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

2005

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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.

[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.

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.

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: 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).

5.3. MITCNL

Participants: Dominique Chapelle [correspondant], Marina Vidrascu.

[2] CardioSense3D
[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.

5.4. Heart simulation package

Participants: 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 post-processing, ease of interfacing with other software (such as for simulating action potential propagation) and provides some very efficient solvers (e.g. Pardiso, UMFPACK).

6. New Results

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

Keywords: *MITC elements, numerical reliability*.

Participants: Dominique Chapelle, Iria Paris, Marina Vidrascu.

This year's effort was focused on investigating the reliability of *triangular* shell elements, which are of key importance in applications, where complex geometries are frequently to be meshed. Indeed, whereas reasonably reliable quadrilateral shell elements (the MITC4 and MITC9 elements, in particular) are available [1], the robustness of triangular elements is still an open problem.

We have assessed the reliability of existing schemes using previously introduced test problems, and we have also designed a new numerical test in order to specifically investigate the impact of MITC procedures on the membrane stiffness of shell elements – a crucial issue as regards their robustness. These tests have shown that a uniformly optimal 6-node MITC isotropic triangular shell finite element is extremely difficult to attain because:

- either numerical locking occurs for bending dominated shell problems when a consistent behaviour is ensured for membrane dominated situations;
- or spurious membrane energy modes are introduced by the mixed formulation.

From now on, we extend our investigations to formulations other than MITC strategies, in particular to mixed *enhanced* procedures.

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.

Prevously, on the structure side, there was a limitation in the size of the problems that could be solved, due to the use of a direct solver [3]. This restriction was lifted this year by introducing a domain decomposition method instead of the direct solver. We use a balanced Neumann-Neumann domain decomposition preconditioner [14]. To effectively use such a preconditioner for fluid-structure interaction problems it is necessary to adapt it as suggested below :

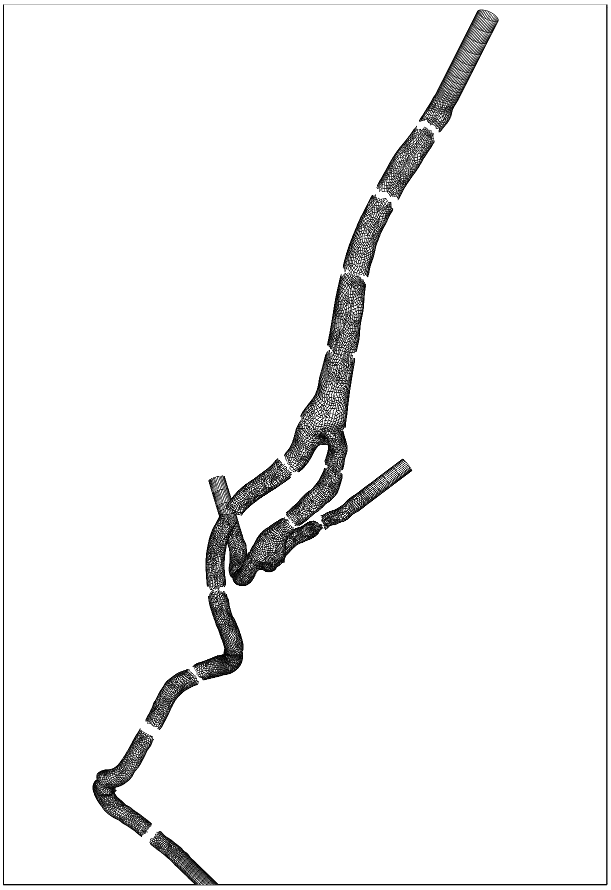

Figure 1. Decomposition of the structure mesh of a realistic carotide

Construction of the coarse space. To build a coarse space we need the degrees of freedom which define rigid modes. We follow M. Barboteu's suggestion [15] and use for all time steps the same degrees of freedom, those of the first tangent stiffness matrix.

Newton-Krylov preconditioner for the fluid-structure interface problem. If a domain decomposition method is used for the structure the solution of the preconditioning step becomes more complicated than for a mono-domain. Indeed, now the factorized stiffness matrix is not available. To avoid increasing the cost of the preconditioning solution we use specific techniques for the solution of iterative problems with multiple right-hand sides based mainly on the use of an optimal startup solution obtained by the projection of the interface problem on the Krylov space associated with previous right-hand sides.

This new algorithm makes possible the solution of problems with a mesh such as the one in figure 1 which was previously out of reach. In addition, there is a spectacular gain in CPU time because the actual implementation of the domain decomposition algorithm takes advantage of the inherent parallelism of the method.

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.

