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Project-Team MC2

Modeling, control and computations

IN COLLABORATION WITH: Institut de Mathématiques de Bordeaux (IMB)

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THEME
Computational models and simulation

Table of contents

Project-Team MC2

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Creation of the Project-Team: July 01, 2007 .

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2. Overall Objectives

2.1. Presentation

The aim of this project is to develop modelling tools for problems involving fluid mechanics in order to explain, to control, to simulate and possibly to predict some complex phenomena coming from physics, chemistry, biology or scientific engineering. The complexity may consist of the model itself, of the coupling phenomena, of the geometry or of non-standard applications. The challenges of the scientific team are to develop stable models and efficient adapted numerical methods in order to recover the main physical features of the considered phenomena. The models will be implemented into numerical codes for practical and industrial applications.
We are interested in both high and low Reynolds number flows, interface and control problems in physics and biology.

Our scientific approach may be described as follows. We first determine some reliable models and then we perform a mathematical analysis (including stability). We then develop the efficient numerical methods, which are implemented for specific applications.

In the next paragraphs, we explain our main goals, we describe our project in terms of development of numerical techniques and we present the team with the competence of the members.

2.1.1. The main goals

2.1.1.1. Modelling

The first goal of the project consists in modelling some complex phenomena. We combine the term model with the three following adjectives: phenomenological, asymptotical and numerical.
Phenomenological : use of ad-hoc models in order to represent some precise phenomena. One example of such modelling process is the construction of nonlinear differential laws for the stress tensor of visco-elastic fluids or for wormlike micelles. Another example is the wall law conditions in microfluidics (fluids in micro-channels) that are often taken heuristically in order to model the slip at the boundary.
In biology, since no fundamental laws are known, the modeling is exclusively phenomenological especially concerning the modeling of tumor growth.
Asymptotical : using asymptotic expansions, we derive simpler models containing all the relevant phenomena. Examples of such a process are the penalization method for the simulation of incompressible flows with obstacles or the analysis of riblets in microfluidics that are used to control the mixing of the fluids. Another example is the use of shallow fluid models in order to obtain fast predictions (Hele-Shaw approximation in microfluidics) or the approximation of thin membranes for the modeling of electroporation of cells.
Numerical : direct numerical tools are used to simulate the modelized physical phenomena. A precise analysis of the models is performed to find out the most convenient numerical method in terms of stability, accuracy and efficiency. A typical example is the POD (proper orthogonal decomposition) and its use in control theory, or in data assimilation in tumor growth, to obtain fast simulations.

2.1.1.2. Analysis and computation

Once the model has been determined, we perform its mathematical analysis. This analysis includes the effect of boundary conditions (slip conditions in microfluidics, conditions at an interface...) as well as stability issues (stability of a jet, of an interface, of coherent structures). The analysis can often be performed on a reduced model. This is the case for an interface between two inviscid fluids that can be described by a Boussinesq-type system. This analysis of the system clearly determines the numerical methods that will be used. Finally, we implement the numerical method in a realistic framework and provide a feedback to our different partners.

2.1.1.3. Applications

Our methods are used in four areas of **applications**.
1)*Interface problems and complex fluids*:

This concerns microfluidics, complex fluids (bifluid flows, miscible fluids). The challenges are to obtain reliable models that can be used by our partner Rhodia (for microfluidics).
2)*High Reynolds flows and their analysis*:
We want to develop numerical methods in order to address the complexity of high Reynolds flows. The challenges are to find scale factors for turbulent flow cascades, and to develop modern and reliable methods for computing flows in aeronautics in a realistic configuration.
3) *Control and optimization*: the challenges are the drag reduction of a ground vehicle in order to decrease the fuel consummation, the reduction of turbomachinery noise emissions or the increase of lift-to-drag ratio in airplanes, the control of flow instabilities to alleviate material fatigue for pipe lines or off-shore platforms and the detection of embedded defects in materials with industrial and medical applications.
4) *Tumor growth*: The challenge is to produce patient-specific simulations starting from medical imaging for growth of metastasis to the lung of a distant tumor.
Our main partners on this project will be :
Industrial: Renault, IFP, CIRA (Centro italiano ricerche aerospaziali), Airbus France and Boeing for high Reynolds flows, optimization and control and Rhodia (biggest french company of chemistry) for interface problems and complex fluids.
Academic: CPMOH (Laboratory of Physics, Bordeaux 1 University) for high Reynolds flows, optimization and control, and Institut Gustave Roussy (Villejuif), University of Alabama at Birmingham and Institut Bergonié (Bordeaux) for tumor growth, optimad (spin-of of the Politecnico de Torino) for simulations of complex flows.

2.1.2. The production of numerical codes

We want to handle the whole process from the modelling part until the simulations. One of the key points is to develop numerical codes in order to simulate the models that are studied with our partners and of course we want to be able to have some feed-back toward the experiments.
i)*Multi-fluid flows and interface problems:*
We perform 2D and 3D simulations of multi-fluid flows using level set methods and mixture models. This includes non newtonian flows such as foams or wormlike miscella. The applications are microfluidics, porous media and complex fluids.
ii) *Modeling of tumor growth:*
Tumor growth in our 3D numerical model includes a cell-cycle, diffusion of oxygen, several population of cells, several enzymes, molecular pathways, angiogenesis, extracellular matrices, non-newtonian effects, membrane, effects of treatments, haptotaxy, acidity. We perform data assimilation processes starting from medical imaging.
iii) *2D and 3D simulations at high Reynolds number:*
We develop various computational methods: multi-grid techniques, vortex methods. The possible applications are turbulence, the flow around a vehicle, the stress on a pipe-line (the penalization method is used in order to take into account the obstacles).
iv) *Fluid structure interactions:*
2D and 3D interaction of a mobile rigid body with a fluid thanks penalty methods.

From a technical point of view, our work is organized as follows. We have build a platform (called **eLYSe**) using only cartesian, regular meshes. This is motivated by the following: we want to address interface problems using level set methods and to take into account obstacles by the penalization method. For these interface problems, we will have to compute the curvature of the interface with high precision (in microfluidics, the surface tension is the leading order phenomenon). The level set technology is now very accurate on structured meshes, we therefore made this choice. However, we want to address cases with complex geometry and/or obstacles. We will therefore systematically use the penalization method. The idea is to have an uniform format for the whole team that consists of several boxes:
1) Definition of the geometry and of the penalization zones.
2) Specification of the model (bifluid or not, Newtonian or not, mixing or not, presence of membranes etc...)
3) The boundary conditions that have to be imposed by a penalization operator.
4) The solvers.

5) Graphic interface.
As said before, the interface problems and the interaction with a membrane will be handled by level set methods as well as the shape optimization problem. So this platform will be dedicated to direct numerical simulation as well as to shape optimization and control.

The main effort concerning modelling will concern points 2) and 3) (model and boundary conditions). We do not plan for the moment to make special research effort on the solver part and we will use the solvers available in the literature or already developed by the team.

This platform will have two roles: the first one will be to allow a comprehensive treatment for the simulation of complex fluids with interface, membranes, adapted to the world of physical-chemistry and microfluidics and for solving shape optimization problems. The second role will be to keep a set of numerical modules that will be devoted to more specific applications (for example multi-grid methods or vortex methods for the study of turbulence). We therefore need to have some unified standards for the geometry or the graphic interface but it is of course hopeless to consider 3D turbulence and low-Reynolds flows in a micro-channel with the same code !

