INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Project-Team Macs

Modeling, Analysis and Control for Computational Structural Dynamics

Paris - Rocquencourt

THEME NUM

Activity Report

2008

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1. Team

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2. Overall Objectives

2.1. Introduction

Numerical simulation has become a widespread tool in engineering. This fact is particularly noteworthy in the field of solid and structural mechanics which has given birth to finite element methods. In industrial design processes, experimenting and simulation go hand in hand, but the balance is increasingly shifted towards simulation, resulting into reduced costs and time to market.

In this general context, the objectives of the Macs project are to address new challenges arising from:

- the need to develop numerical procedures which are *reliable* and well-adapted to *industrial applications*;
- the emergence of *active mechanics* (e.g. control and optimisation) enabling the design of thinner and lighter (hence cheaper) structures, for which innovative modeling and discretization approaches are required.

These research directions benefit from a strong scientific environment and background at INRIA in the fields of numerical analysis and scientific computing (with a well-established record in structural mechanics), as well as in automatic control.

We also emphasize that – in the recent years – we have started to investigate some such issues more particularly related to biomechanical modeling.

2.2. Highlights of the year

Macs is part of the European project euHeart, which started in June 2008, and more specifically in charge of one workpackage, see Section 7.2.1.

Furthermore, we participated in an ANR proposal entitled Epsilon, which will be funded starting in January 2009. The scientific work has already begun, and is described in Section 6.2.

3. Scientific Foundations

3.1. Formulation and analysis of effective and reliable shell elements

Thin structures (beams, plates, shells...) are widely considered in engineering applications. However, most experts agree that the corresponding discretization procedures (finite elements) are not yet sufficiently reliable, in particular as regards shell structures. A major cause of these difficulties lies in the numerical locking phenomena that arise in such formulations [1].

The expertise of the team in this area is internationally well-recognized, both in the mathematical and engineering communities. In particular, we have strongly contributed in analysing – and better explaining – the complex locking phenomena that arise in shell formulations [1]. In addition, we have proposed the first (and only to date) shell finite element procedure that circumvents locking [21]. However, the specific treatment applied to avoid locking in this procedure make it unable to correctly represent membrane-dominated behaviors of structures (namely, when locking is not to be expected). In fact, a "perfect shell element" – namely, with the desired reliability properties mathematically substantiated in a general framework – is still to be discovered, whereas numerous teams work on this issue throughout the world.

Another important (and related) issue that is considered in the team pertains to the design and analysis of numerical procedures that are adapted to industrial applications, i.e. that fulfill some actual industrial specifications. In particular, in the past we have achieved the first mathematical analysis of "general shell elements" – which are based on 3D variational formulations instead of shell models – these elements being among the most widely used and most effective shell elements in engineering practice.

3.2. Stability and control of structures

Stability of structures is – of course – a major concern for designers, in particular to ensure that a structure will not undergo poorly damped (or even unbounded) vibrations. In order to obtain improved stability properties – or to reach nominal specifications with a thinner a lighter design – a control device (whether active, semi-active, or passive) may be used.

The research performed in the team in this area – other than some prospective work on robust control – has been so far primarily focused on the stability of structures interacting with fluid flows. This problem has important applications e.g. in aeronautics (flutter of airplane wings), in civil engineering where the design of long-span bridges is now partly governed by wind effects, and in biomechanics (blood flows in arteries, for instance). Very roughly, the coupling between the structure and the flow can be described as follows: the structural displacements modify the geometry of the fluid domain, hence the fluid flow itself which in turn exerts an action on the structure. The effects of structural displacements on the fluid can be taken into account using ALE techniques, but the corresponding direct simulations are highly CPU-intensive, which makes stability analyses of such coupled problems very costly from a computational point of view. In this context a major objective of our work has been to formulate a simplified model of the fluid-structure interaction problem in order to allow computational assessments of stability at a reasonable cost.

