



INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

*Project-Team Opale*

*Optimization and Control, Numerical  
Algorithms and Integration of  
Multidisciplinary Complex P.D.E. Systems*

*Sophia Antipolis - Rhône-Alpes*

THEME NUM

*Activity*  
*R* *eport*

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# 1. Team

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# 2. Overall Objectives

## 2.1. Research fields

Optimizing a complex system arising from physics or engineering covers a vast spectrum in basic and applied sciences. Although we target a certain transversality from analysis to implementation, the particular fields in which we are trying to excel can be defined more precisely.

From the *physical analysis* point of view, our expertise relies mostly in Fluid and Structural Mechanics and Electromagnetics. In the former project Sinus, some of us had contributed to the basic understanding of fluid mechanical phenomena (Combustion, Hypersonic Non-Equilibrium Flow, Turbulence). More emphasis is now given to the coupling of engineering disciplines and to the validation of corresponding numerical methodology.

From the *mathematical analysis* point of view, we are concerned with functional analysis related to partial-differential equations, and the functional/algebraic analysis of numerical algorithms. Identifying the Sobolev space in which the direct or the inverse problem makes sound sense, tailor the numerical method to it, identify a functional gradient in a continuous or discrete setting, analyze iterative convergence, improve it, measure multi-disciplinary coupling strength and identify critical numerical parameters, etc constitute a non-exhaustive list of mathematical problems we are concerned with.

Regarding more specifically the *numerical aspects* (for the simulation of PDEs), considerable developments have been achieved by the scientific community at large, in recent years. The areas with the closest links with our research are:

1. *approximation schemes*, particularly by the introduction of specialized Riemann solvers for complex hyperbolic systems in Finite-Volume/Finite-Element formulations, and highly-accurate approximations (e.g. ENO schemes),
2. *solution algorithms*, particularly by the multigrid, or multilevel and multi-domain algorithms best-equipped to overcome numerical stiffness,
3. *parallel implementation and software platforms*.

After contributing to some of these progress in the former project Sinus, we are trying to extend the numerical approach to a more global one, including an optimization loop, and thus contribute, in the long-term, to modern scientific computing and engineering design. We are currently dealing mostly with *geometrical optimization*.

*Software platforms* are perceived as a necessary component to actually achieve the computational cost-efficiency and versatility necessary to master multi-disciplinary couplings required today by size engineering simulations.

## 2.2. Objectives

The project has several objectives : to analyze mathematically coupled PDE systems involving one or more disciplines in the perspective of geometrical optimization or control; to construct, analyze and experiment numerical algorithms for the efficient solution of PDEs (coupling algorithms, model reduction), or multi-criterion optimization of discretized PDEs (gradient-based methods, evolutionary algorithms, hybrid methods, artificial neural networks, game strategies); to develop software platforms for code-coupling and for parallel and distributed computing.

Major applications include : the multi-disciplinary optimization of aerodynamic configurations (wings in particular) in partnership with Dassault Aviation and Piaggio Aero France; the geometrical optimization of antennas in partnership with France Télécom and Thalès Air Défense (see Opratel Virtual Lab.); the development of *Virtual Computing Environments* in collaboration with CNES (French Space Research Agency) and the European Airframe Company EADS (Common Research Center).

## 3. Scientific Foundations

### 3.1. Numerical Optimization of PDE systems

**Keywords:** *Partial Differential Equations (PDEs), Proper Orthogonal Decomposition (POD), finite volumes/elements, geometrical optimization, gradient-based/evolutionary/hybrid optimizers, hierarchical physical/numerical models, multi-point/multi-criterion/multi-disciplinary optimization, optimum shape design, shape parameterization.*

Optimization problems involving systems governed by PDEs, such as optimum shape design in aerodynamics or electromagnetics, are more and more complex in the industrial setting.

In certain situations, the major difficulty resides in the costly evaluation of a functional by means of a simulation, and the numerical method to be used must exploit at best the problem characteristics (regularity or smoothness, local convexity).

In many other cases, several criteria are to be optimized and some are non differentiable and/or non convex. A large set of parameters, sometimes of different types (boolean, integer, real or functional), are to be taken into account, as well as constraints of various types (physical and geometrical, in particular). Additionally,

today's most interesting optimization pre-industrial projects are multi-disciplinary, and this complicates the mathematical, physical and numerical settings. Developing *robust optimizers* is therefore an essential objective to make progress in this area of scientific computing.

In the area of numerical optimization algorithms, the project aims at adapting classical optimization methods (simplex, gradient, quasi-Newton) when applicable to relevant engineering applications, as well as developing and testing less conventional approaches such as Evolutionary Strategies (ES), including Genetic or Particle-Swarm Algorithms, or hybrid schemes, in contexts where robustness is a very severe constraint.

In a different perspective, the heritage from the former project Sinus in Finite-Volumes (or -Elements) for nonlinear hyperbolic problems, leads us to examine cost-efficiency issues of size shape-optimization applications with an emphasis on the PDE approximation; of particular interest to us:

- best approximation and shape-parameterization,
- convergence acceleration (in particular by multi-level methods),
- model reduction (e.g. by *Proper Orthogonal Decomposition*),
- parallel and grid computing; etc.

### 3.2. Geometrical optimization

In view of enhancing the robustness of algorithms in shape optimization or shape evolution, modeling the moving geometry is a challenging issue. The main obstacle between the geometrical viewpoint and the numerical implementation lies in the basic fact that the shape gradients are distributions and measures lying in the dual spaces of the shape and geometrical parameters. These dual spaces are usually very large since they contain very irregular elements. Obviously, any finite dimensional approach pertains to the Hilbert framework where dual spaces are identified implicitly to the shape parameter spaces. But these finite-dimensional spaces sometimes mask their origin as discretized Sobolev spaces, and ignoring this question leads to well-known instabilities; appropriate smoothing procedures are necessary to stabilize the shape large evolution. This point is sharp in the “narrow band” techniques where the lack of stability implies to reinitialize the underlying level equation at each step.

The mathematical understanding of these questions is sought via the full analysis of the continuous modeling of the evolution. How can we “displace” a smooth geometry in the direction opposite to a non smooth field, that is going to destroy the boundary itself, or its smoothness, curvature, and at least generate oscillations.

The notion of *Shape Differential Equation* is an answer to this basic question and it rises from the functional analysis framework to be developed in order to manage the lack of duality in a quantitative form. These theoretical complications are simplified when we are back to a Hilbert framework, which in some sense, is possible, but to the undue expense of a large order of the differential operator implied as duality operator. This operator can always be chosen as an *ad hoc* power of an elliptic system. In this direction, the key point is the optimal regularity of the solution to the considered system (aerodynamical flow, electromagnetic field, etc.) up to the moving boundary whose regularity is itself governed by the evolution process.

We are driven to analyse the fine properties concerning the minimal regularity of the solution. We make intensive use of the “extractor method” that we developed in order to extend the I. Lasiecka and R. Triggiani “hidden regularity theory”. For example, it was well known (before this theory) that when a domain  $\Omega$  has a boundary with continuous curvatures and if a “right hand side”  $f$  has finite energy, then the solution  $u$  to the potential problem  $-\Delta u = f$  is itself in the Sobolev space  $H^2(\Omega) \cap H_0^1(\Omega)$  so that the normal derivative of  $u$  at the boundary is itself square integrable. But what does this result become when the domain boundary is not smooth? Their theory permitted for example to establish that if the open set  $\Omega$  is convex, the regularity property as well as its consequences still hold. When the boundary is only a Lipschitzian continuous manifold the solution  $u$  loses the previous regularity. But the “hidden regularity” results developed in the 80's for hyperbolic problems, in which the  $H^2(\Omega)$  type regularity is never achieved by the solution (regardless the

boundary regularity), do apply. Indeed *without regularity assumption on the solution  $u$* , we proved that its normal derivative has finite energy.

In view of algorithms for shape optimization, we consider the continuous evolution  $\Omega_t$  of a geometry where  $t$  may be the time (governing the evolution of a PDE modeling the continuous problem); in this case, we consider a problem with dynamical geometry (non cylindrical problem) including the dynamical free boundaries. But  $t$  may also be the continuous version for the discrete iterations in some gradient algorithm. Then  $t$  is the continuous parameter for the continuous *virtual* domain deformation. The main issue is the validity of such large evolution when  $t$  is large, and when  $t \rightarrow \infty$ . A numerical challenge is to avoid the use of any “smoother” process and also to develop “shape-Newton” methods<sup>1</sup>. Our evolution field approaches permit to extend this viewpoint to the topological shape optimization<sup>2</sup>.

