Scalable BDDC Algorithms for Cardiac Electromechanical Coupling

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1 Introduction

The spread of electrical excitation in the cardiac muscle and the subsequent contraction-relaxation process is quantitatively described by the cardiac electromechanical coupling model. The electrical model consists of the Bidomain system, which is a degenerate parabolic system of two nonlinear partial differential equations (PDEs) of reaction-diffusion type, describing the evolution in space and time of the intra- and extracellular electric potentials. The PDEs are coupled through the reaction term with a stiff system of ordinary differential equations (ODEs), the *membrane model*, which describes the flow of the ionic currents through the cellular membrane and the dynamics of the associated gating variables. The mechanical model consists of the quasi-static finite elasticity system, modeling the cardiac tissue as a nearly-incompressible transversely isotropic hyperelastic material, and coupled with a system of ODEs accounting for the development of biochemically generated active force.

The numerical approximation of the cardiac electromechanical coupling is a challenging multiphysics problem, because the space and time scales associated with the electrical and mechanical models are very different, see e.g. Chapelle et al. [2012], Sundnes et al. [2014]. Moreover, the discretization of the model leads to the solution of a large nonlinear system at each time step, which is often decoupled by an operator splitting techniques into the solution of a large linear system for the electrical part and a nonlinear system for the mechanical part.

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While several studies in the last decade have been devoted to the development of efficient solvers and preconditioners for the Bidomain model, see e.g. Plank et al. [2007], Pavarino and Scacchi [2008], Zampini [2014] and the recent monograph by Colli Franzone et al. [2014], a few studies have focused on the development of efficient solvers for the quasi-static cardiac mechanical model, see Vetter and McCulloch [2000], Rossi et al. [2012], Gurev et al. [2011].

In this paper, we present new numerical results for a Balancing Domain Decomposition by Constraints (BDDC) preconditioner, first introduced in Dohrmann [2003], here embedded in a Newton-Krylov (NKBDDC) method, introduced in Pavarino et al. [2015] for the nonlinear system arising from the discretization of the finite elasticity equations. The Jacobian system arising at each Newton step is solved iteratively by a BDDC preconditioned GMRES method. We report here the results of three-dimensional numerical tests on a BlueGene/Q machine, showing the scalability of the NKBDDC mechanical solver.

2 Cardiac Electromechanical Models

a) Mechanical model of cardiac tissue. We denote by $\mathbf{X} = (X_1, X_2, X_3)^T$ the material coordinates of the undeformed cardiac domain $\widehat{\Omega}$, by $\mathbf{x} = (x_1, x_2, x_3)^T$ the spatial coordinates of the deformed cardiac domain $\Omega(t)$ at time t, and by $\mathbf{F}(\mathbf{X}, t) = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}$ the deformation gradient. The cardiac tissue is modeled as a nonlinear hyperelastic material satisfying the steady-state force equilibrium equation

$$\mathrm{Div}(\mathbf{FS}) = \mathbf{0}, \qquad \mathbf{X} \in \widehat{\Omega}. \tag{1}$$

The second Piola-Kirchoff stress tensor $\mathbf{S} = \mathbf{S}^{pas} + \mathbf{S}^{vol} + \mathbf{S}^{act}$ is the sum of passive, volumetric and active components. The passive and volumetric components are defined as $S_{ij}^{pas,vol} = \frac{1}{2}\left(\frac{\partial W^{pas,vol}}{\partial E_{ij}} + \frac{\partial W^{pas,vol}}{\partial E_{ji}}\right) \quad i,j = 1,2,3,$ where $\mathbf{E} = \frac{1}{2}(\mathbf{C} - \mathbf{I})$ and $\mathbf{C} = \mathbf{F}^T\mathbf{F}$ are the Green-Lagrange and Cauchy strain tensors, W^{pas} is an exponential strain energy function (derived from Eriksson et al. [2013]) modeling the myocardium as a transversely isotropic hyperelastic material, and $W^{vol} = K\,(J-1)^2$ is a volume change penalization term accounting for the almost incompressibility of the myocardium, with K a positive bulk modulus and $J = det(\mathbf{F})$.

