INRIA

INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Project-Team MACS

Modeling, analysis and control in computational structural dynamics

Paris - Rocquencourt

Theme : Observation, Modeling, and Control for Life Sciences

Activity Report

2010

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1. Team

Research Scientists
Dominique Chapelle [Team Leader DR, HdR]
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Philippe Moireau [on secondment from “Corps des Mines”]
Jacques Sainte-Marie [associate researcher, CETMEF/LNH]

Technical Staff
Marc Fragu
Jérémie Foulon

PhD Students
Sofiene Hendili
Alexandre Imperiale [beginning October]
Radomir Chabiniok
Asven Gariah
Daniele Trimarchi

Post-Doctoral Fellows
Maya de Buhan [beginning December]
Nicolae Cindea [beginning September]

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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 past five years – we have increasingly investigated specific topics pertaining to biomechanical modeling.

2.2. Highlights

- Release of the second edition of the book “The Finite Element Analysis of Shells – Fundamentals”, by D. Chapelle and K.J. Bathe, see [15];
- Approval of new European project (FP7, IP category) entitled VPH-Share, intended to provide an info-structure for the Virtual Physiological Human Initiative, to be started in April 2011;
- First public release of the Verdandi data assimilation library, see Section 5.7.

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 [15].

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 [15]. In addition, we have proposed the first (and only to date) shell finite element procedure that circumvents locking [18]. 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, 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 [17]. 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; tires; 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. FELISCE

Participants: Dominique Chapelle, Jérémie Foulon, Philippe Moireau, Marina Vidrascu.

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.

5.2. heartLab

Participants: Dominique Chapelle, Radomir Chabiniok, Philippe Moireau [correspondant], Jacques Sainte-Marie.

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 50,000 lines), and is used within the INRIA teams involved in heart modeling.

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 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 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.

5.3. MITCNL

Participants: Dominique Chapelle, Marina Vidrascu [correspondant].

The package MITCNL is a set of subroutines that implements the triangular MITC3, MITC6 and quadrilateral MITC4 and MITC9 shell elements for large displacements [15]. 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. MODULEF

Participants: Dominique Chapelle, Marina Vidrascu [correspondant].

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/).

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

Participants: Dominique Chapelle [correspondant], Philippe Moireau, Marina Vidrascu.

OpenFEM (http://openfem.sourceforge.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).

5.6. SHELDDON

Participants: Dominique Chapelle, Marina Vidrascu [correspondant].

SHELDDON (SHELls and structural Dynamics with DOmain decomposition in Nonlinear analysis) is a finite element library based on the Modulef package which contains shell elements, nonlinear procedures and PVM subroutines used in domain decomposition or coupling methods.

5.7. Verdandi

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

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

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.

6. New Results

6.1. Modeling and estimation in biomechanics

6.1.1. An energy-preserving muscle tissue model: formulation and compatible discretizations

Participants: Dominique Chapelle, Philippe Moireau, Patrick Le Tallec [Ecole Polytechnique], Michel Sorine [SISYPHE].

In this work we propose a muscle tissue model – valid for striated muscles in general, and for the myocardium in particular – based on a multi-scale physiological description. This model extends and refines an earlier-proposed formulation by allowing to account for all major energy exchanges and balances, from the chemical activity coupled with oxygen supply to the production of actual mechanical work, namely, the biological function of the tissue. We thus perform a thorough analysis of the energy mechanisms prevailing at the various scales, and we proceed to propose a complete discretization strategy – in time and space – respecting the same balance laws. This will be crucial in future works to adequately model the many important physiological – normal and pathological – phenomena associated with these energy considerations. The paper presenting this work is currently in press for the *International Journal of Multiscale Computational Engineering* [6].

6.1.2. General coupling of porous flows and hyperelastic formulations – From thermodynamics principles to energy balance

Participants: Dominique Chapelle, Philippe Moireau.

We formulate a general poromechanics model – within the framework of a two-phase mixture theory – compatible with large strains and without any simplification in the momentum expressions, in particular concerning the fluid flows. The only specific assumptions made are fluid incompressibility and isothermal conditions. Our formulation is based on fundamental physical principles – namely, essential conservation and thermodynamics laws – and we thus obtain a Clausius-Duhem inequality which is crucial for devising compatible constitutive laws. We then propose to model the solid behavior based on a generalized hyperelastic free energy potential – with additional viscous effects – which allows to represent a wide range of mechanical behaviors. The resulting formulation takes the form of a coupled system similar to a fluid-structure interaction problem written in an Arbitrary Lagrangian-Eulerian formalism, with additional volume-distributed interaction forces. We achieve another important objective by identifying the essential energy balance prevailing in the model, and this paves the way for further works on mathematical analyses, and time and space discretizations of the formulation. This work was submitted to *Journal of Elasticity* [16].

6.1.3. External tissue support and fluid-structure simulation in blood flows

Participants: Philippe Moireau, Nan Xiao [Stanford], Matteo Astorino [REO], C. Alberto Figueroa [Stanford], Dominique Chapelle, Charles A. Taylor [Stanford], Jean-Frédéric Gerbeau [REO].

