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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 - Méditerranée - Grenoble - Rhône-Alpes

THEME NUM

Activity Report

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1. Team

Head of project-team
Jean-Antoine Désidéri [DR, INRIA Sophia Antipolis, HdR]

Vice-head of project-team
Toan Nguyen [DR, INRIA Rhône-Alpes, HdR]

Administrative assistant
Montserrat Argente [INRIA Sophia Antipolis]

Research Scientists
Régis Duvigneau [CR, INRIA Sophia Antipolis]
Abderrahmane Habbal [Maître de Conférences, University of Nice–Sophia Antipolis, HdR]
Jean-Paul Zolésio [DR, CNRS, HdR]

Post-doctoral fellow
Praveen Chandrashekarappa [INRIA Sophia Antipolis]
Jichao Zhao [INRIA Sophia Antipolis, until August 2007]

Doctoral students
Badr Abou El Majd [University of Nice–Sophia Antipolis, until March 2007]
Louis Blanchard [Ecole des Mines]
Benoit Chaigne [University of Nice–Sophia Antipolis]
Abdou Wahidi Bello [University of Cotonou, Cotonou (Benin); Mai-Dec. 2007]

Student interns
Jean-Georges Moineau [École Centrale de Paris, July-October]
Daniele Varone [IMAFA Master, University of Nice-Sophia Antipolis, May 15-September 15]

External collaborators
John Cagnol [MdC, Pôle Léonard de Vinci, HdR]
Raja Dziri [Université de Tunis, HdR]
Michel Delfour [Centre de Recherches Mathématiques, Montréal, HdR]
Jacques Périaux [UPC, Barcelona, Spain; TEKES Distinguished Professor, Univ. Jyväskyla, Finland, HdR]
Jan Sokolowski [Institut Poincaré, University of Nancy, HdR]

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 excell can be defined more precisely.

From the *physical analysis* point of view, our expertise relies mostly on 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 methodologies.

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, tailoring the numerical method to it, identifying a functional gradient in a continuous or discrete setting, analyzing iterative convergence, improving it, measuring multi-disciplinary coupling strength and identifying 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 progresses 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 and Chinese partners (ACTRI).

2.3. Highlights of the year

This year, a new partnership with industry was launched with the R & D *Automotive Applications Centre* of Arcelor Mittal in Montataire, France. This partnership is related to the optimization of steel (automobile) elements with respect to mechanical criteria (crash, fatigue). The project team was solicited to audit the GEAR2 optimization team in Montataire [56]. Additionally, a student interm from Arcelor, J.-G. Moineau, was hosted and directed at INRIA for a four-months period.

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 large 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 requires 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 arises 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 return 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 Ω 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 Ω 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 Ω_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 a large evolution when t is large, and when $t \to \infty$. A numerical challenge is to avoid the use of any "smoother" process and also to develop "shape-Newton" methods [60]. Our evolution field approaches permit to extend this viewpoint to the topological shape optimization ([63]).

We denote $G(\Omega)$ the shape gradient of a functional J at Ω. 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_Ω which turns out 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 Γ) 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: $< \mathcal{A}\phi, \phi > \geq |\phi|_H^2$ where H denotes a root space. We consider the following problem: given Ω_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 first been proved 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 $t \to \infty$) 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 field 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 [2], [12], [1].

3.3. Integration platforms

Developing grid computing for complex applications 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, aerostructure 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 militate in favour of 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 the OPALE project since its very beginning. A software integration platform has been designed by the OPALE project for the definition, configuration and deployment of multidisciplinary applications on a distributed heterogeneous infrastructure [62]. 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. [64].

The main difficulty still remains however in the deployment and control of complex distributed applications on grids by the end-users. Indeed, the deployement 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 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. However, it still 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. It is currently deployed within the Collaborative Working Environments Unit of the DG INFSO F4 of the European Commission. It is planned to include Chinese partners from the aeronautics sector in 2007 to set up a project for FP7.

4. Application Domains

4.1. 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 relates to software platforms for code coupling.

4.2. Electromagnetics

In the context of shape optimization of antennas, we can split the existing results in two parts: 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 part 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 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 unbouded 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. 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.

4.3. Biology and medecine

A particular effort is made to apply our expertise in solid and fluid mechanics, shape and topology design, multidisciplinary optimization by game strategies to biology and medecine. Two selected applications are priviledged : solid tumours and wound healing.

Opale’s objective is to push further the investigation of these applications, from a mathematical-theoretical viewpoint and from a computational and software development viewpoint as well. These studies are led in collaboration with biologists, as well as image processing specialists.

4.4. 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, 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 set up for the development of a distributed computing environment for the deployment of parallel applications concerning the modelling of airfoil optimization techniques on distributed PC-clusters and the parallelization of the corresponding algorithms;
- second, a cooperation has been set up with CNES for the design, implementation and deployment of Grid-based Virtual Computing Environments.

The first aspect implies the parallelisation of the Simplex and 3D multi-level parameterization algorithms and the use of the PC-clusters and other various Linux workstations at INRIA Sophia-Antipolis and Grenoble. This will use 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 is devoted to this aspect. The goal is to design and implement an "upperware" software that is extending the functionalities of current middleware platform to simplify the deployment of complex applications on heterogeneous Grids.

Further, strong implication in European Networks, e.g., AEROCHINA, 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 demonstator of this platform is currently being designed in cooperation with CIMNE (Spain).

5.2. FAMOSA package for Optimum-Shape Design in Aerodynamics

We are developing the FAMOSA code (Full Adaptive Multi-level Optimum Shape Algorithms), designed for shape optimization of 3D aerodynamic bodies. It integrates the following toolboxes:

- a module F-MANAGER managing the communications between the flow solver and the optimizer, by calculating an objective function (based on the results of the flow-simulation) and its gradient, by building metamodels and estimating statistical quantities for robust design;
- a parameterization module BZPARAM implementing a 3D multi-level and adaptive Bézier parameterization (Free-Form Deformation) and 3D mesh-update routines;
- an optimization module OPTIM containing general optimization routines using deterministic as well as semi-stochastic algorithms;
- a module PAROPTI allowing the use of a parallel architectures to instantiate the cost function evaluations.

