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Project-Team mc2

Modelling, control and computations: applications to fluid mechanics and biology

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Theme : Computational models and simulation

Activity Report

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MC2 is an INRIA Project-Team joint with University of Bordeaux (UB1) and CNRS (IMB, UMR 5251)

1. Team

Research Scientist
Michel Bergmann [INRIA, Research Associate (CR)]
Clair Poignard [INRIA, Research Associate (CR)]
Olivier Saut [CNRS, Research Associate (CR)]

Faculty Member
Thierry Colin [Institut Universitaire de France, Team Leader, Professor (Pr), HdR]
Héloïse Beaugendre [University Bordeaux 1, Associate Professor (MCF)]
Charles-Henri Bruneau [University Bordeaux 1, Professor (Pr), HdR]
Mathieu Colin [University Bordeaux 1, Associate Professor (MCF)]
Angelo Iollo [University Bordeaux 1, Professor (Pr), HdR]
Iraj Mortazavi [University Bordeaux 1, Associate Professor (MCF), HdR]
Kévin Santugini [University Bordeaux 1, Associate Professor (MCF)]
Lisl Weynans [University Bordeaux 1, Associate Professor (MCF)]

PhD Student
Julien Dambrine [INRIA, Conseil Régional d'Aquitaine grant, from Oct. 2006 to Dec. 2009]
Federico Gallizio [University of Italy, MIUR grant, from Feb. 2005 to Apr. 2009]
Élodie Jaumouillé [CEMAGREF, from Oct. 2006 to Dec. 2009]
Jean-Baptiste Lagaert [University Bordeaux 1, MESR grant, since Sep. 2008]
Damiano Lombardi [University Bordeaux 1, MESR grant, since Oct. 2008]
Edoardo Lombardi [University Bordeaux 1, MESR grant, since Oct. 2006]
Yong-Liang Xiong [INRIA, CORDI/S, since Nov. 2007]
Jessica Hovnanian [INRIA, ANR CARPEINTER grant, since Oct. 2009]
Delphine Depeyras [CNRS,Renault, from Oct. 2006 to Nov 2009]
Sylvain Bénito [University Bordeaux 1, MENRT grant, from Oct. 2005 to Nov. 2009]
Frédéric Chantalat [INRIA, MESR grant, since Feb. 2006 to Dec. 2009]
Yannick Gorsse [INRIA, 1/2 ANR 1/2 Région, since Oct. 2009]
Marco Cisternino [Politecnico di Torino, MIUR grant, since Jan. 2009]
Gabriele Ottino [cotutelle Politecnico di Torino, from Jan. 2006 to Apr. 2009]
Jessie Weller [University Bordeaux I, MESR grant, from Oct. 2005 to January 2009]
Marie Billaud [INRIA, CATS, from 2 Oct. 2009 to 31 Dec. 2009]
Vincent Huber [INRIA, since Sep. 2009]
Johana Pinilla [University Bordeaux I, MESR grant, since Oct. 2009]
Romain Chassagne [University Bordeaux I, ANR PRO-TIDAL, since Dec. 2007]
Christelle Wervaecke [INRIA, 1/2 INRIA 1/2 AIRBUS, since Sep. 2007]

Post-Doctoral Fellow
Youcef Mammeri [INRIA,since Oct. 2008]
Christophe Picard [INRIA, from Dec. 2007 to Aug. 2009]
Victor Péron [INRIA,ARC C3MB, since Oct.2009]
Thomas Milcent [INRIA, since Sep. 2009]

Administrative Assistant
Patricia Maleyran [INRIA]

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).
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 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.
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) and Saint Gobain for interface problems and complex fluids.
Academic: CPMOH (Laboratory of Physics, Bordeaux 1 University) for high Reynolds flows, optimization and control, and the medical school of Lyon, Institut Gustave Roussy (Villejuif), University of Alabama at Birmingham and Institut Bergonié (Bordeaux) for tumor growth.

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. 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 Simulation (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

We simulated the motion of swimming fishes http://www.math.u-bordeaux1.fr/MAB/mc2/videos/fish2.gif and medusas http://www.math.u-bordeaux1.fr/~bergmann/Videos/jellyfish.gif.

We have simulated tumor growth with data acquired from CT scans.

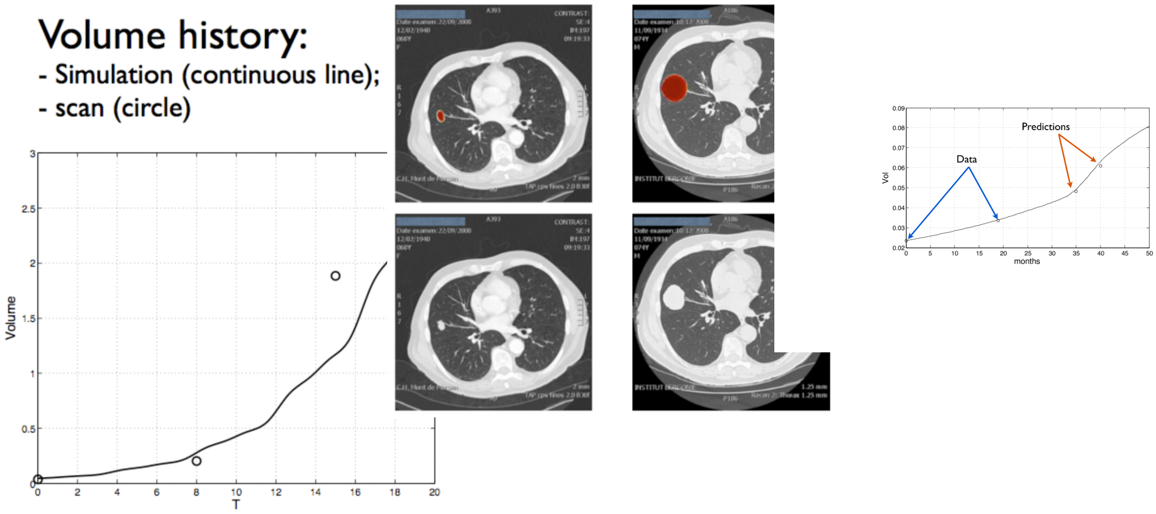

Figure 1.

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 [71] and on instability of lamellar phases [108], [104].
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 [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 [98] where the efficacy of radiotherapy is studied and in [99] 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 [59], [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 [98].

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 [96], see Cottet-Maître [72]. 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 [92] 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 [97] 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.

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 [68]. 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 [60]. 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 [73]. 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 [100] 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 [105]. 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 is the Spalart-Allmaras (S-A) model that contains a destruction term for its eddy viscosity, $\widetilde{\nu}$, proportional to $(\widetilde{\nu}/d)^2$ 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 Δ 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 [75] 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 !

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[1] Reynolds-Averaged Navier-Stokes

[2] Large-Eddy Simulation

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 [64]. 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 [65]. 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 [106] and [107]. 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 [70] 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 [102]. 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 will now present our contribution to the above challenge 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 and application for complex fluids, microfluidics and biology

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

As emphasized above, we need to handle the whole process from the modelling stage until the numerical feedback to the experiments.