b) Mechanical model of active tension. The active component $\mathbf{S}^{act}$ develops along the myofiber direction, $\mathbf{S}^{act} = T_a \frac{\widehat{\mathbf{a}}_l \widehat{\mathbf{a}}_l}{\widehat{\mathbf{a}}_l^T \mathbf{C} \widehat{\mathbf{a}}_l}$, where $\widehat{\mathbf{a}}_l$ is the fiber direction and $T_a = T_a\left(Ca_i, \lambda, \frac{d\lambda}{dt}\right)$ is the biochemically generated active tension, which depends on intracellular calcium concentrations, and the myofiber stretch $\lambda = \sqrt{\widehat{\mathbf{a}}_l^T \mathbf{C} \widehat{\mathbf{a}}_l}$ and stretch-rate $\frac{d\lambda}{dt}$ (see Land et al. [2012]).

c) Electrical model of cardiac tissue: the Bidomain model. We will use the following parabolic-elliptic formulation of the modified Bidomain model on the reference configuration $\widehat{\Omega} \times (0,T)$,

$$\begin{cases} c_m J \dfrac{\partial \widehat{v}}{\partial t} - \mathrm{Div}(J\ \mathbf{F}^{-1} D_i \mathbf{F}^{-T}\ \mathrm{Grad}(\widehat{v} + \widehat{u}_e)) + J\ i_{ion}(\widehat{v}, \widehat{\mathbf{w}}, \widehat{\mathbf{c}}) = 0 \\ -\mathrm{Div}(J\ \mathbf{F}^{-1} D_i \mathbf{F}^{-T}\ \mathrm{Grad}\, \widehat{v}) - \mathrm{Div}(J\ \mathbf{F}^{-1}(D_i + D_e)\mathbf{F}^{-T}\ \mathrm{Grad}\, \widehat{u}_e) = J\ \widehat{i}^{\,e}_{app} \\ \dfrac{\partial \widehat{\mathbf{w}}}{\partial t} - \mathbf{R}_w(\widehat{v}, \widehat{\mathbf{w}}) = 0, \qquad \dfrac{\partial \widehat{\mathbf{c}}}{\partial t} - \mathbf{R}_c(\widehat{v}, \widehat{\mathbf{w}}, \widehat{\mathbf{c}}) = 0. \end{cases} \tag{2}$$

for the transmembrane potential $\widehat{v}$, the extracellular potential $\widehat{u}_e$, and the gating and ionic concentrations variables $(\widehat{\mathbf{w}}, \widehat{\mathbf{c}})$. This system is completed by prescribing initial conditions, insulating boundary conditions, and the applied current $\widehat{i}^{\,e}_{app}$; see Colli Franzone et al. [2016] for further details. The axisymmetric conductivity tensors are given by $D_{i,e}(\mathbf{x}) = \sigma_l^{i,e}\ \mathbf{a}_l(\mathbf{x})\mathbf{a}_l^T(\mathbf{x}) + \sigma_t^{i,e}\ \mathbf{a}_t(\mathbf{x})\mathbf{a}_t^T(\mathbf{x})$, where $\sigma_l^{i,e}$, $\sigma_t^{i,e}$ are the conductivity coefficients in the intra- and extracellular media measured along and across the fiber direction $\mathbf{a}_l, \mathbf{a}_t$.

d) Ionic membrane model and stretch-activated channel current. The functions $I_{ion}(v, \mathbf{w}, \mathbf{c})$ $(i_{ion} = \chi I_{ion})$, $R_w(v, \mathbf{w})$ and $R_c(v, \mathbf{w}, \mathbf{c})$ in the Bidomain model (2) are given by the ionic membrane model introduced by ten Tusscher et al. [2004], available from the cellML depository (models.cellml.org/cellml). χ denotes the cellular surface to volume ratio.

