Parallel Electromechanical model of the heart

M. Vázquez, P. Lafortune, G. Houzeaux, R. Arís

Barcelona Supercomputing Center - Centro Nacional de Supercomputación (BSC-CNS), Spain.
mariano.vazquez@bsc.es,
WWW home page: http://www.bsc.es

Abstract. In this paper, we present a high performance computational electromechanical model of the heart, coupling between electrical activation and mechanical deformation and running efficiently in up to thousands of processors. The electrical potential propagation is modelled by FitzHugh-Nagumo or Fenton-Karma models, with fiber orientation. The mechanical deformation is treated using anisotropic hyper-elastic materials in a total Lagrangian formulation. Several material models are assessed, such as models based on biaxial tests on excised myocardium or orthotropic formulations. Coupling is treated using the Cross-Bridges model of Peterson. The scheme is implemented in Alya, which run simulations in parallel with almost linear scalability in a wide range computer sizes, up to thousands of processors. The computational model is assessed through several tests, including those to evaluate its parallel performance.

Keywords: Computational Electrophysiology, Computational Solid Mechanics, Cardia Mechanics, Parallelization

1 Introduction

This paper continues previous works in Cardiac Computational Mechanics [1–6] that progressively go from Electrophysiology models in simple geometries up to coupled Electromechanical models for subject-specific geometries running in large scale parallel computers. Our objective is not to develop physiological models themselves but to develop computational tools to simulate these complex processes. By "computational tools" it should be understood from the numerical method up to the computer code, including parallelization techniques, ending up in a parallel simulation framework to be used by bio-engineers and medical researchers.

2 The Computational Model

At the organ level, the heart can be described as a Physical system with three mechanical problems: electrical propagation, mechanical deformation and blood flow, coupled in volume (electrical-mechanical) and in surface (mechanical-blood) (Figure 1). In this paper we describe electromechanical simulations, replacing real flow simulation by a simplified Windkessel-like pressure prescription at the epicardium. We next describe the two problems solved and the strategy to couple them togheter.

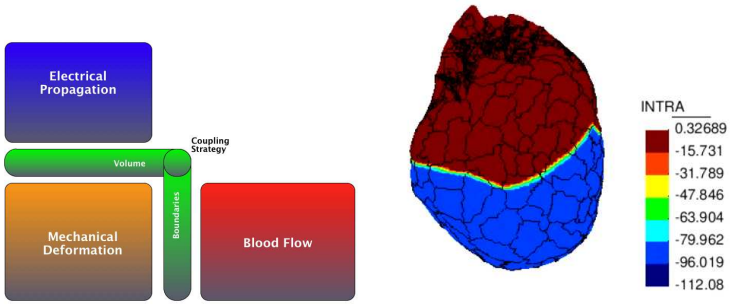

Fig. 1. Description of the heart as a mechanical system (left) and contracting heart, coloured by the propagating excitation potential.

2.1 Electrophysiology

The basic form of the electrical activation potentials ϕ_α propagation equation is[1]:

$$\frac{\partial \phi_\alpha}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial \phi_\alpha}{\partial x_j}\right) + L(\phi_\alpha). \tag{1}$$

Latin subindices counts the space dimension of the problem. Greek subindices counts the number of activation potentials involved, being $\alpha = 1$ for monodomain models and $\alpha = 1, 2$ for bidomain ones, extracellular and intracellular. The equation's right hand side represents the transient macroscopical model, based in the well known *continuum cable equation*. The diffusion term is governed by the diffusion tensor D_{ij}. The equation is set in a fixed reference frame and D_{ij} must describe the cable (i.e. cardiac tissue fibers) orientation in the fixed reference frame. Then, D_{ij} can be written as

$$D_{ij} = C^{-1}_{ik}\ D^{\mathrm{loc}}_{lk}\ C_{lj}, \tag{2}$$

where C_{lk} is the base change matrix from the local fiber-aligned reference frame (a_i, c^1_i, c^2_i) (i.e. one axial vector and two crosswise ones) to the global reference frame. D^{loc}_{lk} is the local diagonal diffusion matrix, whose diagonal components are the axial and crosswise fiber diffusions. $L(\phi_\alpha)$ is a reaction non-linear local term. We present results for FitzHugh-Nagumo and Fenton-Karma models.

2.2 Mechanical Deformation

The local form of the linear momentum balance, to be solved using a Lagrangian (solid mechanics) FEM formulation, is written as

$$\rho_o \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial P_{iJ}}{\partial X_J} + \rho_o B_i, \tag{3}$$

[1] Einstein convention on repeated indexes is used.

which in its weak form is

$$\int_{\Omega_o} \Phi \rho_o \frac{\partial^2 u_i}{\partial t^2} = -\int_{\Omega_o} \frac{\partial \Phi}{\partial x_J} P_{iJ} + \int_{\partial \Omega_o} N_J P_{iJ} \Phi + \int_{\Omega_o} \Phi \rho_o B_i \tag{4}$$

for each space dimension i. P_{iJ}, the nominal stress or first Piola-Kirchoff stress tensor, depends on the second Piola-Kirchoff stress tensor S_{IJ}. Depending on the model, it includes active and passive stresses and a volumetric correction. We present results for a transversally isotropic law, based on Lin-Yin [7] and an orthotropic law based on Holzapfel and Ogden [8].

