INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Project-Team Macs

Modeling, Analysis and Control for Computational Structural Dynamics

Rocquencourt

THEME NUM

Activity Report

2006

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1. Team

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2. Overall Objectives

2.1. Overall Objectives

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.

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) finite element procedure that circumvents locking[1]. 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 and ICEMA2 ARC projects, 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 activation and contraction symptoms. The model we propose is based on a chemically-controlled constitutive law of cardiac myofibre mechanics formulated in the Sosso project-team and consistent with the behavior of myosin molecular motors. 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 (see [2]), considered as given (or measured) data, or as a parameter to be estimated.

[1] D. Chapelle and R. Stenberg. Stabilized finite element formulations for shells in a bending dominated state. *SIAM J. Numer. Anal.*, 36(1): 32-73, 1998.

[2] CardioSense3D

One of our key objectives in this prospective phase was also to survey – and investigate to some extent – the various difficulties to be faced in this global model-data coupling approach, in order to more precisely identify some fundamental (i.e. also going beyond the specific application at hand) research issues in which the team can make important contributions.

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/), with about 100 downloads per month recorded.

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

Participants: Mathieu Alba [team SOSSO2], Dominique Chapelle, Marina Vidrascu [correspondant].

OpenFEM (http://www.openfem.net) is an *opensource* toolbox for finite element analysis (presently for linear structural mechanics only) within the matrix computing environments Matlab and Scilab. This software is developed in a collaboration between Macs and the SDTools company [3]. It was originally developed for Matlab, and then a Scilab version was more recently produced as part of an “ODL”. 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).

In order to improve CPU-time in OpenFEM matrix assembling, we investigated the possibility of **easy parallelization using OpenMP directives**. We performed tests with the OpenMP compatible Intel C compiler (icc). Current distribution of GNU compilers (GCC 3.) are not OpenMP compatible. The next distribution (GCC 4.0) will integrate this feature.
Using the heart package to run tests, the matrix computing time was reduced by **40% for a bi-processor computer** (Intel processors). Following these results, we plan to fully integrate OpenMP features to the OpenFEM toolbox. The code structure has to be adapted to enable OpenMP compatibility.

5.3. MITCNL

Participants: Dominique Chapelle [correspondant], Marina Vidrascu.

[3] SDT

The package MITCNL is a set of subroutines that implements the 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. This year triangular elements (MITC3 and MITC6) were added to the package.

5.4. Heart simulation package

Participants: Mathieu Alba [team SOSSO2], Dominique Chapelle, Marina Vidrascu [correspondant].

In order to obtain simulations of the heart model that we have formulated (see Section 6.3) we developed this package based on OpenFEM and for use with Matlab. The Matlab environment allows powerful postprocessing, ease of interfacing with other software (such as for simulating action potential propagation) and provides some very efficient solvers (e.g. Pardiso, UMFPACK).

The heart simulation code used to produce both healthy and pathological cases is now fully based on the OpenFEM toolbox. This package includes OpenFEM files required to simulate the electromechanical behaviour of the heart, the Matlab script for the simulation code and some data to run simulations. Other Matlab scripts useful to generate files for 3D vizualisation are also given (VTK or ENSIGHT format supported). Refer to figures 1,2