The objective of this work is to address the formulation of an adequate model of the external tissue environment when studying a portion of the arterial tree with fluid-structure interaction. Whereas much work has already been accomplished concerning flow and pressure boundary conditions associated with truncations in the fluid domain, very few studies take into account the tissues surrounding the region of interest to derive adequate boundary conditions for the solid domain. In this paper, we propose to model the effect of external tissues by introducing viscoelastic support conditions along the artery wall, with two – possibly distributed – parameters that can be adjusted to mimic the response of various physiological tissues. In order to illustrate the versatility and effectiveness of our approach, we apply this strategy to perform patient-specific modeling of thoracic aortae based on clinical data, in two different cases and using a distinct fluid-structure interaction methodology for each, namely, an Arbitrary Lagrangian-Eulerian (ALE) approach with prescribed inlet motion in the first case and the coupled momentum method in the second case. In both cases, the resulting simulations are quantitatively assessed by detailed comparisons with dynamical image sequences, and the model results are shown to be in very good adequacy with the data. This work was accepted for publication in *Biomechanics and Modeling in Mechanobiology*.

6.1.4. Trials on tissue contractility estimation from cardiac Cine MRI using a biomechanical heart model

Participants: Radomir Chabiniok, Philippe Moireau, Pierre-François Lesault [Henri Mondor Hospital], Alain Rahmouni [Henri Mondor Hospital], Jean-François Deux [Henri Mondor Hospital], Dominique Chapelle.

In this work we apply specific data assimilation methods in order to estimate regional contractility parameters in a biomechanical heart model, using as measurements *real* Cine MR images obtained in an animal experiment. We assess the effectiveness of this estimation based on independent knowledge of the controlled infarcted condition, and on late enhancement images. Moreover, we show that the estimated contractility values can improve the model behavior in itself, and that they can serve as an indicator of the local heart function, namely, to assist medical diagnosis for the post-infarct detection of hypokinetic or akinetic regions in the myocardial tissue. A short paper was submitted to the *FIMH'11* Conference, and a full paper is being prepared.

6.1.5. Constitutive parameter estimation methodology using tagged-MRI data

Participants: Alexandre Imperiale, Radomir Chabiniok, Philippe Moireau, Dominique Chapelle.

We propose a methodology for performing the estimation of a key constitutive parameter in a biomechanical heart model – namely, the tissue contractility – using tagged-MRI data. We adopt a sequential data assimilation strategy, and the image data is assumed to be processed in the form of deforming tag planes, which we employ to obtain a discrepancy between the model and the data by computing distances to these surfaces. We assess our procedure using synthetic measurements produced with a model representing an infarcted heart as observed in an animal experiment, and the estimation results are found to be of superior accuracy compared to assimilation based on segmented endo- and epicardium surfaces. A short paper presenting this work was submitted to the *FIMH'11* Conference.

6.2. Asymptotic and multiscale modeling

6.2.1. Modeling and simulation of multi-layers mechanical structures

Participants: Marina Vidrascu, Sofiene Hendili.

The collaboration with Françoise Krasucki and Giuseppe Geymonat (Montpellier University) on the modeling of 3D materials connected by stiff interfaces continues within the Epsilon ANR project (Domain decomposition and multi-scale computations of singularities in mechanical structures 7.1.1). In the framework of matched asymptotic expansions we introduced a new effective and robust method to approximate the behavior of a structure containing a thin layer with periodically distributed micro-holes. A surface (in 3D) or a line in (2D) with particular jump conditions thus provide substitutes for the initial problem.

6.2.2. *Multi-scale modeling and simulation of rubber*

Participants: Maya de Buhan, Marina Vidrascu, Antoine Gloria [SIMPAF], Patrick Le Tallec [Ecole Polytechnique].

In collaboration with A. Gloria (project-team SIMPAF) and P. Le Tallec (Ecole Polytechnique), we are currently working on the implementation of a multiscale model for rubber based on the statistical physics description of a network of polymer chains. At the microscopic level the rubber is composed of a network of chains, for which the energy depends only on the average length of the chains. The macroscopic energy will be obtained by minimizing the energy of a representative sample of such chains for a linear deformation of the boundary. The numerical simulations are performed with the Modulef software. The sample of chains is obtained by meshing a stochastic set of points. Meshing tools from the Gamma project-team are used. The edges of the mesh represent the chains. In order to obtain the macroscopic energy, a non linear elasticity problem is solved on each stochastic mesh, and a specific finite element was designed to model the chains. Numerical results are in very good agreement with Treloar's mechanical experiments. The next step is to solve an inverse problem to reconstruct an analytical approximation of the homogenized constitutive law. The numerical tool developed so far allows us to generate as many data as needed to solve this inverse problem. This problem will be addressed in the post-doc of Maya de Buhan. This work is supported by the ARC DISCO (7.1.2).