To facilitate the development of the software and collaborative work between the different developers, a code managing framework based on the SVN version control system has been set up. The code is presently hosted at the inriaGforge.

Moreover, a graphical interface has been developed in order to facilitate the use of the software and allow an easy integration of temporary users and developers.

5.2.1. Flow solver codes

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

Participants: Michele Andreoli [former trainee, update of NS3D], Régis Duvigneau, Aleš Janka [former Post Doctoral Student, update of NS3D], Thibaud Kloczko [Smash Project-Team Post Doctoral Student, NUM3SIS developments], Massimiliano Martinelli [Tropics Project-Team PhD student, development of adjoint solver].

The FAMOSA code is linked to two flow solvers :

- The NS3D flow code originates from Sinus Project-Team and 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;
  - 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.

An adjoint code has been recently developed to compute first and second order derivatives of aerodynamic coefficients with respect to boundary condition parameters (Mach number, angle of attack) or geometry parameters. The code has been obtained by applying the automatic differentiation tool Tapenade (developped by Tropics Project-Team) to the flow solver code (written in Fortran 77). The first order derivatives are computed by solving the adjoint system, that is built by using Tapenade in reverse mode. For the computation of the second derivatives, two strategies can be employed : the use of two successive tangent mode differentiations or the use of the tangent mode on the result of the reverse mode differentiation. The efficiency of these strategies depend on the number of the parameters considered.

- The NUM3SIS code is currently developed by Smash Project-Team. It solves 3D Euler equations on unstructured meshes and includes modules to simulate multiphase flows for steady or unsteady problems. It includes several spatial discretization schemes and explicit or implicit (matrix-free) methods for the temporal discretization.

  The code has been designed for large scale parallel computations using the MPI library.

5.2.2. F-MANAGER (communication between solvers and optimizer):

Keywords: *constraints*, *cost function*, *meta-models*, *statistics*.

Participants: Praveen Chandrashekarappa, Régis Duvigneau, Massimiliano Martinelli [Tropics Project-Team PhD student].

After the flow-simulation for each shape, aerodynamic coefficients are calculated (lift, drag, pressure gradient, etc) and passed to a routine to evaluate the objective function. The objective function is a 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.

The aerodynamic coefficients computed for each shape are stored in a database, that can be used to buid metamodels. These metamodels can then be employed to replace some cost function evaluations or provide additional information (gradient, hessian). Three different metamodels are included:

- Least-squares polynomial approximations
- Radial Basis Functions (RBF) neural networks
- Kriging (Gaussian process)

These metamodels include internal optimization procedures to set some numerical parameters.

For robust design, statistical quantities (such as mean or variance) of the aerodynamic coefficients are estimated on the basis of the metamodels by using classical Monte-Carlo methods, or on the basis of first and second order derivatives of aerodynamic coefficients.

5.2.3. BZPARAM(parameterization):

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

Participants: Michele Andreoli [former trainee], Régis Duvigneau, Aleš Janka [former Post Doctoral Student], Jichao Zhao.

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 represention 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. A multi-level parameterization can be obtained by using the degree elevation property [61].Hence, a set of nested parameterizations can be easily built and used for multi-level optimization strategies.

A routine is being developed, that adapts the initial and perhaps naïve parameterization to the particular problem studied, on the basis of a first approximation of the optimal shape. Basically, it automatically modifies the definition of the deformation basis functions to regularize the deformation field.

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. The FFD technique, which operates a volumic deformation, can also be employed to deform the shape and the mesh simultaneously.

5.2.4. *OPTIM (optimizers):*

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

Participants: Michele Andreoli [former trainee], Yannick Berard [former trainee], Praveen Chandrashekarappa, Régis Duvigneau, Abderrahmane Habbal, Aleš Janka [former Post Doctoral Student], Latifa Oulladji [former trainee].

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 particle swarm optimization (PSO) algorithm;
- the Nelder-Mead simplex algorithm;
- the Torczon multi-directional search algorithm.
- a Sequential Quadratic Programing method (SQP)

The last three routines implement deterministic descent methods. However, due to the multimodality of aerodynamic cost functions, semi-stochastic optimization strategies, such as genetic algorithms of particle swarm optimization, are mandatory for global optimization. Genetic algorithms mimic the evolution of a population, through genetic operators such as selection, crossover and mutation. Particle swarm optimization is inspired from the collective intelligence of birds flocks for food seeking or predators avoiding and is based on underlying rules that enable sudden direction changes, scattering, regrouping, etc.

The most serious disadvantage of semi-stochastic algorithms 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 evaluations are not usefull for the evolutionary process. Therefore, a particular strategy has been developed, called ’inexact pre-evaluation’, that rely on the use of metamodels to provide a cheap estimate of the design performance and select which designs should be evaluated accurately by the flow solver.

5.2.5. *PAROPTI (parallelization):*

Keywords: *MPI*, *parallel computing*.

Participant: Régis Duvigneau.

The shape optimization procedure employ at each iteration independent and simultaneous cost function evaluations, that correspond to different design parameters and/or physical parameters (for robust design). A two-level parallel implementation has been developed, based on the MPI library, to distribute these evaluations on a given number of processors. It results in a significant reduction (quasi linear) of the computational time.

5.3. Numerical Modules for Gradient Computations in Electromagnetics

Participants: Claude Dedeban [France Télécom, La Turbie], Pierre Dubois [former PhD], Jerôme Picard [former engineer], Jean-Paul Zolésio.

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

Additionally, a self-sufficient FORTRAN code is being developed for antenna optimization by parameterized level-set techniques (6.4.9). This code is to be latter interfaced with the code for array antenna optimization (6.4.8).

6. New Results

6.1. Computational methods, numerical analysis and validation

6.1.1. *Numerical simulation of shallow-water equations*

Participants: Abdou Wahidi Bello, Jean-Antoine Désidéri, Aurélien Goudjo [University of Cotonou, Benin], Côme Goudjo [University of Cotonou, Benin], Hervé Guillard [Smash Project Team].

