Isogeometric Overlapping Additive Schwarz Solvers for the Bidomain System

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1 Introduction

The electrical activity of the heart is a complex phenomenon strictly related to its physiology, fiber structure and anatomy.

At the cellular level the cell membrane separates both the intra- and extracellular environments consisting of a dilute aqueous solution of dissolved salts dissociated into ions. Differences in ion concentrations on opposite sides of the membrane lead to a voltage called the *transmembrane potential*, v_M, defined as the difference between the intra- and extracellular potentials, (u_I and u_E). The bioelectric activity of a cardiac cell is described by the time course of v_M, the so called *action potential*. At the tissue level the most complete mathematical model of cardiac electrophysiology is the Bidomain model, consisting of a degenerate reaction-diffusion system of a parabolic and an elliptic partial differential equation modelling v_M and u_E of the anisotropic cardiac tissue, coupled nonlinearly with a membrane model. The multiscale nature of the Bidomain models yields very high computational costs for its numerical resolution. The starting point for a spatial discretization is a geometrical representation that encompasses the required anatomical and structural details, and that is also suitable for computational studies. Detailed models were proposed based on structured grids with cubic Hermite interpolation functions, which enable a smooth representation of ventricular geometry with relatively few elements, see e.g. Smith et al. [2004]. In this study we used an alternative approach based on Isogeometric Analysis (IGA), a novel method for the discretization of partial differential equations introduced in Hughes et al. [2005]. This method adopts the same spline or Non-Uniform Rational B-spline (NURBS) basis functions used to design domain geometries in CAD to construct both trial and test spaces in the discrete variational formulation

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of the differential problem, and provides a higher control on the regularity of the discrete space. The IGA discretization of the Bidomain model in space and semi-implicit (IMEX) finite differences in time lead to the resolution at each time step of a large and very ill-conditioned linear system. Since the iteration matrix is symmetric semidefinite, it is natural to use the preconditioned conjugate gradient method.

We have developed and analyzed an overlapping additive Schwarz preconditioner for the isogeometric discretization of the cardiac Bidomain model. We have proved that the resulting solver is scalable and optimal in the ratio of subdomain/overlap size. Several tests confirm the theoretical bound on three-dimensional NURBS domains. We note that Isogeometric overlapping Schwarz preconditioners were first introduced in Beirão da Veiga et al. [2012] for scalar elliptic problems, while multilevel Schwarz preconditioners for FEM discretizations of the Bidomain system were studied in Pavarino and Scacchi [2008].

2 The Bidomain Model

The macroscopic Bidomain representation of cardiac tissue volume is obtained by considering the superposition of two anisotropic continuous media the intra- (I) and extra- (E) cellular media, coexisting at every point of the tissue and separated by a distributed continuous cellular membrane; see Pennacchio et al. [2005] for a derivation of the Bidomain model from homogenization of cellular model. 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, see LeGrice et al. [1995]. The anisotropy of the intra- and extracellular media is described by the orthotropic conductivity tensors $D_I(x)$ and $D_E(x)$, see e.g. Colli Franzone et al. [2005]. We denote by Ω the bounded physical region occupied by the cardiac tissue and introduce a parabolic-elliptic formulation of the Bidomain system. Given an extra-cellular applied stimulus per unit volume I^E_{app}, we seek the transmembrane and the extracellular potentials, v_M and u_E, respectively, and the gating variable w satisfying the system

$$\begin{cases} c_m \frac{\partial v_M}{\partial t} - \mathrm{div}(D_I \nabla (v_M + u_E)) + I_{ion}(v_M, w) = 0 & \text{on } \Omega \times (0,T) \\ -\mathrm{div}((D_I + D_E)\nabla u_E) - \mathrm{div}(D_I \nabla v_M) = I^E_{app} & \text{on } \Omega \times (0,T) \\ \frac{\partial w}{\partial t} - R(v_M, w) = 0 & \text{on } \Omega \times (0,T) \end{cases} \quad (1)$$

with insulating boundary conditions, suitable initial conditions on v_M, u_E and w, while c_m is the membrane capacitance per unit volume. The nonlinear reaction term I_{ion}, the ionic current of the membrane per unit volume, and the ODE system for the gating variables are given by the chosen ionic

membrane model. Here we will consider the (LR1) membrane model by Luo and Rudy [1991]. The system uniquely determines v_M, while u_E is defined only up to a same additive time-dependent constant, chosen by imposing $\int_\Omega u_E \, \mathrm{d}\mathbf{x} = 0$.

