Activity Report 2013

Team M3DISIM

Mathematical and Mechanical Modeling with Data Interaction in Simulations for Medicine

RESEARCH CENTER
Saclay - Île-de-France

THEME
Modeling and Control for Life Sciences

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Team M3DISIM

Keywords: Scientific Computation, Finite Elements, Data Assimilation, Inverse Problem, Virtual Physiology, Fluid-structure Interaction

Creation of the Team: 2013 January 01.

1. Members

Research Scientists
Dominique Chapelle [Team leader, Inria, Senior Researcher, HdR]
Sébastien Imperiale [Inria, Researcher, from Sep 2013]
Philippe Moireau [Inria]

External Collaborator
Daniele Trimarchi [Engineer with Coventor Inc., from Feb 2013 until Dec 2013]

Engineers
Matthieu Caruel [Inria, supported by FP7 VP2HF project]
Sébastien Gilles [Inria]
Alexandre Imperiale [Inria, supported by FP7 VPH-SHARE project]

PhD Students
Bruno Burtschell [Inria, supported by FP7 VPH-SHARE project, from Oct 2013]
Annabelle Collin [Inria]

Post-Doctoral Fellow
Karine Mauffrey [Inria, supported by FP7 VP2HF project]

Visiting Scientist
Vera Damerjian [Univ. Paris Est, from Feb 2013 until Apr 2013]

Administrative Assistant
Hélèna Kutniak [Inria]

Others
Mohamed Ryadh Haferssas [Master's intern, from Apr 2013 until Jul 2013]
Alessandro Felder [Master's intern, from Nov 2013]

2. Overall Objectives

2.1. Highlights of the Year

- Hiring of one new permanent researcher: Sébastien Imperiale (CR2);
- New European project named VP2HF, see 7.2.1.2;
- First paper with experimental validations of our cardiac model, see [13].

3. Research Program

3.1. Multi-scale modeling and coupling mechanisms for biomechanical systems, with mathematical and numerical analysis

Over the past decade, we have laid out the foundations of a multi-scale 3D model of the cardiac mechanical contraction responding to electrical activation. Several collaborations have been crucial in this enterprise,

see below references. By integrating this formulation with adapted numerical methods, we are now able to represent the whole organ behavior in interaction with the blood during complete heart beats. This subject was our first achievement to combine a deep understanding of the underlying physics and physiology and our constant concern of proposing well-posed mathematical formulations and adequate numerical discretizations. In fact, we have shown that our model satisfies the essential thermo-mechanical laws, and in particular the energy balance, and proposed compatible numerical schemes that – in consequence – can be rigorously analyzed, see [4]. In the same spirit, we have recently formulated a poromechanical model adapted to the blood perfusion in the heart, hence precisely taking into account the large deformation of the mechanical medium, the fluid inertia and moving domain, and so that the energy balance between fluid and solid is fulfilled from the model construction to its discretization, see [29].

3.2. Inverse problems with actual data – Fundamental formulation, mathematical analysis and applications

A major challenge in the context of biomechanical modeling – and more generally in modeling for life sciences – lies in using the large amount of data available on the system to circumvent the lack of absolute modeling ground truth, since every system considered is in fact patient-specific, with possibly non-standard conditions associated with a disease. We have already developed original strategies for solving this particular type of inverse problems by adopting the observer stand-point. The idea we proposed consists in incorporating to the classical discretization of the mechanical system an estimator filter that can use the data to improve the quality of the global approximation, and concurrently identify some uncertain parameters possibly related to a diseased state of the patient, see [5], [6], [7]. Therefore, our strategy leads to a coupled model-data system solved similarly to a usual PDE-based model, with a computational cost directly comparable to classical Galerkin approximations. We have already worked on the formulation, the mathematical and numerical analysis of the resulting system – see [3] – and the demonstration of the capabilities of this approach in the context of identification of constitutive parameters for a heart model with real data, including medical imaging, see [1].