3. Scientific Foundations

3.1. Introduction

We are mainly concerned with complex fluid mechanics problems. The complexity consists of the rheological nature of the fluids (non newtonian fluids), of the coupling phenomena (in shape optimization problems), of the geometry (micro-channels) or of multi-scale phenomena arising in turbulence or in tumor growth modeling. Our goal is to understand these phenomena and to simulate and/or to control them. The subject is wide and we will restrict ourselves to three directions: the first one consists in studying low Reynolds number interface problems in multi-fluid flows with applications to complex fluids, microfluidics and biology - the second one deals with numerical simulation of Newtonian fluid flows with emphasis on the coupling of methods to obtain fast solvers.

Even if we deal with several kinds of applications, there is a strong scientific core at each level of our project. Concerning the model, we are mainly concerned with incompressible flows and we work with the classical description of incompressible fluid dynamics. For the numerical methods, we use the penalization method to describe the obstacles or the boundary conditions for high Reynolds flows, for shape optimization, for interface problems in biology or in microfluidics. This allows us to use only cartesian meshes. Moreover, we use the level-set method for interface problems, for shape optimization and for fluid structure interaction. Finally, for the implementation, strong interaction exists between the members of the team and the modules of the numerical codes are used by all the team and we want to build the platform **eLYSe** to systematize this approach.

3.2. Multi-fluid flows and application for complex fluids, microfluidics

Participants: Angelo Iollo, Charles-Henri Bruneau, Thierry Colin, Mathieu Colin, Kévin Santugini.

Multi-fluid flows,microfluidics

By a complex fluid, we mean a fluid containing some mesoscopic objects, *i.e.* structures whose size is intermediate between the microscopic size and the macroscopic size of the experiment. The aim is to study complex fluids containing surfactants in large quantities. It modifies the viscosity properties of the fluids and surface-tension phenomena can become predominant.

Microfluidics is the study of fluids in very small quantities, in micro-channels (a micro-channel is typically 1 cm long with a section of $50\mu m \times 50\mu m$). They are many advantages of using such channels. First, one needs only a small quantity of liquid to analyze the phenomena. Furthermore, very stable flows and quite unusual regimes may be observed, which enables to perfom more accurate measurements. The idea is to couple numerical simulations with experiments to understand the phenomena, to predict the flows and compute some quantities like viscosity coefficients for example. Flows in micro-channels are often at low Reynolds numbers. The hydrodynamical part is therefore stable. However, the main problem is to produce real 3D simulations covering a large range of situations. For example we want to describe diphasic flows with surface tension and sometimes surface viscosity. Surface tension enforces the stability of the flow. The size of the channel implies that one can observe some very stable phenomena. For example, using a "T" junction, a very stable interface between two fluids can be observed. In a cross junction, one can also have formation of droplets that travel along the channel. Some numerical difficulties arise from the surface tension term. With an explicit discretization of this term, a restrictive stability condition appears for very slow flows [71]. Our partner is the LOF, a Rhodia-Bordeaux 1-CNRS laboratory.
One of the main points is the wetting phenomena at the boundary. Note that the boundary conditions are fundamental for the description of the flow since the channels are very shallow. The wetting properties cannot be neglected at all. Indeed, for the case of a two non-miscible fluids system, if one considers no-slip boundary conditions, then since the interface is driven by the velocity of the fluids, it shall not move on the boundary. The experiments shows that this is not true: the interface is moving and in fact all the dynamics start from the boundary and then propagate in the whole volume of fluids. Even with low Reynolds numbers, the wetting effects can induce instabilities and are responsible of hardly predictable flows. Moreover, the fluids that are used are often visco-elastic and exhibit "unusual" slip length. Therefore, we cannot use standard numerical codes and have to adapt the usual numerical methods to our case to take into account the specificities of our situations. Moreover, we want to obtain reliable models and simulations that can be as simple as possible and that can be used by our collaborators. As a summary, the main specific points of the physics are: the multi-fluid simulations at low Reynolds number, the wetting problems and the surface tension that are crucial, the 3D characteristic of the flows, the boundary conditions that are fundamental due to the size of the channels. We need to handle complex fluids. Our collaborators in this lab are J.-B. Salmon, P. Guillot, A. Colin.

The evolution of non-newtonian flows in webs of micro-channels are therefore useful to understand the mixing of oil, water and polymer for enhanced oil recovery for example. Complex fluids arising in cosmetics are also of interest. We also need to handle mixing processes.

3.3. Cancer modeling

Participants: Angelo Iollo, Thierry Colin, Clair Poignard, Olivier Saut, Lisl Weynans.

Tumor growth, cancer, metastasis

As in microfluidics, the growth of a tumor is a low Reynolds number flow. Several kinds of interfaces are present (membranes, several populations of cells,...) The biological nature of the tissues impose the use of different models in order to describe the evolution of tumor growth. The complexity of the geometry, of the rheological properties and the coupling with multi-scale phenomena is high but not far away from those encountered in microfluidics and the models and methods are close.

The challenge is twofold. On one hand, we wish to understand the complexity of the coupling effects between the different levels (cellular, genetic, organs, membranes, molecular). Trying to be exhaustive is of course hopeless, however it is possible numerically to isolate some parts of the evolution in order to better understand the interactions. Another strategy is to test *in silico* some therapeutic innovations. An example of such a test is given in [81] where the efficacy of radiotherapy is studied and in [82] where the effects of anti-invasive agents is investigated. It is therefore useful to model a tumor growth at several stage of evolution. The macroscopic continuous model is based on Darcy's law which seems to be a good approximation to describe the flow of the tumor cells in the extra-cellular matrix [50], [72], [73]. It is therefore possible to develop a two-dimensional model for the evolution of the cell densities. We formulate mathematically the evolution of the cell densities in the tissue as advection equations for a set of unknowns representing the density of cells with position (x, y)

at time t in a given cycle phase. Assuming that all cells move with the same velocity given by Darcy's law and applying the principle of mass balance, one obtains the advection equations with a source term given by a cellular automaton. We assume diffusion for the oxygen and the diffusion constant depends on the density of the cells. The source of oxygen corresponds to the spatial location of blood vessels. The available quantities of oxygen interact with the proliferation rate given by the cellular automaton [81].

A forthcoming investigation in cancer treatment simulation is the influence of the electrochemotherapy [76] on the tumor growth. Electrochemotherapy consists in imposing to the malignant tumor high voltage electric pulses so that the plasma membrane of carcinoma cells is permeabilized. Biologically active molecules such as bleomycin, which usually cannot diffuse through the membrane, may then be internalized. A work in progress (C.Poignard [80] in collaboration with the CNRS lab of physical vectorology at the Institut Gustave Roussy) consists in modelling electromagnetic phenomena at the cell scale. A coupling between the microscopic description of the electroporation of cells and its influence on the global tumor growth at the macroscopic scale is expected. Another key point is the parametrization of the models in order to produce image-based simulations.

The second challenge is more ambitious. Mathematical models of cancer have been extensively developed with the aim of understanding and predicting tumor growth and the effects of treatments. In vivo modeling of tumors is limited by the amount of information available. However, in the last few years there have been dramatic increases in the range and quality of information available from non-invasive imaging methods, so that several potentially valuable imaging measurements are now available to quantitatively measure tumor growth, assess tumor status as well as anatomical or functional details. Using different methods such as the CT scan, magnetic resonance imaging (MRI), or positron emission tomography (PET), it is now possible to evaluate and define tumor status at different levels: physiological, molecular and cellular.

