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Newton-Krylov-BDDC solvers for nonlinear cardiac mechanics

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Abstract

The aim of this work is to design and study a Balancing Domain Decomposition by Constraints (BDDC) solver for the nonlinear elasticity system modeling the mechanical deformation of cardiac tissue. The contraction-relaxation process in the myocardium is induced by the generation and spread of the bioelectrical excitation throughout the tissue and it is mathematically described by the coupling of cardiac electro-mechanical models consisting of systems of partial and ordinary differential equations. In this study, the discretization of the electro-mechanical models is performed by Q1 finite elements in space and semi-implicit finite difference schemes in time, leading to the solution of a large-scale linear system for the bioelectrical potentials and a nonlinear system for the mechanical deformation at each time step of the simulation. The parallel mechanical solver proposed in this paper consists in solving the nonlinear system with a Newton-Krylov-BDDC method, based on the parallel solution of local mechanical problems and a coarse problem for the so-called primal unknowns. Three-dimensional parallel numerical tests on different machines show that the proposed parallel solver is scalable in the number of subdomains, quasi-optimal in the ratio of subdomain to mesh sizes, and robust with respect to tissue anisotropy.

1. Introduction

In this work, we construct and study a Balancing Domain Decomposition by Constraints (BDDC) method for the scalable and efficient parallel solution of the nonlinear elasticity system arising from finite element discretizations of quasi-static cardiac mechanical models.

The spread of the electrical impulse in the cardiac muscle and the subsequent contraction-relaxation process is quantitatively described by the coupling of cardiac electro-mechanical models. 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. Since the focus of the present paper is on scalable solvers for cardiac mechanical models, we consider here a reduction of the Bidomain system, called Monodomain model, which consists of a single nonlinear reaction-diffusion PDE, modeling the evolution in space and time of the transmembrane potential. In both the Bidomain and Monodomain models, the PDEs are coupled through the reaction term with a stiff system of ordinary differential equations (ODEs), the so-called 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

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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 electro-mechanical 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. [15, 49, 50, 62, 9]. Also, the discretization of the model leads to the solution of a large-scale nonlinear system at each time step, which is often decoupled by one of the possible operator splitting techniques into the solution of a large-scale linear system for the electric part and a nonlinear system for the mechanical part.

While several studies in the last decade have been devoted to the development of efficient solvers and preconditioners for the Bidomain and Monodomain models, see e.g. [11, 22, 43, 45, 55, 44, 51, 59, 61, 53, 54, 66, 69, 70] and the recent monograph [12], a few studies have focused on the development of efficient solvers for the quasi-static cardiac mechanical model, see [48, 67] for parallel GMRES solvers and [57, 30, 31, 29] for parallel direct solvers. In our previous work [13], we have developed an Algebraic Multigrid solver for the cardiac mechanical model.

In this paper, we propose a BDDC preconditioner embedded in a Newton-Krylov approach (NKBDDC) for the nonlinear system arising from the discretization of the finite elasticity equations, where the Jacobian system arising at each Newton step is solved iteratively by a BDDC preconditioned GMRES method. BDDC preconditioners are non-overlapping domain decomposition preconditioners first introduced by Dohrmann in [16] for scalar elliptic problems and then analyzed by Mandel et al. [41, 42]. BDDC can be regarded as 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. The primal constraints can be point constraints and/or averages or more general quadrature rules over edges or faces of the subdomains. We remark that we could also consider FETI-DP algorithms, see, e.g., [20, 35] defined with the same set of primal constraints as our BDDC algorithm, since it is known that in such a case the BDDC and FETI-DP operators have the same eigenvalues with the exception of zeros and ones; see [42, 39]. For other non-overlapping domain decomposition methods of FETI and FETI-DP type used in biomechanics, we refer e.g. to [3, 8, 34] and to [33] for nonlinear alternatives.

We present the results of several numerical parallel tests in three dimensions employing up to about 16K processors on two different machines, an IBM BlueGene/Q and a Cray XC40, showing the scalability of the NKBDDC mechanical solver in both scaled and standard speedup tests. Moreover, we investigate the quasi-optimality of the BDDC preconditioner in the ratio H/h of subdomain to mesh sizes, considering in particular the effects of varying the primal degrees of freedom in the BDDC preconditioner. Finally, we study the time evolution of nonlinear and linear NKBDDC iterations during a complete cardiac cycle, simulating the mechanical contraction and relaxation of a wedge of cardiac tissue.

The rest of this paper is organized as follows. In Sec. 2 we introduce the passive and active mechanical models for the cardiac tissue (Sec. 2.1) and the bioelectrical model (Sec. 2.2). In Sec. 3 we describe the discrete nonlinear mechanical system obtained by discretizing the models in time and space and we propose our solving procedure. The BDDC preconditioner for the mechanical solver is constructed in Sec. 3.5, and the results of several parallel numerical tests in three dimensions are presented in Sec. 4.

2. Cardiac electro-mechanical models

2.1. Mechanical model

From a mechanical point of view, the cardiac tissue is modeled as a nonlinear elastic material. Let us denote the material coordinates of the undeformed or reference cardiac domain by $\mathbf{X} = (X_1, X_2, X_3)^T$, the spatial coordinates of the deformed cardiac domain by $\mathbf{x} = (x_1, x_2, x_3)^T$ and the region occupied by the undeformed and deformed (at time t) cardiac domains by $\hat{\Omega}$ and $\Omega(t)$, respectively. We denote by Div the material divergence of a vector and by Grad the material gradient of a scalar field; divergence and gradient for the spatial coordinates are denoted with lowercase operators div and grad . The deformation gradient tensor $\mathbf{F}$ and its determinant are given by

$$\mathbf{F}(\mathbf{X}, t) = \{F_{ij}\} = \left\{ \frac{\partial x_i}{\partial X_j} \quad i, j = 1, 2, 3 \right\}, \quad J(\mathbf{X}, t) = \det \mathbf{F}(\mathbf{X}, t),$$

whereas Cauchy-Green deformation tensor $\mathbf{C}$ and Lagrange-Green strain tensor $\mathbf{E}$ are

$$\mathbf{C} = \mathbf{F}^T \mathbf{F} \quad \text{and} \quad \mathbf{E} = \frac{1}{2}(\mathbf{C} - \mathbf{I}),$$

with $\mathbf{I}$ the identity matrix.

We first assume that the time-dependent inertial term in the governing elastic wave equation may be neglected, see e.g. [32, 68]. Thus, the steady-state force equilibrium equation reads

$$\text{Div}(\mathbf{FS}) = \mathbf{0}, \quad \mathbf{X} \in \hat{\Omega}, \quad (1)$$

where $\mathbf{S}$ is the second Piola-Kirchhoff stress tensor. Given the splitting of the reference domain boundary $\partial \hat{\Omega} = \partial \hat{\Omega}_D \cup \partial \hat{\Omega}_N$, we close the quasi-static mechanical model (1) by imposing a prescribed displacement on a Dirichlet boundary, $\mathbf{x}(\mathbf{X}) = \hat{\mathbf{x}}(\mathbf{X})$, $\mathbf{X} \in \partial \hat{\Omega}_D$ and no traction force on a Neumann boundary, $\mathbf{FSN} = \mathbf{0}$, $\mathbf{X} \in \partial \hat{\Omega}_N$.

