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

2007

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1. Team

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Research scientist (partners)
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Oskar Talcoth [6 months]

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) shell 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 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 activation and contraction symptoms. The model we propose is based on a chemically-controlled constitutive law of cardiac myofibre mechanics[2] 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, 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] J. Bestel, F. Clément and M. Sorine. A biomechanical model of muscle contraction[3], 2208: 1159–1161, 2001.

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 [4]. 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 matrix assembling OpenFEM allows **easy parallelization using OpenMP directives**. Our tests have shown that the matrix computing time is reduced by **40% for a bi-processor computer** (or dual core processor).

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. In 2007 the 2nd version of MITCNL was released and registered with APP. The key new features in this version are the triangular elements and the ability to model junctions using 6 degrees of freedom (3 for displacements and 3 for rotations) at the corresponding nodes.

5.4. HeartLab

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

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

The Matlab procedures of the heart simulator now include both modeling and estimation modules. The implementation was performed with a particular concern for the modularity of the code, 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 which is more actively maintained.

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 data defined within each element, and referencing necessary for boundary conditions and estimation, in particular. These geometries are analytical or come from CT scans of humans or pigs. The mesh operations performed to obtain computational meshes were carried out using the 3Matic package from Materialise, and the Yams and GHS3D software developed in the Gamma team-project.

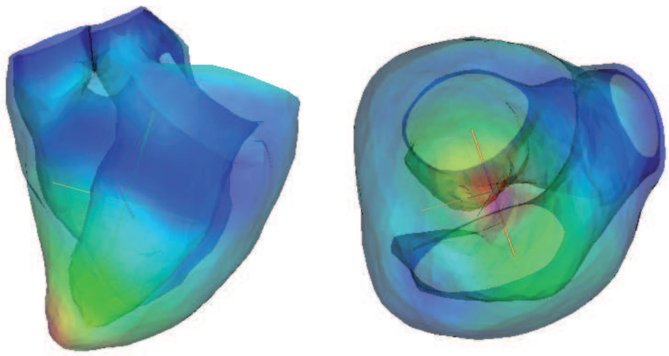

Figure 1. Simulation of the heart on a complete "apex to valve" geometry

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 done in collaboration with Jean-Frédéric Gerbeau[5], Miguel Fernandez[6] and Antoine Gloria[7]. 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.

[5] team REO
[6] team REO
[7] team REO

The problem considered is nonlinear. Last year we started the investigation of a new algorithm which – unlike our previous ones – linearises first and then applies domain decomposition on the tangent problem [8]. This year the new algorithm was succesfully implemented and validated. In addition, this approach was compared to more classical methods and showed its effectiveness when the solid problem is expensive.

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

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

Participants: Radomir Chabiniok, Dominique Chapelle, Philippe Moireau, Elsie Phé [REO], Jacques Sainte-Marie, Oskar Talcoth.

6.2.1. Modeling

6.2.1.1. Fiber interpolation

We derived an intuitive method to prescribe fiber orientation on any heart geometry using different physiological knowledge and constraints. We start from an analytical description of the fiber orientation consistent with physiological considerations and interpolate it on the whole geometry, using additional physiological knowledge around the valves. This interpolation is performed on the surface using a geodesic interpolator, and in the volume using a distance-to-mesh algorithm or harmonic lifting.

6.2.1.2. Perfusion

The perfusion is the phenomenon by which blood reaches organs and tissues starting from the blood vessels, usually to supply nutrients and oxygen. An important 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 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.

The blood flows circulating in the coronaries at the epicardium (cf. Fig. 2) are simulated using a 3D Navier-Stokes model, whereas the drainage in the capillary vessels is represented using a Darcy law. The simulation results are in good agreement with the available physiological data but the modeling of the tissue porosity needs to be refined.