3.3. Modeling and estimation in biomechanics

A keen interest in questions arising from the need to model biomechanical systems – and to discretize such problems – has always been present in the team since its creation. Our work in this field until now has been more specifically focused on the objectives related to our participation in the ICEMA ARC projects and in the CardioSense3D initiative (see Section 7.1.1), namely, to formulate a complete continuum mechanics model of a beating heart, and to confront – or "couple", in the terminology of the INRIA strategic plan – numerical simulations of the model with actual clinical data via a data assimilation procedure.

Our global approach in this framework thus aims at using measurements of the cardiac activity in order to identify the parameters and state of a global electromechanical heart model, hence to give access to quantities of interest for diagnosing electrical activation and mechanical contraction symptoms. The model we propose is based on a chemically-controlled constitutive law of cardiac myofibre mechanics consistent with the behavior of myosin molecular motors [20]. The resulting sarcomere dynamics is in agreement with the "sliding filament hypothesis" introduced by Huxley. This constitutive law has an electrical quantity as an input which can be independently modeled, considered as given (or measured) data, or as a parameter to be estimated.

4. Application Domains

4.1. Application domains

Our researches have natural applications in all sectors of the mechanical industry: car and naval industries; aeronautics and space; civil engineering; tyres; MEMs and nanotechnologies...

We also actively seek new applications in biotechnologies, although of course the economy and structuring of this sector is not as developed yet.

5. Software

5.1. MODULEF

Participants: Dominique Chapelle, Marina Vidrascu [correspondant].

Most of the software developed in our team is integrated in the Modulef library. Modulef is designed to provide building blocks for effective and reliable software development in finite element analysis. Well-adapted rigorous data structures and ease of integration (for new methods or algorithms) are some of its key advantages. Until 1998, Modulef was distributed by the Simulog company within a club structure (for a membership fee). In order to encourage its dissemination, its status was then changed to make it freely available. It can be downloaded at no charge from the INRIA-Rocquencourt web site (http://www-rocq.inria.fr/modulef/).

5.2. OpenFEM: a Finite Element Toolbox for Matlab and Scilab

Participants: Dominique Chapelle, Marina Vidrascu [correspondant].

OpenFEM (http://www.openfem.net) is an *opensource* finite element toolbox for linear and nonlinear structural mechanics within the Matlab and Scilab matrix computing environments. This software is developed in a collaboration between Macs and the SDTools company [1]. Performing finite element analyses within a matrix computing environment is of considerable interest, in particular as regards the ease of new developments, integration of external software, portability, postprocessing, etc. This rather young software is already quite successful in the finite element community (about 300 downloads per month).

5.3. MITCNL

Participants: Dominique Chapelle [correspondant], Marina Vidrascu.

The package MITCNL is a set of subroutines that implements the triangular MITC3, MITC6 and quadrilateral MITC4 and MITC9 shell elements for large displacements [1]. We use it as a basis for new developments of shell elements, in particular within Modulef. It can be easily interfaced with most finite element codes as well. We also license this package to some of our partners for use with their own codes.

5.4. HeartLab

Participants: Dominique Chapelle, Elsie Phé [Reo], Philippe Moireau [correspondant].

The heartLab software is a library written in 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 30000 lines), and is used within the CardioSense3D community.

The code relies on OpenFEM 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 developed in the Reo team-project. In particular, we are now able to include perfusion and electrical coupling with LifeV, using PVM and on the way to update this coupler with MPI.

[1] http://www.sdtools.com

We also included geometric data and tools in the code to define heart anatomical models compatible with the simulation requirements in terms of mesh quality, fiber direction data defined within each element, and 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.

6. New Results

6.1. Modeling and simulation of fluid-structure interaction problems

Keywords: *Newton algorithms*, *fluid-structure interaction*.

Participant: Marina Vidrascu.

This work is performed in collaboration with the Reo team. In the fluid-structure interaction simulations it appears that – even when the geometry is realistic (as when obtained from medical images) – one may observe some global non physiological behavior, such as bending of the blood vessels. To avoid this behavior it is necessary to consider more realistic boundary conditions. We investigated a modeling of the surrounding tissues by viscoelastic support boundary conditions. The first results are very encouraging.