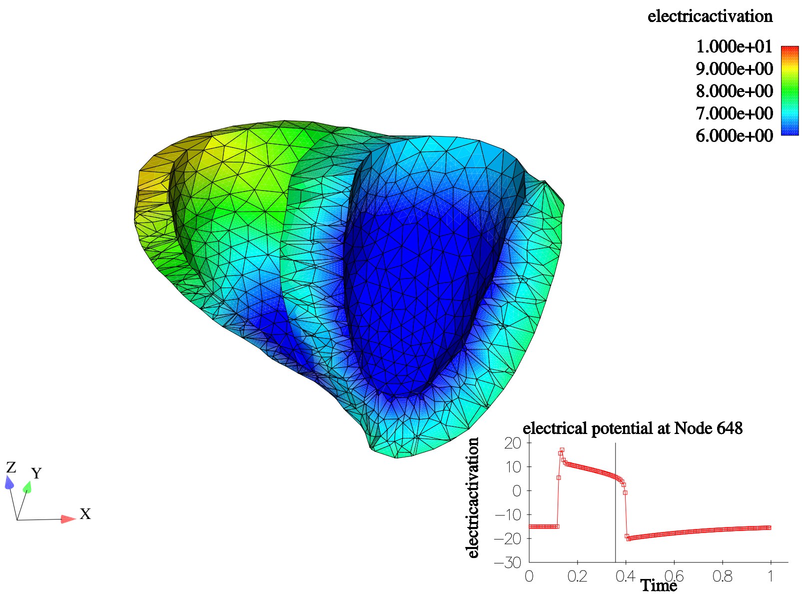

Figure 1. Healthy case

Future work will investigate coupling with other simulation codes based on C/C++ for 3D fluid simulation in ventricles and the inclusion of a more realistic electrical model.

6. New Results

6.1. Design and analysis of effective numerical procedures for structural mechanics

Keywords: *MITC elements*, *numerical reliability*.

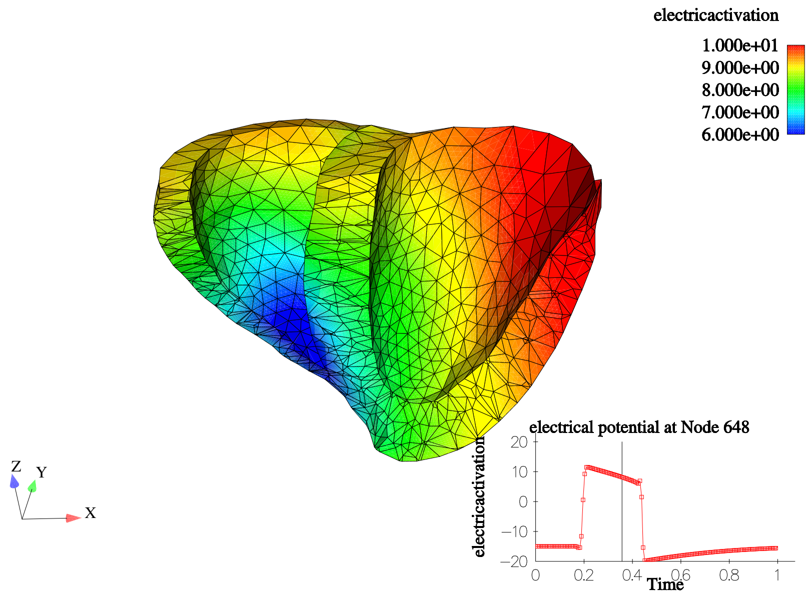

Figure 2. Pathological case Left Branch Block

Participants: Dominique Chapelle, Iria Paris, Lourenço Beirão da Veiga, Marina Vidrascu.

Effective triangular shell elements are of utmost interest in engineering practice, and the MITC6a element – a 6 node biquadratic general shell element of the MITC family – has been shown to significantly reduce the locking phenomena arising in bending dominated behaviours. However, for some specific combinations of midsurface geometry and boundary conditions, the MITC6a element features some non-physical displacement modes with vanishing membrane strain energy. This phenomenon was thoroughly analyzed, and a remedy based on a stabilized bilinear form was proposed. Detailed numerical tests were performed and the results demonstrated the good performance of the proposed method both for membrane and bending dominated problems. This work was published in [10], [8], and concluded the doctoral work of Iria Paris, see [2].

6.2. Modeling and simulation of fluid-structure interaction problems

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

Participants: Patrick Le Tallec, Marina Vidrascu.

This work is done in collaboration with Jean-Frédéric Gerbeau[4] and Miguel Fernandez[5]. The objective is to simulate the mechanical interaction between the blood and the wall of large arteries. The fluid-structure algorithms we use are all based on domain decomposition techniques. This approach allows to formulate the problem on the whole domain and then decompose on a fluid part and a solid part with appropriate coupling conditions. From a practical point of view it is thus possible to use specific fluid, solid and coupling solvers.

[4] team REO
[5] team REO

We investigated a new fluid-solid coupling algorithm. Unlike the previous schemes used, now the linearisation step is performed before domain decomposition. This is an extention of domain decomposition techniques classically used in nonlinear elasticity. An advantage of this approach is that the new algoritm has an intrinsic parallelism. It is now reasonable to consider 3D- shell elements. From the solid side, these models are indeed more expensive than the ones used previously, but they allow to consider more realistic materials for the arteries. For the whole problem the use of a parallel approach implies that the increased complexity in the solid has no consequence on the global execution time.

