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Project-Team mc2

Modeling, control and computations: applications to fluid mechanics.

Futurs

THEME NUM

Activity Report

2007

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1. Team

MC2 has been created in july 2007. We focused the thematics of MC2 on fluid mechanics. We stop (progressively) our activity on laser-plasma interaction. This concerns Mathieu Colin, Thierry Colin and Olivier Saut.

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2. Overall Objectives

2.1. Presentation

The aim of this project is to develop modeling tools for problems of fluid mechanics in order to explain, control, simulate and predict some phenomena coming from physics, chemistry, biology or engineering. The complexity can be in the model itself, in the coupling phenomena, in the geometry or in non-standard applications. The challenges will be to develop stable models and adapted numerical methods that enable us to recover the main physical features and that can be used in realistic situations. With these modeling tools we will construct numerical codes that can be used for practical and industrial applications.

We are interested in high Reynolds number flows, interface and control problems in Physics and biology. Our approach is the following: we first determine some reliable models and then we perform a mathematical analysis (including stability). We develop the numerical methods that are adapted to the specific situations and we implement them on some applications. In the next paragraphs, we explain our main goals using this approach, 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. Modeling

In this context, **modeling** stands for:

Phenomenological : use of ad-hoc models in order to represent some precise phenomena. One example of such models is the construction of nonlinear differential laws for the stress within the context of visco-elastic fluids. Another example is the wall conditions in microfluidics (fluids in micro-channels) that are often taken heuristically in order to model the slip at the boundary, Finally, we also use input/output models in control theory that are useful to model the result of a process without describing it precisely.

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 have fast predictions (Hele-Shaw approximation in microfluidics).

Numerical : direct numerical tools are used to represent the physical phenomena. The choice of the method is not made a priori but after the analysis of the model to find out the most convenient one with respect to stability, accuracy and efficiency. A typical example is the POD (proper orthogonal decomposition) and its use in control theory to obtain fast simulations.

2.1.1.2. Analysis and computation

Once the model has been determined, we want to perform a mathematical analysis on it. 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 (bifluid flows, miscible fluids), tumor growth, complex fluids. 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.

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 for high Reynolds flows, optimization and control and Rhodia (biggest french company of chemistry) for interface problems and complex fluids.

Academic: CPMOH (Laboratory of Physics, Bordeaux 1 University) for high Reynolds flows, optimization and control, and the medical school of Lyon for tumor growth.

2.1.2. The production of numerical codes

We want to handle the whole process from the modeling 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. 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) *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.
iii) *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.

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 in several boxes:
1) Definition of the geometry and of the penalization zones.
2) Specification of the model in itself (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 modeling 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

Stability of jets in micro-channels. Because of surface tension, a jet of one viscous fluid into another is usually unstable (Rayleigh-Plateau instability). The confinement in a micro-channel can change this stability. We have performed a stability analysis of this situation as well as direct computations. Our results perfectly match with experimental situation and we are able to predict the stability diagram.

The control of the flow around a simplified car or truck by the porous interfaces technique give two papers accepted for publication this year. In some cases the drag reduction achieved can reach 30% of the total drag and the mechanisms responsible of these gains are quite well understood. The extension in 3D is under process.

We developed an hybrid method dedicated to predict complex flows in "real time" calculations, or at least to reduce significantly the numerical costs. This method uses both numerical simulations (DNS, LES, *etc*) and reduced order models (ROM) based on a Proper Orthogonal Decomposition (POD)-like formulation. The finality of this hybrid method is to substract the part of the system that is the best modelled to concentrate the numerical effort on what is difficult to forecast, like dynamical bifurcations.

3. Scientific Foundations

3.1. Introduction

We are mainly concerned with complex fluid mechanics problems. The complexity consists in the rheological nature of the fluids (non newtonian fluids), in the coupling phenomena (in shape optimization problems), in the geometry (micro-channels) or in 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 the interface problems and for shape optimization. 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 make this kind of thing systematic.