3 Discretization and numerical methods

Isogeometric space discretization. In the three-dimensional case, our domain Ω, representing the left ventricle, is modeled by a family of truncated ellipsoids. According to the isoparametric approach we discretized the Bidomain system (1) with IGA based on NURBS basis functions, see e.g. Cottrell et al. [2009]. NURBS functions are built from B-spline functions.
In what follows, let $d \geq 2$ be the dimension of the physical domain of interest. For any $\alpha = 1, ..., d$, we introduce the open knot vector, a set of non decreasing real numbers $\Xi_\alpha = \{0 = \xi_{1,\,\alpha}, \xi_{2,\,\alpha}, ..., \xi_{n_\alpha+p+1,\,\alpha} = 1\}$, where p is the order of the B-spline and n_α is the number of basis functions necessary to describe it. Given the knot vector, it is possible to define univariate B-spline basis functions, $B^p_{i,\alpha}(\xi)$, and by tensor product the multivariate B-spline basis functions, $B^p_{i_1,\ldots,i_d}$. Therefore the tensor product spline space living in the parametric domain is

$$\hat{V} := \mathrm{span}\{B^p_{i_1\ldots i_d},\ i_\alpha = 1, ..., n_\alpha, 1 \leq \alpha \leq d\}.$$

Given $\omega_{i_1\ldots i_d}$ the *weights* associated to $\mathbf{C}_{i_1\ldots i_d}$, a mesh of *control points*, we can define the NURBS basis function on the parametric domain

$$R^p_{i_1\ldots i_d}(\xi) = \frac{B^p_{i_1\ldots i_d}(\xi)\omega_{i_1\ldots i_d}}{w(\xi)},$$

with $w(\xi) := \sum_{i_i\ldots i_d}^{n_1\ldots n_d} B^p_{i_1\ldots i_d}(\xi)\omega_{i_1\ldots i_d}$.

Since the single patch domain Ω is a NURBS region, we define a geometrical map $\mathbf{F} : (0,1)^d \to \Omega$ as

$$\mathbf{F}(\xi) = \sum_{i_1=1}^{n_1} ... \sum_{i_d=1}^{n_d} R^p_{i_1\ldots i_d}(\xi)\mathbf{C}_{i_1\ldots i_d},$$

and the physical space V as the span of the pushforward of the NURBS basis functions

$$V := \mathrm{span}\{R^p_{i_1\ldots i_d} \circ \mathbf{F}^{-1}, i_\alpha = 1, \ldots, n_\alpha, 1 \leq \alpha \leq d\}.$$

A semidiscrete problem of (1) is obtained by applying a standard Galerkin procedure. We denote by M the mass matrix, by $A_{I,E}$ the symmetric stiffness matrices associated to the intra- and extra anisotropic conductivity tensors,

respectively.

Time discretization. The time discretization is performed by a decoupled semi-implicit method consisting of the two following steps:

- Given $\mathbf{v}_M^n$, $\mathbf{u}_E^n$ and $\mathbf{w}^n$ at the previous step n, we first solve the ODEs system for the gating and ionic concentration variables. Since the membrane model employed is the LR1, the ODE integration approach is based on the Rush-Larsen method, see Rush and Larsen [1978].
- Once computed $\mathbf{w}^{n+1}$, a semi-implicit scheme is applied to the reaction-diffusion part, see Ascher et al. [1995], i.e., by using the implicit Euler method for the diffusion term, while the nonlinear reaction term I_{ion} is treated explicitly. As a consequence at each time step we need to solve the linear system

$$\begin{bmatrix} \frac{c_m}{\Delta t}M + A_I & A_I \\ A_I & A_I + A_E \end{bmatrix} \begin{pmatrix} \mathbf{v}_M^{n+1} \\ \mathbf{u}_E^{n+1} \end{pmatrix} = \begin{pmatrix} \frac{c_m}{\Delta t}M\mathbf{v}_M^n - \mathbf{i}_{ion}(\mathbf{v}_M^n, \mathbf{w}^{n+1}) \\ \mathbf{I}_{app}^E \end{pmatrix} \quad (2)$$

imposing $\mathbf{1}^T M \mathbf{u_E}^{n+1} = 0$. Due to the ill-conditioning of the iteration matrix and the large number of unknowns required by realistic simulations of cardiac excitation in three-dimensional domains, a scalable and efficient preconditioner is required.