This activity corresponds to A. W. Bello's thesis work in co-direction between the University of Cotonou, Benin, and INRIA, with the support of the French Embassy in Cotonou. The study aims at developing a numerical simulation method of the water network in the city of Cotonou. This network includes a canal connecting Lake Nokoué to the Atlantic Ocean, and various ducts in the city itself. This network is chronically flooded when important rains occur. In our perspective, the simulation code is meant to be used in the future as a control tool to identify ways to prevent flood, or reduce the damages it causes.

The proposed numerical approach consists in simulating the flow by solving the shallow-water equations with topography and friction, as it is customary in estuary-flow-type simulations, by a finite-volume method. The computational domain is the space occupied by water and the floodplains. It is projected on a horizontal plane of reference, and discretized, and the governing equations are integrated on each grid cell. The numerical integration is carried out by a Godunov-type scheme using a two-step Riemann approximate solver of HLLC type which preserves the positivity the water height and which is well adapted to the treatment of the shock waves. To determine the height of the intermediate state in the Riemann solver, we propose an algorithm in a celerity-speeds formulation in which the governing equations are linearized; as a result, the positivity of the height is preserved, and this then allows to compute the speeds of the fastest waves.

The simulation method has been tested on academic problems first to demonstrate its adequacy. Then, a more realistic case has been treated to model the phenomenon of flood in the city of Cotonou (BENIN) by the water risings in the lagoon [49].

6.1.2. Interpolation of Infinite Sequences by Entire Functions

Participant: Jean-Antoine Désidéri.

The study was originally motivated by a theoretical question raised by Warming and Hyett in a famous publication on the *Modified Equation Approach* [65]. Their classical accuracy analysis of a finite-difference method applied to a time-dependent problem implicitly relies on the assumption that a function interpolating the numerical values can be expanded, over an indefinite domain, in Taylor's series of the independent variables x and t. We have established constructively that the problem of interpolation of an arbitrary infinite sequence of real numbers by an *entire* function of x (and possibly t) admits uncountably many solutions. In the case of a single variable, if the values are bounded, the interpolant can be made bounded, and all its derivatives bounded. Besides, the construction is generalized to the interpolation of the values of the function and its derivatives up to an arbitrarily prescribed order (*Hermitian interpolation*). The proposed interpolant depends on a free parameter λ, and its behavior as λ varies is illustrated by a numerical example [28]

6.1.3. Validation of the NUM3SIS flow solver

Participants: Régis Duvigneau, Thibaud Kloczko [Smash Project-Team Post Doctoral Student, NUM3SIS developments].

The new NUM3SIS flow solver is developed by Smash Project-Team for two years. This work has been carried out with the help of a development engineer from DREAM Team in 2006.

A validation study has been carried out by Opale and Smash Project-Teams conjointy to assess the capabilities of the flow solver and compare its performance to the one of NS3D code for various subsonic, transonic and supersonic flows. The computational performance of the NUM3SIS code for large-scale parallel computations has also been tested.

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), as well as algorithmic and software aspects (parallel and grid computing).

These general themes for Opale are given some emphasis this year through the involvement of our project in the ANR/RNTL National Network on Multi-Disciplinary Optimization "OMD” (see paragraph 8.1.1).

6.2.1. Hierarchical (multilevel) and adaptive shape parameterization

Participants: Badr Abou El Majd, Praveen Chandrashekarappa, Jean-Antoine Désidéri, Régis Duvigneau, Abderrahmane Habbal, Jichao Zhao.

6.2.1.1. Algebraic theory of multilevel parametric optimization

With the purpose of developing a basic conceptual model for shape optimization, we have considered the minimization of the quadratic form measuring the square of the distance between a candidate shape and a given target geometry. When solving this problem by a steepest-descent-type optimizer (without special preconditioning), the iteration becomes similar to the classical point–Jacobi iteration applied to a specific linear system, whose matrix reflects the choice of parameterization. This model has been used to support a spectral analysis of the algebraic system under consideration, permitting us to establish a parallel between the present approach and standard geometrical multigrid concepts, identifying in particular the notion of modes and frequency. Thirdly, the analysis suggests us an alternate definition of the *two-level ideal algorithm*, which is classically the theoretical building block of a more general multilevel strategy.

6.2.1.2. Two-level correction algorithms for model problems

Variants of the two-level ideal algorithm for parametric shape optimization have been tested. In the linear case, the method, referred to as the Z' method, employs a permutation operator to rearrange the eigenstructure in such a way that the new high-frequency modes are associated with large eigenvalues. As a result, the classical steepest-descent iteration can be viewed as a Jacobi-type smoother, and standard multilevel strategies be applied. An alternate method is also tested based on odd-even decoupling (L' method). For a linear model problem, both new methods are found efficient and superior to the original formulation, but the Z' method is more robust. Similar numerical results are obtained for a nonlinear model problem by considering the eigensystem of the Jacobian matrix [55].

6.2.1.3. Regularized-two level algorithms for model problems

The three methods considered above have been alternately examined in a more classic way, in terms of singular value decomposition (SVD) and regularizations, for model problems. Numerical results show that regularized two level algorithms are more robust [54].

6.2.1.4. Multilevel shape optimization algorithms and application to 3D aerodynamic Problems

We have proposed to exploit the classical degree–elevation process to construct a hierarchy of nested Bézier parameterizations. The construction yields in effect a number of rigorously–embedded search spaces, used as the support of multilevel shape–optimization algorithms mimicking multigrid strategies. In particular, the most general, *FAMOSA, Full Adaptive Multilevel Optimum Shape Algorithm*, is inspired by the classical *Full Multigrid Method*.

The *FAMOSA* method has been applied to the context of three–dimensional flow for the purpose of shape optimization of a transonic aircraft wing (pressure–drag minimization problem). This complex iterative strategy has been compared with the basic one-level method, and with the simple "one-way-up" algorithm based on degree–elevation only (without coarse-parameterization correction steps). The *FAMOSA* method was found superior to both simpler alternatives [22] [26] [44] [29].

