Project-Team mc2

Modeling, control and computations

Bordeaux - Sud-Ouest

Theme : Computational models and simulation
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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 non-linear 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).

**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 three areas of applications.

1) Interface problems and complex fluids:

This concerns microfluidics, complex fluids (bifluid flows, miscible fluids), cancer modelling. The challenges are to obtain reliable models that can be used by our partner Rhodia (for microfluidics) and to get tumor growth models including some mechanics that can be used by Institut Bergonié.

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 consumption, 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.

Our main partners on this project will be:

**Industrial**: Renault, IFP, CIRA (Centro italiano ricerche aeroespaziali), Airbus France and Boeing for high Reynolds flows, optimization and control and Rhodia (biggest french company of chemistry) and Saint Gobain for interface problems and complex fluids.
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 feedback 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. We describe growth of tumors and tumor-
membrane interactions in the same framework. The applications are microfluidics, tumor growth, 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.

iii) 2D and 3D simulations at high Reynolds number:
We develop various computational methods: multi-grid techniques, vortex methods, Detached Eddy Simula-
tion (DES). 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). Another application is to quantify the
performance degradation of a plane wing due to icing.

iv) Flow control and shape optimization:
We develop adjoint codes ranging from potential to 2D Euler and 2D compressible Navier-Stokes equations.
We also develop a code to solve inverse problems on cartesian meshes using penalization on level set methods
for 2D Stokes flows and problems governed by the Laplace equation.

v) 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 will be organized as follows. We will 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!

2.2. Highlights

The simulation around a 3D rotating wind turbine has been performed with the software NONAME (figure 1) on 128 processors using a cartesian grid $350 \times 350 \times 350$. The length of the blades is 5 meters with a chord of 0.7 meter, a LES simulation using smagorinsky model has been done at Reynolds number 10000 (based on the chord). The angular velocity is fixed at 10 turns/minute.

![Figure 1. wind turbine](image)


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. 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 - the last one focuses on flow control and shape optimization.
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 and biology

Participants: Angelo Iollo, Charles-Henri Bruneau, Thierry Colin, Mathieu Colin, Clair Poignard, Kévin Santugini, Olivier Saut.

3.2.1. 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. We have worked on foam drainage [72] and on instability of lamellar phases [104], [98].

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 perform 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 [80]. 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. An ANR project in the nanotechnology program has been obtained in 2006. Our partners in this ANR project are Rhodia, Saint-Gobain and the Ecole Supérieure de Physique-Chimie Industrielle de Paris. An ANR project in the SYSCOM program has been obtained in 2008 concerning the study of complex fluids in microfluidics.
First work has been done on a micro-viscosimeter. The results have been published in [83], [84], [85]. The challenge is to be able to predict the range of parameters in which the coflow will be stable, that is the range of validity of the rheometer. It is therefore necessary to perform time dependent 3D-simulations involving visco-elastic fluids in "T" junctions, in cross junctions and in "Y" junctions. Once the coflow becomes unstable, droplets are created and they can be used in order to measure some reaction rates or to measure some mixing properties. Micro-channels can also be used to simulate experimentally some porous media. 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.

3.2.2. Cancer modelling

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 main challenge is 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 [93] where the efficacy of radiotherapy is studied and in [94] 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 [57], [81], [82]. 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 [93].

One of the main issues is then to couple the system with an angiogenesis process. Of course realistic simulations will be 3D. The 3D model consists of a Stokes system coupled with some transport equations describing the cell populations. We consider several populations of cells evolving in a cell-cycle model describing mitosis. The evolution inside the cell-cycle gives rise to a non divergence-free velocity field. Again, the system has to be coupled with diffusion of oxygen, but also with membranes that can be degraded biologically. These elastic membranes are handled by a level set version of the immersed boundary method of C. Peskin [91], see Cottet-Maître [73]. The perspectives of development in this direction are of course to increase the biological complexity but also to use more realistic models to describe the mechanics of living tissues and to make comparison with real medical cases. One can think to elasto-visco-plastic models for example.

A forthcoming investigation in cancer treatment simulation is the influence of the electrochemotherapy [88] 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 [92] 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.
Concerning lung tumor, we have developed a hierarchy of models for tumor growth. We use here a simplified version of the systems presented in these references. Our prediction relies on parameters estimation using temporal series of MRI or scans. Our approach uses optimization techniques and POD to estimate the parameters of the chosen mathematical model (adapted to the type of cancer studied) that fit the best with the real evolution of the tumor shown on the MRI.