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

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

Participants: Mathieu Alba [team SOSSO2], Frédéric Bourquin, Dominique Chapelle, Philippe Moireau, Jacques Sainte-Marie, Michel Sorine [team SOSSO2], Marina Vidrascu.

6.3.1. Modeling

In the context of the CardioSense3D project (see section 7.1.1), two new aspects of the cardiac modelling have been investigated, namely the perfusion of the cardiac muscle and the simulation of mechanical activity with reduced models.

6.3.1.1. Perfusion

The perfusion is the phenomenon by which blood reaches organs and tissues starting from the blood vessels, usually to supply nutrients and oxygen. We mainly address the problem of drainage 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.

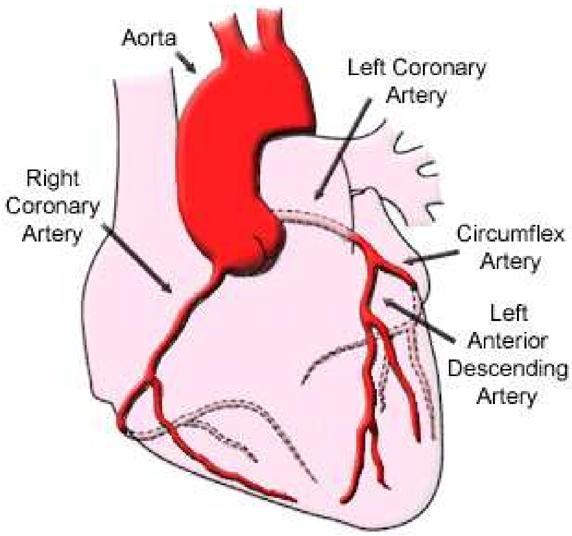

Figure 3. Main coronary arteries (source www.cvphysiology.com).

Considering the whole heart, the complete modeling of blood-tissue interaction leads to prohibitive numerical costs. Moreover, the geometry of the arterioles and veinules being unknown, we are led to considering macroscopic quantities for the fluid and solid parts. Hence, the study of the coupling between the behavior of the blood and the tissue within the framework of poromechanics seems appropriate. We have proposed a preliminary version of a perfusion model including the 3D mechanical model of the myocardium behavior developed in the MACS project, and coupled with a hierarchical structure of vessels ensuring the drainage of blood [9].

In collaboration with the REO team, we aim at improving the proposed model in order to obtain more realistic simulations. We are also investigating the modeling of blood flows in the coronaries circulating at the epicardium (cf. Fig. 3) and the supply of oxygen.

6.3.1.2. Reduced models

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, and in particular the proper orthogonal decomposition [15] and the nonlinear mode decomposition [16] methods. This activity will be further developed in 2007.

6.3.2. Estimation for cardiology

This work is also part of the CardioSense3D “Large Initiative Action”, see Section 7.1.1.

Our objective is to develop robust “data-model coupling algorithms” adapted to an electro-mechanical heart model of the type formulated in [6]. This approach aims at achieving good estimation of the behaviour and physiological parameters of a patient-specific heart, using measurements from medical imaging combined with simulations of the mechanical model. This inverse problem, also called data assimilation, remains very challenging because the current state of the art in the domain is unadapted to our problem. In fact, the heart model is too sensitive and too large to be well inverted by classical Kalman filters or variational assimilation techniques. Hence, the PhD thesis of Philippe Moireau, starting from August 2005, is dedicated to the research on robust and effective state filters inspired from engineering and their extensions to combined state-parameter estimation procedures. In a first step, we have focused on the analysis and justification – by spectral arguments, primarily – of the efficiency of a state filtering strategy based on collocated control. A particular concern was to obtain uniform stabilization with respect to the discretization used in the state filter. In a second step, we have established the global convergence of our state-parameter algorithm, both for the estimation of parameters in the load and in the stiffness. The latter case is much more difficult because the resulting combined state-parameter dynamical system is nonlinear, but we proved local stability. We evaluated our algorithm using a 3D “toy problem", paying particular attention to the choice of measurements – in terms of operator and noise – compatible with the available modalities in medical imaging, see Fig. 4 for the problem description, and Fig. 5 for numerical results. This new methodology is described in [14].