In this context, the present project aims at supporting the decision process of oncologists in the definition of therapeutic protocols via quantitative methods. The idea is to build mathematically and physically sound phenomenological models that can lead to patient-specific full-scale simulations, starting from data collected typically through medical imagery like CT scans, MRIs and PET scans or by quantitative molecular biology for leukemia. Our ambition is to provide medical doctors with patient-specific tumor growth models able to estimate, on the basis of previously collected data and within the limits of phenomenological models, the evolution at subsequent times of the pathology and possibly the response to the therapies.

The final goal is to provide numerical tools in order to help to answer to the crucial questions for a clinician:
When to start a treatment?
When to change a treatment?
When to stop a treatment?
Also we intend to incorporate real-time model information for improving the precision and effectiveness of non-invasive or micro-invasive tumor ablation techniques like acoustic hyperthermia, electroporation, radiofrequency or cryo-ablation.

We will specifically focus on the following pathologies: Lung and liver metastasis of a distant tumor
Low grade and high grade gliomas, meningiomas
Chronic myelogenous leukemia
These pathologies have been chosen because of the existing collaborations between the applied mathematics department of University of Bordeaux and the Institut Bergonié.

Our approach. Our approach is deterministic and spatial: it is based on solving an inverse problem based on imaging data. Models are of partial differential equation (PDE) type. They are coupled with a process of data assimilation based on imaging. We already have undertaken test cases on patients that are followed at Bergonié for lung metastases of thyroid tumors. These patients have a slowly evolving, asymptomatic metastatic disease, monitored by CT scans. On two thoracic images relative to successive times, the volume of the tumor under investigation is extracted by segmentation. To test our method, we chose patients without treatment and for whom we had at least three successive.

3.4. Newtonian fluid flows simulations and their analysis

Participants: Charles-Henri Bruneau, Angelo Iollo, Iraj Mortazavi, Michel Bergmann, Lisl Weynans.

Simulation, Analysis

It is very exciting to model complex phenomena for high Reynolds flows and to develop methods to compute the corresponding approximate solutions, however a well-understanding of the phenomena is necessary. Classical graphic tools give us the possibility to visualize some aspects of the solution at a given time and to even see in some way their evolution. Nevertheless in many situations it is not sufficient to understand the mechanisms that create such a behavior or to find the real properties of the flow. It is then necessary to carefully analyze the flow, for instance the vortex dynamics or to identify the coherent structures to better understand their impact on the whole flow behavior.

The various numerical methods used or developed to approximate the flows depend on the studied phenomenon. Our goal is to compute the most reliable method for each situation.

The first method, which is affordable in 2D, consists in a directly solving of the genuine Navier-Stokes equations in primitive variables (velocity-pressure) on Cartesian domains [59]. The bodies, around which the flow has to be computed are modeled using the penalization method (also named Brinkman-Navier-Stokes equations). This is an immersed boundary method in which the bodies are considered as porous media with a very small intrinsic permeability [51]. This method is very easy to handle as it consists only in adding a mass term U/K in the momentum equations. The boundary conditions imposed on artificial boundaries of the computational domains avoid any reflections when vortices cross the boundary. To make the approximation efficient enough in terms of CPU time, a multi-grid solver with a cell by cell Gauss-Seidel smoother is used.

The second type of methods is the vortex method. It is a Lagrangian technique that has been proposed as an alternative to more conventional grid-based methods. Its main feature is that the inertial nonlinear term in the flow equations is implicitly accounted for by the transport of particles. The method thus avoids to a large extent the classical stability/accuracy dilemma of finite-difference or finite-volume methods. This has been demonstrated in the context of computations for high Reynolds number laminar flows and for turbulent flows at moderate Reynolds numbers [66]. This method has recently enabled us to obtain new results concerning the three-dimensional dynamics of cylinder wakes.

The third method is to develop reduced order models (ROM) based on a Proper Orthogonal Decomposition (POD) [74]. The POD consists in approximating a given flow field $U(x,t)$ with the decomposition

$$U(x,t) = \sum_i a_i(t)\phi_i(x),$$

where the basis functions are empirical in the sense that they derive from an existing data base given for instance by one of the methods above. Then the approximation of Navier-Stokes equations for instance is reduced to solving a low-order dynamical system that is very cheap in terms of CPU time. Nevertheless the ROM can only restitute what is contained in the basis. Our challenge is to extend its application in order to make it an actual prediction tool.

The fourth method is a finite volume method on cartesian grids to simulate compressible Euler or Navier Stokes Flows in complex domains. An immersed boundary-like technique is developed to take into account boundary conditions around the obstacles with order two accuracy.

3.5. Flow control and shape optimization

Participants: Charles-Henri Bruneau, Angelo Iollo, Iraj Mortazavi, Michel Bergmann.

Flow Control, Shape Optimization

Flow simulations, optimal design and flow control have been developed these last years in order to solve real industrial problems : vortex trapping cavities with CIRA (Centro Italiano Ricerche Aerospaziali), reduction of vortex induced vibrations on deep sea riser pipes with IFP (Institut Français du Pétrole), drag reduction of a ground vehicle with Renault or in-flight icing with Bombardier and Pratt-Wittney are some examples of possible applications of these researches. Presently the recent creation of the competitiveness cluster on aeronautics, space and embedded systems (AESE) based also in Aquitaine provides the ideal environment to extend our applied researches to the local industrial context. There are two main streams: the first need is to produce direct numerical simulations, the second one is to establish reliable optimization procedures.
In the next subsections we will detail the tools we will base our work on, they can be divided into three points: to find the appropriate devices or actions to control the flow; to determine an effective system identification technique based on the trace of the solution on the boundary; to apply shape optimization and system identification tools to the solution of inverse problems found in object imaging and turbomachinery.

3.5.1. Control of flows

There are mainly two approaches: passive (using passive devices on some specific parts that modify the shear forces) or active (adding locally some energy to change the flow) control.

The passive control consists mainly in adding geometrical devices to modify the flow. One idea is to put a porous material between some parts of an obstacle and the flow in order to modify the shear forces in the boundary layer. This approach may pose remarkable difficulties in terms of numerical simulation since it would be necessary, a priori, to solve two models: one for the fluid, one for the porous medium. However, by using the penalization method it becomes a feasible task [55]. This approach has been now used in several contexts and in particular in the frame of a collaboration with IFP to reduce vortex induced vibrations [56]. Another technique we are interested in is to inject minimal amounts of polymers into hydrodynamic flows in order to stabilize the mechanisms which enhance hydrodynamic drag.

The active approach is addressed to conceive, implement and test automatic flow control and optimization aiming mainly at two applications : the control of unsteadiness and the control and optimization of coupled systems. Implementation of such ideas relies on several tools. The common challenges are infinite dimensional systems, Dirichlet boundary control, nonlinear tracking control, nonlinear partial state observation.

The bottom-line to obtain industrially relevant control devices is the energy budget. The energy required by the actuators should be less than the energy savings resulting from the control application. In this sense our research team has gained a certain experience in testing several control strategies with a doctoral thesis (E. Creusé) devoted to increasing the lift on a dihedral plane. Indeed the extension of these techniques to real world problems may reveal itself very delicate and special care will be devoted to implement numerical methods which permit on-line computing of actual practical applications. For instance the method can be successful to reduce the drag forces around a ground vehicle and a coupling with passive control is under consideration to improve the efficiency of each control strategy.