The mathematical setting of this problem is well developed since it is similar to that encountered in dynamic meteorology. In the context of tumor growth modeling we intend to pose the problem as the minimization of the distance, in a suitable norm, between the predicted and the observed tumor evolution. The minimization is carried with respect to the uncertain parameters: tumor shape and position, diffusion coefficients, vascularization and mechanical properties of the matter etc. We update the solution each time new data are available. This has the advantage to take heterogeneous data coming from different sources of medical diagnostics into account.

3.3. Newtonian fluid flows simulations and their analysis
Participants: Charles-Henri Bruneau, Angelo Iollo, Iraj Mortazavi, Héloïse Beaugendre, Michel Bergmann, Lisl Weynans.

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.

3.3.1. Numerical methods
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 [67]. 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 [58]. This method is very easy to handle as it consists only in adding a mass term \( \frac{U}{K} \) 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 [74]. This method has recently enabled us to obtain new results concerning the three-dimensional dynamics of cylinder wakes.

The third method is detached-eddy simulation (DES). This is a hybrid technique proposed by Spalart et al. in 1997 [95] as a numerically feasible and plausibly accurate approach for predicting massively separated flows. The aim of DES is to combine the most favorable aspects of both RANS\(^1\) and LES\(^2\) techniques, that is to apply RANS models for predicting the attached boundary layer and LES for time-dependent three-dimensional large eddies [99]. The cost scaling of the method is then affordable since LES is not applied to solve the relatively smaller structures that populate the boundary layer. The base model employed in most of DES applications

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\(^1\)Reynolds-Averaged Navier-Stokes
\(^2\)Large-Eddy Simulation
is the Spalart-Allmaras (S-A) model that contains a destruction term for its eddy viscosity, $\tilde{\nu}$, proportional to $(\tilde{\nu}/d)^2$ where $d$ is the distance to the wall. A subgrid-scale model can then be obtained within the S-A formulation by replacing $d$ with a length scale $\Delta$ directly proportional to the grid spacing. The challenge is then to better understand the coupling between the two models (RANS/LES) and the issues that impact the method to be able to propose developments that increase the robustness of the method.

The fourth method is to develop reduced order models (ROM) based on a Proper Orthogonal Decomposition (POD) [86]. 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.

### 3.3.2. Analysis of the flows

Once simulation of the phenomena are satisfactory it is necessary to properly analyze the data we get. The classical analysis tools such as the Fourier transform, the wavelets [77] or the proper orthogonal decomposition [86] can give various results when used with various parameters. So the aim of this work is, on the one hand to determine the range of the parameters giving reliable results, and on the other hand to find out the statistical laws observed by the flow in configurations uncovered by the theory. Another approach to better evaluate the analysis tools is to use a placebo effect. It is achieved for instance by creating an artificial velocity field where a fundamental characteristic of the flow is not present and by using the classical methods able to detect this characteristic. If the method detects the characteristic it means that it is created by the method itself!

### 3.4. Flow control and shape optimization

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

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.

#### 3.4.1. 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 [63]. 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 [64]. 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.

3.4.2. 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 [79].

A similar procedure is also used in the estimation based on gappy POD, see [100] and [103]. 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.

3.4.3. 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 [69] 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 [87] 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 [97]. 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

- **Microfluidic**
  - computation of bifluid flows : see the thesis of S. Tancogne ([96]) and P. Vigneaux ([101]). 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.
  - emulsions and foam : see the thesis of S. Benito [59]. 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 [71].

- **Cancer Modelling**
– avascular stage: the goal is to develop and implement a 3D model of avascular tumor growth. It is a joint work with B. Ribba, J.-P. Boissel, E. Grenier in Lyon and D. Bresch in Chambéry. O. Saut is responsible for the numerical implementation, Th. Colin for modelling ([16]).
– vascular stage: the goal is to describe the angiogenesis stage. See [60].
– coupling with therapeutics: the goal is to test therapeutic protocols. Joint work with J.-P. Boissel (Clinical Pharmacology Department, Medical School of Lyon) and B. Ribba (Therapeutics in Oncology, Medical school of Lyon) and L.Mir of the CNRS at the Institut Gustave Roussy of Villejuif.
– specific models: investigation of two particular cancer: gliomas (brain tumors) and colorectal cancers. 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/)

4.3. 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 PREEDIT project.
• vortex dynamics: see [78],
• simulation of compressible flows on cartesian grids: see the thesis of Gabriele Ottino’s Thesis [90], 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 [12]. The goal is to use Detached-Eddy Simulation to model turbulent flows around iced bodies.