4.2.1. Microfluidics

4.2.1.1. Modelling of the fluids

If u denotes the velocity of the fluid, p its pressure and σ the stress, one considers the usual Navier-Stokes equations for a bifluid evolution

$$\rho(\partial_t u + u\cdot\nabla u) = \nabla\cdot\sigma - \nabla p - \frac{T}{R}\overrightarrow{n}\delta_I,$$

$$\nabla\cdot u = 0,$$

where δ_I is the Dirac mass on the interface I, R is the curvature radius of the interface, $\overrightarrow{n}$ the normal and T the surface tension coefficient. A rheological law has to be specified for σ. For example, in the case of Newtonian fluids, we have $\sigma = 2\eta D(u)$ where $D(u) = \dfrac{\nabla u + \nabla u^t}{2}$ and $\eta = \eta_1$ in fluid 1, $\eta = \eta_2$ in fluid 2. We will have to handle complex fluids like polymers or miscible fluids. This formulation leads to a large class of models obtained by writing the equations satisfied by the stress tensor σ. It is known for example that normal forces play a key role in the flows of polymers in confined geometries and so this kind of formulation enables us to take into account these subtile effects. For complex fluid, one gives a rheological law of the form $\sigma = F(B)$ with B solution to

$$\frac{\partial B}{\partial t} + (u\cdot\nabla)B - \nabla u^T B - B\nabla u + (1-a)(BD(u) + D(u)B) + H(B) = 2GD(u) - \omega B - D\Delta B \quad (1)$$

that is valid for wormlike micelles, foams or emulsions.

4.2.1.2. Numerical techniques

In order to describe the evolution of the interface we use a level set method [95], [94], [101]: the interface is given as the 0-level set of a smooth function φ satisfying

$$\partial_t\varphi + u\cdot\nabla\varphi = 0.$$

At $t = 0$, φ is the distance to the initial interface. We choose this method for two reasons: the first one is the formation of droplets in microfluidics and the level set method is well adapted to the change of topology. The second reason is the fact that surface tension effects are predominant in microfluidics and one needs to compute the curvature of the interface in a very accurate way. We therefore use high order weno-type schemes in order to solve the equation for φ [89]. These weno-schemes are well adapted to level set methods on cartesian, regular meshes and easily implemented. The main drawback of this kind of mesh is the impossibility to directly take into account a complex geometry but we overcome this difficulty by using the penalization method. This approach can be extended with the same formulation to other physical settings, for example mixing models. In this case, the level set function is replaced by an order parameter φ that evolves through a convection-diffusion equation. An important part of the model is, in this case, the rheological law that gives the stress σ in terms of the velocity and of the order parameter φ.

4.2.1.3. Application 1 : computation of bifluid flows

This study was performed in the thesis of S. Tancogne and P. Vigneaux, defended in 2007. The aim was to investigate with direct numerical simulations, the stability of an interface, the shape of droplets, their velocity, the flow inside a droplet, the formation of a jet. To this end, a Level Set approach was coupled to the resolution of Stokes or Navier-Stokes equations with surface tension.

In the first work, diphasic flows driven by pressure gradient in channels of a few hundred of micrometres square sections were studied. At this scale, the interfacial effects are dominating and the instabilities processes are generally studied from the experimental point of view. The instability is a well-known hydrodynamic instability due to surface tension namely the Plateau-Rayleigh instability. In this work, tridimensional numerical simulations were presented to understand this phenomenon and more generally to study the behaviour of diphasic fluids evolving in square microchannels.

The second work was also dedicated to the numerical simulation of immiscible bifluid flows. A new stability condition induced by surface tension, for low and medium Reynolds numbers where stabilized interfaces can occur, was derived theoretically. Two numerical codes we developed : a two-dimensional cartesian code and a three-dimensional axisymetric code. The results were compared with physical experiments conducted by the LOF laboratory (Rhodia - CNRS) and a good agreement was observed. In particular new mixing dynamics inside microdroplets were brought to the fore.

4.2.1.4. Application 2 : mixing in a micro-channel

In a "Y"-junction, one considers the mixing of two fluids in a micro-channel. An order parameter description is used to obtain reliable models for the mixing. Again, the boundary conditions play a central role. We will address cases like non-flat bottom, surface having complex wetting properties (including patterns involving slipping zones and non-slipping ones). Our main objective is to compare numerically the efficiency of mixing with patterns or with riblets and to determine the shape of the patterns or of the riblets that leads to the best mixing, depending on the fluids that are used. We will compare our results with those obtained in [91], [90] with phase fields models. Finally, these models of mixing will be coupled with reaction equations describing chemistry experiments.

Asymptotics models for mixing in microchannels are derived. The aim is to measure the validity of the so-called Hele-Shaw approximation for various geometry and boundary conditions by performing some numerical simulations. In particular we are interested in passive mixing strategies involving boundary conditions. A simplifed model for wormlike micelles flows in microchannels is also in progress.

As quoted before, we also want to compute mixing oil-water-polymer in a microchannel. Such mixing is used for enhanced oil recovery. The objective here is to model from both a numerical and an experimental point of view the flows in a porous media thanks to microchannels. The measurements that will be obtained could be extrapolated to real scale situations for industrial applications or in macroscopic codes for numerical purpose.

4.2.1.5. Application 3 : models for emulsions and foam

Emulsions and foam have the particularity of being solid (elastic) at low stress and becoming liquid at high stress. We develop new models coming from microscopic considerations in order to properly describe this kind of phenomena. As described above, it consists mainly in giving a relationship between the stress and the hydrodynamical variable. This was the goal of the thesis of S. Benito[11] (advisor C.-H. Bruneau and Th. Colin) and it is a collaboration with C. Gay (Paris 7). The next step will be to use it for modelling in microfluidics and to extend it to other situations, especially to applications in biology (behavior of tissues, of tumor,...)

4.2.1.6. Application 4: a polymer nanotube conglomerate wire

Nanotubes are materials with an enormous tensile strength. However, only short nanotubes can be made at the moment. Making wires made of monolithic nanotubes is completely out of reach at the moment, it is possible to make wires made of several short length nanotubes bound together by a polymer. A work on the production of such wires has begun. A rheological model and numerical results have been achieved in 2D. It is planned to go from 2D to 3D axisymmetric. The extremely elongated shape of the apparatus is an obstacle to a fast numerical convergence. To improve the computational speed, we are planning to use decomposition domain methods. This has been the subjects of the talk in the following conference "WCCM8-ECCOMAS2008" and of the talk[52].

4.2.2. Cancer modelling

It is generally admitted that the process of cancer growth can be divided into two stages. During the avascular stage the cells receive nutrient and oxygen from existing blood vasculature. Avascular tumors can grow until the lack of nutrient and oxygen limits the extension of the initial nodule. An avascular tumor does not contain more than among 10^6 cells. Starving cells have the ability to secrete vessel chemoattractants in order to induce the formation of new blood vessels towards the tumor. This is the the angiogenesis process. When a tumor is able to induce angiogenesis, it can become vascularized. Vascular tumors are much less limited in terms of nutrient and oxygen and can metastasize to distant organs through the newly formed blood vessels. The first stage is of course to work on avascular tumor growth and its numerical study in two and three dimensions. For this purpose, we use a multiscale model using PDEs to describe the evolution of the tumor cell densities. These equations describe the cell cycle (the set of transformations a cell has to undergo in order to divide). The cell division is controlled by environmental factors such as hypoxia and overpopulation. The cancer growth of volume creates a movement with a corresponding velocity. To close our system of equations, we use a Stokes equation on a viscoelastic approach to compute this velocity. The extra-cellular matrix, within which the cells move and duplicate interacts mechanically with the tumor. We use a level set method to describe this matrix and compute its influence on the cell movement (which appears as a source term in the Stokes equation). The evolution of oxygen (used to estimate hypoxia) is led by a stationary diffusion equation.

4.2.2.1. Avascular stage.

For the time being, we have a 3D model of avascular tumor growth. In order to increase the biological information in the model, we have implemented the influence of acidity, several different phenotypes, as well as senescence problems. This code has been imersed in our general setting **eLYSe** in order to be able to work in complex geometries (galactophor canal, glial tumors, ...)

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 ([22]).