6.2.1.5. Parameterization adaption

Parameterization techniques commonly used in aerodynamic shape optimization are essentially general and multi-purpose approaches. As a consequence, they cannot be well suited to a particular shape optimization problem. A new method has been developed that adapts an initial and perhaps naïve parameterization of an aerodynamic shape by the Free-Form Deformation (FFD) technique, to the particular optimization problem to solve, according to a first approximation of the solution. It is based on the optimization of the mapping that defines the FFD coordinates from the lattice coordinates, in order to regularize the displacement of the control points.

This approach was tested on the optimization of the wing shape of a business aircraft. It was shown that parameterization adaption permits to reach shapes of better fitness and also to accelerate the convergence. Especially, it was found that the use of an adapted parameterization of lower degree yields better results than the use of a naïve parameterization of higher degree [27].

6.2.1.6. Combining multilevel algorithms with evolutionary computing

The use of multilevel parameterization strategies in conjunction with evolutionary algorithms is not straightforward, since these methods do not rely on an optimization path that could be split into several parts to solve the problem in different design spaces. Particularly, we have shown in the past that genetic algorithms are not well suited to these strategies.

Therefore a new approach has been developed using Particle Swarm Optimization (PSO) algorithms. Particle swarm optimization is inspired from the collective intelligence of birds flocks for food seeking or predators avoiding and is based on underlying rules that enable sudden direction changes, scattering, regrouping, etc. The developed multilevel algorithm relies on the use of the *swarm memory* to transfer information from one level to the next. This strategy has been found very effective for a simple degree increase strategy. Especially, it was shown that the multilevel algorithm permits to use swarms of smaller size yielding a significant computational time reduction [26].

6.2.1.7. Hybrid multilevel algorithms

Finally, it has been found that that the proposed multilevel parameterization approach defines a suitable framework for hybrid optimization, by combining an evolutionary search in spaces of progressively larger dimension, with a deterministic search in the space of largest dimension.

The application to the optimization of the wing shape of a supersonic business jet has shown that the hybrid approach is far more efficient than deterministic or evolutionary methods alone. Especially, the exploration of the design space as well as the accuracy of the search are improved. This work has been carried out in the framework of the ANR/RNTL National Network on Multi-Disciplinary Optimization "OMD”.

6.2.2. Multidisciplinary Optimization

Participants: Badr Abou El Majd, Praveen Chandrashekarappa, Jean-Antoine Désidéri, Régis Duvigneau, Abderrahmane Habbal, Jean-Pierre Merlet [Coprin Project Team], Jacques Périaux, Zhili Tang [Nanjing University of Aeronautics and Astronautics], Daniele Varone, Jichao Zhao.

6.2.2.1. Multicriterion Aerodynamic Shape Design Optimization and Inverse Problems using Control Theory and Nash Games

Multicriterion design is gaining importance in aeronautics in order to cope with new needs of Society. In the literature, contributions to single discipline and/or single-point design optimization abound. We propose to introduce a new approach combining the adjoint method with a formulation derived from game theory for multipoint aerodynamic design problems. Transonic flows around lifting airfoils are analyzed by Euler computations. Airfoil shapes are optimized according to various aerodynamic criteria. The notion of player is introduced. In a competitive Nash game, each player attempts to optimize its own criterion through a symmetric exchange of information with others. A Nash equilibrium is reached when each player constrained by the strategy of the others, cannot improve further its own criterion. Specific real and virtual symmetric Nash games are implemented to set up an optimization strategy for design under conflict [35].

6.2.2.2. Splitting of territories in concurrent optimization

When devising a numerical shape–optimization method in the context of a practical engineering situation, the practitioner is faced with an additional difficulty related to the participation of several relevant physical criteria in a realistic formulation. For some problems, a solution may be found by treating all but one criteria as additional constraints. In some other problems, mainly when the computational cost is not an issue, Pareto fronts can be identified at the expense of a very large number of functional evaluations. However the difficulty is very acute when optimum-shape design is sought w.r.t. an aerodynamic criterion as well as other criteria for two main reasons. The first is that aerodynamics alone is costly to analyze in terms of functional evaluation. The second is that generally only a small degradation of the performance of the absolute optimum of the aerodynamic criterion alone is acceptable (sub–optimality) when introducing the other criteria.

We have proposed a numerical methodology for the treatment of such problems of concurrent engineering. After completion of the parametric, possibly–constrained minimization of a single, primary functional J_A, approximations of the gradient and the Hessian matrix are available or calculated using data extracted from the optimization loop itself. Then, the entire parametric space (a subset of $\mathbb{R}^{n+1}$) is split into two supplementary subspaces on the basis of a criterion related to the second variation. The construction is such that from the initial convergence point of the primary functional, normalized perturbations of the parameters lying in one of the two subspaces, of specified dimension $p \leq n$, cause the least possible degradation to the primary functional. The latter subspace is elected to support the parameterization of a secondary functional, J_B, in a concurrent optimization realized by an algorithm simulating a Nash game between players associated with the two functionals. We prove a second result indicating that the original global optimum point of the full-dimension primary problem is Pareto-optimal for a trivial concurrent problem. This latter result permits us to define a continuum of Nash equilibrium points originating from the initial single-criterion optimum, in which the designer could potentially make a rational election of operating point [51].

The efficiency of this technique has been illustrated by the optimization of a robot for which various performance criteria and constraints originate from analytical geometry and can be expressed by polynomials or rational functions of (geometrical) design variables. This study has permitted us to initiate a collaboration with the Coprin Project Team that has developed an expertise in optimization by intervals.

6.2.2.3. Coupled fluid-structure optimization using Game Theory

In his thesis, B. Abou El Majd is treating a particular case of concurrent shape–optimization by coupling the drag minimization of a transonic aircraft wing with the reduction of a criterion related to structural design under surface and volume constraints. The structural criterion attempts to equalize over the geometry the stress due to the aerodynamic load. Again, a game strategy is elaborated in which the primitive shape control variables, associated with Bézier control points, are split into two packets, each packet corresponding to the *strategy* of a player in a simulated Nash game.