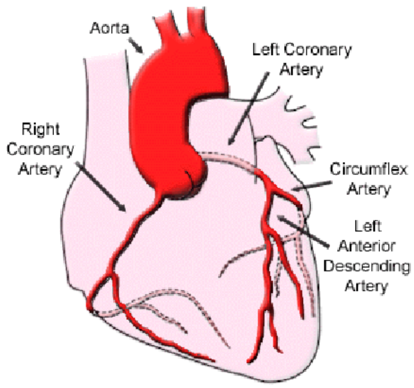

Figure 2. Main coronary arteries (source http://www.cvphysiology.com).

This work is carried out in collaboration with the REO team (I. Vignon). The Navier-Stokes and Darcy codes are developed in the LifeV platform [16], and HeartLab is used for the simulation of the mechanical activity.

6.2.1.3. Reduced models

Another important aspect in the developement of valuable tools for clinical applications is to reduce computational costs. This motivates the analysis and simulation of the heart behavior with techniques leading to reduced size models, and in particular the proper orthogonal decomposition (POD) method [15].

For the mechanical heart model presented in [17], we have studied the size of the POD basis necessary to accurately recover the reference simulation. It seems this can be achieved with approximatively 10 POD modes. Furthermore, the stability of this POD basis with respect to variations of the main mechanical parameters has been demonstrated. The results are presented in [13].

This activity will be further developed in 2008. More specifically, the stability of the POD basis with respect to the variations of the electrical activity will be studied. The objective is also to derive some error estimates between the complete and reduced simulations.

6.2.2. Estimation

6.2.2.1. Filtering procedures for state-parameter estimation

Using the electro-mechanical heart model, our objective is to develop robust "data-model coupling algorithms". This approach aims at achieving good estimation of the behavior and physiological parameters of a patient-specific heart, using measurements from medical imaging in combination with simulations of the mechanical model. This inverse problem – 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 (started in August 2005) is dedicated to the research on robust effective state filters inspired from engineering, and their extensions to combined state-parameter estimation procedures. In the estimation of loading parameters (fully linear for the whole state-parameter observer system) and stiffness parameters (bilinear observer problem) with volume-distributed measurements of the velocity, the complete analysis is now published in [4], see also Figs 3-4. In the case of surface measurements – typically concentrated on the epicardium – the challenge is mostly mathematical, since the classical measurement white noise used in Kalman filtering is not compatible with the physical energy space. Therefore, in order to deal with such measurement errors we have reformulated our state-parameter estimation approach within an H^∞ robust estimation framework. In other words, we are now able to couple our robust state filter with an H^∞ filter on parameters, with a complete analysis of the estimation (including detailed numerical assessments).