4.2.2.2. Vascular stage.

The main goal is to include a part of the model describing the angiogenesis stage. Several possibilities are available. The first one is to use some random walk model that give explicitly the formation of a web of vessels. The main advantage is that the rules of branching are quite easy to impose but the coupling with the biology of the tumors (activators, receptor) is not so clear. The second option is to use continuous PDE's models (similar to those used for chemotaxis) that will give at each point of the model a density of vessels. It is certainly more easy to use biological data with this kind of model but we loose the topological aspect of the web of vessels. The main point will be to compare the influence of both kinds of model on the development of the tumor and try to develop a mixed model ([25]).

4.2.2.3. *Coupling with therapeutics.*

It is one of the goals of our project to use our model to test therapeutic protocols. The influence of two kinds of therapy on tumor growth will be investigated. The first one deal with the influence of anti-angiogenesis drugs. This will studied in collaboration with prof. J.-P. Boissel (Clinical Pharmacology Department, Medical School of Lyon) and B. Ribba (Therapeutics in Oncology, Medical school of Lyon). The second one is the electrochemotherapy, studied in collaboration with L.Mir of the CNRS at the Institut Gustave Roussy of Villejuif. An "ANR Blanc" project proposing a multi-scale modelling of the influence of these cancer treatments (from the molecular scale to the macroscopic scale) has just been submitted. The application to therapeutics innovation is a long term project. We have also started collaborations with H. Fatallah (University of Alabama at Birmingham) and Jean Palussière (Institut Bergonié, Bordeaux).

4.2.2.4. *Mechanical effects*

We have improved our generic model for avascular growth modeling. In our models, advection equations are used to describe the evolution of tumor and healthy cells. The velocity of the movement, which is due to cellular division, was formerly obtained from a Stokes equation or Darcy's law. With these approaches, we were not able to obtain tumor shapes observed in *in vitro* experiments.

We chose to have a more realistic movement : the adhesion between healthy cells shall not be neglected. On the contrary, over the mutations the cancer cells acquire the ability to lower the adhesion with their neighbors. Furthermore, we have accounted for the effect of interstitial liquid between cells (this liquid comes from dead cells for instance). We have chosen to describe the movement of healthy cells as an elastic solid and the movement of interstitial liquid as a Newtonian fluid. The movement of cancer cells is considered as viscoelastic.

4.2.2.5. *Specific models*

Our models were written for a generic type of cancer on purpose. However, each cancer type is particular. Some phenomena are important in one type and can safely be neglected on others. To further validate our models with *in vivo* results, we have to specify our models for some types of cancer. Work has started on gliomas (brain tumors) and colorectal cancers. This is one part of the PhD of J.B. Lagaert and D. Lombardi.

4.2.2.6. *Modelling of electrochemotherapy*

The framework of our research deals with the interactions electromagnetic field/ living tissue, and especially the modelling of the electrochemotherapy. Electrochemotherapy is a cancer treatment, that consists in applying high short voltage pulses to a metastasis in order to increase the tumour permeability to the anti-cancer drugs. This increase of permeability in the living tissue submitted to the high short pulses is the key-point of the electrochemotherapy and a precise description of the involved phenomena is essential. We perform our modelling at two different scales: at the cell scale, we describes the membrane destructuration due to the pulse. In particular, modelling the resealing of the membrane after the electroporation is the main difficulty of the modelling: time-dependent models is necessary and the time scale is very large since the electroporation process occurs within few microseconds, while the resealing takes around an hour. Therefore, on one hand it is necessary to develop accurate approximation of the cell electric model with the help of a rigorous asymptotic analysis and on the other hand we need accurate and robust numerical schemes to solve the involved P.D.E. At the macroscopic scale, the main insight consists in coupling the tumour growth model developed in the team MC2 with the effect of the electrochemotherapy. Here again, a precise description of the field distribution in the tumour is necessary, since the efficacy of the cancer treatment depends on the amount of substance of drugs, that have entered the tumour, and this amount of substance depends whether the tissue is electroporated or not. Therefore, our research consists at the same time in modelling the electric phenomenon in living tissues and performing a rigorous asymptotic analysis on the models in order to simulate accurately the P.D.E

4.2.3. *Inverse problems*

4.2.3.1. *Parameter estimation with the help of low-order models*

Our models are complex and some of their parameters are not recoverable from experimental data. Actually the models described so far give reasonable qualitative results when appropriate sets of parameters are chosen for the simulation. We emphasize that the nature of these models is mostly phenomenological, i.e., they are not derived from first principles of physics but rather they try to reproduce experimental observations. Therefore it is difficult to measure or prescribe the values of the parameters present in the models. We started to design an algorithm to recover these parameters from a sequence of medical images. For instance, temporal sequences of brain MRI are supplied by the Bergonié Institute (Bordeaux). We will determine the parameters that allows to fit in the most accurate way these images. We write an inverse problem to compute these parameters. We resort to a method based on the idea of representing the model solution by means of modes that are obtained by statistical analysis of existing simulations. The less information is available, the more we intend to regularize the inverse problem using this expedient. We write an inverse problem to compute these parameters. The validation of the concept was performed by J.B. Lagaert to determine the vascularization of a tumor from several pictures of cancer cells densities. The extension of this approach and the use of POD models (to shorten computation times) is now one part of the PhD of D. Lombardi.

4.2.3.2. Level-set and penalization for optimal shape design

This task was running for three years already and was completed by solving a number of classical optimization problems which include topology variations, using a cartesian mesh and a penalization method that is second order accurate at the border of the immersed body. This is a major result since penalization methods suffer from a lack of precision on the border, since they are only first order accurate. Indeed, in shape optimization the solution gradients at the border are needed and this improvement is crucial to solve ill-conditioned problems. The method was developed by F. Chantalat[13]. We used this method to recover the vascularization of a model tumor from the knowledge of its shape evolution.

4.3. Newtonian fluid flows simulations and their analysis

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

The simulation of high Reynolds flows has been a strong objective of part of the team these last few years. Accurate and robust approximations have been derived to solve Navier-Stokes equations [68]. Since the first paper on the penalization method [60], the method has been applied in various contexts and has become one of the particularities of our group as it is widely used. We are still working on the development of robust and efficient methods adapted to the problem we want to solve. Besides, combination of classical methods and low order models [103] that are a strong part of our researches give us the opportunity to derive fast methods.
For the analysis of the computed flows and the understanding of the vortex dynamics in laminar and turbulent flows, several paths are followed inspired by original works [76] and [88]. Recent results [74] and [78] show that some significant progress is possible.

4.3.1. Simulation of a synthetic or pulsed jet

Our multigrid solver is robust enough to simulate high Reynolds flows. The aim of this work consists in simulating the flow inside and around an actuator in order to get quantitative data on the real effect of the actuator. This is an ongoing project with Renault and + PSA inside a PREDIT project. Their interests is having reliable data for each actuator made of a hole, a slot and so on ... so as to apply the right action on some parts of a ground vehicle in order to reduce the drag coefficient. C.-H. Bruneau, E. Creusé (Valenciennes, SIMPAF project) and I. Mortazavi are involved.

4.3.2. Analysis of 2D turbulent flows

The Kraichnan-Batchelor classical theory is valid on infinite domains. So the physical as well as the numerical experiments on finite domains yield results that often have significant discrepancies with the theory.

To better analyze the flow, it is important to capture the main components of the flow. For decades the flows were split into coherent structures and noise or background but it appears that the definition of a coherent structure is not so clear. It seems, using wavelet analysis, that a better choice is to distinguish the kernels or solid rotation part of the vortices and the vorticity filaments in 2D turbulence. Their respective role in the development of both inverse energy cascades and direct enstrophy cascades is already shown [77]. These vorticity filaments are a link between vortical structures but also roll up in spirals inside the kernels of the vortices. A careful analysis of these two different components could reveal a different statistical behavior and will help to understand 2D turbulent flows mechanisms. C.H. Bruneau and P. Fischer (external collaborator) use wavelet packets analysis to separate the coherent subfields of a turbulent flow. An interaction function has been derived to locate in the physical space the interactions of vortices that induce strong transfers of enstrophy. This interaction function is now used to find out the physical mechanisms involved in the production of the direct cascade of enstrophy.