For this academic, but very difficult exercise, B. Abou El Majd has shown that a Nash equilibrium could be achieved when using a split of the primitive variables, but only in a very particular case in which the variables in the strategy of the virtual player in charge of reducing the structural criterion are, unsurprisingly, those the most remote from the sensitive shock location. However, the eigensplit proposed in the previous paragraph (here based on the projected Hessian of a RBF-metamodel) revealed far superior, by improving both the iterative convergence of the Nash-equilibrium realization algorithm and the quality of the corresponding aerodynamic solution. B. Abou El Majd experimented with success and documented a number of variants, including unsymmetrical Stackelberg games [22].

6.2.2.4. Metamodel-based optimization

Multidisciplinary optimization is particularly time consuming, since several disciplines and simulation tools are involved in the design procedure. Moreover, communication between the different displines may be tedious in practice, because of the use of different shape representations, meshes, length scales, objective functions, etc.

Therefore, we are currently developing approaches that rely on *metamodels*, i.e. models of models, to accelerate the optimization procedure, facilitate communication among disciplines and provides additional informations such as sensitivities.

Different techniques of metamodeling (polynomial fitting, Radial Basis Functions, Kriging) have been developed and validated on academic problems. Our developments have been particularly focused on the automatic optimization of the internal numerical parameters of the different models[53].

The metamodels have then been used for different purposes :

- Accelerate evolutionary algorithms by replacing some expensive simulations by metamodels. At each generation of the evolution, all individuals are first pre-evaluated using metamodels, and then only a pourcentage of the population (most promising individuals) are exaclty evaluated by simulation. For the Particle-Swarm Optimization (PSO) algorithm, an adaptive method has been proposed, that allows the algorithm to automatically adjust the number of exact evaluations required. A reduction of the CPU cost of factor three has been obtained for a practical test-case in aerodynamics[52], [42].
- Replace the simulation software to estimate statistics using Monte-Carlo methods. In robust design, one intends to estimate the impact of uncertain parameters. Statistics of the performance (expectation, standard deviation) can be estimated for a reasonnable computational cost by using Monte-Carlo methods based on metamodels[50].
- Compute the hessian matrix of the performance with respect to design parameters in order to define a suitable split of territories in multi-disciplinary optimization.

These developements are mainly supported by the OMD project granted by ANR/RNTL.

6.2.2.5. Hybrid algorithms

Derivative-free optimization algorithms are appealing, since they give sense to the expression "one solver = one optimizer".

These algorithms are essentially divided in two families. The first family contains *P*owell-like algorithms developed in the 60s. These methods cannot pretend to perform global optimization. The second family contains evolutionary algorithms, particularly genetic algorithms and evolution strategies. These probabilistic algorithms are designed *t*o perform global optimization. John Holland defined their fundamental principles in 1962 and David Goldberg contributed in popularizing them for practical problems in 1989.

Comparing evolutionary algorithms to classical descent methods using gradient information raises pros and cons, wich are accepted or not depending on the nature of the optimization problem. Evolutionary algorithms are not trapped in local-minimum regions, but require a large number of cost function evaluations. On the contrary, classical descent methods are characterized by a high convergence rate, but they have no way to escape from local-minimum regions. Moreover, gradient computations may yield theorical or computational difficulties.

In 2003, we have implemented a hybridization approach using a local discontinuous approximation based on a classification algorithm, without memory effects from one generation to the next. In the present work, we develop a new variant using a local continuous approximation, so-called “Liszka-Orkisz approximation”, including memory effects. This approach has been applied to a difficult industrial problem concerning preform forming.

6.2.3. Uncertainty estimation and robust design

Participants: Régis Duvigneau, Massimiliano Martinelli [Tropics Project-Team PhD student].

A major issue in design optimization is the capability to take uncertainties into account during the design phase. Indeed, most phenomena are subject to uncertainties, arising from random variations of physical parameters, that can yield off-design performance losses.

To overcome this difficulty, a methodology for *robust design* is currently developed and tested, that includes uncertainty effects in the design procedure, by maximizing the expectation of the performance while minimizing its variance[41].

Two strategies to *propagate the uncertainty* are now under study :

- the use of metamodels to estimate the uncertainties of the objective function from the uncertainties of the input parameters of the simulation tool. During the optimization procedure, a few simulations are performed for each design variables set, for different values of the uncertain parameters in order to build a database used for metamodels training. Then, metamodels are used to estimate some statistical quantities (expectation and variance) of the objective function and constraints, using a Monte-Carlo method[50], [42].
- the use of the automatic differentiation tool Tapenade (developped by Tropics Project-Team) to compute first and second order derivatives of the performance with respect to uncertain parameters. The first order derivatives are computed by solving the adjoint system, that is built by using Tapenade in reverse mode. For the computation of the second derivatives, two strategies can be employed : the use of two successive tangent mode differentiations or the use of the tangent mode on the result of the reverse mode differentiation. The efficiency of these strategies depend on the number of the parameters considered. Once these derivatives have been computed, one can easily derive statistic estimations by integrating the Taylor series expansion of the performance multiplied by the probability density function. This work is carried out in collaboration with Tropics Project-Team.

These strategies are currently tested for the aerodynamic optimization of the wing shape of a business aircraft. The robust design of the wing is performed by reducing the drag mean and the drag variance, under a probabilistic constraint on the lift, for uncertainties on the Mach number and the angle of attack.

6.2.4. Application of sensitivity analysis and optimization algorithms in CFD

Participants: Régis Duvigneau, Michel Visonneau [Laboratoire de Mécanique des Fluides CNRS UMR6598, Nantes].

Recent developments concerning shape optimization in fluid mechanics have been applied to flow control, in order to optimize actuator parameters (e.g. oscillatory jet frequency and position). Promising results have been obtained by optimizing the characteristics of oscillatory/steady jets for stall control for an airfoil[25].

6.2.5. Numerical Shape Optimization of Axisymmetric Radiating Structures

Participants: Benoît Chaigne, Claude Dedeban [France Télécom R & D], Jean-Antoine Désidéri.

This activity aims at constructing efficient numerical methods for shape optimization of three-dimensional axisymmetric radiating structures incorporating and adapting various general numerical advances [66] (multi-level parameterization, multi-model methods, etc) within the framework of the Maxwell equations.