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

Keywords: *Multi-fluid flows*, *biology*, *microfluidics*.

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

3.2.1. Microfluidics

By a complex fluid, we mean a fluid containing some mesoscopic objects, that is to say 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 [54] and on instability of lamellar phases [89], [85].

A new lab (Rhodia LOF) has been built recently in Bordeaux. It is a common lab between the CNRS and Rhodia. One of its goals is to develop experimental tools in order to use microfluidics in Chemistry. 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. Furthermore, one can observe very stable flows and quite unusual regimes that enables us to make more precise 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 3 D simulations covering a large range of situations. For example one wants 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 [63].

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 are showing that this is not the case: 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 G. Cristobal, J.-B. Salmon, M. Joanicot, A. Colin. A grant (ACI) has been obtained on this subject in 2004 and 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.

First work has been done on a micro-viscosimeter. The results have been published in [66], [67], [68].

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. This implies performing 3 D, time dependent 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. Microchanels 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. Tumor growth

The growth of a tumor is also 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.

What are the challenges in this direction? The first one is probably 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 [78] where the efficacy of radiotherapy is studied and in [80] 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 [45], [64], [65] 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 [78].

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 [77], see Cottet-Maître [55]. 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.

3.3. Newtonian fluid flows simulations and their analysis

Keywords: *Analysis*, *Simulation*.

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. But an important point is to well understand the phenomena. 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 solution.

The first method affordable in 2D, is to directly solve the genuine Navier-Stokes equations in primitive variables (velocity-pressure) on Cartesian domains [51]. 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 [46]. 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 [56]. 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 [81] 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 [86]. 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) [69]. 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. *Construction of a fast, hybrid method*

To construct these fast methods, we propose an hybrid method dedicated to predict complex flows in real time calculations, or at least to reduce significantly the numerical costs. This method uses both numerical simulations (DNS, LES, etc) and reduced order models (ROM). A reduced order model is built and integrated in time as long as it is considered to be making a good job. When it is considered to not be adapted any more, it has to be re-actualized using a few solutions of the detailed model (DNS). Using such a process one can see that the greatest part of the simulation is devoted to the reduced order model (POD ROM) so that the whole simulation is greatly accelerated. Physically, we follow the large eddies (POD), and if it is required we can modify them and possibly add smaller eddies (which could be important for controlled flows for example). The POD ROM is considered to be doing a good job while the norm of the Navier-Stokes residuals is less than a given threshold. If not, the POD basis is improved. When the size of the extended basis becomes too large, a new POD compression is performed. The POD basis is thus able to adapt itself to the new dynamic of the flow. In order to improve the effectiveness of the method, we don't actually solve a reduced order model to obtain the temporal coefficients $a(i)$: they are determined using a nonlinear Galerkin method which consists in minimizing the norm of the Navier-Stokes residuals onto the subspace spanned by the POD basis.

Another idea is the coupling between a full order simulation and a reduced order model. The purpose is to reduce the extent of the simulation domain and hence the computational costs. In a broad sense, there exist many applications where far from the boundary, the solution is weakly dependent on the details of the boundary geometry. In such regions, we use a reduced order model based on POD to solve the problem. This approach allows a representation of the solution by a small number of unknowns that are the coefficients of an appropriate Galerkin expansion. Therefore, away from a narrow region close to the boundary of interest, the number of unknowns is drastically reduced. Like all other approaches based on POD, a solution database is necessary to build the Galerkin modes, therefore this method will be useful when many computations for relatively similar cases are to be performed, like for example in fluid structure interaction. The idea of using

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[1] Reynolds-Averaged Navier-Stokes

[2] Large-Eddy Simulation

models that take into account different physical phenomena in different sub-domains is old. We want to renew this approach using a low order model.