4.4. 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 [76] and Yong-Liang Xiang [13] and CH Bruneau and Iraj Mortazavi) [63]. See also project [68] founded by the European Community.
• active control: see the three PhD thesis: M. Buffoni, J. Weller [102], E. Lombardi and FFAST project funded by EU and held by the University of Bristol and AIRBUS UK.
• shape optimization for turbo-machines: See [97].
• 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 [102] and E. Lombardi.
• passive control of flows with porous media: see [65], [62], [61], [89], [66].
• inverse problems in imagery: see [69].

5. Software

5.1. eLYSe

Participant: Olivier Saut [correspondant].
eLYse is a numerical platform used for our computations in Biology (tumor growth), micro-fluidics and complex Newtonian fluid flows. The platform contained 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/~saut/wp/?page_id=201.

- Version: 1
- ACM: ACM J.2 J.3 G.1.8 G.1.10
- AMS: AMS65Z05 35Q92
- Keywords: Modelisation and numerical simulations, Finite volume methods, Level Set approach, Penalization method
- APP: En projet
- Type of human computer interaction: console
- OS/Middleware: Platform developped on Mac OS X architecture.
- Programming language: C++
- Documentation: see doxygen.

### 5.2. Noname

**Participant:**

This code is devoted to the resolution of 3D-flows in fluid mechanics. Navier-Stokes equations are solved on fixed grids and the obstacles are treated by a penalization/level-set method. The numerical method is based on projection schemes of Chorin-Temam’s type. The code is written in C language an use PETSc library for the resolution of linear systems. Using Noname, we are able to deal, for example, with bio-locomotion (optimization of fish like swimming, optimization of airfoil with flaps)

- Version: 1
- Keywords: numerical analyse, fluid mechanics, langage C, PETSc
- Software benefit : simulate a flow around a deformable obstacle, moving into a fluid.
- APP: non
- Patent: non
- Type of human computer interaction: human for the moment
- OS/Middleware: unix, linux, mac os
- Required library or software: PETSc
- Programming language: C/PETSc
- Documentation: in proges
5.3. 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.
  - **NS2D(3D)**: DNS, Finite Difference scheme, Multid solver, parallel MPI.

- 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.

6. New Results

6.1. Multi-fluid flows

- Microfluidics: Drag enhancement and drag reduction in viscoelastic fluid flow around a cylinder according to the amount of dilute polymers in solution. Evolution of three-dimensional bifluid flows in square micro channels. The simulation of immiscible multi-fluids by level-sets and cartesian meshes.

- Microfluidics: 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 introduced a new scheme to overcome this difficulties without changing the complexity of the scheme (PhD in progress).

- Cancer modelling: in 2010, 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.
  
  In particular, we were interested in the prognosis of thyroidal lung nodules. Refractory thyroid carcinomas are a therapeutic challenge owing to some being fast-evolving - and consequently being good candidates for trials with molecular targeted therapies - whilst others evolve slowly. This variation makes it difficult to decide when to treat. In collaboration with Jean Palussière and Françoise Bonichon at the Institut Bergonié (regional center for the fight against cancer), we have developed a diagnostic tool to help physicians predict the evolution of thyroidal lung nodule. For the time being we are only using physical imaging but a work is under way to take functional imaging into account and lift some indetermination on the inverse problem.

  We have also developed a new model for describing the growth of brain tumors. This model takes much more phenomena into account than existing models (typically based on reaction-diffusion equations). This model gives very interesting results on a qualitative point of view. In collaboration with physicians from the CHU Pellegrin, we are now adapting our recovery algorithm to be able to perform patient-based simulations of this model.

  Finally, aside from modeling therapies quantitatively (we have written generic models for chemotherapy and anti-angiogenic treatments), we have started working on the modeling of the electro-chemotherapy in collaboration with the Institut Gustave Roussy (Villejuif, France) and Herlev Hospital (Copenhague, France). Our goal is there to recover the parameters of the growth and therapeutical models (which may be feasible since ECT is not a systemic therapy) in order to improve clinical protocols.
• Modelling of electrochemotherapy: Two articles related to the electrical cell modelling have been done ([20], [50]). 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 variational formulation inherent to the model that leads to new efficient schemes in order to numerically solve the involved P.D.E.