6.4. Structural Health Monitoring: Imaging with distributed sensors

Participants: Grégoire Derveaux, George Papanicolaou [Stanford University], Chrysoula Tsogka [University of Chicago].

The purpose of this work is to locate localized damages in a structure with distributed sensors. This may typically be a crack in an aircraft or some other structure whose integrity we want to monitor. In addition to locating the damage we also want to estimate its size and shape, if possible. One of the difficulties of this problem is that the measured signals do not provide clear arrival times, because of the complexity of the environment. We have developed a robust and stable imaging technique based on the ability of time reversal to take advantage of multipathing (*ie.* the multiple scattering of the waves in the medium). When there are several defects, they can be well separated with the help of the Singular Value Decomposition (SVD) of the matrix of measurements. This SVD can be seen as an optimization of the power distribution allocated to each illuminating sensor.

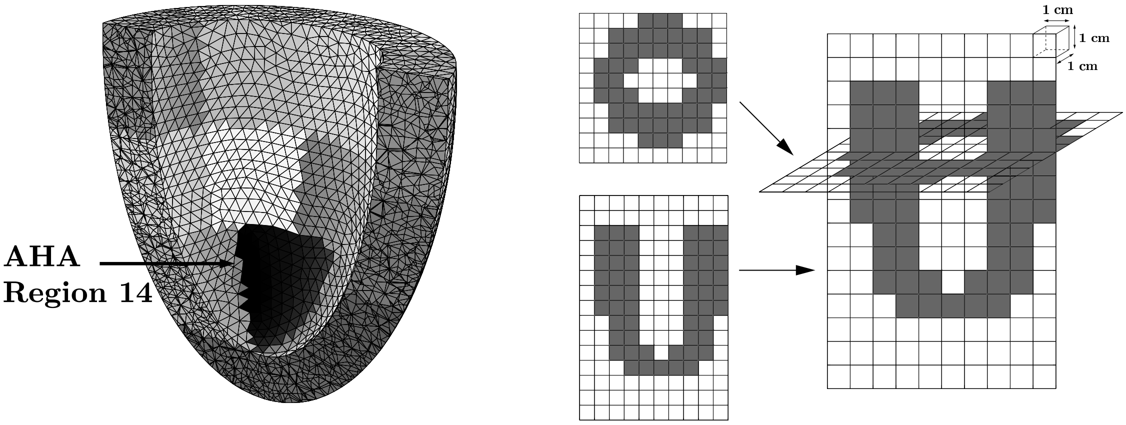

Figure 4. Simplified left ventricule geometry and measurements cells

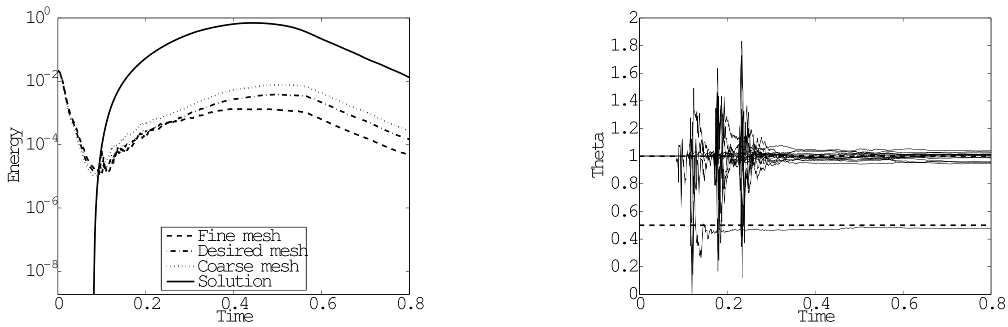

Figure 5. State and parameter convergence in the linear case

This year we have been working on several adaptations of this algorithm:

- Optimization of the waveform, *ie.* the design of the probing signal that is used by each sensor to illuminate the medium.
- Adaptive choice of the receivers to be used when the medium is illuminated by a given emitter. This is particularly useful when the defect to be imaged is extended, w.r.t the central wavelength, because in that case some of the receivers are 'hidden' by the object.