3.3.3. Analysis of the flows

Once a good simulation of the phenomena is obtained it is necessary to properly analyze the data we get. The classical analysis tools such as the Fourier transform, the wavelets [58] or the proper orthogonal decomposition [69] can give various results when used with various parameters. So the aim of this work is, on the one hand to determine the range of the parameters giving reliable results, and on the other hand to find out the statistical laws observed by the flow in configurations uncovered by the theory. Another approach to better evaluate the analysis tools is to use a placebo effect. It is achieved for instance by creating an artificial velocity field where a fundamental characteristic of the flow is not present and by using the classical methods able to detect this characteristic. If the method detects the characteristic it means that it is created by the method itself !

3.4. Flow control and shape optimization

Keywords: *Flow Control*, *Shape Optimization*.

Participants: Charles-Henri Bruneau, Angelo Iollo, Iraj Mortazavi, Frédéric Chantalat, 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 [49]. 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 [50]. 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 [62].

A similar procedure is also used in the estimation based on gappy POD, see [87] and [88]. 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 [53] 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 [70] 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 [83]. 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

Keywords: *Multi-fluid flows*, *biology*, *microfluidics*.

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

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

4.2.1. Modeling 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.

4.2.2. Numerical techniques

In order to describe the evolution of the interface we use a level set method [76], [75], [82]: 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 [72]. 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.

4.2.3. Extensions to mixing models

This approach can be extended with the same formulation to other physical settings. For example, we plan to use 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 will be, in this case, the rheological law that gives the stress σ in terms of the velocity and of the order parameter φ.

For a miscible fluid, we plan to elaborate first a 2D version that will be obtained by a Hele-Shaw approximation: we consider that the vertical variations of the flow are large with respect to the horizontal ones. Taking the mean value in the vertical direction for the horizontal velocity leads to the introduction of a 2D Darcy's law type of model. This will rapidly bring qualitative results that can be compared to experiments.

4.2.4. Application 1 : computation of two newtonian fluids flow in a "T"-junction

This study has been initiated in the thesis of S. Tancogne and P. Vigneaux. The aim is 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. From the technical point of view, this step is necessary in order to select the method that will be implemented in our platform **eLYSe**. Of course, it has to be validated for real situations and we need to do a feed-back to the experiment and try for example to determine the stability of jets, coflows and droplets for large scale of parameters. From the theoretical point of view, the main problem is to prove some linear stability results with a spectral approach.
We need basically one more year to completely validate our results with experiments. The next step is to develop the code **eLYSe** in order to handle complex geometries. A post-doc (funded by ANR) will arrive for two years in october 2007. Permanent researchers involved in this part of the project are C.-H. Bruneau for CFD, O. Saut for computer science and parallel computing, T. Colin and C. Galusinski for the modeling part.

4.2.5. 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 [74], [73] with phase fields models. Finally, these models of mixing will be coupled with reaction equations describing chemistry experiments.

4.2.6. Application 3 : study of droplets

A direct study will consist in computing the flow inside a droplet to be able to quantify the influence of the parameters: velocity of the flow, surface tension... Then this velocity field will be coupled with the mixing models to predict how the mixing can occur in a droplet. Another point of view will be to study numerically the formation of droplets, that is the stability of a jet. All these results will be compared with the experiments done at Rhodia-LOF.

Coupling of mixing in droplets motion will be done within the **eLYSe** framework.

4.2.7. Application 4 : modeling the mixing of oil-water-polymer in a porous medium

As quoted before, we 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.

4.2.8. Application 5 : 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 is the goal of the thesis of S. Benito (advisor C.-H. Bruneau and Th. Colin) and it is a collaboration with C. Gay (CRPP).We need 2 years in order to validate our model and to implement it in 3D situations. The next step will be to use it for modeling in microfluidics and to extend it to other situations, especially to applications in biology (behavior of tissues, of tumor,...)

4.2.9. The application for biological modeling

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. Generally, it is admitted that an avascular tumor does not contain more than 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 called the process of angiogenesis. 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 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.

– *Avascular stage.* For the time being, we have a rough 3D model of avascular tumor growth. In order to increase the biological information in the model, one has to add the influence of acidity, several different phenotypes, as well as senescence problems. We also need to immerse this part of code 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 modeling.