The tensor $\mathbf{S}$ is given by the sum of a passive elastic component $\mathbf{S}^{pas}$, a volumetric component $\mathbf{S}^{vol}$ and a biochemically generated active component $\mathbf{S}^{act}$, i.e.

$$\mathbf{S} = \mathbf{S}^{pas} + \mathbf{S}^{act} + \mathbf{S}^{vol},$$

as done in many previous studies, see e.g. [28, 67, 32]. It is worth mentioning an alternative approach recently proposed in [10] consisting of a multiplicative decomposition of the deformation gradient tensor $\mathbf{F}$ into a passive elastic deformation and an active strain component, see also [1, 48, 57].

Passive component of the stress tensor. The passive component $\mathbf{S}^{pas}$ is computed from a suitable strain energy function W^{pas} and the Green Lagrange strain $\mathbf{E}$ as

$$S_{ij}^{pas} = \frac{1}{2} \left(\frac{\partial W^{pas}}{\partial E_{ij}} + \frac{\partial W^{pas}}{\partial E_{ji}} \right) \quad i, j = 1, 2, 3.$$

A wide variety of strain energy functions W^{pas} have been proposed and adopted in the literature, see e.g. [14, 21, 23, 25, 46, 56, 58, 60, 65].

We recall that the cardiac tissue consists of an arrangement of fibers that rotate counterclockwise from epi- to endocardium, and that have a laminar organization modeled as a set of muscle sheets running radially from epi- to endocardium, e.g. [37, 65]. In the following, we will denote by $\hat{\mathbf{a}}_l$, $\hat{\mathbf{a}}_t$ and $\hat{\mathbf{a}}_n$ the unit vectors of the local fiber coordinate system in the reference configuration. In particular, $\hat{\mathbf{a}}_l$ represents the fiber direction and $\hat{\mathbf{a}}_t$, $\hat{\mathbf{a}}_n$ the two orthogonal cross fiber directions.

In this paper, we choose to model the myocardium as a transversely isotropic hyperelastic material, with the exponential strain energy function given by [67]

$$W = \frac{1}{2} c (e^Q - 1), \quad (2)$$

$$Q = b_{ll} E_{ll}^2 + b_{tn} (E_{nn}^2 + E_{tt}^2 + 2E_{nt}^2) + 2b_{lt} (E_{lt}^2 + E_{ln}^2),$$

where the Lagrange-Green strain tensor is referred to the orthogonal local fiber coordinate system. The material constant c scales the stress, b_{ll} and b_{tn} scale the material stiffness in the fiber and the two cross fiber directions, and b_{lt} scales the material rigidity under shear in the fiber-transverse plane.

Active component of the stress tensor. The contraction of the ventricles results from the active tension generated by the model of myofilaments dynamics activated by calcium. We assume that the generated active force acts in the fiber's direction as [50, 68]; hence, according to [27, Ch. 10], the second Piola-Kirchhoff active stress component is given by

$$\mathbf{S}^{act} = J \mathbf{F}^{-1} \sigma^{act} \mathbf{F}^{-T} = T_a \frac{\hat{\mathbf{a}}_l \otimes \hat{\mathbf{a}}_l}{\hat{\mathbf{a}}_l^T \mathbf{C} \hat{\mathbf{a}}_l}.$$

In this paper, we consider two active tension models, one *stretch and stretch-rate independent* and a second one *stretch and stretch-rate dependent*, defined as follows.

a) Stretch and stretch-rate independent model. We assume as in [47, 21] that the dynamics of biochemically generated active tension T_a depends only on the transmembrane potential v according to this simple twitch-like rule

$$\frac{\partial T_a}{\partial t} = Q_T(v, T_a) = \epsilon(v)(k_{T_a}(v - v_r) - T_a), \quad (3)$$

where $k_{T_a} > 0$ controls the saturated value of T_a for a given potential v and a given resting potential v_r , which is about -80 mV in cardiac cells, see [47, 21] for details.

b) Stretch and stretch-rate dependent model. The biochemically generated active tension T_a is given by the model by Land et al. [36], where the active tension $T_a = T_a(Ca_i, \lambda, \frac{d\lambda}{dt})$ is calcium, stretch and stretch-rate dependent and its dynamics is described by the following system of ODEs:

$$\begin{cases} \frac{dtr}{dt} = k_{tr} \left(\left(\frac{Ca_i}{Ca_{50}(1 + \beta(\lambda - 1))} \right)^{n_{tr}} (1 - tr) - tr \right) \\ \frac{dxb}{dt} = k_{xb} \left(tr_{50} tr^{n_{xb}} (1 - xb) - \frac{1}{tr_{50} tr^{n_{xb}}} xb \right) \\ \frac{dQ_i}{dt} = A_i \frac{d\lambda}{dt} - \alpha_i Q_i, \quad i = 1, 2 \\ T_a = g(Q) h(\lambda) xb, \quad Q = Q_1 + Q_2 \end{cases}, \quad (4)$$

with parameters $k_{tr}, k_{xb}, Ca_{50}, tr_{50} \in (0, 1)$, $n_{tr}, n_{xb}, \beta > 1$, $A_1 < 0$, $A_2 > 0$, $\alpha_1, \alpha_2 > 0$, and where $h : \mathbb{R} \rightarrow \mathbb{R}$ and $g(Q) : \mathbb{R} \rightarrow \mathbb{R}$ are nondecreasing, bounded, Lipschitz functions (see [36] for more details). For sake of compactness, system (4) is rewritten as

$$\begin{cases} \frac{d\mathbf{z}}{dt} = \mathbf{R}_z \left(\mathbf{z}, Ca_i, \lambda, \frac{d\lambda}{dt} \right) \\ T_a = f_{T_a}(\mathbf{z}, \lambda) \end{cases}, \quad (5)$$

where $\mathbf{z} = \{tr, xb, Q_1, Q_2\}$.