4.3.3. Vortex dynamics

For dominated convection flows it is possible to use simplified models such as *point vortex* that are able to follow the trajectory of the vortices. Some improvements of these methods are in progress. One of the most helpful techniques for studying two and three- dimensional vortex dynamics is the identification of the coherent structures which are convected with the flow and concentrate a large amount of the energy and the enstrophy (e.g. [88]). Some works on various strategies have been developed in collaboration with E. Creusé (Valenciennes, SIMPAF project) and with S. Sherwin at Imperial College in London for 2D and 3D flows

A geometrical identification of Coherent Structures in three-dimensional flows is achieved. These studies are especially efficient for an error measurement and cut-off analysis of classical identification techniques. Once the vortices are well identified it is of interest to follow them to detect their interactions and observe the consequence on the whole vortex dynamics. This is a long term program of I. Mortazavi.

4.3.4. Reduced order models

Despite of the good results obtained using a standard ROM,some improvement of ROM based on POD are necessary. Thus, we focused on improving the stability as well as the approximation properties of POD ROM. Due to the energetic optimality of the POD basis functions, few modes are sufficient to give a good representation of the kinetic energy of the flow. But since the main amount of viscous dissipation takes place in the small eddies represented by basis functions that are not taken into account, the leading ROM is not able to dissipate enough energy. It is then necessary to close the ROM by modeling the interaction between the calculated modes and the non resolved modes. Thus, we have developed methods to close the ROM using Navier-Stokes equations residuals and exploiting ideas similar to Streamline Upwind Petrov-Galerkin (SUPG) and Variational Multiscale (VMS) methods. An other drawback of the POD approach is that the POD basis functions are only optimal to represent the main characteristics included in the snapshot database of the flow configuration used to build them. The same basis functions are thus *a priori* not optimal to efficiently represent the main characteristics of other flow configurations. We developed 3 methods to improve the POD solution subspace: (i) a Krylov like method, (ii) an hybrid methods that couple direct numerical simulations and reduced order model simulations, and (iii) using fast optimal sampling of the input system parameter subspace that we called Centroidal Greedy Region (CGR) method. The methods proposed are tested on the two-dimensional confined square cylinder wake flow in laminar regime.

4.3.5. Level-set and penalization for optimal shape design

This task was completed by solving a number of classical optimization problems which include topology variations, using a cartesian mesh and a penalization method that is second order accurate at the border of the immersed body. This is a major result since penalization methods suffer from a lack of precision on the border, since they are only first order accurate. Indeed, in shape optimization the solution gradients at the border are needed and this improvement is crucial to solve ill-conditioned problems. The method was developed by F. Chantalat who will defend his thesis in May 2009.

4.3.6. Simulation of compressible flows on cartesian grids

The first part of this work deals with a particle-grid method used to solve the compressible Euler equations. This method is associated to a level set method in order to solve compressible multifluids flow, and more precisely hydrodynamics instabilities that occur during the first steps of inertial confinement fusion. A numerical implementation of a multilevel technique introduced by Bergdrof, Cottet and Koumoutsakos has been developped in order to adapt locally the accuracy of the computations to the flow. This multilevel technique was mainly used to get a better resolution of the intabilities. A technique to apply limiters on the remeshing step of the particle method developed by Cottet and Magni is being applied presently to the simulation of compressible gaz dynamics. A 3D version of the particle grid method has been implemented. This particle method was extended to the 2D compressible Navier Stokes equations, with a penalization method to impose Dirichlet boundary conditions at the boundary of immersed bodies, that are described by a level set function. This is an exploratory study which is part of a larger project to simulate moving bodies in compressible flows, such as the rotor-stator interaction in turbomachines, buffet or flutter phenomena. This latter subject was the subject of Gabriele Ottino's Thesis [18], 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.

4.3.7. 3D Turbulent Flows

Object: Analysis and development of the DES approach for the simulation of 3D complex turbulent flows (DESGIVRE contract with AIRBUS since January 2008). Co-supervision of Christelle Wervaecke a PhD student supervised by Boniface Nkonga (ScALApplix team).

Details: We are developping a 3D Navier-stokes solver using stabilized finite element methods to solve compressible turbulent flows. We are considering massively separated flows and therefore we propose to use Detached-Eddy Simulation (DES) to model turbulence. Stabilized finite element methods allow us to achieve high order schemes needed in high reynolds turbulence modeling. Programming is under process in the FluidBox platform.

One of the most important challenge in Computational Fluid Dynamics (CFD) is the simulation of turbulent flow. When high Reynolds turbulent flows are combined with complex and large size geometry, computers are no longer enough powerful to deal with Direct Numerical Simulation (DNS), that is to say with the resolution of all the scales of turbulence motion [3]. Thus, at a fixed scale such as computations can be performed, one have to model the unresolved scales of the turbulence. Although there is an important variety of such models, all of them include intrinsically the turbulent viscosity as a parameter or a variable. Numerical schemes always induce an artificial dissipation that it is crucial to control, such as to be always lower to the viscosity obtained by subscale modeling of the turbulence. High order numerical approximations provide a framework where the constraint on the numerical dissipation can be achieved. Finite elements are suitable for the design of high order schemes with compact stencil that are efficient for parallel computing strategies by domain decomposition and messages passing. The main weakness of the classical finite element method (Galerkin) is its lack of stability for advection dominated flows. We consider in this work a compressible Navier-Stokes equations combined with the one equation Spalart Allmaras turbulence model. Therefore, the numerical stability is achieved thanks to the Streamline Upwind Petrov-Galerkin (SUPG) formulation [1]. Within the framework of SUPG method, artificial viscosity is anisotropic and the principal component is aligned with streamlines. The aim is to put sufficient viscosity to get rid of instability and unphysical oscillations without damaging the accuracy of the method. The amount of artificial viscosity is controlled by a stabilization tensor . Besides SUPG method is also used in combination with a shock-parameter term which supplied additional stability near shock fronts [2].

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4.3.8. Porous media

4.3.8.1. Combined finite element - particles discretisation for simulation of transport-dispersion in porous media

Combining finite element together with particle methods provide one of the best compromise for solving transport problem in porous media. Saturated or non-saturated flows are determined by boundary condition and the media permeability. For real terrain, permeability can consist in various almost constant and imbricated zones with complex shapes. Thus, it is of some interest that the boundary between two adjacent zones coincides with a natural mesh interface and that each element is entirely contains in one such zone. Beside this, solving transport equation by means of particle methods offers two distinctive advantages. The method is unconditionally stable when applied to a pure convective equation, and it does not contain any numerical diffusion if the particle trajectories are correctly computed. Therefore the combination of finite elements and particle method appears to be a straightforward application of the principle : “the right method at the right place”.

4.3.8.2. Numerical study of coupling between Richards and transport-diffusion equations in permeable sediment affected by tidal oscillation

We have developed a 2D numerical model that couples Richards equation with transport-diffusion equations of silica and oxygen in beach permeable sediment submitted to tides. The flow into the sediment is described by the Richards’ equation which generalizes the Darcy’s law for variably-saturated porous media. The velocity field and the watertable location, deduced from the numerical resolution of the Richards’equation, are introduced into the transport diffusion-equation of silica and oxygen. Tidal oscillations are modeled as a sinusoidal pressure boundary condition along the beach slope. Both flow characteristics and concentration are solved by finite element method. 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). This work is perfomed in collaboration with UMR CNRS 5805 EPOC (Environnements et Paléoenvironnements OCéaniques).
Help in the supervision of Romain Chassagne PhD student from EPOC.