– *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.

– *Coupling with therapeutics.* It is one of the goals of our project to use our model to test therapeutic protocols. This will be done 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 application to therapeutics innovation is a long term project.

4.2.10. Extensions to chemical engineering and biotechnologies

On a long term period, we want to apply our models to chemical engineering processes, auto-catalysis processes. We are also in contact with some biotechnology companies for production of drugs.

4.3. Newtonian fluid flows simulations and their analysis

Keywords: *Simulation*, *flow analysis*.

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

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 [51]. Since the first paper on the penalization method [46], 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 [84] 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 [59] and [71]. Recent results [57] and [61] show that some significant progress is possible. All these works give rise to the construction of three numerical codes (NSMulti2D, NSMulti3D and NSAnal) that we are going to use and develop further on.

4.3.1. Simulation of a synthetic or pulsed jet

The 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 work is proposed by Renault and PSA inside a PREDIT project for 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 [60]. 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.

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. [71]). 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 ([57]).

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. Detached-eddy simulation

A better understanding of the coupling mechanisms between RANS and LES models is needed. DESGIVRE is a three years project between Airbus and MC2 INRIA Futurs called DES analysis of aircraft performance degradation due to ice accretion. The overall objectives are the following:

- Developing the DES model for the simulation of 3D turbulent flows;
- Discuss the issues that impact the method, including the underlying RANS turbulence model and the simulation design for DES (grids and choice of time steps);
- Use Airbus test cases to answer the following question: is it possible and advisable to use DES to quantify the performance degradation due to icing;
- Analysis of the available post-processing for DES. Draw perspectives on the use of Proper Orthogonal Decomposition (POD) for DES simulations.

It is a three years collaboration of H. Beaugendre with B. Nkonga (ScALApplix).

4.3.5. Reduced order models

We will concentrate on two different problems. For the residuals minimization approach that we propose, we will consider two-dimensional low-Reynolds numbers flows to start with. In particular we will check the robustness of this self-adaptive model by changing the Reynolds number. In the following the robustness will be checked with respect to the application of different control laws. We will concentrate our attention on a posteriori bounds on the error introduced by the low order model.

On the other hand we will continue the study of classical Galerkin models based on POD. The objective will be that of improving the approximation performances of the POD basis in complex three-dimensional flows. Moreover, we will try to develop system identification techniques based on the solution of inverse problems by efficient and robust tools. This will allow us to build calibrated models using O(100) POD modes. This model dimension is out of reach at the moment, but it is a necessary step to identify complex flows. C.H. Bruneau, A. Iollo and one post-doc (M. Bergmann) are working on preliminary studies.

4.4. Flow control and shape optimization

Keywords: *Flow Control*, *Shape Optimization*.

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

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 will model both passive and active control. Passive control will consist in steady devices which do not evolve in time, whereas active control will have 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 are under development in 2D and 3D. A PhD thesis (Delphine Depeyras) has started in October 2006 in collaboration with Patrick Gillieron at Renault Company (advisers CH Bruneau and Iraj Mortazavi) [49].
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 modeling and the numerical issues of such problem. The study is performed in collaboration with CPMOH laboratory in Bordeaux (H. Kellay) [44], [48].
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 [52].
This part of the project concerns C.-H. Bruneau, A. Iollo, I. Mortazavi.

4.4.2. Active control

The effect of a synthetic or a pulsed jet to reduce the drag is studied. First tests in 2D are done for the flow around Ahmed body. The extension both to close loop control and to 3D simulations will come. The aim is to obtain a 30% decrease of the drag coefficient. This is a part of Delphine Depeyras' thesis.
We will derive accurate low-order models based on sophisticated system identification techniques including the effect of boundary actuators. Using this low-order models we will compute an approximate gradient of a stabilization functional with respect to the control parameters. A posteriori bounds on the gradient error will determine a trust region for a descent step in order to ensure convergence. What's more, a state estimate is sought in order to provide the correct feed back to the actuators. A. Iollo and three PhD students (M. Buffoni, E. Lombardi, J. Weller) are involved [47].