4. Application Domains

4.1. Clinical applications

After several validation steps – based on clinical and experimental data – we have reached the point of having validated the heart model in a pre-clinical context where we have combined direct and inverse modeling in order to bring predictive answers on specific patient states. For example, we have demonstrated the predictive ability of our model to set up pacemaker devices for a specific patient in cardiac resynchronization therapies, see [8]. We have also used our parametric estimation procedure to provide a quantitative characterization of an infarct in a clinical experiment performed with pigs, see [1].

5. Software and Platforms

5.1. FELISCE

Participants: Dominique Chapelle, Sébastien Gilles [correspondant], Philippe Moireau.

FELISCE – standing for “Finite Elements for LIfe SCiences and Engineering” – is a new finite element code which the MACS and REO teams have decided to jointly develop in order to build up on their respective experiences concerning finite element simulations. One specific objective of this code is to provide in a unified software environment all the state-of-the-art tools needed to perform simulations of the complex cardiovascular models considered in the two teams – namely involving fluid and solid mechanics, electrophysiology, and the various associated coupling phenomena. FELISCE is written in C++, and may be later released as an opensource library. See https://gforge.inria.fr/projects/felisce/.

5.2. HeartLab

Participants: Matthieu Caruel, Dominique Chapelle, Alexandre Imperiale, Philippe Moireau [correspondant].

The heartLab software is a library written in (64 bits compatible) Matlab and C (mex functions) designed to perform both simulation and estimation (based on various types of measurements, e.g. images) of the heart mechanical behavior. Started in 2006, it is already quite large (about 60,000 lines), and is used within various collaborations.

The code relies on OpenFEM – to which the team has previously contributed, see http://www.openfem.net – for the finite element computations, and the implementation was performed with a particular concern for modularity, since modeling and estimation use the same finite element operators. This modularity also allows to couple the code with other FEM solvers, such as LifeV and Mistral developed in the Reo team-project. In particular, we are now able to include perfusion and electrical coupling with LifeV using PVM, and fluid-structure interaction using Mistral.

We also included geometric data and tools in the code to define cardiac anatomical models compatible with the simulation requirements in terms of mesh quality, fiber direction data defined within each element, and the referencing necessary for handling boundary conditions and estimation, in particular. These geometries are analytical or come from computerized tomography (CT) or magnetic resonance (MR) image data of humans or animals.

We recently incorporated numerous non-linear data assimilation observation operators based on medical imaging post-processing to be able to now perform estimation with a large variety of medical imaging modalities.

5.3. Verdandi

Participants: Dominique Chapelle, Marc Fragu, Vivien Mallet [Clime team], Philippe Moireau [correspondant].

Verdandi is an opensource (LGPL) software library aiming at providing assimilation data methods and related tools. Mainly targeted at large systems arising from the discretization of PDEs, it is intentionally devised as generic, which allows for applications in a wide range of problems (biology and medicine, environment, image processing...). See also the web page http://verdandi.gforge.inria.fr/, with a complete documentation in English. The first stable version (1.0) was released in June 2012 and contains most of the major data assimilation algorithms of both variational and sequential types. The current version (1.5) contains additional estimation algorithm and parallel capabilities. Note that some specific developments are performed with particular regard to cardiac modeling applications, as Verdandi is partly funded by – and distributed within – the VPH-Share project and is now referenced in the peer-reviewed article [16].

- ACM: Mathematical software
- AMS: System theory; control
- Software benefit: Verdandi is the only *generic* data assimilation library
- License: LGPL (2.1 or any later version)
- Type of human computer interaction: Command line and configuration files
- OS/Middelware: Linux, MacOS ou Windows
- Required library or software: Seldon (LGPL, http://seldon.sourceforge.net/)
- Programming language: C++, ISO/IEC 14882: I998(E) Python, version 2.6
- Documentation: Doxygen and utilisation manual in English

6. New Results

6.1. Modeling

6.1.1. Collective effect in molecular motors assembly

Participants: Matthieu Caruel, Jean-Marc Allain [Ecole Polytechnique], Lev Truskinovsky [Ecole Polytechnique].