The optimization problem consists in finding the shape of the structure whose far field radiation fits a target radiation pattern. The target pattern can be expressed in terms of far field, radiated power (norm of the field) or directivity (normalized power).

Two models have been considered for the analysis problem: a simplified approximation model known as "Physical Optics" (PO) for which the far field is known explicitly for a given geometry; a rigorous model based on the Maxwell equations. For the latter, the equations are solved by SRSR, a 3D solver of the Maxwell equations for axisymmetric structures provided by France Télécom R & D.

A parametrical shape optimization based on *Free-Form* deformation (FFD) has been considered. For the PO model, the analytical gradient w.r.t. the FFD parameters has been derived. An exact Hessian has been obtained by Automatic Differentiation (AD) using Tapenade (developed by Tropics Project-Team). Both gradient and Hessian have been validated by finite differences. For the Maxwell equations model, the gradient is computed by finite differences.

Both global and local point of view have been considered for solving the optimization problem. An original multilevel semi-stochastic algorithm [59] showed robustness for global optimization[38]. For local optimization, a quasi-Newton method with BFGS update of the Hessian with linear equality constraints has been developed. A numerical spectral analysis of the projected Hessian or quasi-Hessian for some shapes has exhibited the geometrical modes that are slow to converge. Based on this observation, several multi-level strategies to help this modes to converge have been developed. Successful results have been obtained for both PO and Maxwell model. In addition, it has been observed that better results are obtained when the Bernstein polynomials are replaced by Tchebychev polynomials in the FFD formulation.

In further works we intend to consider a wider class of basis functions in the FFD formulation. A real-case problem for antenna design will be considered, including multi-objective problems.

6.3. Application of shape and topology design to biology and medecine

Participants: Abderrahmane Habbal, Nicholas Ayache [EPIDAURE PROJECT], Grégoire Malandain [EPIDAURE PROJECT], H. Barelli [IPMC], B. Mari [IPMC].

In the framework of a research collaborative action COLOR 2005, involving three research teams specialized in cell biology (IPMC), image processing and mathematical modeling (EPIDAURE and OPALE projects), two test-cases are defined : angiogenesis and wound healing. This latter application is given particular emphasis, since experimental results from biology can be obtained more easily.

Thus, several images and movies are quickly collected from experimental results in biology, concerning monolayer MDCK cell healing. The analysis of these images allows us to observe that the cell migration velocity is constant during the healing.

In order to numerically model the migration, Fisher's model (non-linear parabolic equations) seems relevant to us. Indeed, it is characterized by a constant front velocity. The first results obtained are very promising and confirm the adequacy of Fisher's model. As a consequence of this work, new data are provided to biologists (diffusive coefficients) to describe the behavior of MDCK cells in presence of HGF and inhibitors.

6.4. Mathematical analysis in geometrical optimization

6.4.1. Non cylindrical dynamical system

Participant: Jean-Paul Zolésio.

The optimal control theory is classicaly based on the assumption that the problem to be controled 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 [2]. 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[24]. 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 book.

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. [58].

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.

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

6.4.5. Shape Optimization by Level Set 3D

Participants: Claude Dedeban [France Télécom], Pierre Dubois, Jean-Paul Zolésio.

The *inverse scattering* problem in electromagnetics is studied through the identification or "reconstruction" of the obstacle considered as a *smooth surface* in R^3. Through measurement of the scattered electric field E_d in a zone θ we consider the classical minimization of a functional $\mathfrak{J}$ measuring the distance beetwen E_d and the actual solution E over θ. Then, we introduce the continuous flow mapping T_r, where r is the disturbance parameter which moves the domain Ω in Ω_r. We derive the expression for the shape derivative of the functional, using a $\min \max$ formulation.

Using the Rumsey integral formulation, we solve the Maxwell equation and we compute the shape gradient, verified by finite difference, using the SR3D software (courtesy of the France Telecom company).

Additionally, we have introduced the Level Set representation method in 3 dimensions. This technique, which comes from the image processing community, allows us to construct an optimization method based on the shape gradient knowledge. In this method, the 3D surface, defined by a homogenous triangulation, evolves to reduce the cost functional, easily encompassing certain topological changes. Using this technique, we have studied the inverse problem and evaluated sensibilities w.r.t. quantitative and qualitative criteria.

6.4.6. Shape stabilization of wave equation

Participant: Jean-Paul Zolésio.

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 modeling is foreseen[36].

6.4.6.1. Passive Shape Stabilization in wave equation

We have developed a numerical code for the simulation of the damping of the wave equation in a moving domain. The *cubic shape derivative* has been numerically verified through a new approximation taking care of the non autonomeous oprator in the order reduction technic[36].

6.4.6.2. Active Shape Morphing

The ongoing collaboration on the stability of wave morphing analysis for drones led to new modeling and sensitivity analyses . Any eigenmode analysis is out of the scope for moving domains as we are faced with time depending operators. Then, we develop a new stability approach directely based ont a "Liapounov decay" by active shape control of the wave morphing. This active control implies a backward adjoint variable and working on the linearized state (through the *transverse vector filed* Z which is driven by the Lie brackets) we present a Ricatti-like synthesis for the real time of the morphing.

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, a difficult modeling topic of major importance for our industrial partners.

6.4.8. Array Antennas Optimization

Participants: Louis Blanchard, Jean-Paul Zolésio.

We are developing a new approach for modeling array antennas optimization. This method integrates a Pareto optimization principle in order to account for the array and side lobes but also the antenna behavior. The shape gradient is used in order to derive optimal positions of the macro elements of the array antenna[37].

6.4.9. Parametrized level set techniques

Participants: Louis Blanchard, Jerôme Picard, Jean-Paul Zolésio.