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.
In shape design for turbomachinery we are launching a PhD with the collaboration of Turbomeca, we expect to be able to perform shape optimizations of 3D blades for reduction of noise, using simplified models. A. Iollo is dedicated to this theme with H. Telib [83].

4.4.5. 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.
We are just starting in this direction. F. Chantalat (research engineer) as well as C. Galusinski and A. Iollo work on it. In a long term period we will try to extend to this field some tools we developed for aeronautics [53].

5. Software

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

Keywords: *Multi-fluid flows*, *biology*, *microfluidics*.

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

5.1.1. Microfluidics

This last 3 years 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-symetric 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 include these codes in the platform eLYse.

5.1.2. Biology

The numerical platform eLYSe is maturing. The platform is already used for our biological simulations. Work is still ongoing to finish abstracting the boundary conditions in the 3D version (which was completed for the 2D version). 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.

5.2. Newtonian fluid flows simulations and their analysis

Keywords: *Proper Orthogonal Decomposition*, *Reduced Order Model*, *Simulation*.

Participants: Charles-Henri Bruneau [correspondant], Iollo Angelo, Michel Bergmann.

A parallelized version of 2D and 3D Navier-Stokes solvers are in development.

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.

5.3. Flow control and shape optimization

Keywords: *Control*, *Simulation*, *Vortex Method*.

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

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

Keywords: *Multi-fluid flows*, *biology*, *microfluidics*.

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

6.1.1. Microfluidics

Concerning microfluidics, we now have a 3D code describing the evolution of a diphasic flow in microchannels with "T" junctions. It is based on a level-set method. We are able to compute the formation and the evolution of droplets in a confined environment (see fig. 1). We compute the recirculation in the droplets and in the channel. Two versions of the code are available: in rectangular geometry (real 3D) as well as in the axi-symmetric case. Moreover we have performed a stability analysis of a jet in a microchannel. This analysis relies on a linearization procedure of the Navier-Stokes equations with an interface. We explain the phase diagrams observed experimentally. Concerning mixing in microchannel, we have proved numerically that the Hele-Shaw approximation is valid for shallow channels as long as one is concerned with interdiffusion. For more active mixing, this approximation fails and one has to compute real 3D flows.

We have considered two types of microchannels : a flat bottom with slip boundary conditions and a non-flat bottom with a non-slipping surface.

Bifluid flows with low velocities have to take into account surface tension forces. Numerical difficulties follow, namely for very low flow velocities where numerical parasitic currents appear. An other difficulty concerning low flow velocities is the cost of the numerical stability condition due to surface tension forces. A new stability condition which takes into account all fluid characteristics (density and viscosity) is derived (submitted paper). For low Reynolds (this is the case for our microfluidic applications), this condition degenerates and involves only viscosity [23]. Paul Vigneaux has defended his PhD on July 2007 on this subject.

6.1.2. Biology

New results : cancer growth

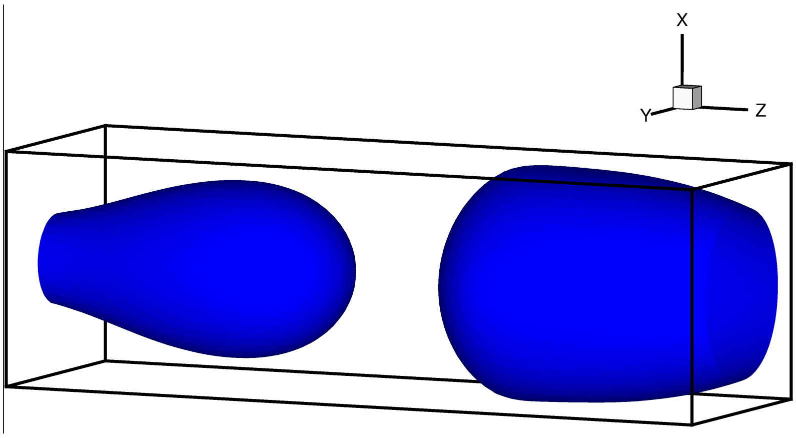

Figure 1. Evolution of droplets in a confined environment.