4.4. Flow control and shape optimization

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

The final application of the simulation and analysis tools developed above is flow optimization and control. The main objectives are drag reduction and suppression of instabilities. A classical approach to achieve such goals is a shape design based on the control theory. This tool is very efficient for steady problems or problems for which the performance does not change much in time but is not robust enough for real time control. The benefits due to the shape improvement, however, soon reach a limit and therefore it is necessary to add control devices that locally modify the flow to provoke global improvements of the flow characteristics. We model both passive and active control. Passive control consists in steady devices which do not evolve in time, whereas active control has an automatic interaction with the flow, based on certain real time physical measurements.

4.4.1. Passive control

The first control is based on the idea of putting a porous interface between the solid body and the fluid. New applications to control the flow around a simplified car geometry have been developed in 2D and 3D. This was the goal of D. Depeyras thesis[15] defended on November in collaboration with Patrick Gilliéron at Renault Company (advisers CH Bruneau and Iraj Mortazavi) [64].

The second control consists in injecting minimal amounts of polymers into hydrodynamic flows in order to stabilize the mechanisms which enhance hydrodynamic drag. A PhD thesis (Yong-Liang Xiong) funded by CORDI has started in november 2007 and deals with the modelling and the numerical issues of such problem. The study is performed in collaboration with CPMOH laboratory in Bordeaux (H. Kellay) [58], [61].

A third approach consists in capturing by appropriately designed cavities large detached structures past bluff bodies. The scopes of this project will be mainly to develop a software tool for designing a flow past a thick airfoil with a trapped vortex assuming that this flow is stable, apart from small-scale turbulence. This project is financed by the European Community [69].
This part of the project concerns C.-H. Bruneau, A. Iollo, I. Mortazavi.

4.4.2. Active control

The coupling of two flow control methods has been studied: a passive control with a wall modification using porous media and an active control with the use of blowing/sucking actuators at car back wall. The aim was to obtain a 30% decrease of the drag coefficient. This was a part of Delphine Depeyras' thesis.

These has been the main objectives of three PhD thesis: M. Buffoni, J. Weller[19], E. Lombardi. The key points that need to be overcome, and that will be attacked in a PhD thesis to be started in 2010, is how to rationally probe the control space in order that the low-order model that is determined has optimal robustness to parameter variation. In particular we will explore a modified version of the Voronoi tessellation with a weight function that is represented by the residual of the Navier-Stokes equations projected on the reduced basis. This activity is performed in the framework of the FFAST project funded by EU and iled by the University of Bristol and AIRBUS UK.

4.4.3. Vortex method

Also, the implementation of novel active control strategies to confined flows (e.g. diffusers) using a vortex-in-cell (VIC) code is recently undertaken. This VIC method is modified in order to implement several closed-loop and open-loop control techniques in a backward-facing step channel geometry. Promising results were achieved for transitional flows (collaboration with E. Creusé (project SIMPAF INRIA Futurs) and A. Giovannini (IMFT)); this is an explorative program of I. Mortazavi.

4.4.4. Shape optimization

The shape optimization problem for turbo-machines consists in finding the blade geometry pertinent to a given work distribution. Within this framework, a model for preliminary blade design can de derived. In this model the blades coincide with a thickness flow surface and their effects on the flow is modeled by volume forces.

The aeroacoustic output of the propeller blade is determined by an integral method. The acoustic problem is formulated for an observer which is fixed to the flight system. In this framework the governing linear acoustics equations are the convected Ffowcs-Wiliams and Hawkings equations.

A set of discrete adjoint equations are then employed to determine the sensitivities of the aeroacoustic characteristics with respect to the design parameters (the work distribution on the blade and the shape of the blad's leading edge). As a Newton method is used in order to find the root of the governing equations of the inverse problem, the gradient can be calculated at nearly no cost. Constraints are introduced by projecting the gradient on the tangent space. Finally, the sensitivities are fed to a gradient based algorithm to optimize performance.
The work on this theme is performed in collaboration with H. Telib [102].

4.4.5. Reduced order models

This is a long standing challenge that we attack from two sides. On the one hand we develop low-order models that are robust to parameter variations using model identification methods. This procedure basically looks for a local approximation of the solution manifold as the control input is varied in a confidence region. The models are accurate enough to permit the control, on a given time horizon, of the Von Karman wake past a square cylinder. We used optimal control theory to minimize the total mean drag for a circular cylinder wake flow in the laminar regime ($Re = 200$). The control parameters are the amplitude and the frequency of the time-harmonic cylinder rotation. In order to reduce the size of the discretized optimality system, a Proper Orthogonal Decomposition (POD) Reduced-Order Model (ROM) is derived to be used as state equation. We then employ the Trust-Region Proper Orthogonal Decomposition (TRPOD) approach, originally introduced by Fahl (2000), to update the reduced-order models during the optimization process. The approach is much less time-consuming since the optimization process is now based only on low-fidelity models. We use a POD ROM for the pressure and velocity fields with an appropriate balance between model accuracy and robustness. The key enablers are the extension of the POD basis functions to the pressure data, the use of calibration methods for the POD ROM and the addition in the POD expansion of several non-equilibrium modes to describe various operating conditions. When the TRPOD algorithm is applied to the wake flow configuration, this approach converges to the minimum predicted by an open-loop control approach and leads to a relative mean drag reduction of 30% at reduced cost.

The second problem we address 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. This subject was pursued by J. Weller, who defended in January 2009, and E. Lombardi who will defend at the beginning of 2010. The control of the wake of the cylinder using local actuators and local measurements was performed at a Reynolds number that is by far higher of the examples found in the literature.

4.4.6. Compressible flow optimization

In collaboration with E. Arian of the mathematics and computing group of Boeing commercial airplanes, it was possible to devise two methods to compute second-order derivatives of relevant functionals in aerodynamics. Moreover it was possible to compute explicit solutions of tha adjoint equation of a simplified compressible flow and validate the methods found. This paves the way to coding such methods in large commercial optimization codes actually used in industry.

4.4.7. Passive control of flows with porous media

Publications: [66], [63], [62], [93], [67].
The idea is to change the shear forces on a solid body using a porous interface on the surface. This induces a significative change in the flow behaviour that yield a drag coefficient reduction up to 30Two papers have been published in 2008 A coupling of this passive control and an active control with closed loop has been also developed. New results have been obtained in 2D these last weeks. This coupling is very efficient, in particular when the passive control cannot be used, for example on a rear window. The extension to 3D flows has been performed. The results will come soon. This was part of D. Depeyras thesis [15].

4.4.8. Inverse problems in imagery

As for inverse problems in imagery, model obstacle problems governed by Laplace and Poisson equations will be considered. Shape detection will be handled by finite differences discretization of the continuous adjoint equations on a cartesian mesh. A level-set function enables the localization of the body by providing the distance of each node from its border. At each step, after determination of the shape-derivative, and alteration of the boundary, fast-marching methods operate a redistanciation process. Both direct and adjoint equations are solved by the GMRES algorithm thanks to a penalization method. An iterative procedure aiming at finding a consistent extension of the solution inside the penalized zone will be added so that the gradient evaluation along the normal, often inaccurate due to the use of this type of mesh can be significantly improved.

Even though level-set methods prove to be quite efficient in terms of dealing with topological changes, such inverse problems appear to be severely ill-posed, causing gradient-based methods to fall into local minima regions. Thus, a study of the choice of the objective function will be carried out showing the relevance of a multiscale approach where large, medium, and small contributions follow one another along iterations in W-shaped cycles.
In the long term, we plan on extending to this field some tools we developed for aeronautics [70].

5. Software

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

Participants: Charles-Henri Bruneau, Thierry Colin [correspondant], Mathieu Colin, Olivier Saut.

5.1.1. Microfluidics

We have built several codes for microfluidics. The forts one deals with bifluid Newtonian flows with surface tensor in channels, "T" junction and cross junction. We have 2D, 3D-axi-symmetric and 3D version. We use a level set method for the evolution of the interface. These codes have been validated with comparison with experiments.