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

Using our heart simulation code (see Section 5.4), we have simulated the electromechanical behavior of the heart for healthy and pathological cases. For healthy cases we calibrated the model using clinical data related to pressure and volume in the ventricles, as well as aortic and mitral flows. We also investigated the ability of our model to represent pathological behaviors like systolic dysfunction as occurs following myocardial infarction or troubles of the electrical propagation (e.g. left bundle branch block). The preliminary results have been confronted with clinical data and presented to cardiologists collaborating in CardioSense3D, and these results indicate good predictive capabilities.

We also worked on elaborating a "methodological chain" to generate a geometrical model compatible with actual anatomical data of the human heart as available in medical imaging see [8]. This is required in order to construct "patient-specific" models, which is needed for diagnosis purposes.

Using the electro-mechanical heart model, our other major objective is to develop robust "data-model coupling algorithms". This approach aims at achieving good estimation of the behaviour and the 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, starting from August, is dedicated to the research on robust and low-cost state filters inspired from engineering and their extensions to combined state-parameter estimation procedures. At this time, we have focused on simplified 1D problems in order to narrow down our strategy. Our main researches concerned the study of collocalised state filtering, its justification in non-linear problems and extension to parameter estimation using in particular the approach of [16].

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 on an aircraft or some other structure whose integrity we want to monitor. In addition

[4] team REO
[5] team REO

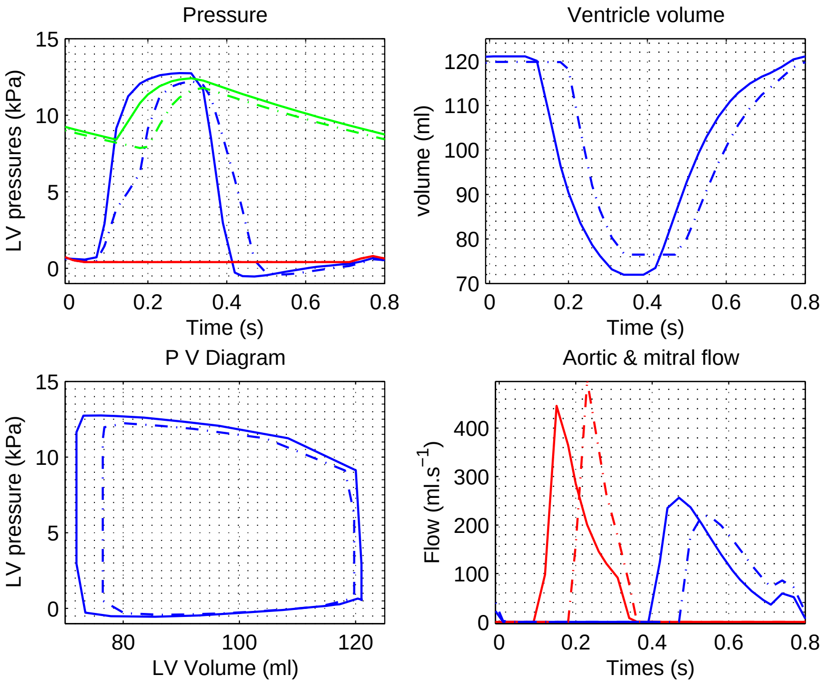

Figure 2. Clinical indicators for regular (solid line) and pathologic (dashed line) case

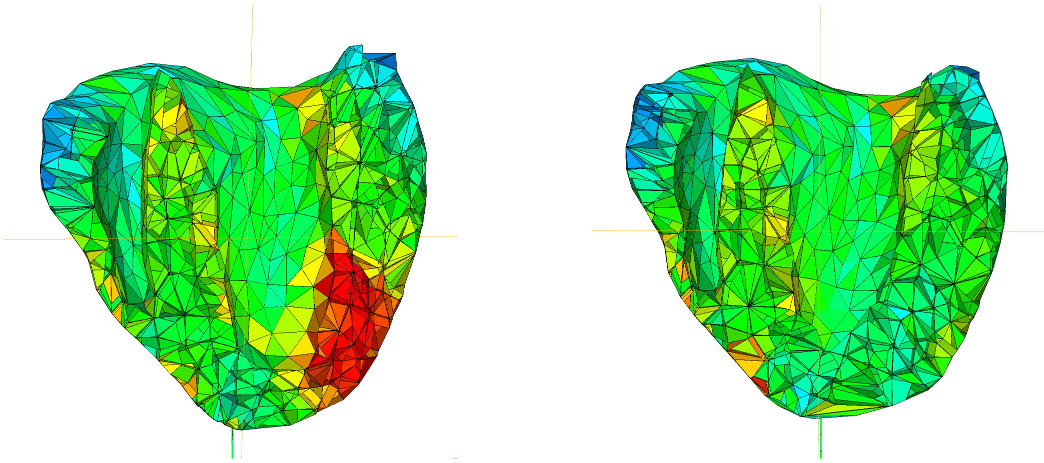

Figure 3. Strains along fibers for a systolic dysfunction (left) and normal cardiac function (right)