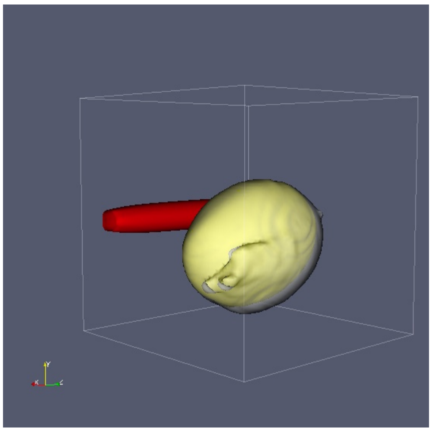

Figure 2. A tumor growing toward a blood vessel in red. Quiescent cells are drawn in grey, dividing cells in yellow. The initial data of this run comes from a scan of a lung tumor.

In 2007, we have continued developing models for tumor growth. The model [79] for avascular growth was improved in three directions:

- **Realistic simulations from medical data and validation:** our simulations are now performed using scans from patients to obtain the initial shape of tumor (as shown on Fig. 2), work has started on the validation of the model using in-vitro and in-vivo experiments. We have contacts within the division of NeuroScience at Rush University to obtain time evolution of brain tumors and in vitro experiments. We also have privileged access to the Centre Leon Berard through one of our co-authors.
- **Distributed computing:** we have adapted some methods of our computational platform (eLYSe) for distributed computing using open standards (MPI).
- **Complexification of the model:** Our model [79] used a Stokes equation to determine the velocity of cells due to cellular division. This basically assumes that cells have a fluidic movement. In order to be more realistic, we have developed a visco-elastic model of the movement. In this new model, healthy cells are considered as solid to model cell-cell adhesion and cancer cells are more liquid. Work is ongoing to add a realistic description of cell-matrix adhesion. The new model also accounts for the acidification caused by cancer cells and its effects on apoptosis. This model was discretized in 2D and the 3D version is being developed. Early simulations show that this model is much closer to the biological processes involved in cancer growth that the previous one.

We have also developed a simplified model for the angiogenic phase of a cancer, where the tumor makes the organism generates blood vessels for its own consumption (when most of its cells are quiescent because of hypoxia). We have developed a simplified continuous model describing the evolution of two angiogenic factor, two endothelial cells types and one anti-angiogenic molecule. This gives at each point the density of endothelial cells using reaction-diffusion and chemotaxy equations. It shall be noted that with a continuous model we lose the topological aspect of the blood network. We are now capable of running simulations of the avascular and angiogenic stages of a tumor. We have started writing a discrete model to compare with the continuous one.

6.2. Newtonian fluid flows simulations and their analysis

Keywords: *Proper Orthogonal Decomposition*, *Reduced Order Model*, *Simulation*.

Participants: Charles-Henri Bruneau [correspondant], Iollo Angelo, Michel Bergmann.

The principal results concerns the analysis of 2D turbulence ([15], [17], [16]). A filtering of numerical solutions of 2D turbulence is achieved by means of wavelet packets and possible biases are analysed. The coexistence of both direct enstrophy cascade and inverse energy cascade are studied computing energy and enstrophy spectra and fluxes.

We are able to simulate a flow control based on synthetic jet actuation in two- as well as three dimensional configurations. This simulation is based on the AERO code developped at INRIA Sophia Antipolis by A. Dervieux and B. Koobus. From these simulations we derive a low-order model including the control effects and give an approximation of the gradient of a flow related cost functional by such low-order model. As for hybrid models, we gave examples of how to couple a low-order model to a full simulation by a Schawrz method in an efficient way. These was shown on compressible flows.