3 Methods

Space and time discretization We discretize the cardiac domain with a hexahedral structured grid T_{h_m} for the mechanical model (1) and T_{h_e} for the electrical Bidomain model (2), where T_{h_e} is a refinement of T_{h_m}. We then discretize all scalar and vector fields of both mechanical and electrical models by isoparametric Q_1 finite elements in space. The time discretization is performed by a semi-implicit splitting method; see Colli Franzone et al. [2016] for further details.

Computational kernels. Due to the discretization strategies described above, the main computational kernels of our solver at each time step are the following:

1- solve the nonlinear system deriving from the discretization of the mechanical problem (1) using an inexact Newton method. At each Newton step, a nonsymmetric Jacobian system $Kx = f$ is solved inexactly by the GMRES iterative method preconditioned by a BDDC preconditioner, described in the next section.
2- solve the symmetric positive semidefinite linear system deriving from the discretization of the Bidomain model by using the Conjugate Gradient

method preconditioned by the Multilevel Additive Schwarz preconditioner developed in Pavarino and Scacchi [2008].

3.1 Iterative Substructuring, Schur Complement System and BDDC Preconditioner

To keep the notation simple, in the remainder of this section and the next, we denote the reference domain by Ω instead of $\widehat{\Omega}$. Let us consider a decomposition of Ω into N nonoverlapping subdomains Ω_i of diameter H_i (see e.g. [Toselli and Widlund, 2004, Ch. 4]) $\Omega = \bigcup_{i=1}^{N} \Omega_i$, and set $H = \max H_i$. As in classical iterative substructuring, we reduce the problem to the interface $\Gamma := \left(\bigcup_{i=1}^{N} \partial\Omega_i\right) \backslash \partial\Omega$ by eliminating the interior degrees of freedom associated to basis functions with support in the interior of each subdomain, hence obtaining the Schur complement system

$$S_\Gamma x_\Gamma = g_\Gamma, \tag{3}$$

where $S_\Gamma = K_{\Gamma\Gamma} - K_{\Gamma I} K_{II}^{-1} K_{I\Gamma}$ and $g = f_\Gamma - K_{\Gamma I} K_{II}^{-1} f_I$ are obtained from the original discrete problem $Kx = f$ by reordering the finite element basis functions in interior (subscript I) and interface (subscript Γ) basis functions. The Schur complement system (3) is solved iteratively by the GMRES method using a BDDC preconditioner M_{BDDC}^{-1}

$$M_{\text{BDDC}}^{-1} S_\Gamma x_\Gamma = M_{\text{BDDC}}^{-1} f_\Gamma. \tag{4}$$

Once the interface solution x_Γ is computed, the internal values x_I can be recovered by solving local problems on each subdomain Ω_i.

BDDC preconditioners represent an evolution of balancing Neumann-Neumann methods where all local and coarse problems are treated additively due to a choice of so-called primal continuity constraints across the interface of the subdomains. These primal constraints can be point constraints and/or averages or moments over edges or faces of the subdomains. BDDC preconditioners were introduced in Dohrmann [2003] and first analyzed in Mandel and Dohrmann [2003]. For the construction of BDDC preconditioners applied to the nonlinear elasticity system constituting the cardiac electromechanical coupling problem, we refer to Pavarino et al. [2015].

4 Numerical Results

We present here the results of parallel numerical experiments run on the IBM-BlueGene/Q machine of Cineca (www.cineca.it). Our FORTRAN90 code is

based on the open source PETSc library, see Balay et al. [2016]. At each Newton iteration of the mechanical solver, the Jacobian system is solved by GMRES preconditioned by the BDDC preconditioner, using as stopping criterion a 10^{-8} reduction of the relative residual l_2-norm. The BDDC method is available as a preconditioner in PETSc and it has been contributed to the library by Zampini [2016. To appear.].

