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COMPUTATIONAL CHALLENGES IN BUILDING MULTI-SCALE AND MULTI-PHYSICS MODELS OF CARDIAC ELECTRO-MECHANICS

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Abstract

Despite the evident multiphysics nature of the heart – it is an electrically controlled mechanical pump – most modeling studies considered electrophysiology and mechanics in isolation. In no small part, this is due to the formidable modeling challenges involved in building strongly coupled anatomically accurate and biophyically detailed multi-scale multi-physics models of cardiac electro-mechanics. Among the main challenges are the selection of model components and their adjustments to achieve integration into a consistent organ-scale model, dealing with technical difficulties such as the exchange of data between electro-physiological and mechanical model, particularly when using different spatio-temporal grids for discretization, and, finally, the implementation of advanced numerical techniques to deal with the substantial computational. In this study we report on progress made in developing a novel modeling framework suited to tackle these challenges.

Keywords

cardiac electrophysiology; cardiac mechanics; bidomain model; Purkinje system; algebraic multigrid

Introduction

Despite the evident multiphysics nature of the heart – it is an electrically controlled mechanical pump – most modeling studies considered electrophysiology and mechanics in isolation. While the vast majority of organ-scale electrophysiological modeling studies ignore mechanical effects, most mechanical modeling studies accounted for electrical activity only in a highly simplistic fashion. Since important regulatory mechanisms in the heart are governed by complex interactions between processes of different physics, a new modeling trend emerged which aims at coupling cardiac electrics and mechanics in a multi-physics model in which multiple scales of biological organization, ranging from sub-cellular mechanisms up to the organ, are accounted for in great biophysical detail.

Building strongly coupled multi-scale multi-physics models of cardiac electro-mechanics poses a series of formidable challenges. First, a set of model components which comprise the organ-scale electro-mechanical model, has to be chosen and complex model adjustments

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have to be made to achieve integration into a consistent organ-scale model. In strongly coupled models a constant exchange of data between electro-physiological and mechanical model is required. Since electrics and mechanics are governed by different time and space constants, different spatio-temporal grids may be used, thus complicating the construction of solver codes, particularly when aiming for massively parallel execution. Finally, the computational burden imposed by such models is significant, necessitating the use of advanced numerical methods and the consequent exploitation of current trend in HPC towards massive parallelization, be it on CPU or GPU clusters. In this study we report on progress made in developing a novel modeling framework suited to tackle these challenges.

Methods

Modeling of cardiac electro-mechanics relies upon discretizations of the bidomain equations to characterize electro-physiology at the tissue scale, and the finite deformation elasticity equation to describe cardiac deformation under mechanical loads and intrinsic active force generation and relaxation. In a strongly coupled multi-physics scenario both sets of equations have to be solved together, necessitating the bidirectional exchange of data between the two physics. The two directions of this coupling loop are referred to as excitation-contraction coupling (ECC) – generated stresses influence the state of deformation – and mechano-electric feedback (MEF) – mechanical stresses or strains influence upon cellular physiology via different mechanisms such as length dependent tension, calcium sensitivity or stretch-activated channels.

Governing equations

The set of equations governing cardiac electro-mechancis is given by

$$\begin{aligned} \nabla \cdot \left(\boldsymbol{\sigma}_i + \boldsymbol{\sigma}_e\right)\mathbf{C}^{-1}\nabla\phi_e &= -\nabla \cdot \boldsymbol{\sigma}_i\mathbf{C}^{-1}\nabla V_m \\ \nabla \cdot \boldsymbol{\sigma}_i\mathbf{C}^{-1}\nabla V_m &= -\nabla \cdot \boldsymbol{\sigma}_i\mathbf{C}^{-1}\nabla\phi_e + \beta I_m \end{aligned} \quad (1)$$

$$I_m = C_m\frac{\partial V_m}{\partial t} + I_{\text{ion}}\left(V_m, \boldsymbol{\eta}\right) \quad (2)$$

$$V_m = \Phi_i - \Phi_e \quad (3)$$

$$\frac{\partial \boldsymbol{\eta}}{\partial t} = f\left(\boldsymbol{\eta}, V_m, \sigma_a\right) \quad (4)$$

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$$\operatorname{div}\boldsymbol{\sigma}(\boldsymbol{u}) = \mathbf{b} \quad (5)$$

