3.71	13
25	1.00	4.02	4.02	13	0.85	3.56	4.18	14
30	<i>out of memory</i>				0.76	3.91	5.14	15
35	<i>out of memory</i>				0.75	4.23	5.60	16
40	<i>out of memory</i>				0.70	4.43	6.27	16

Table 2 contains experimental results of a weak scalability test for the inexact BDDC algorithm on the BlueGene/Q FERMI of CINECA [2]; total number of de-

degrees of freedom (dofs), condition number, number of PCG iterations and solving time per iteration (time/it) in seconds are reported. In the test case, $h=1E-2$, $H/h=30$, $\delta_i=1E-2$ and the number of subdomains N grows in each dimension as reported in the first two columns. Thus, the volume of Ω increases as N increases. Inexact solvers for both local problems and, in parallel, for the coarse problem are used. Results are scalable in the number of iterations and solving time per iteration up to 4K cores and 200 millions degrees of freedom.

Table 2 Weak scalability test for the inexact BDDC method. For each run, number of subdomains and domain decomposition, number of degrees of freedom (dofs), condition number, number of PCG iterations (it) and solving time per iteration are shown. Test case with $h=1E-2$ and $H/h=30$.

N	subd	dofs	$\kappa_2(\tilde{M}_{BDDC}^{-1}\hat{K})$	it	time/it (s)
8	2x2x2	410.758	5.79	13	0.96
64	4x4x4	3.203.226	5.79	13	0.94
512	8x8x8	25.298.674	9.81	15	1.01
4096	16x16x16	201.089.250	11.12	16	1.12

Finally, we report on a test case with coefficients with jumps aligned with Γ , obtained on the x86_64 Linux cluster Matrix of CASPUR [1]. As test case, we consider a 3x3x3 decomposition of Ω , $h=1E-2$, $H/h=15$ and $\delta_i=1E-2$; inexact solvers are used for both local problems, instead the coarse problem is solved exactly with a parallel factorization. Two different checkerboard patterns of discontinuities in the conductivity coefficients are considered; conductivity coefficients are initially set to $\sigma_1^{i,e}=10$, $\sigma_2^{i,e}=1$ and $\sigma_3^{i,e}=0.1$, then the following cases are built given a factor $p > 0$:

- A** Each conductivity coefficient, either intra- or extra-cellular, is multiplied by p in the black subdomains and by $1/p$ in the white subdomains.
- B** Intra-cellular coefficients are multiplied by p in the black subdomains and by $1/p$ in white subdomains; conversely, extra-cellular coefficients are multiplied by $1/p$ in the black subdomains and by p in white subdomains.

Numerical results are summarized in Table 3, with columns labeled according to the previous classification. The condition number and the number of iterations (listed in round brackets) of the inexact BDDC algorithm remain almost constant when we vary the factor p largely in both test cases considered; the ratio between inexact and exact condition number is also shown to highlight the quality of the inexact approach.

References

1. CASPUR HPC home page. <http://hpc.caspur.it>

Table 3 Condition number dependence of inexact BDDC method with coefficient jumps. For each run, condition number and number of iterations in round brackets are shown together with the ratio between condition numbers of the exact and inexact BDDC. Test case with $h=1E-2$, $H/h=15$ and $3 \times 3 \times 3$ subdomains.

p	A		B	
	$\kappa_2(\tilde{M}_{BDDC}^{-1}\hat{K})$	ratio	$\kappa_2(\tilde{M}_{BDDC}^{-1}\hat{K})$	ratio
1	10.47 (20)	1.47	10.47 (20)	1.47
1E1	12.41 (22)	1.46	12.12 (21)	1.49
1E2	12.54 (22)	1.46	13.70 (24)	1.60
1E3	13.75 (23)	1.57	15.13 (24)	1.78

2. CINECA HPC home page. <http://hpc.cineca.it>
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