### 3.2.1. Shape differential equation

We denote  $G(\Omega)$  the shape gradient of a functional  $J$  at  $\Omega$ . There exists  $s \in \mathbb{R}^+$  such that  $G(\Omega) \in H^{-s}(D, \mathbb{R}^N)$ , where  $D$  is the universe (or “hold all”) for the analysis. For example  $D = \mathbb{R}^N$ . The regularity of the domains which are solution to the shape differential equation is related to the smoothness of the *oriented distance* function  $b_\Omega$  which turns to be the basic tool for intrinsic geometry. The limit case  $b_\Omega \in C^{1,1}(\mathcal{U})$  (where  $\mathcal{U}$  is a tubular neighborhood of the boundary  $\Gamma$ ) is the important case.

If the domains are Sobolev domains, that is if  $b_\Omega \in H^r(\mathcal{U})$ , then we consider a duality operator,  $\mathcal{A} \in \mathcal{L}(H^r, H^{-s})$  satisfying:  $\langle \mathcal{A}\varphi, \varphi \rangle \geq |\varphi|_H^2$  where  $H$  denotes a root space. We consider the following problem: given  $\Omega_0$ , find a non autonomous vector field  $V \in C^0([0, \infty[, H^r(D, \mathbb{R}^N)) \cap C([0, \infty[, L^\infty(D, \mathbb{R}^N))$  such that,  $T_t(V)$  being the flow mapping of  $V$ ,

$$\forall t > 0, \mathcal{A}.V(t) + G(T_t(V)(\Omega_0)) = 0$$

Several different results have been derived for this equation under *boundedness* assumptions of the following kind:

$$\text{there exists } M > 0 \text{ so that, } \forall \Omega, \|G(\Omega)\| \leq M$$

The existence of such bound has been proved first for the problem of best location of actuators and sensors, and have since been extended to a large class of boundary value problems. The asymptotic analysis (in time  $t \rightarrow \infty$ ) is now complete for a 2D problem with help of V. Sverak continuity results (and extended versions with D. Bucur). These developments necessitate an intrinsic framework in order to avoid the use of Christoffel symbols and local mappings, and to work at *minimal* regularity for the geometries.

The intrinsic geometry is the main ingredient to treat convection by a vector fields  $V$ . Such a non autonomous vector field builds up a tube. The use of *BV* topology permits these concepts to be extended to non smooth vector fields  $V$ , thus modeling the possible topological changes. The *transverse field* concept  $Z$  has been developed in that direction and is now being applied to fluid-structure coupled problems. The most recent results have been published in three books<sup>3 4 5</sup>.

<sup>1</sup>R. Dziri and J.-P. Zolésio, *Dérivée de forme pour les problèmes non-cylindriques*, INRIA Research Report 4676, December 2002.

<sup>2</sup>C. Ramananjaona and M. Lambert and D. Lesselier and Jean-Paul Zolésio, *Shape reconstruction of buried obstacles by controlled evolution of a level set: from a min-max formulation to numerical experimentation*, in *Inverse Problems*, **17-4**, 2002

<sup>3</sup>M.C. Delfour and J.-P. Zolésio, *Shapes and geometries*, Advances in Design and Control, Analysis, differential calculus, and optimization, SIAM, 2001

<sup>4</sup>B. Kawohl and O. Pironneau and L. Tartar and J.-P. Zolésio, *Optimal shape design*, Lecture Notes in Mathematics, Vol. 1740, 2000.

<sup>5</sup>Shape optimization and optimal design, Lecture Notes in Pure and Applied Mathematics, Vol. 216, Cagnol, John and Polis, Michael P. and Zolésio, Jean-Paul eds., Marcel Dekker Inc., 2001.



### 3.3. Integration platforms

Grids for complex problem solving is one of the priorities of the IST chapter in the 6th Framework Program of the European Community. One of the challenges of the 21st century in the computer science area lies in the integration of various expertise in complex application areas such as simulation and optimisation in aeronautics, automotive and nuclear simulation. Indeed, the design of the reentry vehicle of a space shuttle calls for aerothermal, aerostucture and aerodynamics disciplines which all interact in hypersonic regime, together with electromagnetics. Further, efficient, reliable, and safe design of aircraft involve thermal flows analysis, consumption optimisation, noise reduction for environmental safety, using for example aeroacoustics expertise.

The integration of such various disciplines requires powerful computing infrastructures and particular software coupling techniques. Simultaneously, advances in computer technology advocates the use of massively parallel PC-clusters including thousands of processors connected by high-speed gigabits/sec wide-area networks. This conjunction makes it possible for an unprecedented cross-fertilisation of computational methods and computer science. New approaches including evolutionary algorithms, parameterization, multi-hierarchical decomposition lend themselves seamlessly to parallel implementations in such computing infrastructures. This opportunity is being dealt with by project OPALE since its very beginning. A software integration platform has been designed by project OPALE for the definition, configuration and deployment of multidisciplinary applications on distributed heterogeneous infrastructure<sup>6</sup>. Experiments conducted within European projects and industrial cooperations using CAST have led to significant performance results in complex aerodynamics optimisation test-cases involving multi-elements airfoils and evolutionary algorithms, i.e. coupling genetic and hierarchical algorithms involving game strategies.<sup>7</sup>

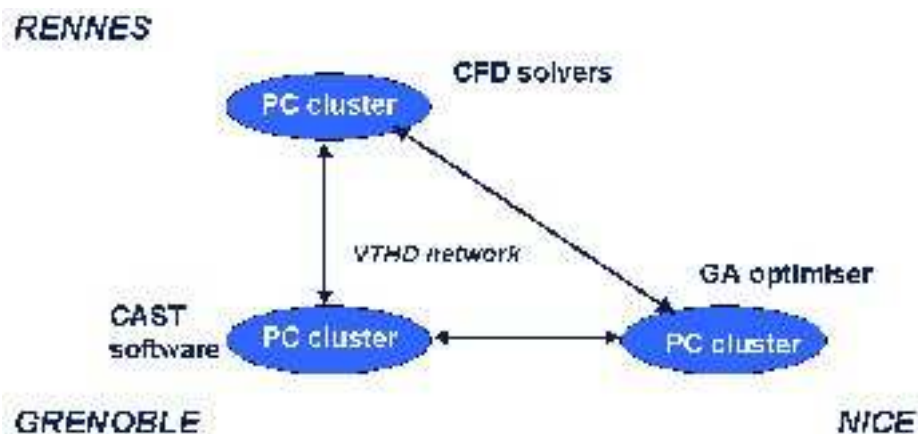


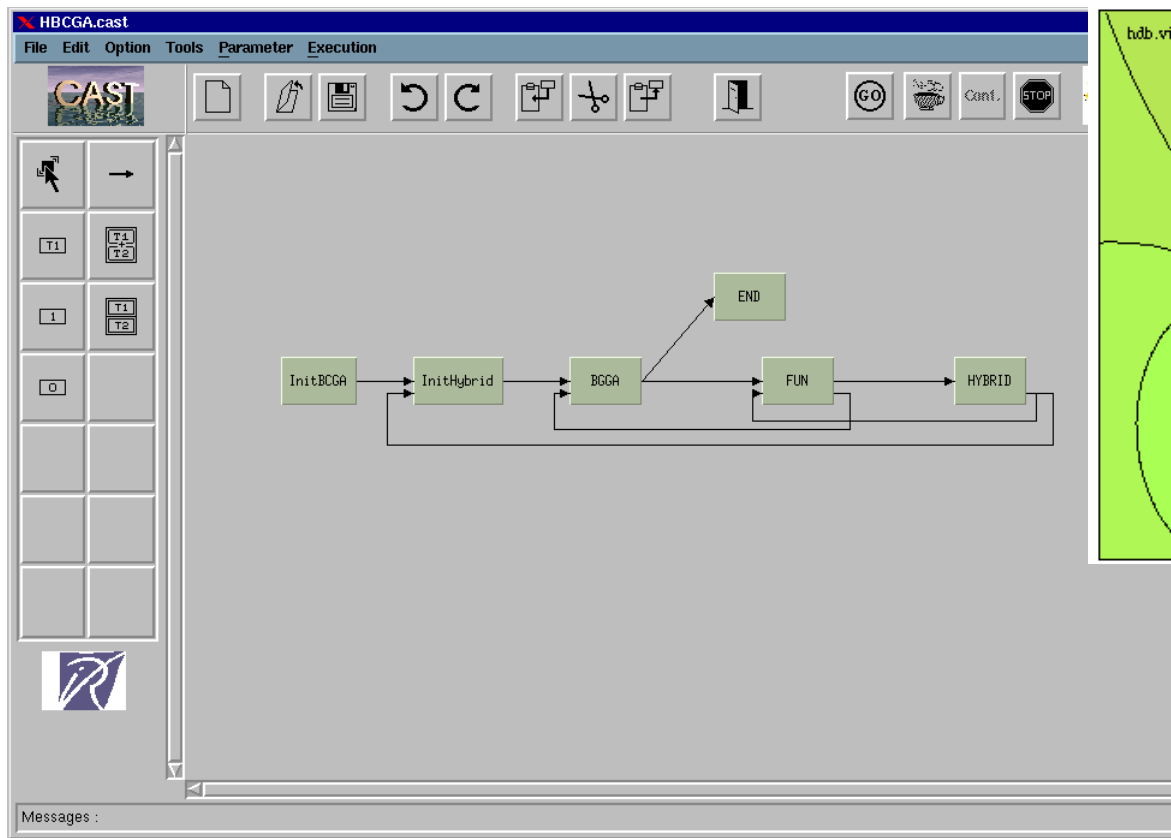
Figure 1. PC Cluster over the VTHD network