3.5.2. System identification

We remark that the problem of deriving an accurate estimation of the velocity field in an unsteady complex flow, starting from a limited number of measurements, is of great importance in many engineering applications. For instance, in the design of a feedback control, a knowledge of the velocity field is a fundamental element in deciding the appropriate actuator reaction to different flow conditions. In other applications it may be necessary or advisable to monitor the flow conditions in regions of space which are difficult to access or where probes cannot be fitted without causing interference problems.

The idea is to exploit ideas similar to those at the basis of the Kalman filter. The starting point is again a Galerkin representation of the velocity field in terms of empirical eigenfunctions. For a given flow, the POD modes can be computed once and for all based on Direct Numerical Simulation (DNS) or on highly resolved experimental velocity fields, such as those obtained by particle image velocimetry. An instantaneous velocity field can thus be reconstructed by estimating the coefficients $a_i(t)$ of its Galerkin representation. One simple approach to estimate the POD coefficients is to approximate the flow measurements in a least square sense, as in [70].

A similar procedure is also used in the estimation based on gappy POD, see [85] and [89]. However, these approaches encounter difficulties in giving accurate estimations when three-dimensional flows with complicated unsteady patterns are considered, or when a very limited number of sensors is available. Under these conditions, for instance, the least squares approach cited above (LSQ) rapidly becomes ill-conditioned. This simply reflects the fact that more and more different flow configurations correspond to the same set of measurements.

Our challenge is to propose an approach that combines a linear estimation of the coefficients $a_i(t)$ with an appropriate non-linear low-dimensional flow model, that can be readily implemented for real time applications.

3.5.3. Shape optimization and system identification tools applied to inverse problems found in object imaging and turbomachinery

We will consider two different objectives. The first is strictly linked to the level set methods that are developed for microfluidics. The main idea is to combine different technologies that are developed with our team: penalization methods, level sets, an optimization method that regardless of the model equation will be able to solve inverse or optimization problems in 2D or 3D. For this we have started a project that is detailed in the research program. See also [62] for a preliminary application.

As for shape optimization in aeronautics, the aeroacoustic optimization problem of propeller blades is addressed by means of an inverse problem and its adjoint equations. This problem is divided into three subtasks:

i) formulation of an inverse problem for the design of propeller blades and determination of the design parameters ii) derivation of an aeroacoustic model able to predict noise levels once the blade geometry and the flow field are given iii) development of an optimization procedure in order to minimize the noise emission by controlling the design parameters.

The main challenge in this field is to move from simplified models [75] to actual 3D model. The spirit is to complete the design performed with a simplified tool with a fully three dimensional inverse problem where the load distribution as well as the geometry of the leading edge are those provided by the meridional plane analysis [84]. A 3D code will be based on the compressible Euler equations and an immersed boundary technique over a cartesian mesh. The code will be implicit and parallel, in the same spirit as what was done for the meridional plane. Further development include the extension of the 3D immersed boundary approach to time-dependent phenomena. This step will allow the designer to take into account noise sources that are typical of internal flows. The task will consist in including time dependent forcing on the inlet and/or outlet boundary under the form of Fourier modes and in computing the linearized response of the system. The optimization will then be based on a direct approach, i.e., an approach where the control is the geometry of the boundary. The computation of the gradient is performed by an adjoint method, which will be a simple "byproduct" of the implicit solver. The load distribution as well as the leading edge geometry obtained by the meridional plane approach will be considered as constraints of the optimization, by projection of the gradient on the constraint tangent plane. These challenges will be undertaken in collaboration with Politecnico di Torino and EC Lyon.

4. Application Domains

4.1. Introduction

We now present our contribution to these above challenges concerning interface problem for complex fluids, direct simulations and analysis, flow control and optimization. From the technical point of view, many productions are common to the different parts of the project. For example, level-set methods, fast-marching procedure are used for shape optimization and for microfluidics, penalization methods are used for high Reynolds flows and for tumor growth. This leads to a strong politic of development of numerical modules.

4.2. Multi-fluid flows

- computation of bifluid flows : see the thesis of S. Tancogne ([83]) and P. Vigneaux ([86]). Stability of an interface, shape of droplets, formation of a jet. Study of the Plateau-Rayleigh instability. Behaviour of diphasic fluids evolving in square microchannels.
- mixing in micro-channel : see the thesis of J. Dambrine [67]. Passive mixing strategies involving boundary conditions. Enhanced oil recovery (study of mixing oil-water-polymer in a microchannel).
- emulsions and foam : see the thesis of S. Benito [52]. Applications in biology : behaviour of tissues, of tumor,....
- polymer nanotube conglomerate wire : it was the subject of a talk in the following conference "WCCM8-ECCOMAS2008" and of the talk [65].

4.3. Cancer modeling

- specific models : investigation of two particular cancer : gliomas (brain tumors), colorectal cancers lung and lever metastasis, brest cancer. This is one part of the PhD works of J.B. Lagaert and D. Lombardi.
- modelling of electrochemotherapy : see ARC C3MB (http://www.math.u-bordeaux1.fr/ArcC3MB/)
- parameter estimations with the help of low order models : see the PhD of J.B. Lagaert and D. Lombardi
- patient-specific simulations
- optimal shape design : the goal is to recover the vascularization of a model tumor from the knowledge of its shape evolution.

4.4. Newtonian fluid flows simulations and their analysis

- simulation of a synthetic or pulsed jet. This is an ongoing project with Renault and PSA inside a PREDIT project.
- vortex dynamics : see [69].
- simulation of compressible flows on cartesian grids : see the thesis of Gabriele Ottino's Thesis [79], who underwent his doctoral studies in conjunction in the MC2 team and at the Politecnico di Torino, and defended in April 2009. He had a grant of the French-Italian university.
- 3D turbulent flows through DESGRIVRE contract with AIRBUS. Thesis of C. Wervaecke [88]. The goal is to use Detached-Eddy Simulation to model turbulent flows around iced bodies.
- porous media : Numerical study of coupling between Richards and transport-diffusion equations in permeable sediment affected by tidal oscillation. See the thesis of R. Chassagne [63]

4.5. Flow control and shape optimization

- passive control : the idea is to put a porous interface between the solid body and the fluid. See the D. Depeyras thesis [68] and Yong-Liang Xiang [90] and CH Bruneau and Iraj Mortazavi) [55]. See also project [60] founded by the Euopean Community.
- active control : see the three PhD thesis: M. Buffoni, J. Weller [87], E. Lombardi and FFAST project funded by EU and iled by the University of Bristol and AIRBUS UK.
- shape optimization for turbo-machines : See [84].
- reduced order models : it consists in designing a non-linear observer that estimates the state of the flow field from a limited number of measurements in the field. The challenge is to reduce as much as possible the information required and to take it from the boundary. See J. Weller [87] and E. Lombardi.
- passive control of flows with porous media : see [57], [54], [53], [78], [58].

- inverse problems in imagery : see [62].

5. Software

5.1. eLYSe

Participants: Olivier Saut [correspondant], Raphael Bahègne, Vincent Huber, Jean-Baptiste Lagaert, Mathieu Specklin.

eLYse is a numerical platform used for our computations in Biology (tumor growth), micro-fluidics and complex Newtonian fluid flows. The platform is divided in two libraries : one is devoted to the modelling equations and the other one includes the numerical solvers. For example, we are able to treat (in 2D and 3D) transport equations, diffusion equations, Navier-Stokes equations, Maxwell system and the interaction fluid-structure by level-set and penalization methods. The solvers are based on finite volume methods on cartesian grids and allow parallel computations. See also the web page http://www.math.u-bordeaux1.fr/~osaut/pages/eLYSe.html.