The next step will be to construct a parallel solver for the Stokes equation with discontinuous coefficient adapted to our framework.

5.1.2. Biology

The numerical platform eLYSe is maturing. All the numerical codes developed on this subject are based on this platform. The platform is also being slightly adapted to have performance on par with a classical discretization on a cartesian mesh at the cost of a small increase of memory use. Some methods of eLYSe were also rewritten to take advantage of distributed architectures. The platform has received the following additions:

- Reorganization of the platform to ease maintenance and extensions. This also permits to completely separate core methods from the mathematical classes.
- New numerical schemes for the solving of Navier-Stokes equations (projection method), advection equations (more conservative schemes), Poisson and heat equations (Ghost Fluid approach, high order method to treat complex geometries...).
- New methods for importing medical images and perform segmentations on these images. The accepted formats are DICOM, Brainweb generated images, PNG, JPG.

5.2. Newtonian fluid flows simulations and their analysis

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

5.2.1. 2D and 3D Navier-Stokes

construction of three numerical codes (NSMulti2D, NSMulti3D and NSAnal) .
A parallelized version of 2D and 3D Navier-Stokes solvers are in development.

5.2.2. ROM

A Hybrid numerical code coupling DNS and Reduced Order Model based on Proper Orthogonal Decomposition is developed. This code is implemented for 2D incompressible NSE, based on the CH Bruneau code. The extension to 3D compressible flows will follow.

Several codes for system identification based on low-order models are now available. They are based on a spectral representation of the inputs and outputs to be identified. These codes allowed us to devise accurate non-linear observers for two-dimensional flows. For three-dimensional complex flows the results still need to be improved.

5.2.3. Coupled transport-diffusion equations

Richards: 2D Finite Element code coupled to transport-diffusion equations of silica and oxygen.
NSdes_SA module in FluidBox the ScAlApplix platform : 3D unstructured Finite Volume/Finite Element code to solve Navier-Stokes equations, parallel computing using MPI.

5.2.4. Particle method for compressible flows

A numerical code implementing a particle method has been implemented in 3D for the compressible Euler equations and in 2D for the compressible Navier-Stokes equations, associated in the latter case with a penalization method and a level-set method to take into account solid obstacles.

5.3. Flow control and shape optimization

Participants: Charles-Henri Bruneau [correspondant], Angelo Iollo, Iraj Mortazavi.

Recent advances in Closed-Loop and Open-Loop flow control using vortex methods for high Reynolds number flows are implemented in a Vortex-In-Cell code in order to apply them easily to various control needs.

6. New Results

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

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

6.1.1. Microfluidics

6.1.1.1. Study of asymptotics models for mixing in microchannels

We have continued with the study of asymptotics models for mixing in microchannels (PhD of J. Dambrine [14] defended in december 2009). We investigate passive mixing which consists in the following assumption : we assume that the flow is driven only by the pressure gradient, and that no other external constraint on the system are taken into account. These approaches involve surface modifications on the top and the bottom of the microchannels. Two kind of microchannels are considered here : the first one is a flat bottom channel with slip boundary conditions derived from chemical patterning; the second one is a non-flat bottom channel with a non-slipping surface The aim is to write simplified models in order to verify the accuracy of the so-called Hele-Shaw approximation. We have also considered a simplified model for wormlike miscelles flows in microchannel.

6.1.1.2. 3D numerical simulations in complex geometries for wormlike micelles

The model that has been used is the classical Johnson-Segelman model. The main difficulties were the numerical complexity of 3D computations as well has the boundary conditions. Concerning the boundary conditions, we had to deal with two different problems. The first one is how can we use Neuman-type boundary conditions with a penalty methods? It is well-know that the penalty method (that is used in order to take into account complex geometries) implies a lack of accuracy. This difficulty can be overcome using the so-called ghost fluid method that has been developed in this context by F. Gibou (University of California at Santa Barbara). F The second point concerning boundary conditions is more conceptual. The question is: what kind of boundary condition can we use for the inlet and the outlet of a channel, of a T-junction. For the inlet, the answer is clear for the velocity field but not for the stress tensor. For the outlet, nothing is clear. J. Dambrine has tested numerically several solutions involving some particular profile. For the inlet, the situation is quite satisfactory, for the outlet, no definitive answer can be given at the time being.

6.1.1.3. Effects of rugosity in microchannels

Usually the Stokes equations that govern a flow in a smooth thin domain (with thickness of order ϵ) are related to the Reynolds equation for the pressure p_{smooth}. In this paper, we show that for a rough thin domain (with rugosities of order ϵ^2) the flow is governed by a modified Reynolds equation for a pressure p_{rough}. Moreover we find the relation $p_{\text{rough}} = K\, p_{\text{smooth}}$ where K is an explicit coefficient depending only on the form of the rugosities and on the viscosity of the fluid. In some sense, we see that the flow may be accelerated using adequate rugosity profiles on the bottom. The limit system is mathematically justified through a variant of the notion of two-scale convergence: The originality and difficulty being the anisotropy in the height profile.

6.1.1.4. Modelling of foams and emulsions.

We have build a model of elasto-visco-plastic system. This model has been implemented in a 2D geometry. The model exhibits some shear-banding behaviour (PhD of Sylvain Benito [11], 3/11/2009). Even if these simulations allow us to obtain some satisfactory phenomena from the numerical point of view, there is a lack of parameter values that have to be used in the numerical codes. It will be one of the main challenges to be able to make some micro-macro coupling in order to be able to parametrize the mode

6.1.1.5. Fast numerical solver for the Laplace and Stokes Equations.

One of the main weaknesses of the computation that we made is its computational coast. We therefore decided to develop a parallel solver for the Laplace and Stokes equations that are adapted to our numerical framework (caratesian grid with penalty methods). It relies on the so-called right-hand-side method: the Laplace equation with non constant coefficient is approximated by a sequence of problem with constant coefficients that converges to the solution. Each problem can be solved on a parallel architecture using a domain decomposition method based on Schwartz algorithm with Aitken acceleration. It has been implemented in 3D for Laplace equation and in 2D for Stokes.

6.1.2. Cancer modelling

6.1.2.1. Modelling of tumor growth.

Tumor angiogenesis is the process by which new blood vessels are formed and enhance the oxygenation and growth of tumors. As angiogenesis is recognized as being a critical event in cancer development, considerable efforts have been made to identify inhibitors of this process. Cytostatic treatments that target the molecular events of the angiogenesis process have been developed, and have met with some success. However, it is usually difficult to preclinically assess the effectiveness of targeted therapies, and apparently promising compounds sometimes fail in clinical trials. We have developed a multiscale mathematical model of angiogenesis and tumor growth. At the molecular level, the model focuses on molecular competition between pro- and anti-angiogenic substances modeled on the basis of pharmacological laws. At the tissue scale, the model uses partial differential equations to describe the spatio-temporal changes in cancer cells during three stages of the cell cycle, as well as those of the endothelial cells that constitute the blood vessel walls. This model is used to qualitatively assess how efficient endostatin gene therapy is. Endostatin is an anti-angiogenic endogenous substance. The gene therapy entails overexpressing endostatin in the tumor and in the surrounding tissue. Simulations show that there is a critical treatment dose below which increasing the duration of treatment leads to a loss of efficacy. This theoretical model may be useful to evaluate the efficacy of therapies targeting angiogenesis, and could therefore contribute to designing prospective clinical trials.

6.1.2.2. Parameter estimation for prediction of tumor growth

We also worked on the system identifications aspects of tumor growth modelling. We were able to predict with small errors the prognostic of tumor growth. 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 the one 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. This problem is solved each time new data is available and has the advantage of taking into account heterogeneous data coming from different sources of medical diagnostics.