Volumetric component of the stress tensor. To model the nearly-incompressibility of the myocardium, we add to the strain energy function a volume change penalization term [67]

$$W^{vol} = K (J - 1)^2, \quad (6)$$

with K a positive bulk modulus, so that the volumetric component S^{vol} can be expressed as

$$S_{ij}^{vol} = \frac{1}{2} \left(\frac{\partial W^{vol}}{\partial E_{ij}} + \frac{\partial W^{vol}}{\partial E_{ji}} \right) \quad i, j = 1, 2, 3.$$

2.2. Bioelectrical model

In the study, the Monodomain model is considered as electrical model together with the Ten Tusscher membrane model [63] on the reference cardiac domain $\hat{\Omega}$ as in [47, 50, 68]. Given an applied current per unit volume $I_{app} : \hat{\Omega} \times (0, T) \rightarrow \mathbb{R}$, and suitable initial conditions $v_0 : \hat{\Omega} \rightarrow \mathbb{R}$, $w_0 : \hat{\Omega} \rightarrow \mathbb{R}$, the Monodomain model finds the transmembrane potential $v : \hat{\Omega} \times (0, T) \rightarrow \mathbb{R}$, the gating variables $w : \hat{\Omega} \times (0, T) \rightarrow \mathbb{R}^{N_w}$ and the ionic concentrations $c : \hat{\Omega} \times (0, T) \rightarrow \mathbb{R}^{N_c}$ such that

$$c_m \frac{\partial v}{\partial t} - J^{-1} \text{Div}(J \mathbf{F}^{-1} D_m \mathbf{F}^{-T} \text{Grad } v) + I_{ion}(v, w, c) = I_{app} \quad \text{in } \hat{\Omega} \times (0, T) \quad (7)$$

$$\frac{\partial w}{\partial t} = R_w(v, w), \quad \frac{\partial c}{\partial t} = R_c(v, w, c), \quad \text{in } \hat{\Omega} \times (0, T) \quad (8)$$

with insulating (Neumann) boundary conditions on $\partial \hat{\Omega}$. $\mathbf{F}$ is the deformation gradient tensor and the functions $I_{ion}(v, w, c)$, $R_w(v, w)$, $R_c(v, w, c)$ are given according to the Ten Tusscher membrane model [63]. This ionic model, available from the cellML repository (<http://models.cellml.org/cellml>), consists of 17 ordinary differential equations modeling the dynamics of the main ionic currents (I_{Na} , I_{to} , I_{Kr} , I_{Ks} , I_{K1} , I_{CaL}) through the membrane of human ventricular myocytes.

The computation of the tensors $\mathbf{F}^{-1}(\mathbf{X}) D_m(\mathbf{x}) \mathbf{F}^{-T}(\mathbf{X})$ must be performed on the reference configuration $\hat{\Omega}$: denoting by $\hat{\mathbf{a}}_l(\mathbf{X})$ the unit vector parallel to the local fiber direction in the reference configuration, it holds

$$(\mathbf{F}^{-1} D_m \mathbf{F}^{-T})(\mathbf{X}) = \sigma_t^m \mathbf{C}^{-1}(\mathbf{X}) + (\sigma_l^m - \sigma_t^m) \frac{\hat{\mathbf{a}}_l(\mathbf{X}) \hat{\mathbf{a}}_l^T(\mathbf{X})}{\hat{\mathbf{a}}_l^T(\mathbf{X}) \mathbf{C}(\mathbf{X}) \hat{\mathbf{a}}_l(\mathbf{X})},$$

where $\sigma_{l,t}^m$ are the Monodomain axisymmetric conductivities, see e.g. [11].

3. Numerical discretization in time and space

3.1. Temporal discretization

The time discretization is performed by a semi-implicit splitting method. For simplicity, we describe the procedure in the case of equal mechanical and electrical time steps, but the two time steps can be chosen independently and usually the electrical time step is smaller in order to properly resolve the steep depolarization wavefront. We describe the time discretization for both the cases of the stretch and stretch-rate independent and dependent models, since they are slightly different. For a review of time discretizations of cardiac models, including IMEX (Implicit - Explicit or semi-implicit) and other splitting methods, we refer to [12, Ch. 7.2].

a) *Stretch and stretch-rate independent model (3).* At each time step,

- 1- given v^n, w^n, c^n, T_a^n , solve the ODEs of the membrane model (8) and active force equation (3) with a first order IMEX method to compute the new $w^{n+1}, c^{n+1}, T_a^{n+1}$

$$\begin{aligned} w^{n+1} &= w^n + \Delta t R_w(v^n, w^{n+1}) \\ c^{n+1} &= c^n + \Delta t R_c(v^n, w^{n+1}, c^n) \\ T_a^{n+1} &= T_a^n + \Delta t Q_T(v^n, T_a^{n+1}), \end{aligned}$$

- 2- given T_a^{n+1} solve the mechanical problem (1) to compute the new deformed coordinates $\mathbf{x}^{n+1}$, providing the new deformation gradient tensor $\mathbf{F}_{n+1}$

$$\text{Div}(\mathbf{F}_{n+1} \mathbf{S}_{n+1}(T_a^{n+1})) = 0, \quad (9)$$

- 3- given $w^{n+1}, c^{n+1}, \mathbf{F}_{n+1}$, and $J_{n+1} = \det(\mathbf{F}_{n+1})$ solve the Monodomain system (7) with a first order IMEX method computing the new electric potentials v^{n+1} , see [11]

$$c_m \frac{v^{n+1}}{\Delta t} - J_{n+1}^{-1} \text{Div}(J_{n+1} \mathbf{F}_{n+1}^{-1} D_m \mathbf{F}_{n+1}^{-T} \text{Grad } v^{n+1}) = c_m \frac{v^n}{\Delta t} - I_{ion}(v^n, w^{n+1}, c^{n+1})$$

b) *Stretch and stretch-rate dependent model (5)*. At each time step,

- 1- given v^n, w^n, c^n at time t_n , solve the ODE system of the membrane model (8) with a first order IMEX method to compute the new w^{n+1}, c^{n+1} :

$$\begin{aligned} w^{n+1} &= w^n + \Delta t R_w(v^n, w^{n+1}) \\ c^{n+1} &= c^n + \Delta t R_c(v^n, w^{n+1}, c^n); \end{aligned} \quad (10)$$

- 2- given the calcium concentration Ca_i^{n+1} , which is included in the concentration variables c^{n+1} , solve the active tension model (5) and the mechanical problems (1) to compute the new deformed coordinates $\mathbf{x}^{n+1}$, providing the new deformation gradient tensor $\mathbf{F}_{n+1}$:

$$\begin{aligned} \mathbf{z}^{n+1} &= \mathbf{z}^n + \Delta t R_z \left(\mathbf{z}^{n+1}, Ca_i^{n+1}, \lambda^{n+1}, \frac{\lambda^{n+1} - \lambda^n}{\Delta t} \right) \\ T_a^{n+1} &= f_{Ta}(\mathbf{z}^{n+1}, \lambda^{n+1}) \\ \text{Div}(\mathbf{F}_{n+1} \mathbf{S}_{n+1}(T_a^{n+1})) &= 0; \end{aligned} \quad (11)$$

- 3- given $w^{n+1}, c^{n+1}, \mathbf{F}_{n+1}$, and $J_{n+1} = \det(\mathbf{F}_{n+1})$ solve the Monodomain system (7) with a first order IMEX method computing the new electric potentials v^{n+1}

$$c_m \frac{v^{n+1}}{\Delta t} - J_{n+1}^{-1} \text{Div}(J_{n+1} \mathbf{F}_{n+1}^{-1} D_m \mathbf{F}_{n+1}^{-T} \text{Grad } v^{n+1}) = c_m \frac{v^n}{\Delta t} - I_{ion}(v^n, w^{n+1}, c^{n+1})$$

We note that our time discretization strategy is based on operator splitting and implicit-explicit methods, thus a CFL condition should be satisfied. However, the accuracy requirements needed to approximate correctly the steep activation wavefront of the heart beat will force us to use time step sizes small enough to satisfy the CFL condition.