Skeletal muscles consist of active material capable of producing force. At the microscale, force is the result of complex interactions between two types of proteins named actin and myosin that work coherently in very large assemblies ($\sim 10^9$). The passive mechanical response of skeletal muscles at fast time scales is dominated by long range interactions inducing cooperative behavior without breaking the detailed balance. This leads to such unusual "material properties" as negative equilibrium stiffness and different behavior in force and displacement controlled loading conditions. Our fitting of experimental data suggests that "muscle material" is finely tuned to perform close to a critical point which explains large fluctuations observed in muscles close to the stall force. See paper [28].

6.1.2. Dimensional reductions of a cardiac model for effective validation and calibration

Participants: Matthieu Caruel, Alexandre Imperiale, Radomir Chabiniok [King's College London], Philippe Moireau, Dominique Chapelle, Yves Lecarpentier [Institut du Cœur].

Complex 3D beating heart models are now available, but their complexity makes calibration and validation very difficult tasks. We thus propose a systematic approach of deriving simplified reduced-dimensional models, in "0D"— typically, to represent a cardiac cavity, or several coupled cavities and in "1D"—to model elongated structures such as muscle samples or myocytes. We apply this approach with an earlier-proposed 3D cardiac model designed to capture length-dependence effects in contraction, which we here complement by an additional modeling component devised to represent length-dependent relaxation. We then present experimental data produced with rat papillary muscle samples when varying preload and afterload conditions, and we achieve some detailed validations of the 1D model with these data, including for the length-dependence effects that are accurately captured. Finally, when running simulations of the 0D model pre-calibrated with the 1D model parameters, we obtain pressure–volume indicators of the left ventricle in good agreement with some important features of cardiac physiology, including the so-called Frank–Starling mechanism, the End-Systolic Pressure–Volume Relationship, as well as varying elastance properties. This integrated multi-dimensional modeling approach thus sheds new light on the relations between the phenomena observed at different scales and at the local versus organ levels. See papers [13], [22].

6.1.2.1. Surface-based electrophysiology modeling and assessment of physiological simulations in atria

Participants: Dominique Chapelle, Annabelle Collin, Jean-Frédéric Gerbeau [Reo Project-Team], Mélèze Hocini [Institut LIRYC - IHU Bordeaux], Michel Haïssaguerre [Institut LIRYC - IHU Bordeaux].

The objective of this work is to assess a previously-proposed surface-based electrophysiology model with detailed atrial simulations. This model – derived and substantiated by mathematical arguments – is specifically designed to address thin structures such as atria, and to take into account strong anisotropy effects related to fiber directions with possibly rapid variations across the wall thickness. The simulation results are in excellent adequacy with previous studies, and confirm the importance of anisotropy effects and variations thereof, see Figure 1. Furthermore, this surface-based model provides dramatic computational benefits over 3D models with preserved accuracy. See paper [23].

6.1.3. Strong convergence results in the asymptotic behavior of the 3D-shell model

Participants: Dominique Chapelle, Annabelle Collin.

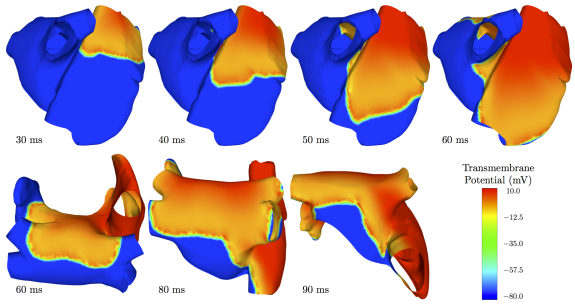

Figure 1. Surface-based modeling of atrial electrophysiology

The objective of this work is to revisit the asymptotic convergence properties – with respect to the thickness parameter – of the earlier-proposed 3D-shell model. This shell model is very attractive for engineering applications, in particular due to the possibility of directly using a general 3D constitutive law in the corresponding finite element formulations. We establish strong convergence results for the 3D-shell model in the two main types of asymptotic regimes, namely, bending- and membrane-dominated behavior. This is an important achievement, as it completely substantiates the asymptotic consistency of the 3D-shell model with 3D linearized isotropic elasticity. See paper [14].