- Version: 0.4
- ACM: ACM J.2 J.3 G.1.8 G.1.10
- AMS: AMS65Z05 35Q92
- Keywords: Modélization and numerical simulations, Finite volume methods, Level Set approach, Penalization method
- APP: En cours
- Type of human computer interaction: console
- OS/Middelware: Platform developped on Mac OS X architecture.
- Required library or software: Petsc (http://www.mcs.anl.gov/petsc/petsc-as/)Vtk (http://www.vtk.org/)Blitz++ (http://c2.com/cgi/wiki?BlitzPlusPlus) (optionnel)Boost (http://www.boost.org/)
- Programming language: C++
- Documentation: doxygen.

5.2. Kesaco

Participants: Olivier Saut [correspondant], Raphael Bahègne, Damiano Lombardi, Mathieu Specklin.

Kesaco is a set of libraries and programs aiming at applications of mathematical modeling in clinical oncology. It features:

- A library of specialized mathematical model describing the growth of different types of cancers (secondary tumors in the lung, gliomas).
- A set of programs useful to validate mathematical models (compute the various behavior they can produce) and to build databases of numerical simulations.
- Segmentation and registration routines to use medical images directly in our numerical codes.
- Calibration methods to recover the parameters of the models using sequences of medical images. Three techniques are implemented (a genetic algorithm, a technique based on reduced order models, a sensitivity technique).

All these routines are adapted to run on a MP architecture. The webpage may be found at http://www.math.u-bordeaux1.fr/~osaut/pages/kesaco.html.

- Version: 0.1
- Keywords: Modélization and numerical simulations
- APP: En cours
- Type of human computer interaction: console
- OS/Middelware: Platform developped on Mac OS X architecture.
- Required library or software: eLYSe, Insight Toolkit (http://www.itk.org)
- Programming language: C++
- Documentation: doxygen.

5.3. NaSCar

Participant: Michel Bergmann [correspondant].

This code is devoted to solve 3D-flows in around moving and deformable bodies. The incompressible Navier-Stokes equations are solved on fixed grids, and the bodies are taken into account thanks to penalization and/or immersed boundary methods. The interface between the fluid and the bodies is tracked with a level set function or in a Lagrangian way. The numerical code is fully second order (time and space). The numerical method is based on projection schemes of Chorin-Temam's type. The code is written in C language and use Petsc (http://www.mcs.anl.gov/petsc/petsc-as/) library for the resolution of large linear systems in parallel.

NaSCar can be used to simulate both hydrodynamic bio-locomation as fish like swimming and aerodynamic flows such wake generated by a wind turbine.

- Version: 1
- Keywords: numerical analyse, fluid mechanics, langage C, PETSc
- Software benefit : simulate a flow around a deformable obstacle, moving into a fluid.
- APP: En cours
- Patent: non
- Type of human computer interaction: human for the moment
- OS/Middelware: unix, linux, mac os
- Required library or software: PETSc item Programming language: C
- Documentation: in progess

5.4. S-MPI-2D-3D

Participants: Charles-Henri Bruneau [correspondant], Khodor Khadra.

The software NS-MPI-2D-3D is a numerical platform devoted to the computation of the incompressible flow around bodies in two or three dimensions modelled by Stokes, Navier-Stokes or Oldroyd-B equations. It is based on finite differences or finite volumes approximations on cartesian grid using the volume penalization method to handle the obstacles. The resolution is achieved by means of the multigrid method. Dirichlet, periodic or artificial boundary conditions are implemented to solve various problems in closed or open domains.

- Version: 3
- Keywords: Numerical simulation of incompressible flows,
- Type of human computer interaction: console
- OS/Middelware: unix, linux, Mac OS X item Programming language: Fortran 95 and MPI
- Documentation: included

5.5. Other MC2 codes

- Penalization techniques on cartesian grids to solve incompressible Navier-Stokes equations
  - **Vortex**: sequential, Vortex In-Cell (VIC) scheme : hybrid vortex methods based on the combination of Lagrangian mesh-free schemes and Eulerian grid based schemes on the same flow region.
  - Unstructured body fitted meshes
  - **Richards** : 2D Unstructured finite element code, implicit solver, sequential, to solve the transport-diffusion equations through a porous media including tidal forcing and mechanisms of diagenesis.
  - development inside **FluidBox** software in collaboration with **BACCHUS**. 2D-3D unstructured meshes, Stabilized Finite Elements method (SUPG), RANS turbulence model, parallel: Domain Decomposition and MPI.
- Immersed boundary techniques for:
  - **Compressible flows** : 2D-3D finite volume scheme for compressible Euler equations with solid obstacles on cartesian grids. 3D code parallelized with MPI
  - **Elliptic problems :** 2 2D-3D finite difference scheme for elliptic interface problems, parallelized with PETSc
  - Electropermeabilization: 2D finite difference scheme, parallelized with PETSc to simulate the electropermeablization of biological cells

6. New Results

6.1. Multi-fluid flows

- Microfluidics : Participants: Charles-Henri Bruneau, Johana Pinilla (PhD), Sandra Tancogne (MCF Reims).
  To handle oil recovery by chemical processes it is useful to better understand the behaviour of multifluids flows in a saturated soil. The porous medium is mimiced by a network of micro channels. The simulation of immiscible multi-fluids flows is then performed by means of the level-sets and the penalization methods to track the interfaces between the fluids and to get rid of the geometry difficulties. In addition the Cox law is added in the model to better move the interfaces during the simulations.
  Concerning visco-elastic fluids in micro-channel, one has often to compute solutions of system for which the viscosity in the stokes part is much smaller than that involved in the extra-stress. In his thesis, V. Huber has constructed a second order scheme solving Stokes equations for a bifluid flow with surface tension on a cartesian grid using a mixte finite volume-finite element approach.

6.2. Cancer modelling

We have improved our generic mathematical models describing tumor growth. These models were then specialized for several types of cancer (thyroidal lung nodules, brain tumors). The algorithm used to recover the parameters of these models from medical images has also been greatly improved and is now adapted to run on HPC architectures.

- Secondary tumors in the lung:

The mathematical models describing the growth of secondary in the lungs have now settled and are well understood. The main focus of the year was to keep on using these models on patient data. New clinical case were selected by clinicians from the Institut Bergonié, there are currently under study. The model is currently able to reproduce the growth observed on 5 clinical cases. In 2011, various improvements to the calibration algorithms were made. The initial seeding of the algorithms was a weak point of the procedure. This has been much improved using a genetic algorithm. A complete rewrite of the routines was done to improve their versatility and efficiency. Previously, the numerical simulations and calibration were performed in 2D (clinicians selected the most relevant slice showing the evolution of the tumor). Work is now ongoing to switch to full 3D computations and calibration.