6.2. Newtonian fluid flows simulations and their analysis

• Simulations of water distribution systems: unsteady water quality modeling and the associated sensitivity equations are solved for water distribution systems. A new solution algorithm is proposed, designed for slow varying velocity and based on a time splitting method to separate and solve efficiently each phenomenon such as advection and chemical reaction. This numerical approach allows simultaneous solution of both the direct problem and the sensitivity equations. Special attention is given to the treatment of advection, which is handled with a total variation diminishing scheme. The general model presented in this study permits global sensitivity analysis of the system to be performed and its efficiency is illustrated on two pipe networks. The importance of the sensitivity analysis is shown as part of the calibration process on a real network. See [27].

• Modelling and simulation of self-propelling movies objects: Modeling and simulation of flows past deformable bodies are considered. The incompressible Navier-Stokes equations are discretized in space onto a fixed cartesian mesh and the displacement of deformable objects through the fluid is taken into account using a penalization 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. 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. See [14].

• 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.

• 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 1D and 2D for Euler and Navier-Stokes compressible equations. The order of convergence of the method is similar to those observed in the literature: second order globally and first order locally, near the interface for Euler equations, and second order locally and globally for Navier-Stokes equations.
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 additional unknowns 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 conditions 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.

- 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. See [40].

- Domain decomposition: 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. The classical Schwarz method was however defined at the continuous level, and similarly, the additive Schwarz preconditioner can also be defined at the continuous level. We provide in this talk a continuous analysis of the additive Schwarz preconditioned operator with a coarse grid in two dimensions. We provide completely explicit constants for the stable decomposition of the continuous additive Schwarz operator with a completely explicit definition of shape regularity. The advantage of having explicit constants is that it opens the way to deal with non shape regular domain decompositions.

- Ice shedding: we are now able to predict ice-shedding trajectories, starting just after the ice break-up [38]. A vortex method is proposed to simulate the interaction of an incompressible flow with rigid bodies, following the innovative approach proposed by Coquerelle et al. A penalization method is used to enforce the no-slip boundary condition inside the solid wall boundaries. Level set functions are used to capture interfaces and compute rigid motions of the solid bodies.

- Turbulent flows: A stabilized finite element (SUPG) method to solve Navier-Stokes equations coupled to the RANS Spalart-Allmaras turbulence model has been developed and validated. 2D high-Reynolds number compressible flows around complex geometries relevant to industrial constraints are now feasible [41] and 3D simulations using domain decomposition and MPI are under process. Unstructured body-fitted meshes around iced 3D airfoil coming from Airbus France (DESGIVRE contract) have been elaborated.

- Porous media: The research goal of R. Chassagne’s thesis (see [11]) concerns the development and application of a 2D reactive transport model for sandy beaches that are subjected to tidal forcing. Recent biogeochemical studies on sandy intertidal have shown that these environments are far more reactive deposits than previously thought. They act as bio-catalytic filters where organic matter is rapidly decomposed. Numerical results will be compared with concentration measured in the Truc Vert beach located along the french Atlantic coast. Our study shows that the residence time of silica in tidal permeable sediment is equal to 7 tidal cycles. The model allows us to test the oxygen demand sensitivity to parameters that govern the properties of the permeable sediment and the tide (permeability, lability of the organic matter, beach slope, tidal amplitude).
6.3. Flow control and shape optimization

- Flow control: Coupling of active and passive control techniques to reduce the drag coefficient of the square-back Ahmed body, see [17]

7. 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.

CARA V AJE project with ADEME (PREDIT Véhicules propres et économiques) 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. DESGIVRE (Airbus)

Participant: Héloïse Beaugendre.

Each year, sudden aircraft performance degradation due to ice accretion causes several incidents and accidents. Icing is a serious and not yet totally mastered meteorological hazard due to supercooled water droplets that impact on aerodynamic surfaces. Icing results in performance degradations including substantial reduction of engine performance and stability, reduction in maximum lift and stall angle and an increase of drag. One of the most important challenges in understanding the performance degradation is the accurate prediction of complex and massively separated turbulent flows. We propose to use DES to analyze and understand the performance degradation due to in-flight icing.

8. Other Grants and Activities

8.1. Regional Initiatives

Participants: Thierry Colin, Mathieu Colin.

We obtained a grant of the Aquitaine district jointly with our partner Rhodia for the years 2007-2010 concerning the modelling and computation of non-newtonien flows in micro-channel in order to study enhance oil recovery.