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_p + \boldsymbol{\sigma}_a \quad (6)$$

$$\boldsymbol{\sigma}_p = J^{-1/3}\overline{\mathbf{F}}\left(2\frac{\partial \Psi}{\partial \mathbf{C}}\right)\overline{\mathbf{F}}^{\mathrm{T}} \quad (7)$$

$$\boldsymbol{\sigma}_a = \sigma_a\left(\overline{\mathbf{f}} \otimes \overline{\mathbf{f}}\right) \quad (8)$$

$$\sigma_a = h\left(V_m, \boldsymbol{\eta}, \lambda, \dot{\lambda}\right) \quad (9)$$

In the bidomain equations (1)-(4) describing electrophysiology, ϕ_i and ϕ_e are the intracellular and extracellular potentials, respectively, $V_m = \phi_i - \phi_e$ is the transmembrane voltage, $\boldsymbol{\sigma}_\mathbf{i}$ and $\boldsymbol{\sigma}_\mathbf{e}$ are the intracellular and extracellular conductivity tensors, respectively, β is the membrane surface to volume ratio, I_m is the transmembrane current density, C_m is the membrane capacitance per unit area, and I_{ion} is the membrane ionic current density which depends on V_m and a set of state variables, $\boldsymbol{\eta}$. Deformation is governed by (5)-(9) with (9) linking electrics and mechanics.

Model Generation

An rabbit ventricular anatomy model was tomographically reconstructed from a MRI dataset [1] using a previously developed mesh generation technique [2]. A rule-based method was employed to assign fiber and sheet orientations [3]. A model of the specialized conduction system was incorporated to obtain realistic activation and repolarization sequences. The Mahajan-Shiferaw model of a rabbit ventricular myocyte was used to describe cellular dynamics [4]. Passive orthotropic material properties of the ventricular myocardium were described by an orthotropic hyperelastic constitutive model. Standard boundary conditions were prescribed for the electrical model. When solving for mechanical deformation, the ventricles were immersed in an elastic medium (Fig. 1). Homogeneous Dirichlet boundary conditions were applied along all surfaces of the container medium, except at the surface facing the base of the ventricles to allow for a larger atrio-ventricular plane displacement. Time-dependent inhomogeneous Neumann boundary conditions were prescribed along the ventricular endocardium, as imposed by the pressure in the ventricular cavities. Active tension development and relaxation were described by the Rice et al model [5]. Active tension was transferred from electrical to the mechanical grid prior to solving the

deformation equation (5). MEF was ignored, i.e. fiber stretch and stretch rate were not fed back into the active tension model.

Numerical Solution

Spatial discretization relied upon the finite element method (FE) where linear tetrahedral elements were used for both electrical and mechanical grid. The same FE grid was used for both problems, thus facilitating an easier exchange of data between the two physics problems. A custom-tailored unsmoothed aggregation algebraic multigrid (AMG) preconditioner for an iterative conjugate gradient (CG) solver was used to solve the deformation equation (5). Scalability benchmarks were performed on both CPUs and GPUs to assess potential and suitability of the numerical setup for solving Eq. (5) relative to other currently used numerical techniques.

Results

Numerical tests were performed on both CPUs and GPUs. A sinus beat was initiated by delivering a stimulus at the His bundle and the ensuing mechanical deformation was computed during the early contraction phase. Performance of the AMG-CG solver and matrix assembly time was monitored for varying core counts (Fig.1).

Discussion

The developed numerical framework for solving both bidomain as well as deformation equation provides adequate performance, allowing to perform electro-mechanically coupled simulations with anatomically detailed models in a tractable fashion. Solver speedups on the GPU were achieved, however, the major compute cost is due to the repeated assembly of the non-linear system. Thus, to speed up mechanics simulations significantly with GPU hardware, the entire FE pipeline has to be executed on the GPU.

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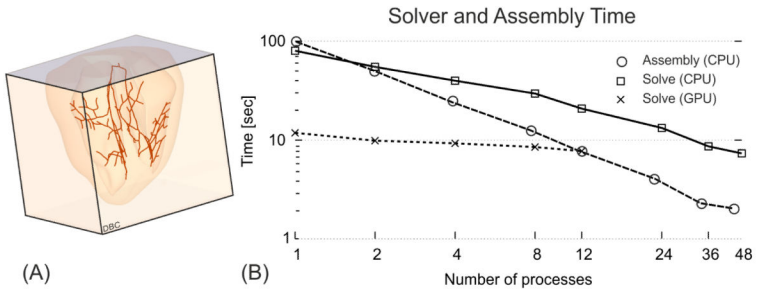

Figure 1.

(A) Benchmark setup showing rabbit ventricles with Purkinje system (red) immersed in an elastic container. Homogeneous Dirichlet boundary conditions (DBC) are applied to all faces of the container, except the blue face close to the base. (B) Strong scaling benchmark results for assembly of stiffness matrices, executed on the CPU, and solver time for both CPU and GPU.