The main drawback still remains however in the deployment and control of complex distributed applications on grids by the end-users. Indeed, the deployment of the computing grid infrastructures and of the applications in such environments still requires specific expertise by computer science specialists. However, the users, which are experts in their particular application fields, e.g. aerodynamics, are not necessarily experts in distributed and grid computing. Being accustomed to Internet browsers, they want similar interfaces to interact

<sup>6</sup>Gia-Toan Nguyen and C. Plumejeaud, *An integration platform for metacomputing applications*, International Conference on Computational Science, P. Sloot and J. Dongarra, Amsterdam, The Netherlands, 2002.

<sup>7</sup>J. F. Wang, *Optimisation Distribuée Multicritère par Algorithmes Génétiques et Théorie des Jeux & Application à la Simulation Numérique de Problèmes d'Hypersustentation en Aérodynamique*, Ph.D. Thesis, Université de Paris 6, 2001

with grid computing and problem-solving environments. A first approach to solve this problem is to define component-based infrastructures, e.g. the Corba Component Model, where the applications are considered as connection networks including various application codes. The advantage is here to implement a uniform approach for both the underlying infrastructure and the application modules. Still however, it requires specific expertise not directly related to the application domains of each particular user. A second approach is to make use of grid services, defined as application and support procedures to standardise access and invocation to remote support and application codes. This is usually considered as an extension of Web services to grid infrastructures. A new approach, which is currently being explored by the OPALE project, is the design of a virtual computing environment able to hide the underlying grid-computing infrastructures to the users. An international collaborative project has been set up in 2003 on this subject involving the OPALE project at INRIA in cooperation with CNES and involving also EADS (Common Research Center) and Datamat (Italy).



(a) CAST Server

(b) Initial and Optimized Mach-number fields

Figure 2. Hybrid Gradient-Genetic Optimization using the demonstration platform developed in the European Project DECISION; note the important shock-strength diminution on the airfoil upper surface

## 4. Application Domains

### 4.1. Scope

**Keywords:** *biology, environment, telecommunications, transportation systems.*

Focused on the development of numerical methods for the optimization of PDE systems and related numerical analysis, mathematical or software issues, the project conducts studies in optimum shape design in aerodynamics (drag, external noise or sonic bang reduction, high-lift configurations, etc.) and electromagnetics (optimal positioning and motion of sensors) in the framework of engineering problems in transport demanding new technologies.

The Rhône-Alpes project component develops software platforms for the treatment of these multi-disciplinary applications by code coupling and distributed computing (*grid computing*).

#### **4.1.1. Aeronautics and Space**

The demand of the aeronautical industry remains very strong in aerodynamics, as much for conventional aircraft, whose performance must be enhanced to meet new societal requirements in terms of economy, noise (particularly during landing), vortex production near runways, etc., as for high-capacity or supersonic aircraft of the future. Our implication concerns shape optimization of wings or simplified configurations.

Our current involvement with Space applications relate to software platforms for code coupling.

#### **4.1.2. Electromagnetics**

In the context of shape optimization of antennas, we can split the existing results in two folds: the two-dimensional modeling concerning only the specific transverse mode TE or TM, and treatments of the real physical 3-D propagation accounting for no particular symmetry, whose objective is to optimize and identify real objects such as antennas.

Most of the numerical literature in shape optimization in electromagnetics belongs to the first class and makes intensive use of the 2-D solvers based on the specific 2-D Green kernels. The 2-D approach for the optimization of *directivity* led recently to historical serious errors due to the modeling defect. There is definitely little hope for extending the 2-D algorithms to real situations. Our approach relies on a full analysis in unbounded domains of shape sensitivity analysis for the Maxwell equations (in the time-dependent or harmonic formulation), in particular, by using the integral formulation and the variations of the Colton and Kreiss isomorphism. The use of the France Telecom software SR3D enables us to directly implement our shape sensitivity analysis in the harmonic approach. Making use of the derivative with respect to the frequency, we derive the derivative of the shape gradient with respect to the frequency (it is a kind of second order derivative). This technique makes it possible, with an adequate interpolation, to retrieve the shape derivatives from the physical vector fields in the time evolution processes involving initial impulses, such as radar or tomography devices, etc. Our approach is complementary to the “automatic differentiation codes” which are also very powerful in many areas of computational sciences. In Electromagnetics, the analysis of hyperbolic equations requires a sound treatment and a clear understanding of the influence of space approximation.

#### **4.1.3. Multidisciplinary couplings**

Our expertise in theoretical and numerical modeling, in particular in relation to approximation schemes, and multilevel, multiscale computational algorithms, allows us to envisage to contribute to integrated projects focused on disciplines other than fluid dynamics or electromagnetics such as biology and virtual reality, image processing, etc., in collaboration with specialists of these fields.

## **5. Software**

### **5.1. CAST**

The main contributions concerning the software platform CAST are twofold :

- first, a technical collaboration within the project has been setup for the development of a distributed computing environment for the deployment of parallel applications concerning the modelling of anti-angiogenesis for solid tumors, based on a Nash equilibrium between antagonistic actors;

- second, a cooperation has been setup with CNES for the design, implementation and deployment of Grid-based Virtual Computing Environments.

The first aspect implied the parallelisation of the original code using MPI and the use of the PC-clusters and other various Linux workstations at INRIA Sophia Antipolis and Grenoble. This work was implemented by Jean Arnaud. It also resulted in the deployment of the CAST distributed software platform on this environment.

The second aspect concerning Virtual Computing Environments resulted in the setup of an industrial collaboration with CNES for the design of seamless application design interfaces on the Grid. Based on current Grid technology and Web Services, a specific doctoral thesis has been started (Lizhe Wang).

Further, strong implication in European Networks, e.g., Promuval, led us to specify with European aircraft manufacturers and research centers the characteristics of a software integration platform for multidisciplinary code validation and verification in aeronautics. A demonstrator of this platform is currently being designed in cooperation with Alenia Aeronautica (Italy) and Cenaero (Belgium).

## 5.2. Numerical Modules for Optimum-Shape Design in Aerodynamics

We are developing an optimization package OBEZ (Optimization with BEZier parameterization) designed for shape-optimization of 3D aerodynamic bodies. It has been applied mostly to a lift-drag minimization in the transonic regime and sonic-bang reduction in supersonics. It integrates the following toolboxes:

- a flow-solver based on the NS3D code (legacy of the SINUS project), together with a calculation of an objective function based on the results of the flow-simulation (pressure field around the aircraft, gradient of pressure, lift and drag coefficient);
- a new parameterization module BZPARAM implementing a black-box 3D Bézier parameterization and 3D mesh-update routines;
- an optimization module containing general optimization routines by a genetic-algorithm and a Nelder-Mead simplex method.

### 5.2.1. NS3D (updates of the code):

**Keywords:** *compressible inviscid or viscous flow, finite volumes, implicit pseudo-time-marching methods, upwind schemes.*

**Participants:** Michele Andreoli [former trainee, University of Pisa], Aleš Janka [former Post Doctoral Student].

The NS3D flow code solves the 3D Euler and Navier-Stokes equations, on general unstructured tetrahedra meshes. The steady flow solution is found as the asymptotic limit of a pseudo-time-dependent process. The code combines the following ingredients:

- a finite volume spatial discretization with an upwind scheme for the discretization of the convective fluxes by the Roe or van Leer splittings;
- an extension to second-order spatial accuracy based on the MUSCL (Monotonic Upwind Scheme for Conservative Laws) approach with flux limiters;
- implicit time-stepping by a simple one-step first-order formula.

The code has been revised and modified, its efficiency and memory requirements improved by changing the sparse-matrix representation scheme. The modifications permit to run flow-simulations past complete aircraft.