We have tested our technique on two test cases; the first one is presented below. Three CT scans were available. The two first CT scans are used for data assimilation (circles on the first figure) and the continuous line is the prediction. The time scale on the x-axis is in weeks. The error on the third CT scan is of the order of one week (and that is pretty good!). On the second figure, we present the comparison between the computation and the image for the last two scans.

For the second test case, four CT scans were available, we have used the two initial images for the prediction. The time scale on the x-axis is in months and the volume is on the y-axis. Again, the circles represent the data obtained from the images and the continuous line represents the prediction. Only the first two circles are used for the prediction.

The numerical simulations are performed with the numerical platform ModCan developed inside the MC2 team for several years.

The discretizations of each equation used in the mathematical models are already implemented in two and three dimensions in the platform. The numerical methods have also been carefully validated on large set of test cases or by comparison with analytical solutions.

6.1.2.3. Modelling of electrochemotherapy

Two articles related to the electrical cell modelling are in preparation. 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.

6.2. Flow control and shape optimization

Participants: Charles-Henri Bruneau [correspondant], Angelo Iollo, Iraj Mortazavi.

6.2.1. Active control for internal and external flows

We firstly worked on a vortex method used to simulate an incompressible two-dimensional transitional flow over a backward-facing step. The simulations are validated for two different Reynolds numbers comparing to previous studies. Two different control strategies are implemented to modify the shedding, the recirculation zone behind the step and the transport in the channel. The first technique consists in using a pulsing inlet velocity and the second one is based on local oscillating jets implemented on the step vertical wall. The influence of these controls on several characteristic functionals related to the flow was carefully investigated. Both, open-loop and closed-loop active control approaches are performed in order to choose the most efficient control methods.

On a second work, a two-dimensional laminar flow past a square cylinder is considered. Actuators placed on the cylinder enable active control by blowing and suction. Proportional feedback control is then applied using velocity measurements taken in the cylinder wake. Projection onto an empirical subspace is combined with a calibration technique to build a low-order model of the incompressible Navier-Stokes equations. This model is used within an optimization method to determine a set of feedback gains which reduces the unsteadiness of the wake at Re = 150. The resulting controlled flows are further characterized by computing the critical Reynolds numbers for the onset of the vortex shedding instability.

6.2.2. Coupling of active and passive control

In the context of D. Depeyras PhD (defended in 2009), the coupling of two flow control methods has been studied: a passive control with a wall modification using porous media and an active control with the use of blowing/sucking actuators at car back wall. The study was made with simplidied car models, in order to reduce the aerodynamic drag.

6.2.3. Compressible flow optimization

The Hessian for the quasi-one-dimensional Euler equations is derived. A pressure minimization problem and a pressure matching inverse problem are considered. The flow sensitivity, adjoint sensitivity, gradient and Hessian are calculated analytically using a direct approach that is specific to the model problems. For the pressure minimization problem we find that the Hessian exists and it contains elements with significantly larger values around the shock location. For the pressure matching inverse problem we find at least one case for which the gradient as well as the Hessian do not exist. In addition, two formulations for calculating the Hessian are proposed and implemented for the given problems. Both methods can be implemented in industrial applications such as large scale aerodynamic optimization.

6.3. Flows simulations

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

6.3.1. Analysis of 2D-turbulence

Two-dimensional turbulence admits two different ranges of scales: a direct enstro- phy cascade from the injection scale to the small scales and an inverse energy cascade at large scales. It has already been shown in previous papers that vortical structures are responsible for the transfers of energy upscale while filamentary structures are responsi- ble for the forward transfer of the enstrophy. We propose an original mathematical tool, the interaction function, for studying the space localization of the enstrophy fluxes. It is defined using an orthogonal two-dimensional wavelet decomposition.

6.3.2. Simulation of turbulent flows

In the context of the co-supervision of Christelle Wervaecke, a PhD student supervised by Boniface Nkonga, we are developping a 3D Navier-stokes solver using stabilized finite element methods to solve compressible turbulent flows. We are considering massively separated flows and therefore we propose to use Detached-Eddy Simulation (DES) to model turbulence. Stabilized finite element methods allow us to achieve high order schemes needed in high reynolds turbulence modeling. Programming is under process in the FluidBox platform. Some validations over 2D unstructured grids are performed using MPI for messages passing. Navier-Stokes equations combined with the one equation Spalart Allmaras turbulence model are solved thanks to two differents methods, with our SUPG scheme and with a finite volume scheme.The comparison should allow us to exhibit improvements supplied by our finite element method.

In the context of a project initiated during CEMRACS 2008, we studied numerical schemes for anisotropic diffusion problems. Numerous systems of conservation laws are discretized on Lagrangian meshes where cells nodes move with matter. For complex applications, cells shape or aspect ratio often do not insure sufficient accuracy to provide an acceptable numerical solution and use of ALE technics is necessary. We were interested in conduction phenomena depending on velocity derivatives coming from the resolution of gas dynamics equations. We proposed the study of a mock of second order turbulent mixing model combining an elliptical part and an hyperbolic kernel. The hyperbolic part is approximated by finite-volume centered scheme completed by a remapping step. The discretization of the anisotropic parabolic equation on polygonal distorted mesh is based on the scheme proposed by Lipnikov, et al. ensuring the positivity of the numerical solution. We propose an alternative based on the partitioning of polygons in triangles. We show some preliminary results on a weak coupling of hydrodynamics and parabolic equation whose tensor diffusion coefficient depends on Reynolds stresses.

6.3.3. Simulation of water distribution systems

In a first part we presented and validated an improved formulation of the hydraulic network equations that incorporate pressure-dependent leakage in Water Distribution Systems. The formulation was derived from the Navier-Stokes equations and solved using an adequate splitting method. An implicit numerical scheme was used to solve the p-Laplacian equation. The model was validated on a benchmark pipe network.

In a second part, direct water quality modelling and the associated unsteady sensitivity equations, are solved in Water Distribution Systems (WDS). A new solution algo- rithm is proposed, based on a time splitting method to separate and solve efficiently each phenomenon such as advection and chemical reaction. This numerical approach allows a simultaneous solution of both the direct problem and the sensitivity equa- tions. Special attention is given to the treatment of advection, which is handled with a Total Variation Diminishing (TVD) scheme. The general model presented in this study permits a global sensitivity analysis of the system and its efficiency is illustrated on two pipe networks. The importance of the sensitivity analysis is shown as part of a fitting process on a real network.

6.3.4. Improvements of ROM

A first work focuses on improving the stability as well as the approximation properties of Reduced Order Model (ROM) based on Proper Orthogonal Decomposition (POD). The ROM is obtained by seeking a solution that lives in the POD subspace and at the same time minimizes the Navier-Stokes residuals. A modified ROM that directly incorporates the pressure term is proposed. The ROM stabilization makes use of methods based on the fine scale equations. The solution to these equations are approximated using the residuals of the Navier-Sokes equations. The improvement of the POD subspace is performed thanks to an hybrid method that couples direct numerical simulations (DNS) and reduced order model simulations. The methods proposed are tested on the two-dimensional confined square cylinder wake flow in laminar regime.

A second work explores some numerical alternatives that can be exploited to derive efficient low-order models of the Navier-Stokes equations. It is shown that an optimal solution sampling can be derived using appropriate norms of the Navier-Stokes residuals. Then the classical Galerkin approach is derived in the context of a residual minimization method that is similar to variational multiscale modeling. Finally, calibration techniques are reviewed and applied to the computation of unsteady aerodynamic forces. Examples pertaining to both non-actuated and actuated flows are shown.