- Metastasis to the liver of a GIST
  Gastro-Intestinal Stromal Tumors often create metastasis to the liver. We have modeled the response to the treatment of such lesion starting from CT-scans.
- Modeling glioblastomas:
  In 2011, a hierarchy of models describing the growth of brain tumors was developed (and described in a submitted paper) in collaboration with University of Alabama at Birmingham. As we wished to obtain models that could be calibrated from patient data and yet be reasonably accurate, we believe that these models are suitable trade-offs between the simplicity of the SwansonÕs model (the only one used on patient data of brain tumors so far) and the accuracy of more complex models (that cannot really produce quantitative results). In particular, two models were built. The first one allows to study the efficacy of anti-angiogenic therapies. It seems to predict that the efficacy of these treatments is limited, this could be confirmed by a world-wide ongoing clinical study. The second model has been validated and we are trying to recover its parameters for a patient in 3D (which is a rather unique initiative to our knowledge).
- Modelling of electrochemotherapy :
  Two articles related to the electrical cell modelling have been done ([64], [61]) . The first one deals with the influence of the ionic fluxes on the transmembrane voltage potential and on the cell volume. The main insight of the results consists in linking the transmembrane potential with the cell volume: it has been observed experimentally that cells with a low voltage potential do divide, whereas cells with high voltage potential do not, and the obtained relationship between voltage potential and cell volume can provide an explanation. The second article deals with a new model of cell electroporation essentially based on the experimental results of the I.G.R. In this paper we describe precisely the model, which takes into account the main experimental results in the electroporation process, and we present a variationnal formulation inherent to the model that leads to new efficient schemes in order to numerically solve the involved P.D.E.
  The article describing a new electrical model of classical has been accepted in Journal of Math Biology [27]. This new phenomenological model involves much less parameters than the usual models, but it still provides the qualitatively good description of the electroporation. The main feature of this model lies in the fact that it provides an intrinsic behavior of the cell membrane, which seems in accordance with the preliminary experimental results of the IGR partner. We also adapted the finite difference method developed by L. Weynans and M. Cisternino for elliptic interface problems to the electropermeabilization model developed recently by C. Poignard with O. Kavian. The new method has been validated by convergence tests and comparison with other models. We have proven that in one dimension the numerical solution converges to the solution of the exact problem.
- Cell Migration modelling:
  The collaboration with IECB (University of Bordeaux) has continued with the postdocatoral position of Julie Joie. We have obtain a continuous model of cell density evolving on micropatterned polymers. The research report RR 7998 will be published in Math. Biosci. and Eng. A discrete model describing the single cells motility is being written.

We also have started a collaboration with the University of Osaka (Japan), thanks to a PHC Sakura project, on the invadopodia. C. Poignard has been invited at Osaka in februray by Prof. Suzuki and T.Colin and C.Poignard have been at Osaka in september. A model describing the destruction of the extracellular matrix by the MMP enzyme, and then the cell migration has been obtained. R. Mahumet, a PhD student of Prof. Suzuki is developing a code to simulate the model.

6.3. Newtonian fluid flows simulations and their analysis

- Simulations of water distribution systems :Water losses may constitute a large amount of the distributed total water volume throughout water distribution systems. Here, a new model method is proposed that intends to minimize the total water volume distributed through leakage reduction. Our group has worked on the derivation of advection-reaction-diffusion type equations with an explicit relationship between the local pressure and the leakage rate. An original splitting technique to solve this type of hydraulic problem was then achieved. This technique allows pressure-dependent leakage to be taken into account, whereas in most models leakage is assumed to be uniform along a pipe. Finally, a constrained optimization problem was formulated for leakage reduction in WDS. The control variable had the mean of a local head loss and is considered in the Boundary Conditions to avoid dealing with discontinuities in the governing equations. The objective function to minimize was a regularization of the total water volume distributed. Specific operational constraints were added to ensure enough pressure at consumption points. The direct solution for this minimization problem was sought with a Gradient type method. The leakage reduction was proven to be significant in a case study. The percentage of leakage reduced from 24% to 10% in the linear relationship between pressure and leakage flow rate. With other leakage exponents, the same rate of reduction was achieved . The method was applied on a real network in the South-West of France. Controlling the pressure at two different strategic points permits a significant amount of the total distributed water to be saved (5%). This work was performed in collaboration with Cemagref Bordeaux . Future work will consist of applying a sensibility analysis of control location points to optimize the method.
- Incompressible flows : modeling and simulation of moving and deformable bodies. The incompressible Navier-Stokes equations are discretized in space onto a fixed cartesian mesh. The deformable bodies are taken into using a first order penalization method and/or second order immersed boundary method. The interface between the solid and the fluid is tracked using a level-set description so that it is possible to simulate several bodies freely evolving in the fluid. A turbulence model based on Samgorinsky model has been added to the numerical code. The numerical code written in the C langage is massively parallel. The large linear systems (over than 100 millions of dofs) are solved using the Petsc Library. As an illustration of the methods, fish-like locomotion is analyzed in terms of propulsion efficiency. Underwater maneuvering and school swimming are also explored. We were able to simulate the three-dimensional flow about a swimmer for realistic physical configurations. Another application is the turbulent 3D flow around complex wind turbine (see http://www.math.u-bordeaux1.fr/~mbergman and http://www.math.u-bordeaux1.fr/MAB/mc2/analysis.html for simulation movies). Wake flows generated by boat propellers are also modeled and simulated.
  We recently take in account a simplified elasticity model of the swimmer (elastic caudal tail of a fish). Some elastic parameters allows to increase the swimming efficiency around 20%-30%. Recent developments on multiphase flows have been performed. We are able to simulate water/air interactions with interface regularization. The interface with a boat is also taken into account. See http://www.math.u-bordeaux1.fr/~mbergman for simulations.
- Turbulence flow on an hemisphere : Participants: Charles-Henri Bruneau, Patrick Fischer (MCF Bordeaux 1), Yong Liang Xiong (PostDoc)
  ANR Cyclobulle lead by Hamid Kellay Soap hemi-bubble film experiments have shown some links between the formation of vortices when the hemi-bubble is heated at the equator and the formation of tornados in the earth atmosphere. Two-dimensional simulations using a stereographic map are used to compare to these experimental results and confirm the results when Coriolis force and heat source terms are added.

- Compressible flows: Immersed boundary methods. We are concerned with immersed boundary methods, i.e., integration schemes where the grid does not fit the geometry, and among this class of methods, more specifically with cartesian grid methods, where the forcing accounting for the presence of boundaries is performed at the discrete level. We have developed a simple globally second order scheme inspired by ghost cell approaches to solve compressible flows, inviscid as well as viscous. In the fluid domain, away from the boundary, we use a classical finite-volume method based on an approximate Riemann solver for the convective fluxes and a centered scheme for the diffusive term. At the cells located on the boundary, we solve an ad hoc Riemann problem taking into account the relevant boundary condition for the convective fluxes by an appropriate definition of the contact discontinuity speed. This method can easily be implemented in existing codes and is suitable for massive parallelization. It has been validated in two dimensions for Euler and Navier-Stokes equations, and in three dimensions for Euler equations. The order of convergence is two in L^2 norm for all variables, and between one and two in L^∞ depending on the variables. The 3D code has been parallelized with MPI. The case of a moving solid has been tested (flapping wing) and gives results for the drag and the lift in agreement with the references in the literature.
  The Oldroyd B constitutive model is used to study the role of the viscoelasticity of dilute polymer solutions in two-dimensional flows past a bluff body using numerical simulations. This investigation is motivated by the numerous experimental results obtained in quasi two dimensional systems such as soap film channels. The numerical modeling is novel for this case and therefore a comprehensive comparison is carried out to validate the present penalization method and artificial boundary conditions. In particular we focus on flow past a circular object for various values of the Reynolds number, Weissenberg number, and polymer viscosity ratio. Drag enhancement and drag reduction regimes are discussed in detail along with their flow features such as the pattern of vortex shedding, the variation of lift as well as changes in pressure, elongational rates, and polymer stress profiles. A comprehensive study of the flow behavior and energy balance are carefully carried out for high Reynolds numbers. Flow instabilities in both numerical and experimental results are discussed for high Weissenberg numbers .
- Elliptic problems: We have developed a new cartesian method to solve elliptic problems with immersed interfaces. These problems appear in numerous applications, among them: heat transfer, electrostatics, fluid dynamics, but also tumour growth modelling, or modelling of electric potential in biological cells This method is second order accurate in the whole domain, notably near the interface. The originality of the method lies on the use of additionnal unknows located on interface points, on which are expressed flux equalities. Special care is dedicated to the discretization near the interface, in order to recover a stable second order accuracy. Actually, a naive discretization could lead to a first order scheme, notably if enough accuracy in the discretization of flux transmission condtions is not provided. Interfaces are represented with a distance level-set function discretized on the grid points. The method has been validated on several test-cases with complex interfaces in 2D. A parallel version has been developed using the PETSC library.
- Simulations of fluid-solid interactions : The interaction of an elastic structure and an fluid occurs in many phenomena in physics. To avoid the difficulty of coupling lagrangian elasticity with an eulerian fluid we consider a whole eulerian formulation. The elasticity of the structure is computed with retrograde caracteristics which satisfy a vectorial transport equation. We derive the associated fluid-structure models for incompressible and compressible media. The equations are discretized on a cartesian mesh with finite differences and finite volumes schemes. The applications concern the bio-locomotions and the study of air-elastic interaction.
- Vortex methods : The aim of this work is to couple vortex methods with the penalization methods in order to take advantage from both of them. This immersed boundary approach maintains the efficiency of vortex methods for high Reynolds numbers focusing the computational task on the rotational zones and avoids their lack on the no-slip boundary conditions replacing the vortex sheet method by the penalization of obstacles. This method that is very appropriate for bluff-body flows is validated for the flow around a circular cylinder on a wide range of Reynolds numbers. Its validation