Since a 1981 NATO study from the University of Iowa, we know how to define the speed vector field whose flow mapping is used to build the level set of a time-dependent smooth function F(t,x) in any dimension. We consider the Galerkin approach when F(t,.) belongs to a finite dimensional linear space of smooth functions over the fixed domain D. Choosing an appropriate basis (eigenfunctions, special polynomials, wavelets, ...), we obtain F(t,.) as a finite expansion over the basis with time-dependent coefficients. The Hamilton-Jacobi equation for the shape gradient descent method applied to an arbitrary shape functional (possessing a shape gradient) yields a non linear ordinary differential equation in time for these coefficients, which are solved by the Runge-Kutta method of order four. This Galerkin approximation turns to be powerful for modeling the *topological changes* during the domains evolution. Jerome Picard has developed a code which is used by L.Blanchard (in the OpRaTel collaboration). Also they have together developed a code for an optimal partionning procedure which is working on the same Galerkin principle but avoiding the use of calculus which would have been developed by the brut force technique. Indeed, if the optimal partionning of a domain (e.g. an antenna) consisted in finding a decomposition by 100 subdomains, the level set approach would lead to 100 Hamilton Jacobi equations. We introduced the concept of "multi-saddle" potential function $F(t,x)$ and through the Galerkin technique we follow the evolution of the saddle points. This technique has been succesfully understood thanks to the various testing developed by J. Picard and will be exploited in OpRaTel collaboration by L. Blanchard and F. Neyme (Thales TAD). The work of Jerome Picard has been very interactive and very important to understand this multi-saddle procedure which turns out to be very delicate in the parameters tuning. We developed a mathematical analysis to justify that trials-error method and some existence results have been proved for the crossing of the singularity associated with the toplogical change in the Galerkin approximation (here the finite dimensional character is fundamental)[37].

6.4.10. Shape Metrics

Participants: Louis Blanchard, Jean-Paul Zolésio.

We characterize the geodesic for the Courant metric on Shapes. The Courant Metric is described in the book [2]. It furnishes an intrinsic metric for large evolutions. We use the extended weak flow approach in the Euler setting[48].

It is extended to larger class of sets and using the *transverse flow mapping* (see the book) we derive *evolution equation* which caracterises the Geodesic for that differentiable metric.

Applications are beeing developed for Radar image analysis as well as for various non cylindrical evolution problems including real time control for array antennas.

6.5. Virtual computing environments

Participant: Toan Nguyen.

Based on the previous work on Virtual Computing Environments until 2006, the OPALE project/team is working on Virtual Collaborative Platforms which are specifically adapted to Multiphysics Collaborative projects. This is in particular studied in the framework of the European AEROCHINA support action. The approach considers not only code coupling for multiphysics applications in aeronautics, but includes also interactions between participant teams, knowledge sharing through numerical databases and communication tools using Wikies. The design of a proof of concept demonstrator is planned in the AEROCHINA2 project, started in October 2007[46], [47], [45]. Indeed, large scale multiphysics problems are expected to be orders of magnitude larger than existing single discipline applications, like weather forcast which involve ocean and atmosphere circulation, environmental disaster prevention and emergency management. New computing technologies are therefore required. Among these technologies are wide area networks and distributed computing, using cluster and grid-based environments. It is clear that large supercomputers, PC-clusters and, to a limited extent wide area grids, are currently used for demanding e-science applications, e.g., nuclear and flight dynamics simulation. It is not so clear however what approaches are currently the best for developing multiphysics applications. We advocate the use of an appropriate software layer called upperware, which, combined with cluster and grid-based techniques, can support their uptake by the users when running multidisciplinary codes and business software, e.g., decision support tools. This paves the way for "Virtual Collaborative Platforms"[34], [57]. Unlike Wikis and othercollaborative tools widely accepted for document editing, virtual collaborative platforms are used to deploy distributed and parallel multiphysics simulation tools that require the use of remote software, databases and vizualization tools. Their execution may be controlled and monitored by distributed workflow systems that may hierarchically composed. Work in progress is done on this subject in partnership with other participants to European projects, e.g., PROMUVAL, AEROCHINA.

7. Contracts and Grants with Industry

7.1. Optimum-shape design in aerodynamics and multidisciplinary extensions

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.

7.2. Optimization in electromagnetics

- France Télécom (La Turbie); two contracts:
  - *Optimization of antennas*, which has partially supported L. Blanchard's thesis;
  - *Shape Optimization Codes Platform by Hierarchical Methods*, which partially supports B. Chaigne's thesis.
- Thalès (Bagneux) : optimization of the most dangerous trajectories in radar applications.

7.3. Optimized Steel Solutions

This year, a new partnership with industry was launched with the R & D *Automotive Applications Centre* of Arcelor Mittal in Montataire, France. This partnership is related to the optimization of steel (automobile) elements with respect to mechanical criteria (crash, fatigue). The project team was solicited to audit the GEAR2 optimization team in Montataire [56]. Additionally, a student interm from Arcelor, J.-G. Moineau, was hosted and directed at INRIA for a four-months period.

8. Other Grants and Activities

8.1. National and Regional Initiatives

8.1.1. RNTL Network

Opale participates in the RNTL[1] Project "OMD" for multi-disciplinary optimization (see http://omd.lri.fr). This project was set-up by the CNRT Aéronautique. The involvement of Opale includes two major lines of investigation developed by Post-Doctoral researchers:

1. To establish the status of multilevel strategies in shape optimization;
2. To develop efficient techniques for hierarchical model coupling for optimum-shape design in Aerodynamics.

This contract provides the grant supporting the post-doctoral studies of P. Chandrashekarappa and J. Zhao.

8.1.2. 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.

[1] RNTL: *Réseau National des Technologies Logicielles* (National Network for Software Technologies, a program supported by the National Agency for Research (ANR))

More specifically, the classical problem of frequency allocation is a main activity. 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).

8.2. International Networks and Working Groups

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. Collaboration with Finland

T. Nguyen was invited to the University of Jyvaskyla in Finland on 25-26 september 2007 : talk to the FiDiPro DESIGN meeting "Collaborative Platforms for Multiphyics Design Applications". T. Nguyen was invited to collaborate with the CSC, Finnish IT Center for Science in Helsinki, by M. Jari Jarvinen, Development Director at CSC. He was also invited to theVTT, Technical Research Center of Finland, to give a talk on computational science.