After the flow-simulation for each shape, aerodynamic coefficients are calculated (lift, drag, pressure gradient) and passed to a routine to evaluate the objective function. The objective function is the measure of quality of the shape, it usually combines target values of aerodynamic coefficients together with penalties originating from geometrical constraints (volume, thickness). Several objective functions have been implemented for a lift-drag optimisation in the transonic regime and a sonic-bang minimization in the supersonic regime, with or without geometrical constraints.

### 5.2.2. BZPARAM:

**Keywords:** *Free-form deformation, elliptic solvers, moving mesh, tensorial 3D Bezier, torsional springs.*

**Participants:** Michele Andreoli, Aleš Janka.

The parameterization module BZPARAM manages, during the optimization process, the deformations of 3D shapes and of the corresponding tetrahedral computational mesh. It accounts for the possible *a priori* geometrical constraints (fixed parts of the shape, angles, or thicknesses) and uses a representation of the optimized shape by a condensed parametric vector  $\mathbf{x} \in \mathbb{R}^N$  ( $N$  small) containing just an active set of degrees of freedom of the shape deformation. Such a parametric vector  $\mathbf{x}$  can then be passed to a general optimization algorithm operating in  $\mathbb{R}^N$ .

The developed BZPARAM module implements the Free-Form Deformation with a 3D tensorial Bézier parameterization. It can perform the degree elevation while recalculating the new parametric vector  $\mathbf{x}' \in \mathbb{R}^{N'}$  corresponding to shapes before the degree elevation.

Mesh-deformation routines are being developed within this module to update the 3D computational mesh around the deformed objects. The objective is to move rapidly the existing nodes of the mesh to follow (large) mesh deformations, while preserving mesh quality and local mesh metrics (boundary layers). Experiments were performed with torsional-spring pseudo-elasticity model and with elliptic solvers.

### 5.2.3. Optimization module:

**Keywords:** *genetic algorithm, hybridization, reduced models, simplex method.*

**Participants:** Michele Andreoli [simplex algorithm and validation], Yannick Berard [former trainee, hybridization in PIKAIA], Abderrahmane Habbal [hybridization in PIKAIA], Aleš Janka [simplex algorithm and validation], Latifa Oulladji [former trainee, new genetic operators in AG2D].

The optimization module contains some general optimization algorithms which minimize a given objective function in a parametric space  $\mathbb{R}^N$ . The implemented algorithms are:

- a binary-coded genetic algorithm based on AG2D (legacy of the SINUS project), with modified genetic operators;
- a real-coded genetic algorithm based on PIKAIA, with a gradient-based hybridization;
- a Nelder-Mead simplex algorithm.

The Genetic algorithms operate on a set (population) of shapes (individuals) to produce an artificial evolution. Their task is to modify (evolve) shapes towards the optimal shape by using three main genetic operators: *selection* (of best-fitted individuals), *cross-over* (recombination of the selected individuals to obtain new shapes), and *mutation* (random changes in shapes). The shape parametric vector  $\mathbf{x}$  is coded either in a fixed precision scheme (binary-coded) or in a floating point scheme (real-coded). Accordingly, the genetic operators operate either on a set of bits (0/1's) or on a set of real numbers.

The most serious disadvantage of an ordinary genetic algorithm is the necessity to evaluate fitness (objective) functions for a large number of shapes. Each evaluation of fitness function comprises at least one simulation of the flow problem in 3D. At the same time, most of the shapes are rejected during the evolutionary process. Therefore, simplified models for fitness evaluation, permitting to reject unsatisfactory shapes without necessitating the 3D flow simulation, are of interest. A new algorithm has been developed based on the genetic algorithm with real coding PIKAIA (public domain software) employing a first-order gradient interpolation of fitness values on subsets (clusters) of the current population.

#### 5.2.4. NS3D-VSAERO:

**Keywords:** *hierarchy of flow solvers, multi-point optimization, panel method.*

**Participants:** Aleš Janka, Dario Pinelli [Piaggio Aero Industries].

A coupling of two different flow solvers for two flow regimes is currently under development in collaboration with PIAGGIO Aero (Italy).

For CPU-time reasons, we have been using within NS3D only the cheapest Euler flow model for compressible inviscid flows. A shape optimization using this simplified model neglecting viscous effects is known, however, to give super-critical optimal shapes which are not optimal with respect to the non-simplified physical laws (viscous, turbulent, with a boundary-layer model).

One standard approach to avoid erroneous optimal shapes is to increase the complexity of the mathematical flow model in NS3D, and this leads to a substantial increase of computational effort in the flow solution phase. As an alternative, we are currently integrating to the optimization loop a commercial 3D panel method solver VSAERO with an enhanced boundary layer model (courtesy of PIAGGIO Aero), which accounts for the viscosity and turbulence effects, but whose validity is limited to subsonic regimes.

By coupling the inviscid transonic Euler code (NS3D) with the subsonic panel code including a boundary layer model, in the framework of a multi-criteria optimization, we would like to filter-out the non-physical optimal shapes while maintaining the CPU-cost at a reasonable level.

### 5.3. Numerical Modules for Gradient Computations in Electromagnetics

**Participants:** Claude Dedebean [France Télécom, La Turbie], Pierre Dubois, Jean-Paul Zolésio.

Shape gradients with respect to 3D geometries in electro-magnetic fields are computed by numerical code developments peripheral to the France Télécom SR3D code for the solution of the Maxwell equations. These developments, combined with interpolation in the frequency domain, allow to compute the derivative w.r.t. the frequency.

## 6. New Results

### 6.1. Computational methods, numerical analysis and validation

#### 6.1.1. Model reduction in fluid dynamics

**Participants:** Guillermo Artana [University of Buenos Aires], Juan D'Adamo [University of Buenos Aires], Jean-Antoine Désidéri.

In this work, we construct reduced dynamical models for an incompressible turbulent external flow. The model is devised from a set of particle image velocimetry (PIV) measurements, using the velocity field data obtained in previous experiments. The Proper Orthogonal Decomposition (POD) is a technique which allows the extraction of the significant modes of a flow. It permits to identify modes without any *a priori* hypothesis, and these are ordered by their associated level of energy. The POD modes are used to formulate a dynamical system which only contains the main features of the flow, a low order dynamical system (LODS). This is achieved by means of a Galerkin projection of the Navier-Stokes Equations, thus obtaining a system of ordinary differential equations describing the main aspects of the flow without demanding excessive computational requirements [47].

Numerical model reduction is developed for its own sake, but also in view of computational efficiency in future complex multi-disciplinary optimization involving fluid dynamics by *hierarchical* algorithms.

#### 6.1.2. Multi-disciplinary validation

**Participants:** Alain Dervieux [Project-Team Tropics], Jean-Antoine Désidéri, Toan Nguyen, Jacques Périaux.



The computational resources available today are pushing the computational community towards complex multi-disciplinary problems, in which the numerical validation issue of coupled models is very difficult, and still relatively unexplored. In this area, we participate in the European Project PROMUVAL (see *International Networks*) aimed at identifying the elements related to physical modeling, numerical methods and software environments, that such computational situations will necessitate, for a set of coupled problems of great importance in Aeronautics (turbulence, aero-acoustics, thermal problems, etc).

## 6.2. Numerical algorithms for optimization and optimum-shape design

Our research themes are related to optimization and control of complex multi-disciplinary systems governed by PDEs. They include algorithmic aspects (shape parameterization, game strategies, evolutionary algorithms, gradient/evolutionary hybridization, model reduction and hierarchical schemes), theoretical aspects (control and domain decomposition) and software aspects.

### 6.2.1. Shape parameterization, hierarchical (multilevel) algorithms, adaptivity.

**Participants:** Jean-Antoine Désidéri, Badr Abou El Majd, Aleš Janka, Dario Pinelli [Piaggio Aero Industries].

We are concerned with the general problem consisting of minimizing a functional constrained by a PDE state equation subject to a shape-dependent boundary condition. The prototype 2D test problem is the optimization of an airfoil shape immersed in a two-dimensional flow (of Eulerian type in the simplest case) to reduce drag; the shape is then subject to certain geometrical constraints (specified endpoints, vertical tangent at leading edge, given area, etc). In general applications, the field, or distributed state, is computed by some standard PDE approximation method (e.g. of finite-volume type) over a mesh, one boundary of which is optimized in shape, via *design parameters* in number much less than the boundary gridpoints. The shape is thus formally represented, prior to mesh-discretization, by a *parameterization* here specifically chosen to be of Bézier type, based on *control points* whose abscissas are prescribed, and ordinates optimized according to some physical criterion.