is now extended to moving obstacles (axial turbine blades) and three-dimensional bluff-bodies (flow around a sphere). See [77]. Moreover, using the global properties of the penalization method, this technique permits to include porous media simultaneously in the flow computation. We aim to adapt the porous media flows to our new method and to apply it in order to implement passive control techniques using porous layers around bluff-bodies.

- Domain decomposition : Domain decomposition methods are a way to parallelize the computation of numerical solutions to PDE. To be efficient, domain decompositions methods should converge independently on the number of subdomains. The classical convergence result for the additive Schwarz preconditioner with coarse grid is based on a stable decomposition. The result holds for discrete versions of the Schwarz preconditioner, and states that the preconditioned operator has a uniformly bounded condition number that depends only on the number of colors of the domain decomposition, and the ratio between the average diameter of the subdomains and the overlap width. Constants are usually non explicit and are only asserted to depend on the "shape regularity" of the domain decomposition.
  two years ago, we showed the result holds the additive Schwarz preconditioner can also be defined at the continuous level and provided completely explicits estimates. Last year, we established that a similar result also holds for non shape regular domain decompositions where the diameter of the smallest subdomain is significantly smaller than the diameter of the largest subdomain. The constants are also given explicitely and are independent of the ratio between the diameter of the largest sudomain and the diameter of the smallest subdomain.
  This year, we have studied explored new coarse spaces algorithms for domain decomposition methods. Coarse spaces are necessary to get a scalable algorithm whose convergence speed does not deteriorate when the number of subdomains increases. For domains decomposition methods with discontinuous iterates, we showed that continuous coarse spaces can never be an optimal choice. As an alternative, we introduced both the use of discontinuous coarse spaces(DCS) and a new coarse space algorithm using these discontinuous coarse spaces.

6.4. Flow control and shape optimization

- Flow control : Participants: Charles-Henri Bruneau, Iraj Mortazavi, Emmanuel Creusé (Lille), Patrick Gilliéron (Paris).

  An efficient active control of the two- and three-dimensions flow around the 25 degrees rear window Ahmed body has been performed. A careful theoretical and numerical study of the trajectories of the vortices allows to adapt the control in order to improve its efficiency and get a better drag reduction.

6.5. Calculation of Ice Chunk Trajectory

- Participants: Héloise Beaugendre, Ramesh Yapalparvi.
  In this work, calculation of trajectories of ice chunk are carried out at varying values of ratio of density of ice piece to that of the ambient fluid. Proper Orthogonal Decomposition with Interpolation (PODI) method is then applied on snapshots of trajectories simulated by computational fluid dynamics. Snapshots of trajectories are obtained based on cartesian grids, penalization, and level sets. The extracted POD modes from snapshots are then used to reconstruct solutions and capabilities of POD with interpolation are demonstrated on ice trajectory calculations for flow around iced airfoil and cylinder for density ratio's that are not part of the snapshot set.

7. Bilateral Contracts and Grants with Industry

7.1. Program PREDIT

Participants: Charles-Henri Bruneau, Iraj Mortazavi.

Program PREDIT ADEME with Renault and Peugeot. The aim of this program is the work on drag reduction in order to decrease the fuel consumption.

7.2. Renault

Participants: Charles-Henri Bruneau, Iraj Mortazavi.

CARAVAJE project with ADEME (PREDIT Véhicules propres et économes) notified october 24th 2008. Collaboration with Renault and Peugeot, two PME and 3 labs to reduce the drag coefficient of a ground vehicle. 95 k euros for 3 years.

7.3. Plastic Omnium

Participant: Iraj Mortazavi.

The MC2 team works actually with the Plastic Omnium company in order to study the flow behaviour around square back ground vehicles (like buses, camions,...) using LES and DNS techniques. The main target of this collaboration is to identify the structures of velocity fields that generate aerodynamical losses, in order to design drag reduction control strategies using pulsed or synthetic jets. In the framework of this project, we also want to compute accurately instantaneous velocity fields, with high velocities. The computations should be performed on long time for complex geometries. A part of this work is included in the PhD thesis of Yoann Eulalie.

7.4. Contracts with Industry

Thierry Colin is Scientific consulting for the CEA CESTA. The CEA is funding the thesis of M. Latige and a grand of 30 k euros has been obtained.

Angelo Iollo is consulting with OPTIMAD engineering.

7.5. Grants with Industry

CIFRE - Conventions Industrielles de Formation par la REcherche - with VALEOL (VALOREM Group)

8. Partnerships and Cooperations

8.1. Regional Initiatives

Angelo Iollo is belongs to the Aerospace Valley committee IGPC. He is monitoring the project ECOSEA for the fnrae http://www.fnrae.org/.

8.2. National Initiatives

8.2.1. ANR MANIPHYC

Participants: Charles-Henri Bruneau, Thierry Colin.

Simulations of complex fluids.

Collaboration with Rhodia-Lof and University of Lyon 1, 2008–2012.

8.2.2. ANR CARPEiNTER

Participants: Héloïse Beaugendre, Michel Bergmann, Charles-Henri Bruneau, Angelo Iollo [Leader Project], Lisl Weynans.

Cartesian grid, penalization method, complex flow. The P.I. is Angelo Iollo. See http://www.math.u-bordeaux1.fr/CARPEINTER/

8.2.3. ANR CYCLOBULLE

Participants: Charles-Henri Bruneau, Yong Liang Xiang.

The formation and dynamics of long lived coherent structures in atmospheric flows can be mimicked by soap film experiments on an hemisphere heated at the equator. The aim of this work is to simulate such flows and to compare both to the experiments and to the known data of various tornados.