6.2. Modeling and simulation of multy-layers mechanical structures

Keywords: *multi-scale mechanical structures*, *shells*.

Participants: Dominique Chapelle, Michele Serpilli, Marina Vidrascu.

We started a collaboration with Françoise Krasucki and Giuseppe Geymonat (Montpellier University) on the modeling of 3D materials connected by stiff interfaces. The first simplified model considers two elastic bodies coupled by a strong thin material layer for which the asymptotic behavior can be analysed when the stiffness grows [19]. This problem is difficult to solve directly with 3D models because the thin layer requires a very fine mesh, and furthermore the difference in elastic coefficients induces numerical difficulties. Introducing a variational limit problem allows to substitute the thin layer with a "material surface" which – in this case – is modeled by a shell. Our study will focus on effective numerical methods to solve this problem. A specific shell element was developed to model this material surface. An alternative to the direct solution of this problem is to formulate an appropriate domain decomposition technique. This work is in progress and is the subject of Michele Serpilli's postdoc. In addition, we will participate in the Epsilon ANR project (Domain decomposition and multi-scale computations of singularities in mechanical structures) which will start next January.

6.3. Modeling and estimation of the electromechanical behavior of the heart

Keywords: *active mechanics*, *biomechanics*, *data assimilation*.

Participants: Radomir Chabiniok, Dominique Chapelle, Asven Gariah, Philippe Moireau, Elsie Phé [Reo], Jacques Sainte-Marie.

6.3.1. Modeling

6.3.1.1. Modeling of the cardiac tissue

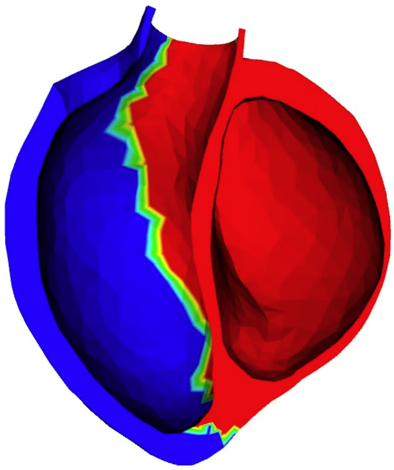

Figure 1.

Complete electrical and mechanical simulation of a heart beat with pathological condition (collaboration with Reo team)

The following research directions have been investigated.

- Validation of the tissue model using experimental data of a papillary muscle contraction. The data are provided by the team of Y. Lecarpentier (Kremlin-Bicêtre hospital), on rat muscle samples. This is useful to validate the tissue model independently of the other ingredients of the complete heart model (fibre directions, blood circulation modeling, boundary conditions...)
- Validation of the complete heart model using animal data with an induced myocardial infarct. Animal experiments will be performed to obtain data – images, ECGs and some pressures, in particular – for healthy and infarcte hearts. The objectives are the following:
  - validation of the 3D model of the physiological heart;
  - adjustment of the parameters of the model to simulate clinically relevant myocardial infarction;
  - formulation of a long term mathematical model predicting morphological remodeling and functional changes of the heart after a myocardial infarction.

  The data will be acquired by the radiological department of the Henri Mondor hospital in a collaboration with A. Rahmouni and J.F. Deux (Henri Mondor), with the participation of J. Garot (Centre Hospitalier Jacques Cartier, Massy).
- Direct cardiac simulations using human data: modeling of the infarct and of conduction disorders with the perspective of therapy optimization. This is a joint work with the Asclepios team (INRIA Sophia-Antipolis) and King's College London, see submitted paper [18].

6.3.1.2. Perfusion

Perfusion is the phenomenon by which blood coming from the blood vessels reaches cells in the tissues, in particular to supply nutrients and oxygen. We mainly address the problem of fluid circulation, whereas the nutrition can be represented by a simplified O_2/CO_2 exchange mechanism. Another aspect of the perfusion is the regulation of the cardiac function with respect to the physical activity of the body.