The values of the Bidomain electrical conductivity coefficients used in all the numerical tests are $\sigma_l^i = 3.0$, $\sigma_l^e = 2.0$, $\sigma_t^i = 0.315$, $\sigma_t^e = 1.35$, all in $m\Omega^{-1}cm^{-1}$. The parameter values in the transversely isotropic strain energy function are chosen as in the original work Eriksson et al. [2013]. The domains used in the simulations model are wedges of the ventricular wall. They are either slabs or truncated ellipsoidal domains; for details on the dimensions, see Pavarino et al. [2015]. The myocardial fibers are modeled to rotate intramurally linearly with the depth of the ventricular wall for a total amount of 120^o.

		V		VE		VEF		VEm		VEmF	
procs.	dof	lit	time	lit	time	lit	time	lit	time	lit	time
slab domains											
256	105903	94	1.0	42	0.9	38	1.1	32	1.2	26	1.2
512	209223	90	1.1	40	1.1	37	1.3	32	1.5	26	1.5
1042	413343	86	1.4	38	1.6	36	1.9	30	2.1	24	2.2
2048	807003	85	2.2	38	2.9	36	3.5	30	3.9	24	4.1
4096	1604043	84	5.2	39	6.6	-	-	-	-	-	-
8192	3188283	88	16.7	-	-	-	-	-	-	-	-
ellipsoidal domains											
256	105903	475	3.3	180	2.3	168	2.6	119	2.5	106	2.4
512	209223	533	4.2	191	2.8	174	3.3	126	3.0	109	3.0
1042	413343	558	5.8	173	4.0	158	4.6	125	4.7	106	4.9
2048	807003	674	9.4	179	6.3	169	7.5	130	7.2	107	7.5
4096	1604043	686	15.9	176	12.3	-	-	-	-	-	-

Table 1 Weak scaling test on slab and ellipsoidal domains. Mechanical solver with GMRES-BDDC and different choices of primal constraints: vertices (V), vertices + edges (VE), vertices + edges + faces (VEF), vertices + edges + edge moments (VEm), vertices + edges + edge moments + faces (VEmF). Fixed local mechanical mesh: $5 \times 5 \times 5$ elements. Local mechanical problem size = 648. The table reports the number of processors (procs., that equals the number of subdomains), the total number of degrees of freedom (dof), the average GMRES-BDDC iterations per Newton iteration (lit) and the average CPU time in seconds per Newton iteration (time). The missing results (denoted by -) correspond to out-of-memory runs.

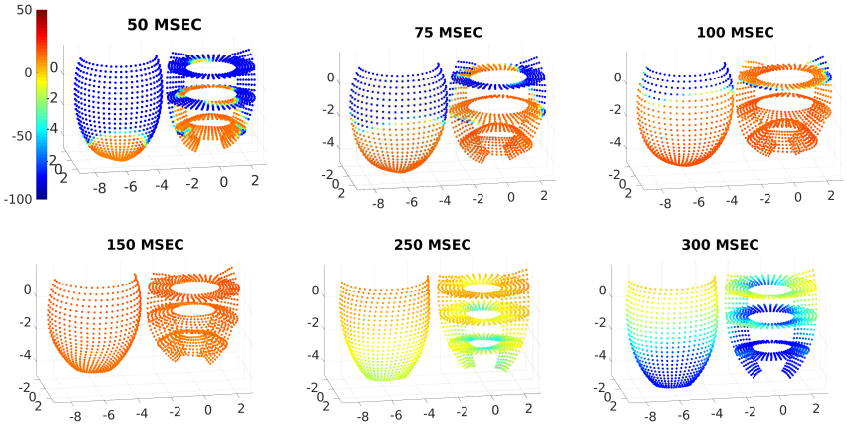
Test 1: weak scaling. We first consider a weak scaling test on slab and truncated ellipsoidal domains of increasing size. The number of subdomains (processors) is increased from 256 to 8192, with the largest domain being a slab or a truncated half ellipsoid. The physical dimensions of the domains are chosen so that the electrical mesh size h is kept fixed to the value of about $h = 0.01\ cm$ and so that the local mesh on each subdomain is fixed ($20 \cdot 20 \cdot 20$).