2.3 Coupling

Most of the EC coupling formulation use the assumption that active stress (T) is generated along the muscle fiber direction. Then, the total Cauchy stress is expressed by [10]:

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_{passive} + T(\lambda, [Ca^{2+}]) \boldsymbol{f} \otimes \boldsymbol{f} \tag{5}$$

where $\boldsymbol{f}$ is a unit vector align with the fiber in the current configuration. If λ_f is the muscle fiber stretch and $\boldsymbol{f}_0$ is the fiber in the reference configuration, it can be expressed by:

$$\lambda_f \boldsymbol{f} = \boldsymbol{F} \boldsymbol{f}_0 \tag{6}$$

The muscle fiber stretch is defined by the ratio of the current length over the initial length of the sarcomere ($1.9\ \mu m$). Hunter *et al.* [11] suggest a simple model based on steady state data at different constant level of activation and extension ratio (see also [8, 12]):

$$T = \frac{[Ca^{2+}]^n}{[Ca^{2+}]^n + C_{50}^n} T_{max}(1 + \beta(\lambda_f - 1)) \tag{7}$$

where C_{50} is the value of the intracellular calcium concentration for 50% of T_{max}, n is a coefficient controlling the shape of the curve and T_{max} is the maximum isometric active tensile stress developed at $\lambda_f = 1$. Experiments shows that T_{max} is a linear function of λ with β being the non-dimensional slope $dT/d\lambda$ [11]. This parameter represents the dependency of the force on the sarcomere length. The force increases with the stretch of the fiber, since the number of overlapping myosin/actine bending site increases. The fluctuation of the free calcium ions concentration follows this relation:

$$[Ca^{2+}](t) = [Ca^{2+}]_{max}(t/\tau_{Ca}) exp(-t/\tau_{Ca}) \tag{8}$$

2.4 Parallelization

The simulation models presented here are implemented in the Alya System, conceived for simulating complex computational mechanics problems in parallel. Alya is designed from scratch to take profit of parallel architectures with two premises: programming flexibility and parallel efficiency. In order to have an efficient algorithm to run on thousands of processors, some important aspects of the parallelization must be carefully treated: mesh partitioning, node numbering and communication scheduling. These issues will be discussed at the conference presentation.

3 Conclusions

We present a high performance computational electromechanical model of the heart that includes coupling between electrical activation and mechanical deformation, capable of running efficiently in up to thousands of processors meshes of millions of elements. The computational model is assessed through several numerical tests for different electrophysiology, mechanical and coupling models.

References

1. D. Gil, J. Garcia-Barnes, M. Vázquez, R. Arís and G. Houzeaux Patient-Sensitive Anatomic and Functional 3D Model of the Left Ventricle Presented at the *8th. World Congress on Computational Mechanics (WCCM8) 5th European Congress on Computational Methods in Applied Sciences and Engineeering (ECCOMAS 2008)*. Venice, Italy. 2008
2. M. Vázquez, R. Arís, A. Rosolen and G. Houzeaux A High Performance Computational Electrophysiology Model Presented at the *8th. World Congress on Computational Mechanics (WCCM8) 5th European Congress on Computational Methods in Applied Sciences and Engineeering (ECCOMAS 2008)*. Venice, Italy. 2008
3. F. Rubio, M. Hanzich, R. Arís, G. Houzeaux and M. Vázquez. Parallel Computational Electrophysiology in Cell/B.E. Processors, Presented at *COMPBIOMED Conference*, Swansea, UK. 2009.
4. M. Vázquez, R. Arís, P. Lafortune, P. Villar, G. Houzeaux, D. Gil, J. Garcia-Barnes, M. Ballester and F. Carreras. Massively parallel eletrcomechanical model of the heart., Presented at *CMBBE Conference*, Valencia, Spain. 2010.
5. M. Vázquez, R. Arís, G. Houzeaux, P. Villar, P. Lafortune, C. Labarta, D. Gil, J. Garcia-Barnes, M. Ballester and F. Carreras. A massively parallel electro-mechanical model of the heart for large-scale simulations Presented at the *IV European Conference on Computational Mechanics*, Paris, France. 2010.
6. M. Vázquez, R. Arís, G. Houzeaux, R. Aubry, P. Villar, J. Garcia-Barnes, D. Gil and F. Carreras. A massively parallel computational electrophysiology model of the heart. *International Journal for Numerical Methods in Biomedical Engineering*. 2010. Published online in Wiley Online Library (wileyonlinelibrary.com). DOI: 10.1002/cnm.1443.
7. D. H. Lin and F.C Yin. A multiaxial constitutive law for mammalian left ventricular myocardium in steady-state barium contracture or tetanus. *J Biomech Eng.*, 120(4), 1998.
8. Gerhard A. Holzapfel and Ray W. Ogden. Constitutive modelling of passive myocardium: a structurally based framework for material characterization. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 367(1902):3445-3475, 2009.
9. Hiroshi Watanabe, Seiryo Sugiura, Hidenobu Kafuku, and Toshiaki Hisada. Multiphysics simulation of left ventricular filling dynamics using fluid-structure interaction finite element method. *Biophysical Journal*, 87(3):2074-2085, 2004.
10. Gerhard A. Holzapfel. *Computational Biomechanics of Soft Biological Tissue*, volume 2 of *Encyclopedia Of Computational Mechanics*, chapter 18, pages 605–635. John Wiley & Sons, Chichester, 2004.
11. P. J. Hunter, M. P. Nash, and G. B. Sands. *Computational Electromechanics of the Heart*, pages 345–407. Computational Biology of the Heart. John Wiley and Sons, London, 1997.
12. A. Hung, K. Mithraratne, M. Sagar, and P. Hunter. Multilayer soft tissue continuum model: Towards realistic simulation of facial expressions. *WORLD ACADEMY OF SCIENCE, ENGINEERING AND TECHNOLOGY*, 54, June 2009.