We recall that the linear system (2) is equivalent to the elliptic variational problem: given $f \in L^2(\Omega)$,

$$\text{find } u \in U \text{ such that} \quad a_{bido}(u, z) = (f, z_M) \quad \forall z = [z_M,\, z_E] \in U,$$

where $U := V \times \tilde{V}$, with $\tilde{V} := \{u_E \in V \,:\, \int_\Omega u_E = 0\}$, while for the definition and the properties of the bilinear form a_{bido} see Pavarino and Scacchi [2011].

4 Overlapping Schwarz preconditioners

In this section, we construct an isogeometric overlapping additive Schwarz preconditioner for the Bidomain system, using the general framework developed in Beirão da Veiga et al. [2012] for a model elliptic problem, and in Pavarino and Scacchi [2008] for the Bidomain system discretized using FEM. For $\alpha = 1, ..., d$, we define a decomposition of the reference interval $\hat{I}$ selecting from the open knot vector Ξ_α a subset of $N_\alpha + 1$ nonrepeated interface knots $\{\xi_{i_{m_\alpha},\alpha}, m_\alpha = 1, ..., N_\alpha + 1 | \xi_{i_1,\alpha} = 0,\ \xi_{i_{N_\alpha+1},\alpha} = 1\}$. Thus, the closure of $\hat{I}$ can be decomposed into N_α intervals $\hat{I}_{m_\alpha,\alpha} := (\xi_{i_{m_\alpha},\alpha}, \xi_{i_{m_\alpha+1},\alpha})$, assuming that they have a similar diameter on order H. For each of the interface knots there exists at least one index $s_{m_\alpha,\alpha}$ such that $2 \le s_{m_\alpha,\alpha} \le n_\alpha - 1$ and so that the support of the basis function $B^p_{s_{m_\alpha,\alpha}}$ intersects both $\hat{I}_{m_\alpha-1,\alpha}$ and $\hat{I}_{m_\alpha,\alpha}$.

Let r be an integer counting the basis functions shared by adjacent subdomains. We are able to define N_α subspaces $\{\hat{V}_{m_\alpha,\alpha}\}_{m_\alpha=1}^{N_\alpha}$ forming an over-

lapping decomposition of the B-spline univariate space, $\hat{V}$, as

$$\hat{V}_{m_\alpha,\alpha} := \text{span}\{B^p_{j,\alpha}(\xi) | s_{m_\alpha,\alpha} - r \leq j \leq s_{m_\alpha+1,\alpha} + r\} \quad m_\alpha = 1, ..., N_\alpha.$$

We build the coarse space $\hat{V}_{0,\alpha}$ from the partition of $\hat{I}$. Let

$$\Xi_{0,\alpha} = \{\xi_{1,\alpha}, ..., \xi_{p,\alpha}, \xi_{i_1,\alpha}, \xi_{i_2,\alpha}, ..., \xi_{i_{N_\alpha-1},\alpha}, \xi_{i_{N_\alpha},\alpha}, \xi_{i_{N_\alpha+1},\alpha}, ..., \xi_{i_{N_\alpha+p+1},\alpha}\}$$

an open knot vector and let $\{\overset{\circ}{B}{}^p{}_{i,\alpha}\}_{i=1}^{N_{0,\alpha}}$ be the corresponding $N_{0,\alpha}$ basis functions, then the coarse space is

$$\hat{V}_{0,\alpha} = \text{span}\{\overset{\circ}{B}{}^p{}_{i,\alpha}, \quad i = 1...N_{0,\alpha}\}.$$

In more than one dimension, we proceed by using tensor product. Let $N := \prod_1^d N_\alpha$, for $m = 1, ..., N$ the local and the coarse subspaces are then

$$\hat{V}_m \equiv \hat{V}_{m_1,...,m_d} := \text{span}\{B^p_{i_1,...,i_d},\ s_{m_\alpha} - r \leq i_\alpha \leq s_{m_\alpha+1} + r,\ \alpha = 1, ..., d\};$$
$$\hat{V}_0 := \text{span}\{\overset{\circ}{B}{}^p{}_{i_1,...,i_d}, \quad i_\alpha = 1...N_{0,\alpha},\ \alpha = 1, ..., d\}.$$