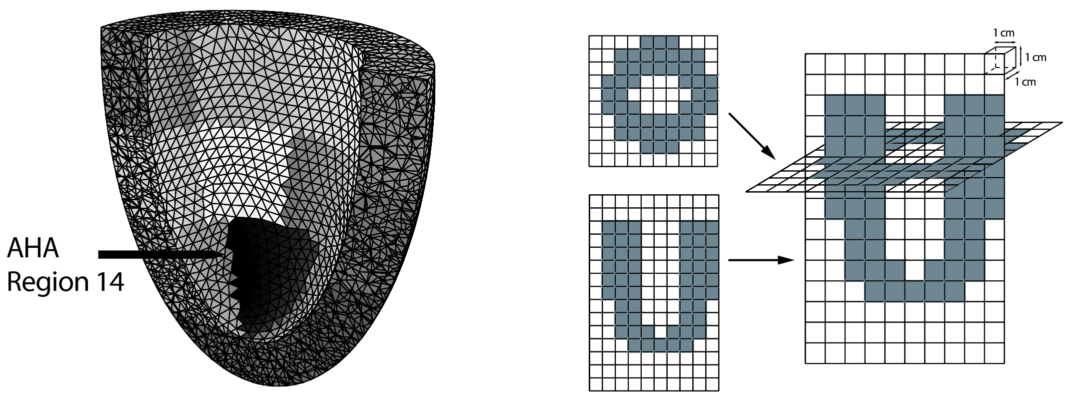

Figure 3. Simplified left ventricule geometry and measurements cells

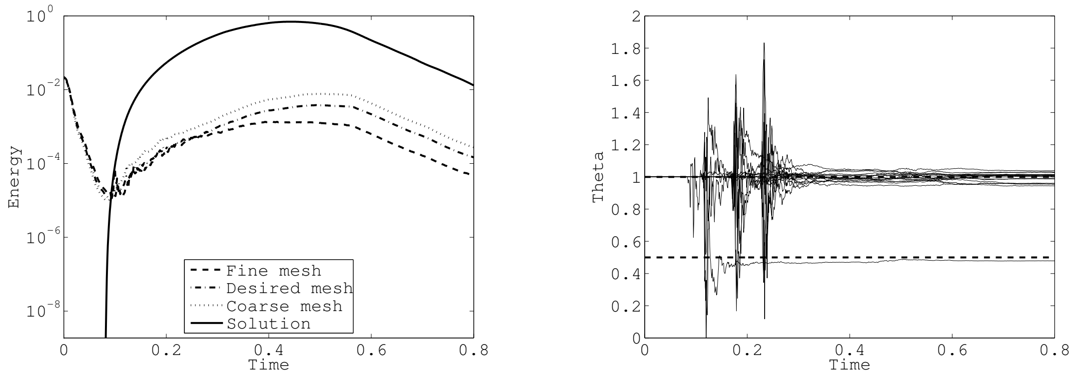

Figure 4. State and parameter convergence in the linear case

- we expect better performance in nonlinear estimation, since UKF seems to be more robust than Extended Kalman Filter in mechanical parameter estimation, as demonstrated in [18];
- the numerical implementation of UKF avoids the computation of tangent quantities.

Another work in progress concerns the formulation of state filters applicable when the measurements are not Lagrangian velocities. We derived a robust collocated filter which can be used with measured Lagrangian displacements, and we are in the process of extending this approach to Eulerian measurements using model-image distances as employed in some image analysis methods.

6.2.2.2. Ultrasound image simulations for the assessment of optical flow tracking

This was the topic of O. Talcoth's Master's thesis [14], cosupervised by E. Angelini (ENST), D. Chapelle and P. Moireau. In order to evaluate the possibilities of using an optical flow (OF) algorithm in a cardiac data assimilation context, three-dimensional cardiac ultrasound images were simulated using an electro-mechanical model of the human heart and a signal processing simulation framework. Several extensions to an existing ultrasound simulation method were proposed and implemented: 1) The acquisition geometry was changed from Cartesian to spherical. 2) The spatial resolution was improved by performing local convolutions. 3) The echoegeneity parameters were optimised using the Kolmogorov-Smirnov test. 4) Specular reflections were modeled. The simulated images were processed by the OF and the estimated movements were compared to the true ones from the heart model. Different norms used to measure the OF errors were discussed. Although simple movements yielded good results, the OF did not perform well when more complicated movements were examined. A probabilistic model for the OF results was proposed permitting an improvement of the OF method to be suggested.

6.3. Structural Health Monitoring: Imaging with distributed sensors

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

The purpose of this work is to locate some 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 in this problem is that the measured signals do not provide clear arrival times, because of the complexity of the environment.

This year we have been working on the investigation of the following algorithms:

- A coherent interferometric algorithm that computes an image based on the correlation of the measured traces in the frequency inside a “coherent” bandwidth. This bandwidth is a parameter of the algorithm which is typically smaller than the pulse bandwidth. It yields lower resolution images, but the images are stable with respect to changes in the complexity of the background.
- Adaptive choice of the illuminating pulse to be used, based on the minimization of a sparsity norm of the image produced – typically the bounded variation norm.
- Adaptive selective focusing based on the singular value decomposition of the response matrix in the frequency domain. Again, the choice of subspace signals for each frequency is done by minimizing the norm of the image produced.
- Use of the Green function of the background. Application to a “full” migration algorithm.