Considering the whole heart, the complete modeling of blood-tissue interaction leads to prohibitive numerical costs. Moreover, the geometry of the smallest arteries and veins is unknown. Thus we consider macroscopic quantities for the fluid and solid parts, and the modeling of the coupling between the blood and the tissue within the framework of poromechanics seems appropriate.

The blood flows in the coronary arteries located at the epicardium are simulated using a 3D Navier-Stokes model, while the drainage in the capillary vessels is represented using a Darcy law. The model previously obtained has been refined. In particular the two constitutive laws, namely the muscular contraction law and the Darcy flow now derive from a suitable definition of the free energy of the porous system. The formulation thus-obtained has been validated for classical test cases and its further calibration is in progress.

This work is carried out in collaboration with the Reo team (I. Vignon & J.F. Gerbeau). The Navier-Stokes and Darcy codes are developed in the LifeV library [22], whereas for the simulation of the mechanical activity we use the HeartLab code.

6.3.1.3. Model reduction

Another aspect of the development of valuable tools for clinical applications is to reduce computational costs. This is the reason why we are interested in the analysis and simulation of the mechanical behavior of the heart with techniques leading to reduced size models.

We have first investigated the POD technique (Proper Orthogonal Decomposition). The preliminary results obtained in [23] have been extended by A. Gariah [15].

This activity will be further developed in 2009. A. Gariah has started a Phd thesis (November 2008) on model reduction. The approach is to examine model reduction in the scope of control theory and filtering techniques. The objective is to obtain error estimates between the complete and reduced simulations for a given category of models – e.g. reaction diffusion type or hyperbolic type problems.

6.3.2. Estimation in cardiology

Using the electro-mechanical heart model, our objective is to develop robust "data-model coupling algorithms". This approach aims at achieving an estimation of the behavior and of the physiological parameters of a patient-specific heart using measurements from medical imaging in combination with simulations of a biomechanical model. This inverse problem, called data assimilation, is very challenging because the current state of the art is unadapted to our problem. In fact, the heart model is too sensitive and too large to be adequately estimated by classical Kalman filters or variational assimilation techniques. Hence, the PhD thesis of Philippe Moireau – started in 2005 – is dedicated to the research on robust and low-cost state filters inspired from engineering and their extensions to combined state-parameter estimation procedures. In our previous work we were able to jointly estimate the state and parameters with a specific combination of Kalman filter on the parameters and DVF (direct velocity feedback) filter on the state. This method was fully analyzed in the case of linear systems – with respect to the state and the parameters – but featured some restrictions:

- the DVF state filter requires velocity measurement, whereas in practice only displacements are available in general.
- the derivation of such Kalman filters in a non-linear framework leads to the Extended Kalman Filter (EKF) which is not very efficient and requires the computation of new tangent operators in the code.

To circumvent these difficulties, we proposed two original extensions. On the one hand, we formulated a new filter which uses displacement measurements and ensures the decrease of the error energy with a rate comparable to that provided by the DVF filter. The main idea in order to control the energy error is to take advantage of the fact that the state filter is an *in silico* observer, so in this second order dynamical system we can incorporate a control on the equation that initially gives the velocity as the time derivative of the displacement. The resulting filter can be extended for a nonlinear model and observation operator. Hence, we showed that this filter allows to directly estimate the complete position of the beating heart using only contour measurements. These results are presented in a paper submitted to Inverse Problems [16]. This also provides new insight and ideas regarding model-based image segmentation. The performance of this new filtering approach was further demonstrated using realistic synthetic data in a collaboration with the Geometrica Project-Team [17].

On the other hand we obtained a reduced-order version of the so-called Unscented Kalman Filter (UKF) filter, generalizing an idea proposed in the original paper of [24]. This allows to use a UKF filter – instead of EKF – in the parameter estimation stage of our approach. The UKF filter is well-known for its robustness, and it avoids the computation of new tangent operators – such as the derivatives of the model with respect to parameters – by using only adequately sampled particle trajectories.