One particularity of SHM compared to other imaging areas, as in geophysics or medical imaging, is that the structure without defect is known before the defect appears. So it is possible to get the response of the structure without defect. This is called the baseline. In principle one could subtract the baseline to the response when a defect has appeared, so that one can get the response coming from the defect only. But this subtraction cannot be perfect, as the structure has changed between two data acquisitions. We are currently investigating a stable way of using the difference between those two signals in order to image the defect.

6.5. Mechanics of the cell: Modeling of the cell membrane

Participants: Dominique Chapelle, Grégoire Derveaux.

The mechanical structure of a cell is essentially constituted by the *cytoskeleton* and the *plasma membrane*. The former is a complex network of 1D proteic filaments that provides its rigidity to the cell and transport means for molecules. The role of the plasma membrane is to provide a semi-permeable frontier to the cell, whose shape can be easily remodeled. The recent development of nanotechnologies, as for instance the Atomic Force Microscope, allows the investigation of the mechanical behavior at the scale of one cell. Therefore there is a growing need for accurate models of those structural elements. To begin with, we are interested in the modeling of the membrane. To date, it seems that there are few models of this object. On the one hand, there exist mechanical models based on a local behavior, described with one stiffness parameter. On the other hand, there exist numerical simulations based on a viscoelastic modeling of classical elastic membranes.

We have formulated a model of the plasma membrane in the framework of continuum mechanics. The model is based on both Lagrangian and Eulerian approaches. On the one hand, the movement of the surface itself is described by a parametrized time dependent function (Lagrangian description). On the other hand, the movement of fluid particles inside this membrane is described by their velocity and by the density of particles at each point (Eulerian approach). The equations of the movement are given by conservation of momentum, conservation of mass and the transport equation of the surface. Using the same formalism as for thin shell problems, the stress tensor is decomposed into membrane and flexural stresses. To start with, the latter is neglected, which leads to a pure membrane constitutive law. We have proposed a numerical scheme for the approximation of this model in the incompressible case. We are currently working on the implementation of this numerical method.

7. Other Grants and Activities

7.1. National projects

7.1.1. CardioSense3D

Participants: Mathieu Alba [team SOSSO2], Dominique Chapelle, Grégoire Derveaux, Philippe Moireau, Marina Vidrascu.

CardioSense3D[6] 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 Sosso2, but other academic, industrial and clinical partners are closely associated in this action.

[6] http://www-sop.inria.fr/CardioSense3D/

7.1.2. ACI CONSTRUCTIF (COuplage de coNcepts pour la Surveillance de sTRUCTures mécaniques InFormatisées - Coupling of concepts for the surveillance of computerised mechanical structures)

Participants: Frédéric Bourquin, Dominique Chapelle.

This project[7] coordinated by the SISTHEM team (IRISA) is part of the “ACI Sécurité Informatique”[8] and was launched in September 2003 (for 3 years). The objectives are:

- the coupling of statistical models of sensor data with models of the physical phenomena governing the instrumented structures for monitoring purposes;
- the investigation of the combined use of multidisciplinary approaches – namely, statistical inference, data assimilation, finite element model updating and optimization methods – with a view to diagnosing and localising damage.

7.2. International projects

7.2.1. RTN Project “SMART”

Participants: Michel Bernadou, John Cagnol, Dominique Chapelle, Marina Vidrascu.

This project[9] – an RTN project of the fifth European Framework Program – started in November 2002 (for 4 years). The aim is to foster research and to provide training for researchers in the field of new materials and adaptive systems. “New materials” is used here as a generic term for “functional” materials whose physical or chemical properties are used in the design of control elements yielding smart systems. The scientific objectives of the research are to develop efficient mathematical methods and numerical tools for modelling, control and numerical simulation.

This network project is coordinated by ESIEE[10], MACS being the other French member out of a total of 11 members from 8 European countries.

7.2.2. Other long-term collaborations

- Collaboration on numerical locking with MIT and ADINA R&D (Klaus-Jürgen Bathe);
- Collaboration on structural health monitoring with G. Papanicolaou (Stanford) and C. Tsogka (Chicago).