3.2. Spatial discretization

We use a structured hexahedral grid τ_{hm} for the nonlinear elasticity system (1) and a structured hexahedral grid τ_{he} for the Monodomain model (7), assuming that τ_{he} is a refinement of τ_{hm} . We then discretize all scalar and vector fields of both mechanical and electrical models by isoparametric Q_1 finite elements in space. Our NKBDDC method, described in the next sections, and the results provided in the present paper apply also to unstructured tetrahedral meshes and irregular partitions obtained from automatic mesh partitioners, as already demonstrated in the original BDDC paper by Dorhmann [16] and in several subsequent BDDC works.

In the volumetric energy, we consider a bulk modulus $K = 200kPa$, so that the tissue is only moderately almost-incompressible and our pure displacement formulation of the non-linear elasticity equations is still appropriate. For larger values of K , volumetric locking would affect both the accuracy of the numerical solution and the robustness of the iterative solver (described in the following). In such cases, we should adopt a mixed formulation with both displacements and pressures (see [7]) or a B-bar method (see [26, 18]).

3.3. Computational kernels

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

- 1- solve the nonlinear system

$$G(\mathbf{x}^{n+1}) = 0, \quad (12)$$

deriving from either one of the discretizations (9) or (11) of the mechanical problem (1) with exponential strain energy function (2) by using an inexact Newton method. At each Newton step, a nonsymmetric Jacobian system

$$Kx = f, \quad (13)$$

is solved inexactly by the GMRES iterative method preconditioned by the BDDC, described in the next section. The resulting Newton-Krylov-BDDC nonlinear solver (NKBDDC) is the main focus of our numerical investigation.

- 2- solve the symmetric positive definite linear system deriving from the discretization of the Monodomain model (7) using the Conjugate Gradient method preconditioned by the Block Jacobi (BJ) preconditioner with Inexact ILU(0) local solvers for the local problems on the subdomains. While the efficient solution of the Bidomain model requires more sophisticated preconditioners (such as Algebraic Multigrid [55, 54], Multilevel Schwarz [51], Balancing Neumann-Neumann [69] or BDDC preconditioners [70]), the adopted strategy has proven to be very effective [11] to solve the Monodomain model.

3.4. Non-overlapping Domain Decomposition

To keep the notation simple, in the following of this section and in the next one, we will denote the reference domain by Ω instead of $\hat{\Omega}$. Let us consider a decomposition of Ω into N non-overlapping subdomains Ω_i of diameter H_i (see e.g. Toselli and Widlund [64, Ch. 4])

$$\Omega = \bigcup_{i=1}^N \Omega_i,$$

and the interface among them

$$\Gamma := \left(\bigcup_{i=1}^N \partial\Omega_i \right) \setminus \partial\Omega.$$

We then define $H = \max H_i$.

Using a block Cholesky technique, we can eliminate the interior degrees of freedom associated to basis functions with support in the interior of each subdomain, hence obtaining an explicit formula for the inverse of (13)

$$K^{-1} = \begin{pmatrix} I & -K_{II}^{-1}K_{I\Gamma} \\ 0 & I \end{pmatrix} \begin{pmatrix} K_{II}^{-1} & 0 \\ 0 & S_{\Gamma}^{-1} \end{pmatrix} \begin{pmatrix} I & 0 \\ -K_{\Gamma I}K_{II}^{-1} & I \end{pmatrix}, \quad (14)$$

where

$$S_{\Gamma} = K_{\Gamma\Gamma} - K_{\Gamma I}K_{II}^{-1}K_{I\Gamma} \quad (15)$$

is the Schur complement matrix, and with K_{II} , $K_{I\Gamma}$, $K_{\Gamma I}$, and $K_{\Gamma\Gamma}$ obtained by reordering the finite element basis functions in interior (subscript I) and interface (subscript Γ) basis functions.

The focus of non-overlapping Domain Decomposition methods is on constructing efficient preconditioners for the Schur complement system, being the elimination of the interior degrees of freedom an embarrassingly parallel step which can be accomplished by solving a block diagonal problem, with blocks associated to the subdomains. The application of our non-overlapping preconditioner consists in using formula (14) where S_{Γ}^{-1} is replaced by a suitable preconditioner, in our case the BDDC.

3.5. Balancing Domain Decomposition by Constraints

Balanced Domain Decomposition by Constraints (BDDC) preconditioners are 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 by Dohrmann [16] and first analyzed by Mandel, Dohrmann and Tezaur [41, 42]. We refer to the domain decomposition monograph by Toselli and Widlund [64, Ch. 6] for a detailed treatment of Neumann-Neumann, FETI and FETI-DP algorithms, see also [20, 35, 39]. FETI-DP methods are closely related to BDDC methods having the same set of primal constraints, since in this case the two families of methods exhibit essentially the same spectrum, except for possible 0 and 1 eigenvalues.

Subspace decompositions. We denote by V the Q_1 finite element space used for the displacement discretization and by $V^{(i)}$ the local discrete space defined on the subdomain Ω_i that vanish on $\partial\Omega_i \cap \partial\Omega_D$. We then split the local space into a direct sum of its interior (I) and interface (Γ) subspaces $V^{(i)} = V_I^{(i)} \oplus V_{\Gamma}^{(i)}$ and we define the associated product spaces by

$$V_I := \prod_{i=1}^N V_I^{(i)}, \quad V_{\Gamma} := \prod_{i=1}^N V_{\Gamma}^{(i)}.$$

The functions in V_{Γ} are generally discontinuous across Γ , while our finite element approximations are not. Therefore, we also define the subspace

$$\widehat{V}_{\Gamma} := \{\text{functions of } V_{\Gamma} \text{ that are continuous across } \Gamma\}.$$

We also need an intermediate subspace

$$\widetilde{V}_{\Gamma} := V_{\Delta} \oplus \widehat{V}_{\Pi},$$

defined by further splitting the interface (subscript Γ) degrees of freedom into primal (subscript Π) and dual (subscript Δ) degrees of freedom, where:

a) $\widehat{V}_\Pi$ is a subspace consisting of functions which are continuous at selected *primal* variables, which can be the subdomain basis functions associated with subdomains' corners and/or edge/face basis functions with a constant value at the nodes of the associated edge/face. In order to simplify the formulas and keep the exposition compact, we assume that a change of basis has been performed and each primal variable correspond to an explicit degree of freedom; see [39].

b) $V_\Delta = \prod_{i=1}^N V_\Delta^{(i)}$ is the product space of the local subspaces $V_\Delta^{(i)}$ of *dual* interface functions that vanish at the primal degrees of freedom.

Choice of primal constraints. The choice of primal degrees of freedom is fundamental for the construction of efficient BDDC preconditioners. One of the simplest choices consists of taking as primal degrees of freedom those associated with the subdomain corners. Such choice is not always sufficient to obtain scalable and fast preconditioners and this has motivated the search for richer primal sets that may yield faster preconditioners in terms of number of iterations, but at the expense of higher computational costs, due to larger coarse problems that would be generated using edge and/or face based primal degrees of freedom, see e.g. [64, 35].