The decomposition of the NURBS space V and therefore of U in the physical domain is trivial:
$U_m := V_m \times V_m$ and $U_0 := V_0 \times \tilde{V}_0$ with

$$V_m \equiv V_{m_1,...,m_d} := \text{span}\{R^p_{i_1,...,i_d} \circ \mathbf{F}^{-1},\ s_{m_\alpha} - r \leq i_\alpha \leq s_{m_\alpha+1} + r,\ \alpha = 1, ..., d\};$$
$$V_0 := \text{span}\{\overset{\circ}{R}{}^p{}_{i_1,...,i_d} \circ \mathbf{F}^{-1},\ i_\alpha = 1...N_{0,\alpha},\ \alpha = 1, ..., d\} \quad \text{and} \quad \tilde{V}_0 := V_0 \cap \tilde{V}.$$

We are now able to construct a two-level overlapping Additive Schwarz method for the Bidomain system (2). We remark that $U_0 \subset U$, whereas U_m is not a subset of U, $m = 1, ..., N$. We define therefore the interpolation operators $\mathbf{I}_m : U_m \to U$ as

$$\text{given } u = (v_M,\ u_E) \in U_m,\ \mathbf{I}_m u = (\mathbf{I}_{m,M} u, \mathbf{I}_{m,E} u) := (v_M, u_E - \frac{1}{|\Omega|} \int_\Omega u_E),$$

whereas $\mathbf{I}_0 : U_0 \to U$ is simply the embedding operator. We define the local projectors operators $\widetilde{\mathbf{T}}_m : U \to U_m$ for $m = 0, ..., N$ by

$$a_{bido}(\widetilde{\mathbf{T}}_m u, v) = a_{bido}(u, \mathbf{I}_m v) \quad \forall v \in U_m.$$

Defining $\mathbf{T}_m = \mathbf{I}_m \widetilde{\mathbf{T}}_m$, the 2-level Overlapping Additive Schwarz (OAS) operator is then

$$\mathbf{T}_{OAS} := T_0 + \sum_{m=1}^{N} \mathbf{T}_m.$$

We have the following result about the convergence rate bound, see Charawi [2014].

Theorem 1. *Under the assumptions that the parametric mesh is quasi-uniform and the overlap index r is bounded from above by a fixed constant, the condition number of the preconditioner operator T_{OAS} is bounded by*

$$\kappa(\mathbf{T}_{OAS}) \leq C\left(1+\frac{H}{\delta}\right), \tag{3}$$

where $\delta := h(2r+2)$ is the overlap parameter and C is a constant independent of h, H, N and δ but not of p and the regularity k.

5 Numerical results

Numerical results presented in this section refer to the 3D Bidomain problem on a portion of the truncated ellipsoid, representing a simplified ventricular geometry. The IGA discretization with mesh size h and polynomial degree p and regularity k is carried out by in MATLAB, using the library GeoPDEs, De Falco et al. [2011]. The domain is decomposed in N overlapping subdomains of characteristic size H and overlap index r.

Table 1 shows the scalability of the 2-level OAS preconditioner for a 3D NURBS domain decomposed into an increasing number of subdomains, such that their size are fixed $\frac{H}{h} = 4$, $p = 3$, $k = 2$ and $r = 0, 1$. The simulation is run for 30 time steps, 1.5 ms, and the condition number is estimated using the usual Lanczos' method. As expected the 1-level preconditioner (without coarse problem) has a condition number growing with N, and the performances of the 2-level OAS improve when increasing the overlap size. Additional results, for $p = 3, 2$ and $k = p - 1$, are plotted in Fig.1, and confirm that the condition number, κ, of the 2-level preconditioned problem grows linearly with the increasing ratio $\frac{H}{h}$, as predicted by (3) using minimal overlap ($r = 0$).

Finally, Fig. 2 compares the variation of the condition number and iteration count during a complete heartbeat (300 ms) by using 1- and 2-level OAS solvers or unpreconditioned Conjugate Gradient. These variations are strictly related to the time step size (Δt), that changes according to the adaptive strategy described in Colli Franzone et al. [2005], following the different phases of a ventricular action potential. In this test the number of the subdomains is $6 \times 6 \times 5$ and the ratio $\frac{H}{h} = 4$. We can note that the depolarization is the most intense computationally phase, nevertheless OAS solvers keep the condition number quite uniform for all the duration of the cycle. As expected, the 2-level greatly improves the conditioning of the problem.