8.2.4. ANR INTCELL

Participants: Thierry Colin, Olivier Saut, Clair Poignard.

The members T.Colin, C.Poignard and O.Saut are involved in the consortium INTCELL directed by P.LEVEQUE (XLIM), and which begun in December 2010. This mutlidisciplinary project, composed of four partners (XLIM laboratory, Vectorology and Anticancer therapies team at the IGR, EDAM and MC2) aims at studying the electropermeabilization by nanopulses at the subcellular level. The goal is to develop new electrical devices and accurate models to understand the electropermeabilization of the cytoplasm constituents such as the nuclear envelop or the mitochondrial membrane, based on the experiments and on the simulations of molecular dynamics.

8.2.5. ANR MEMOVE

Participants: Mathieu Colin, Thierry Colin, Angelo Iollo, Clair Poignard, Olivier Saut, Lisl Weynans.

Part of the team (M.Colin, T.Colin, A.Iollo, C.Poignard, O.Saut and L. Weynans) are involved in the consortium MEMOVE coordinanted by MC2 (coordinator C. Poignard), and which begins at the begining of 2012. This consortium is composed of four partners (the Vectorology and Anticancer therapies team at the IGR, the bioengineering laboratory AMPERE of Lyon and the Department of mathematics of Versailles). It aims at developing electropermeabilization models from the cell scale to the tissue scale. This project focuses on quite long pulses (from micro- to milli-pulses) compared with the ANR consortium INTCELL that has begun in december 2010. The main goal is to provide multi-scale modelling of "classical" eletroporation, in order to obtain numerical tools that can help from one side the biologists to understand the electropermeabilization process when "non standard" pulses are applied, and from the other side it eventually aims at providing tools for the physicians to optimize the pulse delivering when the electrochemotherapy is used.

8.2.6. PEPS CaRaMel3d

- Program: PEPS Idex-CNRS
- Project acronym: CaRaMel3d
- Project title: Calibration et Recalage sur l'Imagerie Médicale
- Duration: 07/2012-07/2013
- Coordinator: Olivier Saut
- Other partners: Institut Bergonié, CHU Pellegrin (Bordeaux),
- Abstract: Les médecins de l'Institut Bergonié (centre régional de lutte contre le cancer) s'intéressent à l'évaluation de l'agressivité de métastases dans le poumon. Les modèles mathématiques spatiaux développés par des mathématiciens de l'IMB permettent de décrire la croissance d'une tumeur solide plus ou moins fidèlement. Pour adapter ces modèles à un patient, il faut développer des méthodes pour trouver des valeurs raisonnables de leurs paramètres. Ces modèles calibrés peuvent alors fournir une prédiction numérique de l'évolution des nodules. Une collaboration entre ces deux équipes a déjà permis de développer un modèle et une technique de calibration qui permet d'évaluer cette agressivité en utilisant des coupes 2D. Même si ces résultats sont encourageants, l'aspect 3D de la croissance n'est pas pris en compte. L'objectif de ce projet est de prendre en compte cette 3ème dimension en développant pour cela de nouveaux algorithmes de recalage et de calibration en vue d'une application pratique.

8.3. European Initiatives

8.3.1. FP7 Projects

8.3.1.1. FFAST

Title: FUTURE FAST AEROELASTIC SIMULATION TECHNOLOGIES
Type: COOPERATION (TRANSPORTS)
Instrument: Specific Targeted Research Project (STREP)
Duration: January 2010 - December 2012
Coordinator: University of Bristol (Saint Pierre And Miquelon)
Others partners: University of Bristol, irias, TU Delft, Politecnico di Milano, Numeca, EADS, DLR, Airbus, University of Cap Town, csir, Optimad
See also: http://www.bris.ac.uk/aerodynamics-research/ffast/
Abstract: The FFAST project aims to develop, implement and assess simulation technologies to accelerate future aircraft design. These technologies will demonstrate a step change in the efficiency and accuracy of the dynamic aeroelastic "loads process" using unique critical load identification methods and reduced order modelling. The outcome from the project will contribute to the industrial need to reduce the number of dynamic loads cases analysed, whilst increasing the accuracy and reducing the cost/time for each unsteady aeroelastic analysis performed compared to the current approach. Unsteady loads calculations play an important part across much of the design and development of an aircraft, and have an impact upon the concept and detailed structural design, aerodynamic characteristics, weight

8.4. International Initiatives

- Collaboration with Hassan Fathallah, Neuro-oncoly and mathematics, University of Alabama at Birmingham. We work on numerical modeling of brain tumor.
- Collaborations with Luca Zannetti, Politecnico di Torino; Simone Camarri, Universita di Pisa; Eyal Arian, Boeing Commercial Airplanes.
- PHC Sakura on cancer modeling with University of Osaka. (12Keur for 2 years) Collaboration with the University of Osaka on the modeling of the cell migration in cancer.

9. Dissemination

9.1. Scientific Animation

Thierry Colin is elected as a member of the national committee of the French Universities (CNU). It is a national structure that has in charge a peer review of the carriers of mathematicians in France.

Charles-Henri Bruneau is member of the executive board of the international conferences on CFD. Selection of the 270 abstracts recieved for the next conference in Hawaii july 2012.

Angelo Iollo is managing the national ANR research project Carpeinter.

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

All Professors and Associate Professors teach 192 hours per year.

Licence : Modélisation et calcul scientifique, 32H, L2, Université Bordeaux 1, France (Michel Bergmann)
Licence : Initiation au langage de programmation Fortran 90, 28H, ENSEEIRB-MATMECA, France (Michel Bergmann)
Master : approximation des EDP 2, 28h, M1, Université Bordeaux 1, France (Michel Bergmann)
Master : electrical modelling of biological cells, 32H, M2, Université Bordeaux 1, France (Clair Poignard)

9.2.2. Supervision

PhD & HdR :

HdR: O. Saut, Contributions en optique non-linéaire et en modélisation de la croissance tumorale en vue des applications cliniques, Université Sciences et Technologies - Bordeaux I, September 2012

M. Cisternino, A parallel second order Cartesian method for elliptic interface problems and its application to tumor growth model, Université Sciences et Technologies - Bordeaux I and Politecnico di Torino, April 2012

PhD: Y. Gorsse, Méthode cartésienne pour les fluides compressibles et l'élasticité non-linéaire autour d'obstacles, November 2012

J. Hovnanian, Modélisation, Simulation et contrôle d'écoulement autour d'obstacle déformables, December 2012

PhD: V. Huber, Numerical modelling of complex bifluid flows, September 2012

J. Pinilla, , Modélisation et simulation à l'échelle du pore de la récupération assistée des hydrocarbures par injection de polymères, December 2012

PhD in progress : F. Cornelis is a medical doctor of the Institut Bergonié. He is a radiologist practicing CT-Scans, MRI but also local mini-invasive treatments (interventional radiology). He spends one day a week to prepare a PhD on the modelling aspects of his work. started 2010

PhD in progress : X. Jin, Etude et conception d'une éolienne, started 1st May 2011, supervisors : Angelo Iollo and Michel Bergmann

PhD in progress : M. Leguebe, Electroporation modelling at the cell scale, started 1st october 2011, supervisors : Thierry Colin and Clair Poignard

PhD in progress : M. Lattige, (co-director G. Gallice, CEA CESTA). Numerical modeling of ablation. started october 2010

PhD in progress, started October 2011: F. Bernard, V. Pianet

PhD in progress, started October 2012: A. De Bauer, J. Jouganous, G. Lefevre, H. Ung.

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