Restriction and scaling operators. In order to define our preconditioners, we will need the following restriction and interpolation operators represented by matrices with elements in the set $\{0, 1\}$:

$$\begin{aligned} R_{\Gamma\Delta} : \widetilde{V}_\Gamma &\longrightarrow V_\Delta, & R_{\Gamma\Pi} : \widetilde{V}_\Gamma &\longrightarrow \widehat{V}_\Pi, \\ R_\Delta^{(i)} : V_\Delta &\longrightarrow V_\Delta^{(i)}, & R_\Pi^{(i)} : \widehat{V}_\Pi &\longrightarrow \widehat{V}_\Pi^{(i)}, \end{aligned} \quad (16)$$

where $\widehat{V}_\Pi^{(i)}$ is the local subspace of *primal* interface functions. We will also need the standard counting functions of the Neumann–Neumann methods and in particular their pseudoinverses $\delta_i^\dagger(x)$ defined at each degrees of freedom x on the interface of subdomain Ω_i by

$$\delta_i^\dagger(x) := \frac{1}{\mathcal{N}_x}, \quad (17)$$

with $\mathcal{N}_x$ the number of subdomains sharing x . We remark that the novel BDDC deluxe scaling introduced in [17] and studied in [6] could be used here, as well as other scalings for anisotropic coefficients, see e.g. [38, 69, 70]. Here for simplicity we confine ourselves to BDDC with classical scaling. We then define scaled local restriction operators $R_{D,\Delta}^{(i)}$ by multiplying the sole nonzero element of each row of $R_\Delta^{(i)}$ by $\delta_i^\dagger$, and we define

$$R_{D,\Gamma} := \text{the direct sum } R_{\Gamma\Pi} \oplus R_{D,\Delta}^{(i)} R_{\Gamma\Delta}. \quad (18)$$

The BDDC preconditioner. We denote by $K^{(i)}$ the local stiffness matrix restricted to subdomain Ω_i . By partitioning the local degrees of freedom into interior (I), dual (Δ), and primal (Π) degrees of freedom, $K^{(i)}$ can be written as

$$K^{(i)} = \begin{bmatrix} K_{II}^{(i)} & K_{\Gamma I}^{(i)T} \\ K_{\Gamma I}^{(i)} & K_{\Gamma\Gamma}^{(i)} \end{bmatrix} = \begin{bmatrix} K_{II}^{(i)} & K_{\Delta I}^{(i)T} & K_{\Pi I}^{(i)T} \\ K_{\Delta I}^{(i)} & K_{\Delta\Delta}^{(i)} & K_{\Pi\Delta}^{(i)T} \\ K_{\Pi I}^{(i)} & K_{\Pi\Delta}^{(i)} & K_{\Pi\Pi}^{(i)} \end{bmatrix}.$$

Using the scaled restriction matrices defined in (16) and (18), the BDDC preconditioner can be written as

$$M_{\text{BDDC}}^{-1} = R_{D,\Gamma}^T \widetilde{S}_\Gamma^{-1} R_{D,\Gamma}, \quad (19)$$

where

$$\tilde{S}_\Gamma^{-1} = R_{\Gamma\Delta}^T \left(\sum_{i=1}^N \begin{bmatrix} 0 & R_\Delta^{(i)T} \end{bmatrix} \begin{bmatrix} K_{II}^{(i)} & K_{\Delta I}^{(i)T} \\ K_{\Delta I}^{(i)} & K_{\Delta\Delta}^{(i)} \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ R_\Delta^{(i)} \end{bmatrix} \right) R_{\Gamma\Delta} + \Phi S_{\Pi\Pi}^{-1} \Phi^T. \quad (20)$$

The first term in (20) is the sum of local solvers on each subdomain Ω_i , with Neumann data on the local dual nodes and with the local primal degrees of freedom constrained to vanish. The second term is a coarse solver for the primal variables, that we implemented as in [39, 5, 52] by using the coarse matrix

$$S_{\Pi\Pi} = \sum_{i=1}^N R_{\Pi}^{(i)T} \left(K_{\Pi\Pi}^{(i)} - \begin{bmatrix} K_{\Pi I}^{(i)} & K_{\Pi\Delta}^{(i)} \end{bmatrix} \begin{bmatrix} K_{II}^{(i)} & K_{\Delta I}^{(i)T} \\ K_{\Delta I}^{(i)} & K_{\Delta\Delta}^{(i)} \end{bmatrix}^{-1} \begin{bmatrix} K_{\Pi I}^{(i)T} \\ K_{\Pi\Delta}^{(i)T} \end{bmatrix} \right) R_{\Pi}^{(i)}$$

and a matrix Φ which maps primal degrees of freedom to interface variables

$$\Phi = R_{\Gamma\Pi}^T - R_{\Gamma\Delta}^T \sum_{i=1}^N \begin{bmatrix} 0 & R_\Delta^{(i)T} \end{bmatrix} \begin{bmatrix} K_{II}^{(i)} & K_{\Delta I}^{(i)T} \\ K_{\Delta I}^{(i)} & K_{\Delta\Delta}^{(i)} \end{bmatrix}^{-1} \begin{bmatrix} K_{\Pi I}^{(i)T} \\ K_{\Pi\Delta}^{(i)T} \end{bmatrix} R_{\Pi}^{(i)}.$$

The columns of Φ represent the coarse basis functions, defined as the minimum energy extension of the primal constraints into the subdomains with respect to the original bilinear form.

Remark 1. It is well-known that BDDC and FETI-DP preconditioners for compressible linear elasticity problems satisfy a scalable quasi-optimal condition number bound (see e.g. [64, Ch. 6.4])

$$\text{cond}(M_{\text{BDDC}}^{-1} S_\Gamma) \leq C \left(\frac{H}{h} \right) \left(1 + \log \frac{H}{h} \right)^2, \quad (21)$$

with $C(\frac{H}{h}) = \alpha$ constant for sufficiently rich coarse spaces and $C(\frac{H}{h}) = \alpha \frac{H}{h}$ for the minimal primal space spanned by the degrees of freedom defined at subdomain corners. Due to the more complex nonlinear elasticity problem (1) based on an exponential strain energy function (2), we could not prove a similar GMRES bound for the convergence rate of our nonsymmetric NKBDDC preconditioned operator. Nevertheless, the numerical results presented in the next section indicate that our NKBDDC method is scalable and quasi-optimal.