6.4. Other activities

Participants: Marie-Odile Bristeau [BANG], Jacques Sainte-Marie.

Another research activity dealing with the modeling of free surface flows and the coupling between hydrodynamic and biology is carried out in collaboration with the BANG team (M.-O. Bristeau and B. Perthame). The detailed description of the corresponding results is given in the activity report of the BANG team, see [3].

7. Other Grants and Activities

7.1. National projects

7.1.1. CardioSense3D

Participants: Radomir Chabiniok, Dominique Chapelle, Elsie Phé [Reo], Philippe Moireau, Marina Vidrascu.

CardioSense3D[2] is a 4-year Large Initiative Action launched in 2005 and funded by INRIA, which focuses on the modeling and estimation of the heart electro-mechanical behaviour. This action follows the 4-year ICEMA project. The core members of CardioSense3D are the INRIA project-teams Asclepios, Macs, Reo and Sysiphe, but other academic, industrial and clinical partners are closely associated in this action. See Section 6.3 for the detailed results obtained by Macs in this framework.

7.2. International projects

7.2.1. euHeart

The euHeart Project[3] is a European FP7 project of the IP category. It combines seventeen industrial, clinical and academic partners, whose collective goal is the development of individualized, computer-based, human heart models. Using comprehensive, patient-specific data as the basis for their design, these models will provide insight into the origin and progression of specific disease patterns, including those associated with heart failure, heart rhythm disorders, coronary artery disease, and aortic disease.

Within this project, the Macs team is more specifically in charge of coordinating one workpackage entitled “Biophysical model personalisation”, which consists in developing some methodological and software tools to solve the inverse problems of concern in the applications considered in the project. In this framework we already organized a two days workshop in Paris in October to present some methodological guidelines and discuss the participants’ needs.

[2] http://www-sop.inria.fr/CardioSense3D/
[3] http://www.euheart.eu/

7.2.2. *Other long-term collaborations*

- Collaboration on numerical locking with MIT and ADINA R&D (K.J. Bathe);

8. Dissemination

8.1. Various academic responsibilities

Dominique Chapelle:

- Vice-chairman of INRIA-Rocquencourt Project Committee, and chairman of the CR2 recruitment committee;
- Member of the editorial boards of “Computers & Structures” and “M2AN”;
- Elected member of the board of SMAI;
- Elected treasurer of GAMNI (“Groupement pour l’Avancement des Méthodes Numériques de l’Ingénieur”) and chairman of the GAMNI thesis award committee;
- Co-organizer of the joint INRIA - Paris 5 “Myocardial modeling” seminar[4].
- Member of the AERES evaluation committee for Poems team (UMR 27-06).

8.2. Teaching activities

- Dominique Chapelle: Master’s course “Numerical analysis for cardiac mechanics” (joint Paris 6 and Polytechnique M2 program).
- Dominique Chapelle and Philippe Moireau: lecturers at EMS-SMI Summer School “Mathematical and Numerical Models for the Cardiovascular System”, August 2008, Cortona, Italy.
- Philippe Moireau: course “The Finite Element Method”, at ENSTA, Fall 2008.

8.3. Participation in conferences, workshops and seminars

Dominique Chapelle

- Invited speaker at conferences: CIM’08 (February 19–22, Porto), ESOF’08 (July 18-21, Barcelona), JFR’08 (Oct. 27th, Paris).
- Speaker at CRM-INRIA-MITACS meeting (May 5–9, Montréal) and Eccomas conference (July 2008, Venice).
- Seminars: Univ. Besançon (Oct. 10th), Medicen (Nov. 6th), Geometrica (Nov. 11th).
- Thesis committees: Alexandre Nassiopoulos (ENPC), Shen Ming (CityU, Hong Kong, referee), Michele Serpilli (Montpellier), Arnaud Münch (Besançon, HDR).