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

Participants: Dominique Chapelle, Grégoire Derveaux.

Cells are the fundamental elements of life. They can be isolated – as for bacteria – or part of a complex multicellular organism. The contents of cells are circumscribed by a thin membrane called the plasma membrane. The emergence of nanosciences technology – and in particular the Atomic Force Microscope (AFM) – allows today for investigating the fine mechanical phenomena at this level. During the last ten years, there has been a growing interest in the analysis of the mechanical behavior of the cell – and more particularly of cell membranes.

Plasma membranes are very thin structures with thickness 4 to 5 nm for an overall size of 10 to 100 microns. They consist of two layers of lipid molecules and have original properties: their behavior may be described by both structural mechanics (bending and streching) and fluid mechanics (lipid molecules constituting the two membrane layers can move within each layer so shear stresses only arise from viscosity, unlike classical membranes). Mechanical descriptions available in the literature essentially consider local aspects. Numerical simulations seem to be limited to the use of viscoelasic models of classical membranes and do not address the fluid properties of plasma membranes. Another approach is molecular dynamics, but it is necessarily restricted to very small time and space scales.

Hence, it seems that a global modeling taking into account this hybrid behavior of the plasma membrane is still lacking. So we have formulated a model of this original thin structure in the general framework of continuum mechanics, using a partly Lagrangian and partly Eulerian description. This allows for modeling both solid and fluid properties of the plasma membrane. On the one hand, the motion of the surface is described using a parametrized function. On the other hand, the behavior of the fluid particles inside the membrane is represented by their velocity and by the density at each point. The equations governing these 3 unknowns are conservation of mass, conservation of momentum and transport of the surface. As in shell theory, the stress tensor is decomposed into an in-plane term and a flexural term. Neglecting the latter, we obtained a first incompressible membrane model, similar to Navier-Stokes equations defined on a moving two-dimensional surface. For the numerical approximation we formulated a low-order mixed method. The implementation of this numerical method has been performed.

This first step allows a preliminary assessment of our modeling approach. The objective is now to successively add into the model some terms that were neglected in the first step: nonlinearities, construction of a flexural term in the constitutive law, etc.

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[8] 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 6.2 for the detailed results obtained by MACS in this framework.

7.2. International projects

7.2.1. Other long-term collaborations

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

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[9].

8.2. Teaching activities

- Dominique Chapelle: Master's course "Numerical analysis for cardiac mechanics" (joint Paris 6 and Polytechnique M2 program).
- Grégoire Derveaux:
  - Course "*Scientific Computing: hyperbolic equations*" at ENSTA, June 2007;
  - Course "*Scientific Computing: finite element method*" at ENSTA, Fall 2007.
- Philippe Moireau: course "Introduction to the discretization of PDEs", at ENSTA.

8.3. Participation in conferences, workshops and seminars

Dominique Chapelle

- Speaker at FIMH'07 Conference, Salt Lake City, USA, June 2007.

Grégoire Derveaux

- Speaker at SMAI2007, Praz-sur-Arly, France, June 2007.
- Speaker at the "9th US National Congress on Computational Mechanics", San Francisco, USA, July 2007.

[8] http://www-sop.inria.fr/CardioSense3D/
[9] http://www.math-info.univ-paris5.fr/map5/-Seminaires

Philippe Moireau

- Participant at FIMH'07 Conference, Salt Lake City, USA, June 2007.

Marina Vidrascu

- Seminar at Univ. Montpellier, March 22nd
- Speaker at the "9th US National Congress On Computational Mechanics", San Francisco, July 23–26
- Speaker at the "Journée en l'honneur d'Alain Perronnet", Paris 6, November 5th
- Participant in "Journées nationales des ARCs 2007" (Rennes, October 1–2).

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Year Publications

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Miscellaneous

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