#### 6.2.1.1. Hierarchical (multilevel) algorithms.

We exploit the classical *degree-elevation process* [53] to construct an *a priori hierarchy of embedded Bézier parameterizations* as the support of a number of multi-level optimization algorithms, including one inspired from the *Full Multi-Grid* concept, and referred to as the *Full and Adaptive Multi-Level Optimum-Shape Algorithm (FAMOSA)*. Our construction yields rigorously-nested optimization search spaces. The framework allows us also to propose ways to employ *reduced models*, as well as to construct *hybrid optimizers* (combining gradient-based with evolutionary algorithms) [39] [41].

#### 6.2.1.2. Aerodynamic optimization of three-dimensional geometries.

A versatile parameterization technique has been developed for 3D shape optimization in aerodynamics. Special attention is paid to construct a hierarchical parameterization by progressive enrichment of the parametric space. After a brief review of possible approaches, the free-form deformation framework was elected for a 3D tensorial Bézier parameterization. The classical degree-elevation algorithm applicable to Bézier curves is still valid for tensor products, and its application yields a hierarchy of embedded parameterizations. A drag-reduction optimization of a 3D wing in transonic regime has been carried out by applying the Nelder-Mead simplex algorithm and a genetic algorithm. The new parameterization including degree-elevation is validated by numerical experimentation and its performance assessed [39] [45].

#### 6.2.1.3. Adaptivity.

A shape optimization in aerodynamics can benefit greatly in conditioning by adaption, at regular intervals, of the parameterization supporting the shape representation. From the knowledge of an approximate optimal shape, one considers the set of all Bézier parameterizations of same degree that approximate the shape in the sense of least squares. One elects the parameterization associated with the most regular control polygon (least total variation). We have provided all the details of the formulation, that is very close to our initial works but relies on a lesser number of numerical quadratures most of which are realized by fourth-order formulas. We

have proposed a shape-optimization test-case originating from calculus of variations. This surrogate “physical optimization” has allowed us last year, at moderate cost, to demonstrate the convergence of the algorithm coupling the pseudo-physical optimization with the Bézier parameterization adaption, and to assess its merit [50].

Adaptivity is a key element to achieve fast convergence of the shape-optimization algorithm. Thus, we continue to explore this issue in the course of B. El Majd’s thesis work, for three-dimensional flow applications.

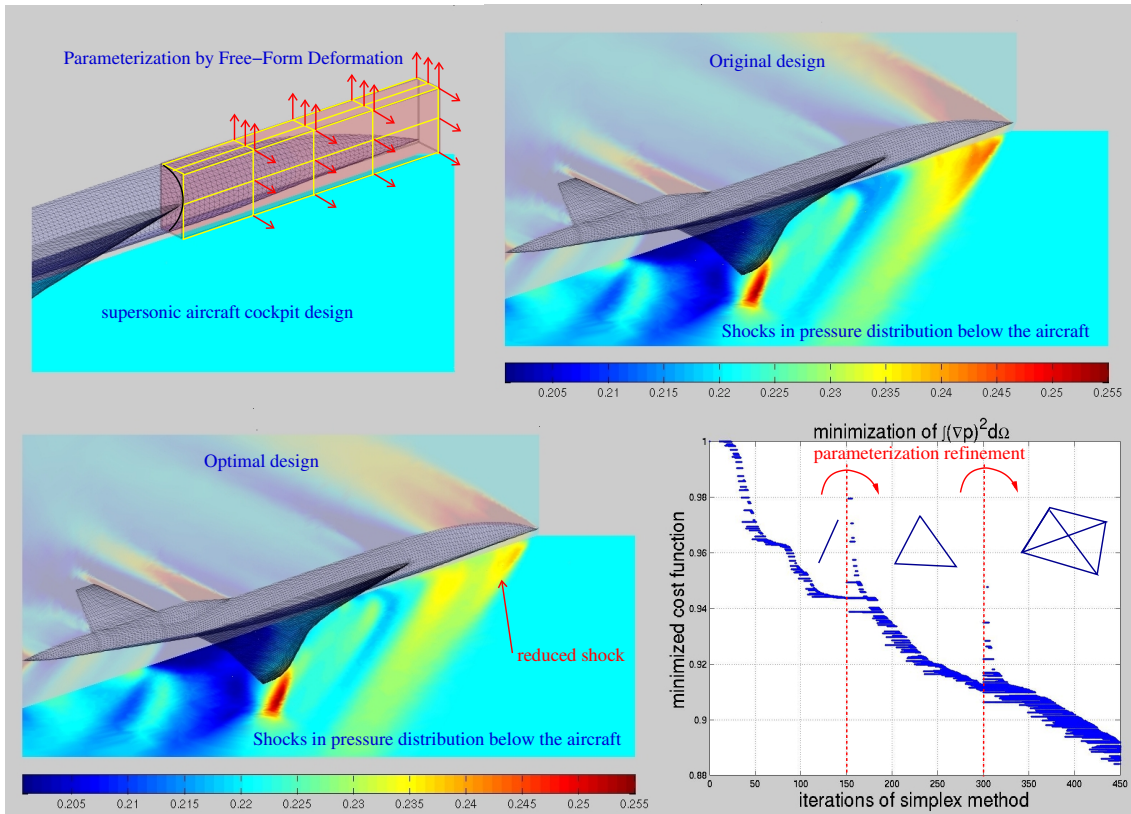


Figure 3. Shape optimization of a supersonic business-jet geometry for external noise reduction; << Free-Form Deformation >> parameterization in the nose region of a generic geometry (courtesy of Dassault Aviation); initial supersonic flow (pressure field); optimized flow demonstrating reduced shock attached to the nose; convergence history of a multilevel simplex method using successive degree elevations. Technical elements: mesh: 173526 nodes, 981822 tetrahedra (for the half-geometry); flow solver: NS3D solver, inviscid option, Roe FDS; flow conditions:  $M_\infty = 1.8$ ,  $\alpha = 1^\circ$ ; parameterization and optimizer: free-form deformation of cockpit region in tensor form (length  $\times$  height  $\times$  span), Nelder-Mead simplex method, degree elevation every 150 iterations applied 3 times: 2-1-1 for 6 active d.o.f., 3-1-1 for 12 active d.o.f., 3-2-2 for 30 active d.o.f. of shape deformation.

### 6.2.2. Inverse Shape Optimization Model Problems and Application to Aerodynamic Reconstruction

**Participants:** Jean-Antoine Désidéri, Jean-Paul Zolésio.

Another aspect of validation is code certification, a process by which we gain confidence in the ability of the numerical method to solve (or optimize) satisfactorily the P.D.E. model. This requires in particular the success



of grid-convergence experiments, but not only. In the context of shape optimization methods, disposing of reduced shape optimization model problems may be very useful:

- to develop and test shape-optimization numerical algorithms in a simplified context bearing appropriate geometrical characteristics, e.g. parameterization adaption, multilevel algorithms, etc;
- to adapt a shape-optimization numerical algorithm to a 'meta-model', e.g. a neural network to improve convergence or P.O.D. to reduce cost;
- to construct purely-geometrical penalty functions in an inverse-problem formulation;
- to test multidisciplinary coupled optimization algorithms by partial verification: only one "real" model and  $n - 1$  "reduced" models at a time.

For this purpose, we have developed formulations of problems of calculus of variations permitting in particular the reconstruction of arbitrary airfoils. The functional we considered has the form:

$$\mathcal{J}(y(t)) = \frac{p^\alpha}{\mathcal{A}} \quad (\text{for fixed } x(t))$$

where

$$p = \int_0^1 \sqrt{x'(t)^2 + y'(t)^2} \omega(t) dt, \quad \mathcal{A} = \int_0^1 y(t) x'(t) \omega(t) dt$$

( $\alpha > 1$ ;  $\omega(t) > 0$ ).

We proved the following results [27]:

- Direct problem – The functions  $x(t)$  and  $\omega(t)$  being fixed:
  - for  $\alpha \geq 2$ , the functional is strictly convex;
  - there exists a critical  $\alpha_0$  ( $1 \leq \alpha_0 \leq 2$ ), such that the minimization problem is ill-posed for  $\alpha < \alpha_0$ , and unimodal for  $\alpha > \alpha_0$ ;
  - if  $\omega(t) \equiv 1$ ,  $\alpha_0 = 2$ .
- Inverse problem – Basically, if  $x(t)$  is monotone increasing, and  $y(t)$  unimodal:
  - then some exponent  $\alpha > 1$ , and some positive and  $\mathcal{C}^1$  function  $\omega(t)$  can be constructed to make the functional unimodal, the global minimum being realized by the associated shape.
  - Asymptotics have been established.
  - Numerical experiments illustrate these results, but indicate a certain sensitivity to the normalization (scaled data are recommended).

### 6.2.3. Game strategies and Variability of Boundary conditions in Optimization

**Participants:** Jean-Antoine Désidéri, Toan Nguyen, Jacques Périaux, Zhi Li Tang [former Opale Post. Doct. fellow, currently at Dassault-Aviation/UPMC Scientific Pole].