to locating the damage we also want to estimate its size and shape, if possible. One of the difficulties of the problem is that the measured signals do not provide clear arrival times, because of the complexity of the environnment. We have been working on a robust and stable imaging technique based on the ability of time reversal to take advantage of the multipathing (*ie.* the multiple scattering of the waves in the medium) [11], [7]. 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.

We are currently working on the optimization of the waveform, *ie.* the design of the probing signal that is used by each sensor to illuminate the medium. We are also investigating some strategies for the sensor deployment, based on the (partial) knowledge of the structure.

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. The role of the plasma membrane is to provide a semi-permeable boundary to the cell, whose shape can be easily remodeled. The recent development of nanotechnologies, as for instance the Atomic Force Microscope, allows for investigating the mechanichal behaviour at the scale of one cell. Therefore, there is a growing need for accurate models of those structural components. To begin with, we are interested in the modeling of the membrane for which existing models are scarce and very limited. On the one hand, there exist mechanical models representing a local behavior, typically described with one “stiffness parameter”. On the other hand, numerical simulations are frequently performed based on a viscoelastic modeling of classical elastic membranes, which does not take into account the major specificities of cell membrane behaviour. We are currently working on the elaboration of a specific model of the plasma membrane, considered as a continuous medium that has both solid and fluid properties.

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 Epidaure, Macs, Reo and Sosso2, but other academic, industrial and clinical partners are closely associated to this action.

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;

[6] http://www-sop.inria.fr/CardioSense3D/
[7] http://www.irisa.fr/sisthem/index-fr.htm
[8] http://acisi.loria.fr/

- 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).

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");

8.2. Teaching activities

- Grégoire Derveaux :
  - Course: *The scalar wave equation: mathematical analysis and numerical resolution*, at Ecole National Supérieur des Techniques Avancées (ENSTA), Fall 2005.
  - Course: *Scientific Computing*, at ENSTA, Fall 2005.
- Marina Vidrascu : Course "*Mathematical fundamentals of the finite element method*" at Ecole Supérieure d'Ingénierie Léonard de Vinci.

[9] http://www.esiee.fr/smart-systems/index.php
[10] http://www.esiee.fr/en/index.php

8.3. Participation in conferences, workshops and seminars

Dominique Chapelle

- Invited plenary speaker at: 2nd Symposium on Modelling of Physiological Flows (Lisbon), Third MIT Conference on Comput. Mechanics, Workshop on Thin Structures (Naples);
- Organizer of FreeFEM-OpenFEM day (23 sept., with G. Allaire) at IHP, Paris;
- Seminars at Ecole Polytechnique (27 May) and Imati (Pavia, Italy, 28 and 30 June);
- Expert for EDF prospective ("Défi Simul2010") and evaluation (group SINETICS/I23).

Grégoire Derveaux

- "8th Annual Landmine Basic Research Technical Review Meeting and Workshop", Springfield, Viginia (Jan. 12-13 2005)
- "ARO-MURI Workshop on "Adaptive Sensing and Waveform Design", Atlanta, Georgia (Aug. 2-3 2005)
- "CIRM Workshop on Radiative transport and diffusion-approximation: From theory to applications", CIRM, Marseille. (Sept. 5-9 2005)
- "5th International Workshop on Structural Health Monitoring", Stanford University, California. (Sept. 12-14 2005)

Philippe Moireau

- "Functional Imaging and Modeling of the Heart FIMH 2005", Barcelona June 2-4, 2005
- Speaker at the "Third M.I.T. Conference on Computationnal Fluid and Solid Mechanics". June 14-17, 2005.

Iria Paris

- Mid-term review European Network HPRN-CT-2002-00284, Lisbon, 21-22 July 2005
- Speaker at the "Workshop on Smart Systems" (Network HPRN-CT-2002-00284: *New Materials, Adaptive Systems and Their Nonlinearities. Modelling, Control and Numerical Simulation*.), Berlin, 10-12th October 2005

Marina Vidrascu

- Speaker at the "16th International Conference on Domain Decomposition Methods", New York, January 2005
- Invited speaker at "8th Workshop on Biomaterials and Biomechanics: Fundamentals and Clinical Applications", Essen, September 2005

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Miscellaneous

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