8. Dissemination

8.1. Various academic responsibilities

Dominique Chapelle:

- Vice-chairman of INRIA-Rocquencourt Project 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”);

[7] http://www.irisa.fr/sisthem/index-fr.htm
[8] http://acisi.loria.fr/
[9] http://www.esiee.fr/smart-systems/index.php
[10] http://www.esiee.fr/en/index.php

8.2. Teaching activities

- Grégoire Derveaux: Course *Scientific Computing,* at ENSTA, Fall 2006.
- Marina Vidrascu: Course “*Mathematical fundamentals of the finite element method*” at Ecole Supérieure d’Ingénierie Léonard de Vinci.

8.3. Participation in conferences, workshops and seminars

Dominique Chapelle

- Seminars: Poems 23 Febr., Cermics 15 March.
- Conferences: CSSM 2006 Lisbon (keynote, 5–9 June), CIMPA-ISFMA School Shanghai (invited, 7–18 August), “MAP5 Scientific Day” Paris (invited, 14 Dec.).
- Organizer of CEA-EDF-INRIA Summer School on Data Assimilation (26 June – 7 July).
- Thesis committees: C. Poutous (Pau, referee, 25 Oct.), I. Paris (Paris 6, supervisor, 28 Nov.).
- Participant in CISM Summer School on Biomechanics (Udine, 11–15 Sept.).

Grégoire Derveaux

- 151st Meeting of the Acoustical Society of America, Providence, USA, 5–9 June 2006.
- Participant in CISM Summer School on Biomechanics (Udine, 11–15 Sept.).

Philippe Moireau

- Assistant-lecturer at CEA-EDF-INRIA Summer School on Data Assimilation (26 June – 7 July).
- Participant in CISM Summer School on Biomechanics (Udine, 11–15 Sept.).

Iria Paris

- Seminar at CERMICS, 15 March 2006.
- European Conference on Smart Systems Rome, 26–28 October 2006.

Jacques Sainte-Marie

- Assistant-lecturer at CEA-EDF-INRIA Summer School on Data Assimilation (26 June – 7 July).

Marina Vidrascu

- Thesis committee: M. Barboteu (Perpignan, 22 May).
- Participant in CISM Summer School on Biomechanics (Udine, 11–15 Sept.).
- Participant in Journées nationales des ARC 2006 (Grenoble, 17–18 Oct.).

9. Bibliography

Major publications by the team in recent years

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Year Publications

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[2] I. PARIS. *Robustesse des éléments finis triangulaires de coque*, Ph. D. Thesis, Université Pierre et Marie Curie - Paris VI, 26 Nov 2006.

Articles in refereed journals and book chapters

[3] G. DERVEAUX. *Space time mesh refinement methods (chapter 6)*, in "Effective Computational Methods in Wave Propagation", V. A. DOUGALIS, J. EKATERINARIS, N. KAMPANIS (editors). , to appear, CRC Press, 2006.

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[5] G. DERVEAUX, G. PAPANICOLAOU, C. TSOGKA. *Time reversal imaging for distributed sensor networks*, in "The Journal of the Acoustical Society of America", In press, 2006.

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Publications in Conferences and Workshops

[8] L. BEIRÃO DA VEIGA, D. CHAPELLE, I. PARIS SUAREZ. *A stabilized MITC6 triangular shell element*, in "Proceedings of European Conference on Smart Systems, Rome, 26–28 October 2006".

[9] J. SAINTE-MARIE, R. CIMRMAN, E. ROHAN. *Excitation-contraction coupling and perfusion in the heart*, in "Mathematics, Finite Elements and Applications (MAFELAP2006)", J. WHITEMAN (editor). , 2006.

Miscellaneous

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[13] D. CHAPELLE, I. PARIS. *Detailed assessment of MITC6 elements*, In preparation.

[14] P. MOIREAU, D. CHAPELLE, P. LE TALLEC. *Joint state and parameter estimation for distributed mechanical systems*, In preparation.

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[16] O. THOMAS, C. TOUZÉ. *Large amplitude forced vibrations of thin shallow spherical shells : reduced order models at resonance and mode coupling*, in "2nd International Conference on Nonlinear Normal Modes and Localization in Vibrating Systems", 2006.