We have tested a number of “splits of territory”, identified as portions of an airfoil shape, allocated to virtual players competing in a Nash game, each one optimizing a different criterion in a multi-point aerodynamic optimization and until an equilibrium is reached. The technique is effective, and very cost-efficient compared to the construction of a complete Pareto equilibrium, but obviously less general, but in a design loop it realizes feasible trade-offs between criteria [40].

Current aspects of this research includes the following two topics [46]:

1. comparing the 2-D and 3-D results obtained by the capture of non dominated airfoil shape solutions of the Pareto front of a multi objective design optimization of subsonic-transonic flow using a Navier-Stokes code and structured meshes;
2. increasing the stability of the solution under uncertainty of boundary and environment conditions via robust design using a Navier Stokes solver.

## 6.3. Application of shape and topology design to biology and medicine

A particular effort is made towards the application to biology and medicine of solid and fluid mechanics, shape and topology design, multidisciplinary optimization by game strategies ; domains of expertise which were successfully applied to other fields. Two selected applications are privileged : solid tumours and wound healing.

The objective is to continue the investigation of these applications, from a mathematical-theoretical viewpoint as well as from a computational and software development viewpoint.

Collaboration with biologists is ongoing (Biochemistry lab, Nice) and is intended to be extended (to e.g. Oncology research institutes such as Lacassagne, Nice). Contacts and first meetings were also held with INRIA projects specialized in image processing (e.g. Epidaure, INRIA Sophia Antipolis). Collaboration with such projects seems is mandatory, particularly in view of a biological validation of the computational results.

Wound healing rises multiscale and homogenization theoretical and numerical questions. Games for tumoural anti-angiogenesis rise questions related to existence of equilibria, efficiency among others. Moreover, these two applications need validation with respect to the genuine biological phenomena. These to-do's can be achieved by means of Ph.D. theses. A particular attention will be paid in the next two years to the setup of a computational biology thesis subject, for which Region PACA's grants will be solicited.

### 6.3.1. Anti-angiogenesis for solid tumours

**Participants:** Jean Arnaud, Abderrahmane Habbal, Toan Nguyen.

An original approach based on game theory framework was proposed to model anti-angiogenesis. It relies on a competition between two density functions which are intended to represent respectively activators and inhibitors of angiogenesis.

To illustrate our approach, we defined a theoretical game (competition) between a porous medium and a structure governed by linear elasticity. The problem was formulated as a topology static design with complete information game, for which existence of a Nash equilibrium was proved. We assumed that activators would act to provide the tumor with an optimal drainage network, while the inhibitors would try to keep the structural compliance of the extra cellular matrix as low as possible (or try to minimize the drainage of the blood vessels network in the case of zero-sum version).

A dedicated software was developed, based on proprietary routines, Modulef finite element library, and a third party optimization package. The numerical results clearly characterize the multiplicity of feeding channels as an optimal response of the activators to optimally distributed inhibitors (see Figure 4).

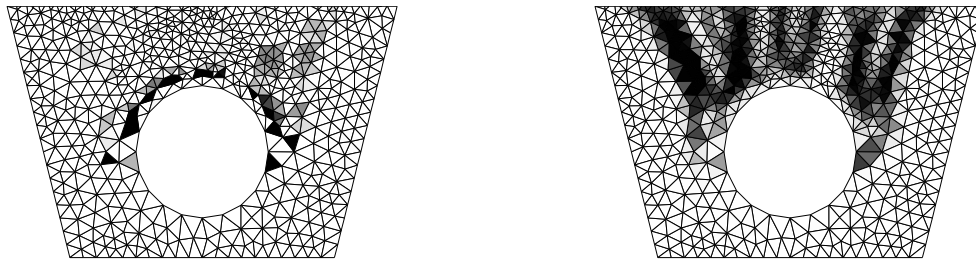


Figure 4. Distribution of antagonistic actors: anti-angiogenesis proteins (left); proteins facilitating angiogenesis (right)

This study is however based on simplified modeling and assumptions. Many improvements should be considered.

First, the dynamic growth of the tumor must be taken into account, and more generally a *dynamical system* based on an incomplete information game is more likely to be closer to the actual angiogenesis process.

Then, the fundamental assumptions on the nature of *objectives* targetted by angiogenesis and anti-angiogenesis should be validated, confronting numerical results to biological data.

Another important direction of validation is related to the determination of actual rheological data as well as models of interaction between pro- and anti-angiogenesis factors.

From the computational viewpoint, our next goal is to run realistic three dimensional calculations coupling porous media and elasticity models. In this respect, the MPI parallelization of the program was implemented by Opale team of INRIA Grenoble, as a mandatory step for computational efficiency.

### 6.3.2. Wound healing

**Participants:** L. Almeida [Dept. of Mathematics, University of Nice], A. Habbal, S. Noselli [Dept. of Biochemistry, University of Nice].

Wound healing involves many complex coordinated biological, chemical and mechanical processes. Wound contraction, the biomechanical phenomenon by which the wound boundaries are drawn inwards, is an essential feature in the healing of these wounds. Currently, available drugs which monitor the contraction do not generally lead to a satisfactory remodeled dermis.

In collaboration with L. Almeida and S. Noselli our long term goal is to develop mathematical models and computational tools that can help the biologist to a better understanding of the impact of particular biological factors on the wound healing. Moreover, developing relevant mathematical models is a necessary preamble to design, using mathematical control and optimization techniques, optimally targetted drugs. In this view, Dorsal Closure of the *Drosophila* is known to be a very practical relevant live-model of mammalian tissue repair, on which we have focused our efforts.

We have introduced an original mathematical model based on systems of nonlinear parabolic equations with a singular term which models the *zipping* effect. A fortran program based on finite differences method was implemented, and several numerical experiments were achieved, providing first results showing effective closure of the curve modeling the margins, these are boundaries between the lateral ectoderm and the amnioserosa cells (see Figure 5).

The above models are however based on geometry information only, while the biological process obviously involves at least some mechanics. So, we considered a completely different approach, based on the idea that margins could be modeled as soft one-dimensional thin shells, under quasi-static membrane-bending elastic regime, with adhesive contact. A fortran program based on finite element method was developed, and

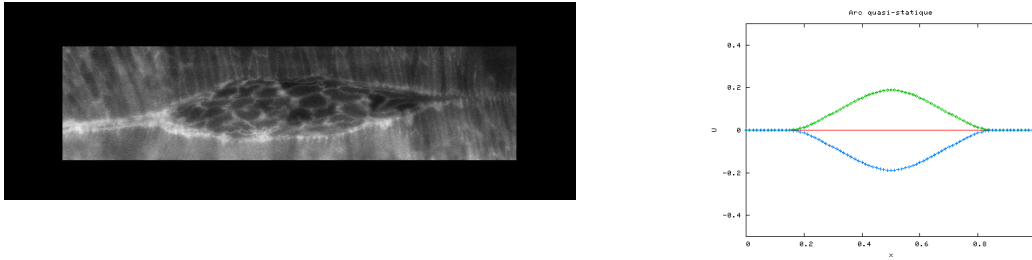


Figure 5. A mechanical model for healing (right) compared with a photograph

numerical results were recently obtained. They show closure dynamics of the margins subject to mechanical loads which are very conforming to the closure observed by confocal microscopy of real *Drosophila* embryo. Now, both a geometry-based model and a mechanical model are at hand, along with their computational implementations. Considering these very basic features, many future development directions are sought :

- In collaboration with image processing experts, extract margins dynamics from experimental movies led at the biochemistry lab. in order to compare to computational results, and more important, to achieve the mechanical parameters identification (data calibration) of our mechanics model ;
- Is bending relevant, is quasi-static regime sufficient or should we go into second order dynamics?
- Is there any possible generalization to biological thin shells under closure and zipping dynamics?
- We have now at hand experimental data of the two scales pertaining to the cell and the tissue. Is there a room for homogenization to apply? What is the relevance of a multiscale modeling?
- Genetic mutation can lead to unusual distribution and behaviour of e.g. filipodes, responsible for the zipping. We intend to study what best distribution of filipodes would lead to best (in some sense) closure, and then what genetic operation would lead to this best distribution. This challenging question would be a first step into a *computational drug design process*.

## 6.4. Mathematical analysis in geometrical optimization

### 6.4.1. Non cylindrical dynamical system

**Participant:** Jean-Paul Zolésio.

The optimal control theory is classically based on the assumption that the problem to be controlled has solutions and is well posed when the control parameter describes a whole set (say a closed convex set) of some functional linear space. Concerning moving domains in classical heat or wave equations with usual boundary conditions, when the boundary speed is the control parameter the existence of solution is questionable. For example with homogeneous Neumann boundary conditions the existence for the wave equation is an open problem when the variation of the boundary is not monotonic. We derive new results in which the control forces the solution to exist.