4. Numerical results

In this section, we present the results of parallel numerical experiments performed on the IBM-BlueGene/Q machine Fermi (<http://www.cineca.it/en/content/fermi-bgq>) of the CINECA Consortium and on the novel Cray XC40 machine Shaheen [24] of KAUST. While the reported mathematical quantities such as nonlinear and linear iterations remain the same for the same run on the two machines, the reported CPU times are not directly comparable due to the different architectures of the two machines. Our code is built on top of the FORTRAN90 wrappers of the open source PETSc library [4], a widely used suite of routines for the solution of linear and nonlinear PDEs for distributed memory systems developed and maintained by the Argonne National Laboratory. At each time step, the nonlinear mechanical system is solved by an inexact (since the Jacobian system is solved inexactly by GMRES) Newton method employing a line search Newton update with cubic backtracking, see [4, Ch. 5]. The mechanical solution at the previous time step is used to start the next Newton process which is then stopped when the reduction of the relative residual l_2 -norm is lower than 10^{-4} . At each Newton iteration, the nonsymmetric Jacobian system is solved

iteratively by GMRES preconditioned by the BDDC preconditioner, with zero initial guess and stopping criterion a 10^{-8} reduction of the relative residual l_2 -norm. In the current implementation of the BDDC shipped with the PETSc library, each subdomain is assigned to an MPI process. In the present study, the direct solution of local problems involved in the static condensation step (14) and in the application of the BDDC preconditioner (20) is performed using the PETSc sequential LU factorizations. The BDDC coarse problem is solved in parallel using the parallel LU factorization provided either by SuperLU_DIST [40] or by MUMPS [2] packages.

Our use of structured grids allow us to use PETSc DMDA objects and very regular subdomain partitions that are very well balanced. Nevertheless, our NKBDCC method would apply also to unstructured tetrahedral meshes and irregular partitions obtained from automatic mesh partitioners, as already demonstrated in the original BDDC paper by Dorhmann [16] and in several subsequent BDDC works. These works have proven that the same scalability and quasi-optimality properties also hold for unstructured meshes and complex geometries with irregular (automatic) partitions, albeit with a higher computational cost due mostly to more expensive data management subroutines. We plan to extend our study to unstructured meshes and automatic subdomain partitions in a future study.

Parameter calibration. For simplicity, we assume that the electrical and mechanical behavior of the cardiac tissue is transversely isotropic or axisymmetric with respect to the local fiber direction. The values of the Monodomain electrical conductivity coefficients used in all the numerical tests are obtained as $\sigma_{l,t}^m = \frac{\sigma_{l,t}^i \sigma_{l,t}^e}{\sigma_{l,t}^i + \sigma_{l,t}^e}$, where the Bidomain conductivity coefficients are the following:

$$\begin{aligned} \sigma_l^i &= 3.0 \text{ m}\Omega^{-1}\text{cm}^{-1} & \sigma_l^e &= 2.0 \text{ m}\Omega^{-1}\text{cm}^{-1} \\ \sigma_t^i &= 0.31525 \text{ m}\Omega^{-1}\text{cm}^{-1} & \sigma_t^e &= 1.3514 \text{ m}\Omega^{-1}\text{cm}^{-1}. \end{aligned}$$

This choice of parameters yields physiological propagation velocities of the electrical excitation wavefront along and across fiber of about of 0.05 and 0.03 cm ms^{-1} , see e.g. [12] (here and in the following ms denotes milliseconds). The parameter values in the transversely isotropic strain energy function (2) are chosen as in the original work [67], i.e. $c = 1.76 \text{ kPa}$, $b_{ll} = 18.5$, $b_{tt} = b_{nn} = b_{tn} = b_{nt} = 3.58$, $b_{lt} = b_{ln} = 1.63$ and $K = 200 \text{ kPa}$. Unless explicitly stated, the active tension model used in the following tests is the twitch-like rule (3).

Computational domains. The domains used in the simulations models wedges of the ventricular wall. They are either slabs of size $[a_1 \ a_2] \times [b_1 \ b_2] \times [c_1 \ c_2]$ (with specific values given below), or truncated ellipsoidal domains described by the parametric equations

$$\begin{cases} x = a(r) \cos \theta \cos \phi & \phi_{\min} \leq \phi \leq \phi_{\max}, \\ y = b(r) \cos \theta \sin \phi & \theta_{\min} \leq \theta \leq \theta_{\max}, \\ z = c(r) \sin \theta & 0 \leq r \leq 1, \end{cases}$$

where $a(r) = a_1 + r(a_2 - a_1)$, $b(r) = b_1 + r(b_2 - b_1)$, $c(r) = c_1 + r(c_2 - c_1)$, and $a_1 = 1.5$, $a_2 = 2.7$, $b_1 = 1.5$, $b_2 = 2.7$, $c_1 = 4.4$, $c_2 = 5$ are given coefficients (all in cm) determining the main axes of the ellipsoid; see Fig. 1 for some examples.

Fiber structure. For slab domains, the fiber direction $\mathbf{a}_l(\mathbf{x})$ and the other two principal axes at a point $\mathbf{x}$ in the canonical cartesian reference system $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$, are given by

$$\mathbf{a}_l(\mathbf{x}) = \mathbf{e}_1 \cos \alpha(r) + \mathbf{e}_2 \sin \alpha(r), \quad \mathbf{a}_t = \mathbf{e}_3, \quad \mathbf{a}_n(\mathbf{x}) = \mathbf{e}_1 \sin \alpha(r) - \mathbf{e}_2 \cos \alpha(r),$$

where the fiber rotation angle is $\alpha(r) = \frac{2}{3}\pi(1-r) - \frac{\pi}{4}$, with $r = (x_3 - c_1)/(c_2 - c_1)$, yielding a 120° fiber rotation. For an ellipsoidal domain, the fiber direction $\mathbf{a}_l(\mathbf{x})$ at a point $\mathbf{x}$ in a local ellipsoidal

Figure 1: Top: slab and ellipsoidal domains for the weak scaling test (drawn with half subdomains in each direction). Bottom: plots of GMRES-BDDC iterations counts for the slab (left) and ellipsoidal (right) domains from Table 1.

reference system $(\mathbf{e}_\phi, \mathbf{e}_\theta, \mathbf{e}_r)$, is given by

$$\mathbf{a}_l(\mathbf{x}) = \mathbf{e}_\phi \cos \alpha(r) + \mathbf{e}_\theta \sin \alpha(r), \quad \text{with} \quad \alpha(r) = \frac{2}{3}\pi(1-r) - \frac{\pi}{4}, \quad 0 \leq r \leq 1,$$

i.e. the fibers rotate intramurally linearly with the depth for a total amount of 120° .

procs	dof	Slab domains						Ellipsoidal domains					
		V		VE		VEF		V		VE		VEF	
		lit	time	lit	time	lit	time	lit	time	lit	time	lit	time
256	105903	96	0.31	41	0.44	37	0.44	473	0.74	165	0.91	150	0.81
512	209223	93	0.44	40	0.42	37	0.50	566	1.50	185	0.99	163	1.14
1024	413343	90	0.52	38	0.58	34	0.63	598	2.15	177	1.60	153	1.67
2048	807003	96	0.66	38	0.74	34	0.96	644	3.11	180	2.14	158	2.63
4096	1633023	88	0.95	38	1.12	29	1.33	589	5.00	181	3.45	154	4.17
8192	3188283	89	1.50	36	1.92	29	2.74	626	28.33	192	6.49	167	7.89
16384	6491583	88	2.38	33	3.38	26	5.40	796	33.24	189	11.19	148	14.06

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). Fixed local mechanical mesh: $5 \times 5 \times 5$ elements. Local mechanical problem size = 648. Table with the number of processors (procs.), 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).