6.3.5. Penalization method

The aim of our work is to combine penalization and level-set methods to simulate compressible and incompressible flows, and to perform inverse or shape optimization on uniform cartesian meshes. Special care is devoted to the solution of the governing equations in the vicinity of the penalized regions. Methods have been introduced to increase the accuracy of the discretization, by the mean of the penalization term or by modifying the numerical fluxes at the interface. Another essential feature of the optimization technique proposed is the shape gradient preconditioning. This aspect turns out to be crucial since the problem is infinite dimensional in the limit of grid resolution. Examples pertaining to model inverse problems and to shape design for Stokes flows are been discussed, demonstrating the effectiveness of this approach.

6.3.6. Simulations of fluid-solid interaction

Modeling and simulation of two-dimensional flows past deformable bodies is considered. The incompressible and compressible 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 penalisation 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. The application considered are notably fish-like swimming and insect flight. The propulsion efficiency for different swimming modes is investigated. Some control problems related to underwater manouvering and school swimming are also explored. Two PhD have begun in the context of these studies in September 2009 (Yannick Gorsse and Jessica Hovnanian).

Incompressible and compressible 2D Navier Stokes sequential code including penalization and level set methods have been written. Body motions are computed from aerodynamic forces and torques.

In order to model in flight icing and particularly ice-shedding, a vortex method for the simulation of the interaction of an incompressible flow with rigid bodies is used to compute the trajectories of ice chunks. The method is based on a penalization technique where the system is considered as a single flow. The bodies around which the flow is computed are modeled using the so-called penalization method or Brinckman-Navier-Stokes equations in which the bodies are considered as porous media with a very small intrinsic permeability.

The geometry is described using level-sets. Challenging points are first to increase the accuracy of boundary conditions using penalization and second to put turbulence models to achieve realistic simulations. Code development is under process.

6.3.7. Porous media

Task 1 An hybrid particle level-set method for convection-diffusion problems in porous media is investigated with I. Mortazavi and S. Huberson (LEA Poitiers).
Details: In this work a particle level-set method is coupled to a streamline technique in order to obtain accurate approximations of transport-diffusion problems in porous media. The convective part is resolved using a modified streamlines technique and the diffusion is approximated taking advantage from a level-set framework applied to particle methods. Several bench tests are then simulated to validate the new method.
Task 2 Numerical coupling between hydrodynamic and geochemical process in variably saturated coastal permeable sediments. Collaboration with EPOC UMR CNRS 5805 from Bordeaux I University (EPOC: Environnements et Paléoenvironnements OCéaniques). Co-supervision of Romain Chassagne a PhD student from EPOC.
Details: We have developed a 2D numerical model that couples Richards' equation with transport-diffusion equations of silica and oxygen in beach permeable sediment submitted to tides. The flow into the sediment is described by the Richards' equation which generalizes the Darcys law for variably-saturated porous media. The velocity field and the watertable location, deduced from the numerical resolution of the Richards equation, are introduced into the transport diffusion-equation of silica and oxygen. Tidal oscillations are modeled as a sinusoidal pressure boundary condition along the beach slope. Both flow characteristics and concentration are solved by finite element method. 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).

6.4. Other studies

Participants: Mathieu Colin, Thierry Colin.

Publications [32], [30].
Since MC2 has been created, we stop progressively the activity on laser-plasma interaction. However we present here a few results obtained in 2009.

Short pulses approximation in dispersive media: we derive various approximations for the solutions of nonlinear hyperbolic systems with fastly oscillating initial data. We first provide error estimates for the so-called slowly varying envelope, full dispersion, and Schrödinger approximations in a Wiener algebra; this functional framework allows us to give precise conditions on the validity of these models; we give in particular a rigorous proof of the "practical rule" which serves as a criterion for the use of the slowly varying envelope approximation (SVEA). We also discuss the extension of these models to short pulses and more generally to large spectrum waves, such as chirped pulses. We then derive and justify rigorously a modified Schrödinger equation with improvedfrequency dispersion. Numerical computations are then presented, which confirm the theoretical predictions.

Stability of solitary waves for a system of nonlinear Schrodinger equations with three wave interaction: In this paper we consider a three components system of nonlinear Schrödinger equations related to the Raman amplification in a plasma. We study the orbital stability of scalar solutions of the form $(e^{2i\omega t}\varphi, 0, 0)$, $(0, e^{2i\omega t}\varphi, 0)$, $(0, 0, e^{2i\omega t}\varphi)$, where φ is a ground state of the scalar nonlinear Schrödinger equation.

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, Delphine Depeyras.

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. 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 action

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.

8.2. National actions

8.2.1. ANR Scan2

Participants: Charles-Henri Bruneau, Thierry Colin.

The projet is with Rhodia (and Saint Gobain) 2006-2009. The aim is to compute flows in microfluidics. We focus on the formation of droplets, the stability of jets and more generally on stability of interface in microchannels for the elaboration of specific devices.

8.2.2. ANR MANIPHYC

Keywords: *Simulations of complex fluids*.

Participants: Charles-Henri Bruneau, Thierry Colin.

Collaboration with Rhodia-Lof and University of Lyon 1, 2008–2011.

8.2.3. ANR COMMA

Keywords: *algorithms*, *models*, *multi-physics problems*, *multi-scale problems*.

Participant: Iraj Mortazavi.

The P.I. is Georges-Henri Cottet (Grenoble).

See also the web page http://www-lmc.imag.fr/COMMA/.

8.2.4. ANR CARPEiNTER

Keywords: *Cartesian grid*, *complex flow*, *penalization method*.

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

The P.I. is Angelo Iollo.

8.2.5. ANR CORMORED

Keywords: *Low-order model*.

Participants: Michel Bergmann, Angelo Iollo.

The P.I. is L. Cordier (Poitiers).

8.2.6. Grant with the Aquitaine District.

Keywords: *Complex fluids*.

Participants: Charles-Henri Bruneau, Mathieu Colin, Thierry Colin.

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

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), hôpital 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.

In collaboration with Houston (2008–2010). Parallel computation tools for complex fluids and biology.

8.4. International actions

8.4.1. VORTEX CELL

Keywords: *Vortex cell method*.

Participant: Angelo Iollo.

The P.I. is Sergei I. Chernyshenko (Imperial College, London) with Southampton University.

VortexCell2050 will deliver a new technological platform combining the two cuttingedge technologies, the trapped-vortex and the active flow control. The project outcomes will serve the designers of the next-generation thick-wing aircraft. Success of VortexCell2050 will ensure European Aeronautical Sector a leadership in a small but critical area, the importance of which will grow in the future with an increase in aircraft size. VortexCell2050 exploitation route involves the application of the new technological platform to a relatively small High-Altitude Long-Endurance aircraft.

8.4.2. 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 had the visti of Eyal Arian, from Boeing company of Seattle (Shape optmization), M. Garbey, from University of Houston (parallel computing for biology medicine), S.Manaa, Mosul University and Duhok University (POD for turbulence flow).

9. Dissemination

9.1. Organization of workshops

- Organization of a workshop on cancer: interdisciplinary research in Modelling, Simulation and surgery of tumors, the methodist hopital, Houston, Texas USA, Dec 3–4, 2009.
- A cemacs project during summer 2009 on modelling tumor growth.

9.2. New positions for former members

Former PhD students:

Sylvain Benito: ATER, Ecole Central de Nantes.
Marie Billaud: Post-doc at CELIA.
Frederic Chantalat: Contract with ADERA(Bordeaux).
Julien Dambrine: Post-doc, Université Paris V.
Delphine Depeyras: In formation for the industry private sector.
Federico Gallizio: Optimad: engineering company spin off Politecnico di Torino.
Élodie Jaumouillé: Cemagref. Post-doc at CERFACS. starting february 2010.
Edoardo Lombardi: Optimad: engineering company spin off Politecnico di Torino.
Gabriele Ottino: Research Engineer at CFD enginering in Genoa.
Jessie Weller: Post-doc at Politecnico di Torino.

Former MC2 Post-doc:

Christophe Picard Assistant professor ENSIMAG, Grenoble.

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