### 6.4.2. Shape Optimization theory

**Participants:** Michel Delfour, Jean-Paul Zolésio.

The ongoing collaboration with the CRM in Montreal (mainly with Professor Michel Delfour) led to several extensions to the theory contained in the book *Shape and Geometry* (SIAM 2001) . In that direction 6 papers have been published or accepted for publication. The emphasis is put on two main aspects: in order to *avoid* any relaxation approach but to deal with real shape analysis we extend existence results by the introduction of several new families of domains based on fine analysis. Mainly *uniform cusp* condition, *fat* conditions

and *uniform non differentiability* of the oriented distance function are studied. Several new compactness results are derived. Also the fine study of *Sobolev domains* leads to several properties concerning boundaries convergences and boundaries integral convergence under some weak global curvature boundness.

#### 6.4.3. Control of Coupling fluid-structure devices

**Participants:** Marwan Moubachir, John Cagnol, Raja Dziri, Jean-Paul Zolésio.

The use of the transverse vector field governed by the Lie bracket enables us to derive the “first variation” of a free boundary. This result has led to the publication of a note at the *Comptes Rendus of Academy of Sciences* (presented by Roland Glowinski), and a book, as well as a conference paper at the TC7 IFIP conference in July 2003 and in the three IFIP working conferences in Scuola Normale Sup. di Pisa (January 04), Lisbon (June 04), Jyväskylä (July 04).

An alternate approach to fluid-structure has been developed with P.U.L.V. (J. Cagnol) and the University of Virginia (I. Lasiecka and R. Triggiani, Charlottesville) on stabilization issues for coupled acoustic-shell modeling. [51].

#### 6.4.4. Shape Gradient in Maxwell Equations

**Participants:** Pierre Dubois, Jean-Paul Zolésio.

It is well known that in 3D scattering, the geometrical singularities play a special role. The shape gradient in the case of such a singularity lying on a curve in 3D space has been derived mathematically and implemented numerically in the 3D code of France Télécom.

A communication has been presented at ECCOMAS 2004 Conference.

This work with P. Dubois is potentially applicable to more general singularities.

#### 6.4.5. Frequency Derivative (harmonic regimes)

**Participants:** Jean-Pierre Damiano [Electronic Lab., University of Nice], Claude Dedeban [France Télécom], Pierre Dubois, Jean-Paul Zolésio.

These works extend the ongoing collaboration with France Telecom and the Electronic Laboratory of the University of Nice. The main results have been presented in two international conferences ( [52] and ECCOMAS 2004).

#### 6.4.6. Shape stabilization of wave equation

The former results by J.P. Zolésio and C. Trucchi have been extended to more general boundary conditions in order to derive shape stabilization via the energy “cubic shape derivative”. Further extension to elastic shell intrinsic modelling is foreseen.

#### 6.4.7. OpRaTel Electronic-Laboratory

**Participants:** Marwan Moubachir, Jean-Paul Zolésio.

The collaboration with France Télécom and Thales led to the creation of an “e-lab”. Our activity is divided in two main themes:

- development of models of array antennas for telecommunication purposes; a patent will shortly be deposited;
- frequency allocation (M. Moubachir), a difficult modeling topic of major importance for our industrial partners.

## 6.5. Virtual computing environments

**Participants:** Lizhe Wang, Toan Nguyen.

The advantages demonstrated by grid-computing infrastructures and complex problem solving environments are fundamental in terms of raw computing power and massive storage media. Indeed, they allow parallel and distributed computing of demanding applications that can now be deployed on thousands of connected processors and they can connect petabytes of data through tens gigabits/sec networks at affordable cost.

So far, however, there seems to be some reluctance from the industry to use these environments because they require expertise in the computer science field which is currently not yet widely available on the job market [49]. Users have become in the last decade experts in the manipulation of Web browsers to access inter-continental mass of data and execute remotely located pieces of code transparently. Unfortunately, grid computing environments are still far from providing these seamless and flexible interfaces. New concepts and interfaces are therefore required to alleviate these shortcomings.

One approach that is currently being explored by the OPALE project is the definition of virtual computing infrastructures by which users will be able to define their specific computing environment and use it with their own ad-hoc procedures. This requires the design and implementation of powerful middleware services implemented on top of existing grid environments. The goal is to provide standardised services and the corresponding procedures to help the users specify the resources and computing environment they need to run the complex (and soon, multidisciplinary) applications they currently execute. This implies the design of generic graphic problem solving interfaces, of the implementation of enabling middleware and of ad-hoc interfaces on top of existing grid environments. An international consortium has been set up on this subject, including twelve corporate and academic research institutions, as well as industry partners from Italy, Great Britain, Greece, Cyprus and France. The OPALE project is one of the founding members of this consortium.

This is part of Lizhe Wang doctoral thesis work on *Virtual Computing Environments*.

The CAST platform has also been ported on the Sophia Antipolis cluster and several other Linux workstations in Grenoble with the purpose of developing a grid computing environment for biomedical applications with A. Habbal in Sophia Antipolis. An anti-angiogenesis simulation has thus been parallelised by Jean Arnaud and is being ported on this grid computing environment.

## 7. Contracts and Grants with Industry

### 7.1. Contracts

#### 7.1.1. *Optimum-shape design in aerodynamics and multidisciplinary extensions*

- *Self-Adaptive Parameterization for multidisciplinary optimum-shape design*, with Dassault Aviation, St Cloud.
- *Aerodynamic Generic-Wing Shape Optimization for a Business Aircraft*, with Piaggio Aero France; this contract reinforces a cooperation initiated through a Local Cooperative Action (COLORS) on “Hierarchical Parameterizations”, and complements the set up of B. Abou El Majd Doctoral’s program financed by the PACA Region. Additionally, it is being consolidated by a Cooperation Agreement with CIRA (Centro Italiano per la Ricerche Aerospaziale), Capua, under finalization.

#### 7.1.2. *Optimization in electromagnetics*

- France Télécom (La Turbie): optimization of antennas;
- Thalès (Bagneux) : optimization of the most dangerous trajectories in radar applications.



## 8. Other Grants and Activities

### 8.1. National and Regional Initiatives

#### 8.1.1. E-Lab Opratel

The collaboration with France Télécom and Thalès Défense led to the creation of the e-lab OPRATEL in which we develop models for array antennas for telecommunication purposes.

More specifically, the classical problem of frequency allocation is closely examined. This problem results in a very acute technological challenge today due to the numerous systems operating concurrently (interference of radar, surveillance systems, telephone, radio, television, domestic electronics, electromagnetic noise of WIFI, etc.). Since the channels are limited, special techniques are envisaged to support these systems (orthogonal waves, coding, dynamic occupation of the spectrum).

#### 8.1.2. Local Cooperative Action: *Hierarchical Shapes for optimization in Aerodynamics*

The OPALE project launched jointly with the GALAAD project a Local Cooperative Action (COLORS) “Hierarchical Shapes for optimization in aerodynamics” in order to initiate a cooperation with Piaggio Aero France, Nice (see <http://www-sop.inria.fr/opale/>). This year, the project has permitted to finance the visit of N. G. Pavlidis (Computational Intelligence Laboratory, University of Patras, Greece) hosted by the Galaad Project, who studied applications of *Particle-Swarm Optimization* (PSO) algorithms to shape optimization problems.

Originally, this initiative facilitated the financing by the Region of a doctoral thesis on related topics (B. Abou El Majd). This cooperation initially related to aerodynamics and geometrical tools to interface with CAD systems, is meant to be extended to other engineering fields demanding advanced computational tools, such as structural design.

### 8.2. International Networks and Working Groups

**Participants:** Jean Arnaud, Jean-Antoine Désidéri, Toan Nguyen, Jacques Périaux.

The OPALE project is involved in European interest groups on code validation and mathematical modelling, and in international cooperations on optimum-shape design.

#### 8.2.1. European Accompanying Measures Promuval

This European project coordinated by CIMNE, Barcelona, is a follow-up of FLOWnet, with an extended scope. It started in December 2002 at INRIA Sophia Antipolis, and its main objective is to prospect methods and tools for the validation of multi-physics codes. The development of the project consists in collecting available data on a database and prospecting new models, new numerical methods and validation tools which will be necessary for the Verification and Validation (“V and V”) of multi physics codes. Since several disciplines are interfacing numerically a pilot integrated platform is proposed by the Grenoble project’s component (as workpackage leader) to provide a cooperative environment for knowledge sharing. Several new mathematical methods and models have also been suggested by the OPALE project (as another workpackage leader) in order to achieve a good matching of information at interfaces (maintaining numerical accuracy of each discretized discipline, in particular). Several Working Groups focused on multiphysics applications have been set up to discuss these new lines of V and V: aeroelasticity, thermal flows, aeroacoustics and Flight Dynamics couplings.