4.1. Weak scaling test

We first consider a weak scaling test on slab and truncated ellipsoidal domains of increasing size, run on the Cray XC40 machine Shaheen. The number of subdomains (processors) is increased from 256 to 16384, with the largest domain being a slab or a truncated half ellipsoid with parameters $\phi_{min} = -\pi/2$, $\phi_{max} = \pi/2$, $\theta_{min} = -3\pi/8$, $\theta_{max} = \pi/8$. 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 thousands degrees of freedom for the case with 256 subdomains to about 6.5 millions degrees of freedom for the case with 16384 subdomains. In the BDDC preconditioner, we have considered three choices of primal constraints associated with vertices (V), vertices and edge averages (VE), and vertices, edge and face averages (VEF). 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 are reported in Table 1, for both slab (left columns) and ellipsoidal (right columns) domains. The same experimental results are also reported in Fig. 1 as functions of N for the slab (left) and ellipsoidal (right) domains, for a graphical comparison. Both the nonlinear Newton iterations (not shown) and linear GMRES iteration (lit) are completely scalable, except for the primal choice V in the ellipsoidal test. We remark that the scalability of the GMRES iterations is achieved by the use of the BDDC preconditioner. For both slab and ellipsoidal tests, the BDDC iteration counts are largest for the vertex primal choice V as expected; the introduction of additional edge averages (VE) reduced the number of iterations by more than a factor 2. A further reduction is achieved by also considering the face averages (VEF). The iteration counts are much higher in the ellipsoidal tests than in the slab tests, due to the domains curvature and mesh non-uniformity. In spite of the scalability of the iteration counts, the CPU times are not scalable, particularly for high core counts, where the solution of the BDDC coarse problem becomes a bottleneck. In the slab tests, the best CPU times are given by the primal choice V, even if it requires more iterations, followed by the cases VE and VEF. In the ellipsoidal tests the

procs.	VE			VEF		
	lit	time	speedup	lit	time	speedup
64	58	80.1	1	57	82.9	1
128	53	28.9	2.77 (2)	47	29.8	2.78 (2)
256	88	11.4	7.03 (4)	75	11.6	7.15 (4)
512	87	5.5	14.56 (8)	75	5.7	14.54 (8)
1024	59	3.7	21.65 (16)	43	3.7	22.40 (16)

Table 2: Strong scaling test on a truncated ellipsoidal domain. Mechanical solver with GMRES-BDDC and different choices of primal constraints: vertices + edges (VE) and vertices + edges + faces (VEF). Fixed global mechanical mesh: $96 \times 96 \times 24$ elements. Total mechanical size = 705675. In the Table are reported the number of processors (procs.), the average GMRES iterations per Newton iteration (lit), the average CPU time in seconds per Newton iteration (time) and the speedup with respect to the 64 processor run. The ideal speedup is reported in brackets.

timings increase considerably, due to the higher linear and nonlinear (not shown) iteration counts; the best CPU times are given by the choice VE, followed by VEF and V (except in the smallest test with 256 cores). These timings indicate that additional code optimization is required in order to exploit the iteration counts scalability to obtain improved and scalable timings.

4.2. Strong scaling test

We then report on a strong scaling test run on the BlueGene/Q machine Fermi of CINECA using the Land-Niederer active tension model (4). The three-dimensional cardiac domain considered is a truncated half ellipsoid (with parameters $a_1 = b_1 = 1.5$, $c_1 = 4.4$, $a_2 = b_2 = 2.7$, $c_2 = 5$, all in cm, and $\phi_{min} = -\pi/4$, $\phi_{max} = \pi/4$, $\theta_{min} = -\pi/4$, $\theta_{max} = \pi/8$). modeling a half of the left ventricular wall, discretized by a fine electrical mesh of $384 \cdot 384 \cdot 96$ Q_1 finite elements. The mechanical mesh size is four times larger than the electrical one in each direction, thus the mechanical elements are $96 \cdot 96 \cdot 24$ resulting in 705675 degrees of freedom. The number of subdomains (processors) increases from 64 to 1024 whereas the number of degrees of freedom per subdomain is reduced as the number of subdomains increases. Results are reported for the primal choices VE and VEF. As in the previous test, the physical dimensions of the truncated ellipsoidal domain are chosen so that the electrical mesh size h is kept fixed to the value of about $h_e = 0.01$ cm and the simulation is run for 10 time steps of size $\tau_e = 0.05$ ms during the excitation phase.

Table 2 reports the GMRES iterations (lit), the CPU times and speedup of the mechanical solver. The speedup is defined with respect to the 64 processors run as

$$speedup(procs.) := \frac{time(64)}{time(procs.)}.$$

The GMRES iterations are completely scalable, since they remain bounded when the number of processors increases. A superlinear speedup has been observed, and it can be attributed to the reduction of the computational times for backward and forward substitutions needed by the direct solvers used for the static condensation step in (14) and in the application of the BDDC preconditioner (20). The use of additional face primal constraints did not improve the convergence rate of the linear solvers. We observe that the increase of GMRES iterations in the 256 and 512 processor runs with respect to the 1024 processor run could be due to the different aspect ratios of the subdomains, i.e. to the varying ratio H/h in the condition number bound (21) that we conjectured to hold in Remark 1. We finally remark that these results outperform those obtained with an Algebraic Multigrid solver, presented in our previous publication [13].

		V		VE		VEF	
H/h	dof	lit	time	lit	time	lit	time
		slab domains					
5	105903	94	1.0	42	1.0	38	1.1
7	282663	117	3.0	44	2.8	41	3.1
9	591519	138	7.9	46	7.1	42	7.7
11	1069335	158	20.0	48	17.5	45	18.8
13	1752975	180	46.5	49	39.5	48	42.3
15	2679303	202	98.4	53	82.7	51	87.3
		ellipsoidal domains					
5	105903	475	3.3	180	2.3	168	2.6
7	282663	574	8.3	189	5.0	176	5.5
9	591519	598	18.8	197	11.3	187	12.2
11	1069335	856	54.3	219	26.7	193	27.2
13	1752975	840	109.4	222	57.0	203	58.5
15	2679303	-	-	231	114.5	211	116.7

Table 3: Quasi-optimality test on slab and ellipsoidal domains. Mechanical solver with GMRES-BDDC and different choices of primal constraints: vertices (V), vertices + edges (VE) and vertices + edges + faces (VEF). Fixed number of processors = 256. Number reported are the ratio H/h , the total mechanical degrees of freedom (dof), the average GMRES-BDDC iterations per Newton iteration (lit) and the average CPU time in seconds per Newton iteration (time).

Figure 2: Quasi-optimality test on slab (left) and ellipsoidal (right) domains. Mechanical solver with GMRES-BDDC and different choices of primal constraints: vertices (V), vertices + edges (VE) and vertices + edges + faces (VEF). Fixed number of processors = 256. Plot of the GMRES-BDDC iteration counts for the slab (left) and ellipsoidal (right) domains.