6.1.4. Mechanical modeling and numerical methods for poromechanics: Applications to cardiac perfusion

Participants: Bruno Burtschell, Dominique Chapelle, Philippe Moireau.

We have previously formulated a rather general modeling framework of poromechanics – formulations that combine solid and fluid components to represent the behavior of a porous medium – to take into account large deformations and rapid fluid flows, see [29]. This allows to consider, in particular, the application of blood perfusion within the cardiac tissue, which – indeed – features these specific complex phenomena, out of the scope of classical poromechanical models. One of our major objectives now, within the PhD of Bruno Burtschell, is to propose and assess some associated relevant numerical schemes, which requires special care regarding both space and time discretizations. In a first stage, in order to ease numerical prototyping and assessments, an axisymmetric reduction of the model has been formulated, and some existing algorithms of fluid-structure interaction have been implemented within this axisymmetric framework (in FreeFEM++). The rationale is that our poromechanics formulations feature some rather deep similarities to so-called Arbitrary-Lagrangian-Eulerian (ALE) fluid-structure formulations, hence the latter are considered as a natural starting point for further extensions.

6.1.5. Personalized modeling for cardiac amyloidosis diagnosis

Participants: Alessandro Felder, Dominique Chapelle, Philippe Moireau, Jean-François Deux [Hôpital Henri Mondor], Thibault Damy [Hôpital Henri Mondor].

Cardiac amyloidosis is a condition induced by pathological deposition of amyloid proteins within muscle tissue and nerves, thus severely impairing the cardiac function and often requiring cardiac transplantation as the only available treatment. Our objective here in a first stage is to use our previously developed patient-specific modeling methodologies to analyse some clinical cases – based on actual patient data – to better apprehend the impact of the pathology on biomechanical properties. Further perspectives include the modeling of the protein deposition and associated tissue remodeling in order to predict the disease evolution in a patient-specific context. This work is performed in collaboration with medical doctors from Hôpital Henri Mondor (Créteil).

6.2. Model-Data Interaction

6.2.1. State observers of a vascular fluid-structure interaction model through measurements in the solid

Participants: Cristobal Bertoglio [Reo Project-Team], Dominique Chapelle, Miguel Angel Fernández [Reo Project-Team], Jean-Frédéric Gerbeau [Reo Project-Team], Philippe Moireau.

We analyze the performances of two types of Luenberger observers – namely, the so-called Direct Velocity Feedback and Schur Displacement Feedback procedures, originally devised for elasto-dynamics – to estimate the state of a fluid-structure interaction model for hemodynamics, when the measurements are assumed to be restricted to displacements or velocities in the solid. We first assess the observers using hemodynamics-inspired test problems with the complete model, including the Navier-Stokes equations in Arbitrary Lagrangian-Eulerian formulation, in particular. Then, in order to obtain more detailed insight we consider several well-chosen simplified models, each of which allowing a thorough analysis – emphasizing spectral considerations – while illustrating a major phenomenon of interest for the observer performance, namely, the added mass effect for the structure, the coupling with a lumped-parameter boundary condition model for the fluid flow, and the fluid dynamics effect *per se*. Whereas improvements can be sought when additional measurements are available in the fluid domain in order to more effectively deal with strong uncertainties in the fluid state, in the present framework this establishes Luenberger observer methods as very attractive strategies – compared, e.g., to classical variational techniques – to perform state estimation, and more generally for uncertainty estimation since other observer procedures can be conveniently combined to estimate uncertain parameters. See paper [11].