Radomir Chabiniok

- Participant in course “Mathematical and Numerical Models for the Cardiovascular System”, EMS-SMI Summer School, August 17-30, Cortona, Italy.
- Participant in course “Advanced Methods in Cardiovascular Magnetic Resonance Imaging”, European Society for Magnetic Resonance in Medicine and Biology, September 25–27, Rome, Italy.
- Participant in MediTech meeting “Imaging and Measurements in Biomechanics”, October 2–3, Paris.

[4] http://www.math-info.univ-paris5.fr/map5/-Seminaires

Philippe Moireau

- Speaker at “Equations aux dérivées partielles et applications”, March 25–29 2008, Hammamet.
- Speaker at MediTech meeting “Imaging and Measurements in Biomechanics”, October 2–3, Paris.
- Speaker at Séminaire Poems, February 21 2008.

Jacques Sainte-Marie

- Seminar at Compiègne University of Technology: Kinetic equations for the modeling of free surface flows - Modeling, numerics and data assimilation, November 2008.
- Speaker at 12th International Conference on Hyperbolic Problems, University of Maryland.

Marina Vidrascu

- Speaker at Eccomas conference, July 2008, Venice.

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Year Publications

Articles in International Peer-Reviewed Journal

[2] E. AUDUSSE, M. BRISTEAU, B. PERTHAME, J. SAINTE-MARIE. *An Exchanging Mass Multilayer Saint-Venant System for Shallow Water flows. Derivation and numerical validation*, Submitted.

[3] M. BRISTEAU, J. SAINTE-MARIE. *Derivation of a non-hydrostatic shallow water model; Comparison with Saint-Venant and Boussinesq systems*, in "Discrete Contin. Dyn. Syst. Ser. B", vol. 10, n^o 4, 2008, p. 733-759.

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Invited Conferences

[7] D. CHAPELLE. *La météo du coeur*, in "Journées Françaises de Radiologie 2008, conférence invitée".

[8] D. CHAPELLE. *Modeling and estimation of the cardiac electromechanical activity*, in "ESOF'08, invited conference".

Workshops without Proceedings

[9] E. AUDUSSE, M. BRISTEAU, J. SAINTE-MARIE. *A new multilayer Saint-Venant System - Derivation and Numerical Validation*, in "12th International Conference on Hyperbolic Problems, University of Maryland", 2008.

[10] D. CHAPELLE. *Modeling and computations of shells: conference in the honor of Michel Bernadou*, in "ECCOMAS'08".

[11] M. VIDRASCU. *Shell based robust numerical procedures for the solution of real-life problems: conference in the honor of Michel Bernadou*, in "IACM ECCOMAS, Venice, Italy", 30 june-4 july 2008.

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[12] M. FERNÁNDEZ, J. GERBEAU, A. GLORIA, M. VIDRASCU. *A partitioned Newton method for the interaction of a fluid and a 3D shell structure*, RR-6623, Rapport de recherche, 2008, http://hal.inria.fr/inria-00315765/en/.

Other Publications

[13] D. CHAPELLE. *Fundamental and applicative challenges in the modeling and computations of shells: an overview*, CIM'08, invited conference.

[14] D. CHAPELLE, M. FERNÁNDEZ, J. GERBEAU, P. MOIREAU, N. ZEMZEMI. *Numerical simulation of the electromechanical activity of the heart*, Submitted to FIMH'09.

[15] A. GARIAH. *Réduction de modèle pour la simulation de l'activité électromécanique cardiaque (in french)*, Master Thesis in Applied Mathemtics, Ecole Nationale des Ponts et Chaussées & Laboratoire J.-L. Lions, Univ. Paris VI, France, 2008.

[16] P. MOIREAU, D. CHAPELLE, P. LE TALLEC. *Filtering for distributed mechanical systems using position measurements: Perspectives in medical imaging*, Submitted to Inverse Problems, 2008.

[17] P. MOIREAU, D. CHAPELLE, M. YVINEC. *Cardiac motion extraction from images by filtering estimation based on a biomechanical model*, Submitted to FIMH'09.

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