7. Other Grants and Activities

7.1. National Initiatives

7.1.1. *Epsilon*

The Epsilon project is an ANR project entitled "Domain decomposition and multi-scale computations of singularities in mechanical structures". The members are Ecole Polytechnique, I3m at Montpellier, Laga at Paris-Nord and INRIA. INRIA is particularly involved in the modeling and simulation of an assembly of structures containing a very thin layer embedded in a 3D structure. Sofiene Hendili PhD student (co-supervised by Montpellier and INRIA) spent the first year with the EPI MACS in Rocquencourt..

7.1.2. *DISCO*

DISCO[2] (du DIScret au COntinu pour les polymères réticulés) is an INRIA ARC. The members are EPI SIMPAF and MACS from INRIA, Ecole polytechnique, ESPCI, and the Max Planck Institute for Mathematics in the Sciences (Leipzig). The aim of this project is a multi scale modeling and simulation of reticulated polymers.

7.2. European Initiatives

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.

[2] http://chercheurs.lille.inria.fr/~gloria/DISCO.html
[3] http://www.euheart.eu/

7.3. International Initiatives

7.3.1. Other long-term collaborations

- Collaboration on numerical locking with MIT and ADINA R&D (K.J. Bathe);
- Collaboration with CVBRL Stanford (C. Taylor) on cardiovascular modeling and estimation.

8. Dissemination

8.1. Animation of the scientific community

Dominique Chapelle:

- Member of the editorial boards of “Computers & Structures” and “M2AN”
- Elected member of the board of SMAI (until June)

8.2. Teaching

- Asven Gariah: Scilab hands-on sessions at Paris 6, Fall 2010
- Philippe Moireau: course “Introduction to the discretization of Partial Differential Equations” at ENSTA, Spring 2010
- Philippe Moireau: course “The Finite Element Method” at ENSTA, Fall 2010
- Jacques Sainte-Marie: course “Waves and vibrations in continuum mechanics” at ENSTA

8.3. Participation in conferences, workshops and seminars

Dominique Chapelle

- C++ advanced Course (INRIA, Jan. 25-26 and Febr. 5)
- Speaker at WCCM’10 (Sydney, July), WCB’10 (Singapore, August), CARI’10 (Yamoussoukro, Oct.)
- Seminars: Univ. Oxford (Jan. 28th), PARCC (June 16th), Collège de France (Nov. 5th), INSERM U637 (Montpellier Nov. 18th)
- PhD jury N. Cindea (Nancy, March 29th), habilitation J. Sainte-Marie (Paris 6, Dec. 2nd)

Radomir Chabiniok

- Speaker at WCB’10 (Singapore, August)

Asven Gariah

- Workshop “Méthodes de réduction de modèle dans le calcul scientifique”, ECN Journées scientifiques CSMA (Sept.)

Sofiane Hendili

- Annual meeting of PhD students I2S (Montpellier, June 10)
- Seminar of the ACSIOM team from I3M Montpellier (Nov. 16)

Jérémie Foulon

- C++ advanced Course (INRIA, Jan. 25-26 and Febr. 5)
- Introduction to parallel computing (INRIA, Febr. 3-4)

Philippe Moireau

- Speaker at WCCM'10 (Sydney, July), WCB'10 (Singapore, August)
- Invited speaker at the French Conference in Data Assimilation (Grenoble, Dec. 8-9)
- Seminars: PARCC (June 16th), INSERM U637 (Montpellier Nov. 18th)

Jacques Sainte Marie

- C++ advanced Course (INRIA, Jan. 25-26 and Febr. 5)
- Seminar at Univ. Franche-Comté (Nov.) "Du système de Saint-Venant aux équations de Navier-Stokes à densité variable. Modélisation, interprétation cinétique et simulations"

Marina Vidrascu

- C++ advanced Course (INRIA, Jan. 25-26 and Febr. 5)
- Speaker at ECCM2010 (Paris, May)
- Speaker in special session "Analyse, contrôle et approche numérique en mécanique des solides" at 10ème Colloque Franco-Roumain de Mathématiques Appliquées, (Poitiers, Aug. 26-31)
- Seminars: Ancona (Italy, June 30th), Sophia-Antipolis (Nov. 27th)

9. Bibliography

Publications of the year

Doctoral Dissertations and Habilitation Theses

[1] J. SAINTE-MARIE. *Models and numerical schemes for free surface flows. Beyond the Saint-Venant system*, U. Pierre et Marie Curie Paris 6, 2010, Habilitation à Diriger des Recherches.

Articles in International Peer-Reviewed Journal

[2] E. AUDUSSE, M.-O. BRISTEAU, M. PELANTI, J. SAINTE-MARIE. *Approximation of the hydrostatic Navier-Stokes system for density stratified flows by a multilayer model. Kinetic interpretation and numerical validation.*, in "J. Comp. Phys.", 2010, Submitted.

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Scientific Books (or Scientific Book chapters)

[15] D. CHAPELLE, K. BATHE. *The Finite Element Analysis of Shells – Fundamentals*, Second, Springer, 2011.

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