6.2.2. Improving Efficiency of Data Assimilation Procedure for a Biomechanical Heart Model by Representing Surfaces as Currents

Participants: Alexandre Imperiale, Alexandre Routier [Aramis Team], Philippe Moireau, Stanley Durrleman [Aramis Team].

We adapt the formalism of currents to compare data surfaces and surfaces of a mechanical model and we use this discrepancy measure to feed a data assimilation procedure. We apply our methodology to perform parameter estimation in a biomechanical model of the heart using synthetic observations of the endo- and epicardium surfaces of an infarcted left ventricle. We compare this formalism with a more classical signed distance operator between surfaces and we numerically show that we have improved the efficiency of our estimation justifying the use of state-of-the-art computational geometry formalism in the data assimilation measurements processing. See paper [24].

6.2.3. Optimal observer for parabolic problems

Participants: Karine Mauffrey, Philippe Moireau.

We aim at proposing optimal observers strategies for reconstructing the solution of general systems of PDEs using avalaible observations, including both wave-type equations and heat-like equations. The main objective of this work is to present a self-contained analysis. For a general parabolic system, we have established the exponential stability of the operator occurring in the equation satisfied by the error between the target and the optimal observer. The proof relies on two major hypotheses: an observability inequality satisfied by the observation operator and a controllability property for the modeling error operator by which model noises enter the dynamics (controllability property which is related to the invertibility of the solution of the associated infinite dimensional Riccati equation). The next questions we want to tackle are the discretisation of the model and the construction of a reduced Kalman filter.

7. Partnerships and Cooperations

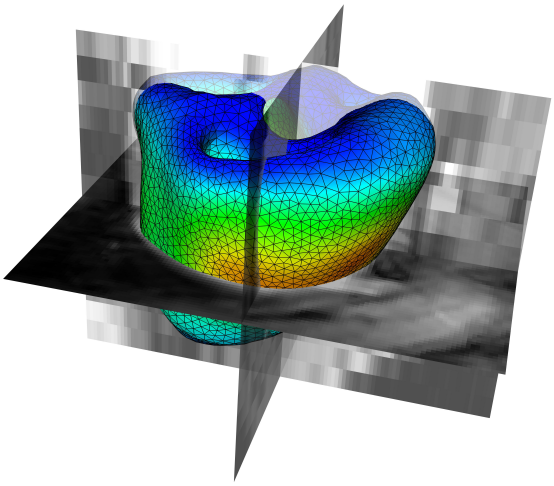

Figure 2. Heart model immersed in MR image data

7.1. Regional Initiatives

The team is part of the Mechanics and Living Systems Initiative (Opération Mécanique et Systèmes du Vivant), a joint operation – focused on biomechanical modeling – between the LadHyx and LMS labs (CNRS and Ecole Polytechnique), and Inria.

7.2. European Initiatives

7.2.1. FP7 Projects

7.2.1.1. VPH-Share

Title: VPH-Share

Type: COOPERATION

Defi: Towards sustainable and personalised healthcare

Instrument: Integrated Project

Objectif: Virtual Physiological Human

Duration: March 2011 - February 2015

Coordinator: Univ. Sheffield (UK)

Other partners: Cyfronet (Cracow), University College London, Istituto Ortopedico Rizzoli (Bologna), NHS, IBM Israel, Univ. Auckland, Agència d'Informació, Avaluació i Qualitat en Salut (Barcelona), Biocomputing Competence Centre (Milano), Universitat Pompeu Fabra (Barcelona), Philips Research, TUE (Eindhoven), Sheffield Teaching Hospitals, Atos Origin (Madrid), the Open University (UK), Univ. Vienna, King's College London, Empirica (Bonn), Fundació Clínic (Barcelona), Univ. Amsterdam

See also: http://vph-share.org/

Abstract: VPH-Share aims at developing the organisational fabric (the infostructure) and integrate the optimised services to expose and share data and knowledge, to jointly develop multiscale models for the composition of new VPH workflows, and to facilitate collaborations within the VPH community. Within this project, the Macs team is in charge of developing some high-performance data assimilation software tools.