4.3. Quasi-optimality test

We then consider a quasi-optimality test on slab and ellipsoidal domains running on the Blue-Genie/Q machine Fermi of CINECA. The number of subdomain (processors) is kept fixed to 256, and the mesh is refined. Thus the number of local unknowns increases by increasing the ratio H/h as indicated in Table 3. The number of mechanical degrees of freedom increases from 100 thousands

to 2.6 millions. Primal spaces considered are V, VE, and VEF. The simulation is run for 10 time steps of 0.05 ms during the excitation phase.

The results reported in Table 3 show that, with only vertices as primal unknowns, the GMRES iterations grow faster than with the richer coarse spaces. When the ratio H/h is large, the best choice in terms of CPU time is vertices + edges (VE) as primal unknowns. GMRES iterations counts are also plotted in Figure 2 as functions of H/h for the slab (left) and ellipsoidal (right) domains, indicating a linear growth of the iteration counts with the ratio H/h .

	V			VE			VEF		
strain energy	nit	lit	time	nit	lit	time	nit	lit	time
axisymmetric	3	412	2.67	3	209	3.43	3	205	5.02
orthotropic	3	306	2.06	3	160	2.69	3	148	3.83

Table 4: Axisymmetric vs. Orthotropic strain energy functions. BDDC primal constraints (V, VE, VEF); Newton iterations at the last time step $t=50$ ms (nit); GMRES-BDDC iteration per Newton step (lit); CPU times in seconds for the entire Newton solve.

4.4. Axisymmetric vs Orthotropic strain energy function

In this test, we study the dependence of our BDDC solver on the choice of the strain energy function. We consider an axisymmetric and an orthotropic law, with the parameters reported in [19]. The ventricular domain is a truncated ellipsoid discretized by an electrical mesh of $512 \times 256 \times 64$ Q1 finite elements. The mechanical mesh is eight times coarser than the electrical, with a grid of $64 \times 32 \times 8$ finite elements. Thus, the unknowns of the Monodomain linear system are 8552960, while the unknowns of the finite elasticity system are 57024. The number of subdomains and processors is kept fixed to 256. Primal spaces considered are V, VE, and VEF. The simulations last for 50 ms after the onset of stimulation and run on the Cray XC40 Shaheen of KAUST.

The results reported in Table 4 refer to the last time step at $t=50$ ms, when the mechanical contraction process is in a computationally intensive phase. The results indicate that the NKBDDC solver is quite robust with respect to the strain energy function considered. The Newton iterations are always 3, while in this particular case, the orthotropic law requires less linear iterations than the axisymmetric one. For both laws, the linear iterations are highest with the primal choice V, are reduced by about half with the choice VE and slightly further reduced by the choice VEF, while the CPU times are smallest with V and increase with VE and VEF.

	Newton iterations				GMRES-BDDC iterations				CPU time			
	per time step				per Newton step				per time step			
	m	aver.	M	total	m	aver.	M	total	m	aver.	M	total
V	1	3.5	6	7083	10	615.5	7485	$1.23 \cdot 10^6$	2.6	24.5	222.8	$5.76 \cdot 10^4$
VE	1	3.5	6	7083	10	617.7	9221	$1.23 \cdot 10^6$	2.6	24.6	272.2	$5.78 \cdot 10^4$
VEF	1	3.5	6	7083	6	517.4	6313	$1.03 \cdot 10^6$	2.6	25.4	225.2	$5.94 \cdot 10^4$

Table 5: Whole heartbeat simulation. From left to right: BDDC primal constraints (V, VE, VEF); Newton iterations per time step (minimum (m), average (aver.), maximum (M)) and total; GMRES-BDDC iteration per Newton step (minimum (m), average (aver.), maximum (M)) and total; CPU times per time step (minimum (m), average (aver.), maximum (M)) and total.

Figure 3: Whole heartbeat simulation. Mechanical deformation of the cardiac domain at selected time instants. The colors denote the value of the transmembrane potential v at each point, ranging from resting (blue) to excited (red) values. The values on the axis are expressed in centimeters.

4.5. Whole heartbeat simulation

We now present the results of a whole heartbeat simulation on 1024 processors using the Land-Niederer active tension model (4) and run on the BlueGene/Q machine Fermi of CINECA. The domain is a truncated half ellipsoid discretized with a $96 \times 96 \times 24$ mechanical mesh (705675 dof) nested in a $384 \times 384 \times 96$ electrical mesh (28755650 dof). Fig. 3 reports the transmembrane potential distributions on the deforming cardiac domain at nine selected time instants during the heartbeat, while Fig. 4 shows the activation time (ACTI), repolarization time (REPO) and action potential duration (APD) distributions on the epicardial, midmyocardial and endocardial surfaces of the ellipsoidal domain in the reference configuration. Below each panel are reported the minimum, the maximum, and the step (in ms) of the displayed map.

The time evolution of the GMRES and Newton iterations displayed in Fig. 5 show that the most difficult phase for the mechanical solver occurs at 100 ms after the stimulus during the plateau phase of the heartbeat, when the contraction is maximal. Table 5 reports the average (per time step) and total number of Newton iterations, the average (per Newton step) and total number of GMRES iterations, the average (per time step) and total CPU times. In terms of CPU time, the results reported in Table 5 indicate that the BDDC preconditioners with V and VE coarse spaces are the most effective, even if the BDDC with VEF coarse space attains the best performance in

terms of total number of linear iterations.

Figure 4: Whole heartbeat simulation. Activation (ACTI), repolarization (REPO) time and action potential duration (APD) distributions on the epicardial, midmyocardial and endocardial surfaces of the reference domain. Below each panel are reported the min, max and step in ms of the displayed map. The values on the axis are expressed in centimeters.

5. Conclusion

We have developed a scalable solver for the cardiac electromechanical coupling. The parallel solver is based on solving the nonlinear system deriving from the discretization by finite elements of the quasi-static mechanical model with a Newton-Krylov-BDDC (NKBDDC) method, where the linear Jacobian system is solved by GMRES, preconditioned by a BDDC preconditioner. Three-dimensional parallel numerical tests have shown that the proposed method is scalable in the number of subdomains, quasi-optimal in the ratio of subdomain to mesh sizes, and robust with respect to tissue anisotropy. Moreover, the scalability of the solver is independent of the active tension model employed.

Further developments of this study should include: the extension to the more complex Bidomain model of bioelectrical activity instead of the Monodomain model; the investigation of more sophisticated scaling functions in the BDDC preconditioner, such as the deluxe scaling, and of adaptive

Figure 5: Whole heartbeat simulation. time evolution of total GMRES-BDDC iteration (top left), GMRES-BDDC iteration per time step (top right), Newton iterations per time step (bottom left), timings of Newton solves per Newton iteration (bottom right).

choices of primal BDDC constraints; the comparison of the proposed NKBDDC method with non-linear BDDC or FETI-DP techniques; the use of more efficient Krylov solvers like BiCG-STAB (since the Jacobian seems to be positive definite); the validation of our results on unstructured meshes and irregular subdomain partitions.

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