The mechanical mesh size is four times smaller than the electrical one in each direction, thus on each subdomain the local mechanical mesh is $5 \cdot 5 \cdot 5$. The discrete nonlinear elasticity system increases from about 100 thousand degrees of freedom for the the case with 256 subdomains to 3 million degrees of freedom for the the case with 8192 subdomains. Motivated by the results of our previous study (Pavarino et al. [2010]) of BDDC methods for almost incompressible linear elasticity, we have considered several choices of primal constraints in our BDDC preconditioner: subdomain vertices (V), vertices + edges (VE), vertices + edges + faces (VEF), vertices + edges + edge moments (VEm), vertices + edges + edge moments + faces (VEmF). The simulation is run for 10 electrical time steps of size $\tau_e = 0.05\ ms$ during the excitation phase and for 2 mechanical time steps of size $\tau_m = 0.25\ ms$.

The results regarding the mechanical solver reported in Table 1 show that the linear GMRES iteration (lit) are completely scalable due to the use of the BDDC preconditioner, as well as the nonlinear Newton iterations (not shown), while the cpu times increase with the number of processors. This is due to the superlinear cost of the coarse problem and will require further research with a three-level BDDC preconditioner. For slab domains, even if the number of GMRES iterations is the largest, the best choice of primal space in terms of CPU times is the minimal one (V), using only the vertices. For truncated ellipsoidal domains, instead, the GMRES iterations with only vertices as primal space grow considerably, and the best primal choice in terms of timings is vertices + edges (VE).

Test 2: whole heartbeat simulation. We then present the results of a whole heart beat simulation (500 ms, 10000 time steps) on 256 processors. The domain is a truncated ellipsoid discretized with a $96 \times 32 \times 8$ mechanical mesh (86427 dof) nested in a $768 \times 256 \times 64$ electrical mesh (25692290 dof). Fig. 1, top panels, reports the transmembrane potential distributions on the deforming epicardial surface and selected transmural sections of the cardiac domain at six selected time instants during the heartbeat.

We compare our BDDC solver (with only subdomain vertices primal constraints) vs. the widely used parallel AMG preconditioner BoomerAMG provided within the Hypre library (Henson and Yang [2002]); we used the default BoomerAMG parameters without any specific tuning. The Table in Fig. 1, bottom, shows the average GMRES iterations per time step are 821 and 138 for the AMG and the BDDC solver, respectively. The average CPU times per time step are 32 and 3 seconds for the AMG and the BDDC solver, respectively. Thus the BDDC solver yields a reduction of computational costs and cpu times of about a factor 10 with respect to the default AMG preconditioner considered (this gain would probably be reduced by a proper AMG parameter tuning).



prec	Tnit	nit	Tlit	lit	Ttime (s)	time (s)
AMG	6790	3	1642220	232	64578	32.29
BDDC	6790	3	276932	40	6083	3.04

Fig. 1 Whole heartbeat simulation. Top: mechanical deformation of the cardiac domain at six time instants, from 50 to 300 msec. At each instant, the plot shows the transmembrane potential v at each point, ranging from resting (blue, -85 mV) to excited (red, 45 mV) values, on the epicardial surface and on selected transmural sections. The values on the axis are expressed in centimeters. Bottom: table reporting the comparison between the AMG and BDDC preconditioners: total Newton iterations (Tnit), average Newton iterations per time step (nit), total GMRES iterations (Tlit), average GMRES iterations per Newton iteration (lit), total CPU time (Ttime) in seconds, average CPU time per time step (time) in seconds.

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