7.2.1.2. VP2HF

Title: Computer model derived indices for optimal patient-specific treatment selection and planning in Heart Failure

Type: COOPERATION

Defi: ICT for Health, Ageing Well, Inclusion and Governance

Instrument: Specific Targeted Research Project

Objectif: Virtual Physiological Human

Duration: October 2013 - September 2016

Coordinator: King's College London (UK)

Abstract: Heart failure (HF) is one of the major health issues in Europe affecting 6 million patients and growing substantially because of the ageing population and improving survival following myocardial infarction. The poor short to medium term prognosis of these patients means that, treatments such as cardiac re-synchronisation therapy and mitral valve repair can have substantial impact. However, these therapies, are ineffective in up to 50% of the treated patients and involve significant morbidity and substantial cost. The primary aim of VP2HF is to bring together image and data processing tools with statistical and integrated biophysical models mainly developed in previous VPH projects, into a single clinical workflow to improve therapy selection and treatment optimisation in HF.

8. Dissemination

8.1. Scientific Animation

Dominique Chapelle

- Member of the editorial boards of journals *Computers & Structures* and *M2AN*
- Program committee of conference "Functional Imaging and Modeling of the Heart 2013"
- Invited lecturer at conference "Shell Structures - Theory and Applications 2013"
- Member of the Academic Senate of FCS Paris-Saclay

Philippe Moireau

- Reviewer this year for ACOM IJNME JOMP MCCS journals, the Waves conference and the American Control Conference

8.2. Teaching - Supervision - Juries

8.2.1. Teaching

Philippe Moireau

Bachelor's degree: "MA103 - Introduction aux EDP et à leur approximation numérique", 14h, M1, ENSTA ParisTech, France

Master's: "MA201 - La méthode des éléments finis", 3h lectures and 14h classes , M2, ENSTA ParisTech, France

Sébastien Imperiale

Master's: "MA201 - La méthode des éléments finis", 12h, M2, ENSTA ParisTech, France

Post-graduate: "Numerical methods for waves propagation simulations", 4h30, Collège Polytechnique, France

Post-graduate: "Piezoelectric sensor and wave based inverse problems", Summer school on Inverse Problems, Bremen, 1h30, Germany

Annabelle Collin

Oral examination:“Algebra and Geometry”, UPMC, Spring 2012

Bachelor’s degre:“Multivariable Calculus”, UPMC, fall 2012

8.2.2. Supervision

PhD in progress: Annabelle Collin, “Dimensional reduction and electro-mechanical coupling for the modeling of electrophysiology and muscle contraction”, UPMC, started September 2011, advisors D. Chapelle and J.-F. Gerbeau

PhD in progress: Bruno Burtschell, “Mechanical modeling and numerical methods for poromechanics: Applications to cardiac perfusion”, Ecole Polytechnique, started October 2013, advisors D. Chapelle and P. Moireau

PhD defended in December: Alexandre Imperiale, “Image-based observation operators for data assimilation in cardio-mechanics”, UPMC, started October 2010, advisors D. Chapelle and P. Moireau

8.2.3. Juries

Dominique Chapelle: member of PhD committee of S. Marchesseau

Philippe Moireau: member of PhD committee of A.-C. Boulanger

8.3. Popularization

TV News Story “la météo du coeur” (how to predict the heart weather) on France5 “Magazine de la santé” (11 March 2013)

D. Chapelle invited speaker at “Horizon Maths 2013”

9. Bibliography

Major publications by the team in recent years

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Publications of the year

Doctoral Dissertations and Habilitation Theses

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Articles in International Peer-Reviewed Journals

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