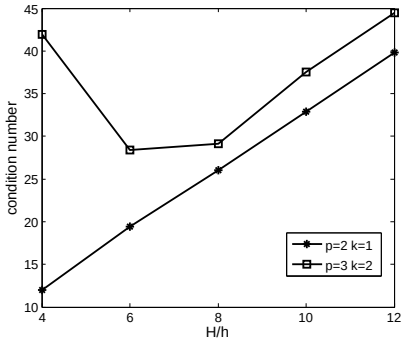

Fig. 1 2-level OAS dependence on $\frac{H}{h}$: plot of κ as a function of $\frac{H}{h}$, for $p = 2, 3$ and $k = p - 1$.

Table 1 OAS preconditioner in 3D ellipsoidal domain. Scalability test:iteration counts (it.), condition number κ and extreme eigenvalues (λ_{max} and λ_{min}) as a function of the number of subdomains N for fixed $H/h = 4$ for unpreconditioned (Unpc.), 1-level and 2-level OAS preconditioners. $p = 3$, $k = 2$ and $r = 0, 1$.

	Unpc.		1-level OAS		2-level OAS			
					r=0		r=1	
N	it.	κ	it.	$\kappa = \lambda_{max}/\lambda_{min}$	it.	$\kappa = \lambda_{max}/\lambda_{min}$	it.	$\kappa = \lambda_{max}/\lambda_{min}$
$2 \times 2 \times 1$	175	4.98e3	21	65=4.0/6.09e-2	12	11.07=4.74/4.12e-1	6	5.24 = 5.00/0.95
$3 \times 3 \times 2$	185	4.44e3	44	331=8.0/2.41e-2	22	32.13=8.60/2.72e-1	9	10.87 = 9.21/0.85
$4 \times 4 \times 3$	206	6.32e3	61	627=8.0/1.27e-2	23	31.90=8.63/2.73e-1	8	9.00 = 9.31/1.03
$5 \times 5 \times 4$	247	8.89e3	78	1020=8.0/7.84e-3	23	32.09=8.64/2.69e-1	8	10.39 = 9.20/0.89
$6 \times 6 \times 5$	297	1.20e4	94	1507=8.0/5.31e-3	23	31.60=8.64/2.27e-1	7	9.16 = 6.95/1.32

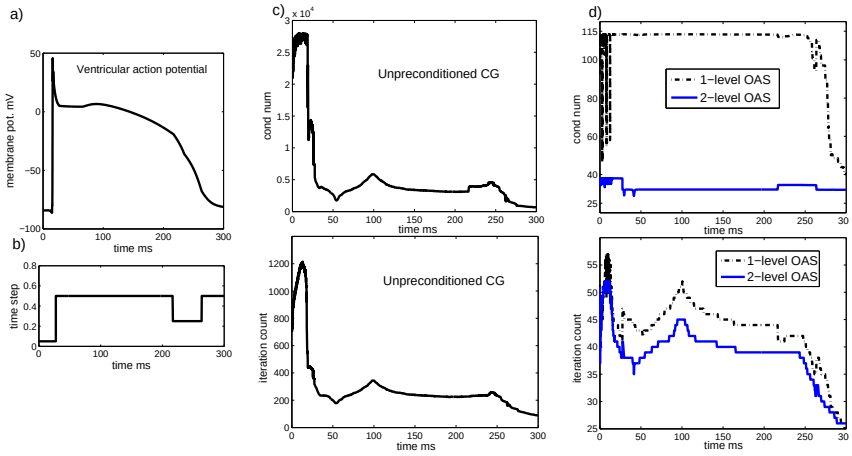

Fig. 2 Complete heart beat. **a)-b):** Variation of the time step size following the phases of a ventricular action potential. **c)-d)**: Time course of κ (upper panels) and iteration count (lower panels) during a heartbeat: comparison between unpreconditioned operator c) and 1- and 2-level OAS d). $N = 6 \times 6 \times 5$, $\frac{H}{h} = 4$, $p = 3$, $k = 2$ and $r = 0$.

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