8.1.1. Grant with the Aquitaine District.


It is a joint grant with Rhodia-LOF that enables us to buy a cluster of 200 processors.

8.2. National Initiatives

8.2.1. ANR MANIPHYC

Participants: Charles-Henri Bruneau, Thierry Colin.

8.2.2. **ANR CARPEINTER**

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

The P.I. is Angelo Iollo. See [http://www.math.u-bordeaux1.fr/CARPEINTER/](http://www.math.u-bordeaux1.fr/CARPEINTER/)

8.2.3. **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 multidisciplinary project, composed of four partners (XLIM laboratory, Vectorology and Anticancer therapies team at the IGR, EDAM and MC2) aims at studying the electropormeabilization by nanopulses at the subcellular level. The goal is to develop new electrical devices and accurate models to understand the electropormeabilization of the cytoplasm constituents such as the nuclear envelop or the mitochondrial membrane, based on the experiments and on the simulations of molecular dynamics.

8.3. **INRIA actions**

8.3.1. **ARC C3MB**

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

The goal of this project is to propose some simulation tools for therapeutic innovation in oncology. The targeted applications are brain tumors (gliomas) as well as lung tumors. The participating members are the INRIA teams MC2 (Bordeaux-Sud-Ouest) and NUMED (Rhône-Alpes), the mathematics department of the university of Versailles, the team EA 3738 “Ciblage thérapeutique en Oncologie”, faculté de médecine Lyon-Sud , Vectorologie physique et nouvelles stratégies antitumorales, UMR 8203 CNRS Institut Gustave-Roussy-Université Paris-Sud. The team is therefore multi-disciplinary. Furthermore, we will work with Institut Bergonié (Bordeaux), hôtel Neuro-Cardio (Lyon) and the hospital of the university of Alabama at Birmingham (neuro-oncology).

We propose to develop a generic multiscale model of tumor growth. This model will allow us to perform qualitative studies concerning the efficacy of several treatment (chemotherapies, anti-angiogenic drugs...). This model will then be specified and adapter to the two types of targeted cancers in order to allow their parametrization. This parametrization will be achieved using a data assimilation process from the medical Imaging (CT Scan, MRI) in order to obtain evolution or optimization prediction of drug delivery that uses the 3D-information that is included in the images.

Another direction is the modeling of electro-chemotherapy. This treatment is studied at the microscopic as well as at the macroscopic levels from both experimental and numerical point of view.

8.3.2. **TEAM CPAIBM**

**Participants:** Thierry Colin, Olivier Saut, Charles-Henri Bruneau.

8.4. International Initiatives

- **FFast**
  **Participants:** Angelo Iollo, Michel Bergmann.

  The aim of the upstream FFAST project is to develop, implement and assess a range of candidate numerical simulation technologies to accelerate future aircraft design. A step change in the efficiency and accuracy of the dynamic aeroelastic “loads process” will be achieved using unique critical load identification methods and reduced order modelling. The numerical simulation technologies to be assessed will include upcoming techniques as well as totally new methods developed within the FFAST project and will produce early release software. This area is critical because in the design of future aircraft there is an industrial need to reduce the number of dynamic loads cases analysed, whilst simultaneously increasing the accuracy and reducing the cost/time for each unsteady aeroelastic analysis. For conventional designs reducing the cost and turn around time of the loads process within the design cycle will lead to significant improvements to product development and manufacture supporting the ACARE 2020 targets. In particular, identifying the flight conditions that give rise to the maximum loads on the aircraft structure and introducing more accurate methods at these conditions will allow the new and innovative designs, required for green aircraft, to be considered more rapidly and at significantly lower risk. In summary, the ultimate objective of FFAST is to achieve the accuracy of the current loads process coupled to high fidelity aeroelastic simulations, with a speed up of two to three orders of magnitude.

8.5. Visitors

We have the visit of M. Ohta from Saitama University (March 2010-March 2011).

9. Dissemination

9.1. Organization of workshops

- Organization of a workshop on on numerical methods for the solution of PDE’s on non-body-fitted grids, Maratea, Italy, 13-15, May 2010.

10. Bibliography

**Major publications by the team in recent years**


Publications of the year

Doctoral Dissertations and Habilitation Theses


Articles in International Peer-Reviewed Journal


Invited Conferences


International Peer-Reviewed Conference/Proceedings


Workshops without Proceedings


Scientific Books (or Scientific Book chapters)


Research Reports


Other Publications


References in notes