The uncertainties of multiphysics simulations and experimentations need to be addressed systematically and managed. The utility of multi-physics modeling and simulation tools will be critical in the accurate and efficient design of modern multidiscipline aircraft systems. In order to reduce uncertainties in multi-physics results the sensitivity of computational data associated to multi-physics uncertainties need to be quantified : it is the road map investigated by PROMUVAL partners to increase the credibility of multidisciplinary design.

A State of the Art Short course on multi-physics codes validation was held in 2004 in Barcelona, as well as a workshop in Athens.

The outcome of this European initiative is a roadmap to multi-disciplinary code validation under finalization.

### 8.2.2. *The HEAVEN Project*

The project participates in the HEAVEN Project proposal (<< Hosting European Applications in a Virtual Environment >>), currently submitted to the EC as part of the IST FP6 program, concerning the << Grids for complex problem solving >> priority. In this proposal, our project is leader of several workpackages including the definition and implementation of the software supporting the virtual computing infrastructure. It is also leader of a test-case workpackage for airfoil optimisation.

Whereas resource co-allocation and dynamic control of distributed applications remains an important objective, a large effort is also currently dedicated to Virtual Computing Environments which are emerging as a new concept encompassing the grid technologies, distributed and parallel computing, as well as business processes for their widespread use in sophisticated technology areas, such as multidisciplinary design and optimisation.

The vision which underpins this approach is that seamless interfaces to distributed and multidisciplinary design are mandatory for the general use of grid technology in engineering, business and education.

In much the same way as the Internet is now available everywhere to everyone today through Web browsers, the focus is here to deliver new applications design methodologies by making the grid technology transparent through Virtual Computing Environments.

These environments, based on graphic interfaces, will rely on grid technology middleware and presumably require specific functionalities for the advanced definition and control of user applications, in particular in multidisciplinary engineering, based on mixed data and workflow management. This is the focus of Lizhe Wang's doctoral thesis. This approach is a joint collaboration with CNES (French National Space Research Center) and EADS (Common Research Center).

The goal is here to define and develop software "upperware" concepts, which will build on current middleware technology for the Grid, in order to provide Virtual Computing Environments. They will be able to support seamlessly application definition in various multidisciplinary fields, including engineering, business and education.

For this objective to be reached, high-level functionalities will be defined and developed for the modular and incremental construction of heterogeneous applications. This will rely on software component models and Web Services to provide simple interfaces that will hide the technicalities of current distributed computing technology, e.g., Corba.

The goal is to mask the technicalities of grid middleware, e.g., Globus, to the casual users, and provide a software layer in charge of high-level tasks concerning the control of grid-based applications (remote control of suspended sub-tasks, analysis of performance bottlenecks, advisory input to the users concerning the distribution of sub-tasks, etc). Several doctoral theses will be necessary to design, develop and test these environments, and one has already started mid-2004 (Lizhe Wang).

### 8.2.3. *European Network of Excellence MACSInet*

The project participates in the European Network of Excellence MACSINET (*Mathematics, Computing and Simulation in Industry Network*) supported by DG XIII et DG XII. This network is a joint initiative by ECCOMAS (*European Community for Computational Methods in Applied Sciences*) and ECMI (*European Community of Mathematics for Industry*). It aims at fostering European initiatives to approach new industrial multi-disciplinary challenges by mathematics and scientific computing. See <http://www.macsinet.org>.

This year the network contributed a prospective document, *Roadmap for Mathematics in European Industry*, largely disseminated in Europe.



### 8.3. Bilateral international cooperations

Chinese-French Institute LIAMA : joint-coordination of the project << Coordination and Optimisation of Hierarchical Methods for the Distributed Numerical Simulation of Nonlinear P.D.E. Problems >> (X. Xu, Institute of Computational Mathematics, CAS, and J.-A. Désidéri) also linked to the University of Nanjing (Dept. of Aeronautics and Astronautics) and the University of Tsinghua (grid computing).

Australian-French network on UAV systems As a follow up of a successful workshop on UAV systems (UAV: Unmanned Aerial Vehicles), which took place in Sydney last July 2003, it was decided by the main actors of this event to set up a French-Australian network on << Innovative technologies for the design of UAV systems >>. The three main themes of this project are : (i) Multi-Disciplinary Optimization (MDO), (ii) Autonomy, control and guidance, and (iii) sensors. The OPALE project is interested in the first topic since it requires new methods and tools for multidisciplinary and multicriterion optimization, and in particular Evolutionary Algorithms (EAs). Several test cases have been proposed for testing new adaptive methods like colony ants, Particle Swarm Optimization (PSO), Neural networks and EAs. To this end, regular information sharing sessions, on-line tools, sharing and exchange of research students between laboratories and institutes are being arranged. An on-line information sharing repository has already been established at : <http://www.aeromech.usyd.edu.au/UAVThinkTank>.

## 9. Dissemination

### 9.1. Education

The members of the OPALE project participate in the Educational effort within different areas at the University of Nice (UNSA).

#### 9.1.1. Master's degree in Mathematics, << Shapes >>

The project OPALE has been involved in the definition of this new Master's degree program dedicated to mathematical aspects of general shapes, and to industrial applications. The project is fully in charge the second term course UEf4 : << Shape Optimization >> (40 hrs) which includes lessons in

- Calculus of Variations, optimal control, domain deformation, domain derivatives and applications (A. Habbal), and
- Industrial motivation and examples, hierarchical parameterization, adaptive Optimization (J.-A. Désidéri).

#### 9.1.2. Ecole Supérieure en Sciences Informatiques (ESSI)

ESSI is an engineering school in computer sciences of UNSA on the Sophia Antipolis campus. A. Habbal teaches the following courses:

- Calculus (first year, 120 hrs)
- Programming mathematics (first year, 40 hrs)
- Numerical Methods in Finance (third year, 30 hrs)

### 9.1.3. Graduate program in Economics, option << Industrial Organization >>

– Game Theory and Economic Applications (A. Habbal, 15 hrs)

## 9.2. Theses and Educational Trainings

The following trainees have been, or are being supervised by the project:

Badr Abou El Majd , University of Nice-Sophia Antipolis; doctoral student (PACA Region scholarship); topic: Hierarchical algorithms and game strategies for the aerodynamic and structural shape optimization of a business jet.

Jean Arnaud , University P. Mendes France, Grenoble; topics: upgrade and port of the CAST software on the PC cluster at INRIA Rhone-Alpes and Sophia-Antipolis (April-June, 2004); parallelization of the anti-angiogenesis simulation of A. Habbal and port on the PC cluster at Sophia-Antipolis (July-August, 2004).

Louis Blanchard , University of Savoie, Chambéry; April-Aug. 2004: Optimal weighting for network antenna; doctoral student since October 2004; topic: design of antennas by optimization and numerical active control.

Pierre Dubois , Ecole des Mines and France Télécom, thesis student (Sophia Antipolis); topic: 3D electromagnetic gradient computations.

Jérôme Picard , University of Savoie, Chambéry; April-Aug. 2004: shape optimization of a reflector; Junior Technical Staff since October 2004.

Lizhe Wang , University J. Fourier, Grenoble; doctoral student; topic: Virtual Computing Environments for the Grid.

## 9.3. Organization of Scientific Events

As the chairman of Working Group IFIP 7.2 *System Modelling and Optimization*, J.P. Zolésio organizes an international workshop twice yearly, this year in July in Jyväskylä (within the ECCOMAS 2004 Conference) and in December at the University of Houston.

## 9.4. Participation in Scientific Committees

- J.-A. Désidéri is a member of << Comité d’Orientation et du Secrétariat Exécutif (COSE) du Réseau de Recherche et d’Innovation Technologique (RRIT) ‘Recherche Aéronautique sur le Supersonique’ >> (<< Steering and Executive Committee (COSE) of the Research and Technology Innovation Network ‘Aeronautical research for supersonics’ >>), and co-animates with C. Michaut, ONERA, the topic on << aerodynamic and optimization >>.
- J.-A. Désidéri is a member of << Comité Scientifique et Technique (CST) auprès du Centre National de Recherche Technologique ‘Aéronautique et Espace’ >> (<< Scientific and Technical Committee of the National Center for Technological Research ‘Aeronautics and Space’ >>), CNRT-AE at Cerfacs, Toulouse.
- J.P. Zolésio is chairman of Working Group IFIP 7.2 *System Modelling and Optimization*.

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