We propose an hybrid method dedicated to predict complex flows in "real time" calculations, or at least to reduce significantly the numerical costs. This method uses both numerical simulations (DNS, LES, *etc*) and reduced order models (ROM) based on a Proper Orthogonal Decomposition (POD)-like formulation.
A reduced order model is built and integrated in time as long as it is considered to make a good job. When it is considered to be not adapted any more, it has to be re-actualiazed using a few solutions of the detailled model (DNS). Using such a process one can see that the greatest part of the simulation is devoted to the reduced order model (POD ROM) so that the whole simulation would be greatly accelerated. Physically, we follow the large eddies (POD), and if it is required we can modify them and eventually add smaller eddies (which could be important for controlled flows for example).

The POD consists to approximate a given flow field $U(x,\,t)$ with the decomposition $\widetilde{U}(x,\,t) = \sum_i a^{(i)}(t)\Phi^{(i)}(x)$. The POD ROM is considered to make a good job while the norm of the Navier-Stokes residuals evaluated from the solution $\widetilde{U}(x,\,t)$ is less than a given threshold. If not, the POD basis $\Phi^{(i)}$ is improved by adding a new mode evaluated as being the orthogonal component of a detailled solution $U(x,\,t)$. When the size of the extended basis becomes greater than a desired threshold, a new POD compression is performed. The POD basis is thus able to adapt itself to the new dynamic of the flow. In order to improve the effectiveness of the method, we actually don't build and solve any reduced order model to obtain the temporal coefficients $a^{(i)}$: they are determined using a nonlinear Galerkin method which consists in minimizing the norm of the Navier-Stokes residuals onto the subspace spanned by the POD basis.
The finality of this hybrid method is to substract the part of the system that is the best modelled to concentrate the numerical effort on what is difficult to forecast, like dynamical bifurcations.

6.3. Flow control and shape optimization

Keywords: *Control*, *Simulation*, *Vortex Method*.

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

Recent advances in Closed-Loop and Open-Loop flow control using vortex methods for high Reynolds number flows are investigated.

We were concerned by passive control of bluff bodies flow ([20], [19], [18]).
We are able to simulate a flow control based on synthetic jet actuation in two- as well as three dimensional configurations. This simulation is based on the AERO code developped at INRIA Sophia Antipolis by A. Dervieux and B. Koobus. From these simulations we derive a low-order model including the control effects and give an approximation of the gradient of a flow related cost functional by such low-order model.

Inverse problems based on level sets for fluids and medical imagery turned out to be a viable tool. We have set up a multiscale method to solve inverse problems and gave examples of topological optimisation for Stokes flows. In turbomachinery design we realised a code that is capable of optimising an aeronautical propeller with a simplified model that takes into account the emitted noise.

7. Contracts and Grants with Industry

7.1. Program PREDIT

Participants: Charles-Henri Bruneau, Patrick Gilliéron, 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. 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.

7.3. Renault

Participants: Charles-Henri Bruneau, Iraj Mortazavi, Delphine Deyperas.

This study is organized around the PhD of Delphine Deyperas that is funded half by Renault and half by the CNRS concerning passive control for the drag reduction.

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 COMMA

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

Participant: Iraj Mortazavi.

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

Voir aussi la page web http://www-lmc.imag.fr/COMMA/.

8.2.2. ANR COBORD

Keywords: *Numerical model for the control on the boundary fluid mechanics and nano optics*.

Participant: Iollo Angelo.

COBORD is devoted to the study of numerical methods allowing the solution of control problems by means of boundary controls through accurate and robust low order models. Using these tools or more classical approaches inverse problems. such as shape optimization or system identification are attacked.

8.3. International actions

8.3.1. 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.

9. Dissemination

9.1. Visitors

We have had the visti of Eyal Arian, Boeing company of Seatle (Shape optmization), and M. Garbey, University of Houston (parallel computing for biology medicine).

9.2. Organization of workshop

We organized a session of the GdR MABEM (Mathematics in Biology) in Bordeaux Dec 6-7 2007.

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