T. Nguyen was invited to the Technology and Innovation Seminar at the University of Jyvaskyla (Finland), 26 september 2007.

8.2.2. Collaboration with China

Project OPALE represents INRIA in the European Aerochina (2005-2006) and Aerochina2 projects(2007-2008)

8.2.3. European project NODESIM

Opale and Tropics Project-Teams participate to the European project NODESIM (NOn DEterministic SIMulation), whose topic is the study of the influence of uncertainty on simulation in aeronautics. Tropics Project-Team is in charge of computing first and second order derivatives of the flow characteristics with respect to uncertain parameters, whereas Opale Project-Team uses these computations to carry out robust design optimization exercises.

8.2.4. Integrated Action Project France-Marroco ANOPIC

A. Habbal is the French responsible for the Integrated Action Project France-Morocco *ANOPIC* : new applications in optimization, inverse problems and control, granted from 2005 to 2008 (7650 euros in 2005). The project is gathering several teams from France (INRIA/OPALE, University of Nice, “École des Ponts et Chaussées” and technical University of Compiègne) and Morroco (Engineering School Mohammedia and “ École des Mines”, University Mohammed V in Rabat, and University Chouaib Doukkali in Settat). The research topic is the mathematical and numerical study of parametric, geometry or topology optimization problems.

This project has supported the organization of the workshop “New Applications, Shape Optimization, and Inverse Problems, PDEs and Applications”, Rabat, Morocco, November 7, 2007, during which J.-A. Désidéri delivered an invited opening lecture.

9. Dissemination

9.1. Education

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

9.1.1. University of Nice (UNSA)

A. Habbal teaches the following courses:

- Introduction to game theory and its application to economy (Master 1, 47hrs)
- Game theory for pollution taxes (Master 2 30hrs)

9.1.2. Ecole Polytechnique Universitaire (EPU), Nice

A. Habbal teaches the following courses ("Information Systems"):

- Numerical Engineering methods (first year, 75 hrs)
- Programming mathematics (first year, 16 hrs)
- Numerical Methods in Finance (third year, 18 hrs)
- Introduction to biomathematics (2nd year, 14hrs)

J.-A. Désidéri and R. Duvigneau teach the following course ("Applied Mathematics and Modelling"):

- Multiscale methods (36hrs)
- Shape optimization (36hrs)

R. Duvigneau teaches the following courses ("Applied Mathematics and Modelling"):

- Numerical Engineering methods (first year, 24 hrs)

9.2. Participation in International Courses

- A. Habbal delivered a lecture at "UNESCO Modèles mathématiques du cancer" (*Mathematical Models of Cancer*), Tunis, march 2007.
- J.-P. Zolésio delivered the short-course: "Controle Optimal des systèmes non autonomes" (*Optimal Control of Non-Autonomous Systems*) at the University of Monastir, Tunisia.

9.3. 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.

Abdou Wahidi Bello, University of Cotonou; topic: Finite-volume methods for the shallow-water equations with application to the simulation of the flow in the ducts system of the city of Cotonou, Benin.

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.

Benoît Chaigne, University of Compiègne; topic: shape optimization of axisymetric reflectors in electromagnetism.

Jean-Georges Moineau, Ecole Centrale de Paris; topic: Adapting a Design of Experiment for an Optimized Steel Solution.

Nouredine Moussaid, "École Mohammedia" Engineering School of Rabat, Marroco; topic: Nash games in topological optimization.

Babacar Ndiaye, University of Nice; topic: Mathematical modeling of cellular migration.

Daniele Varone, University of Nice; topic: split of territories to optimize a robot.

9.4. Organization of Scientific Events

The OPALE project-team (with A. Dervieux, TROPICS project-team) organized the 42nd Applied Aerodynamics Colloquium, INRIA Sophia Antipolis, April 19-21, 2007, whose theme has been: Multidisciplinary Couplings and Optimization.

The OPALE project-team organized the 4th French-Finnish seminar at INRIA Grenoble, "Computational Science: Understanding and Solving Multiphysics Problems for Industry and Society with Large Scale Simulation", 10-12 May 2007.

9.5. Participation in Scientific Committees

- 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.-A. Désidéri has been the Delegate of the Directorate for International Relations in the Sophia Antipolis Unit (until October 2007). This responsability has consisted in participating in hosting a large number of foreign delegations visiting the unit, participating in the organizational activities of the Directorate including juries (such as the jury for the INRIA Associated Teams Program), and in disseminating information related to cooperation programs within the unit.
- J.-A. Désidéri has been appointed "ONERA Collaborator" at the French National Research Establishment for Aerospace (ONERA), for a duty of one day per month. This appointment is made with the Optimization Group of the DSNA (Directorate for Numerical Simulation of Flowfields and Aeroacoustics).
- A. Habbal is member of the specialists board for sections 25-26-27 in IUFM of Nice.
- A. Habbal is member of the executive board of "Ecole Polytech Nice".
- T. Nguyen is member of the Advisory Board of the French-Finnish Association for Scientific Research.
- T. Nguyen was member of the Scientific and Technical Committee of the Workshop NUAA-Europe held at the Nanjing University of Aeronautics and Astronautics de Nanjing (PR China), 22-24 october 2007.
- J.P. Zolésio is chairman of Working Group IFIP 7.2 *System Modelling and Optimization*.

9.6. Invited or keynote lectures

- *Algorithms for Efficient Shape Optimization in Aerodynamics and Coupled Disciplines*, 42e Colloque d'Aérodynamique Appliquée, Optimisation et Couplages Multidisciplinaires, INRIA Sophia Antipolis, April 19-21 (J.-A. Désidéri).
- *Shape Optimisation in Aerodynamics: Multi-Level Parametric Approaches*, ERCOFTAC Introductory Course to Design Optimisation, Trieste, Italy, April 18-20, 2007 (J.-A. Désidéri).
- *Aero-Structural Optimization of a Wing Shape by an Adapted Game Strategy*, Aerochina Workshop, Barcelona, April 25-27 (J.-A. Désidéri).
- *Split of Territories in Concurrent Engineering*, 4th French-Finnish Seminar, "Computational Sciences: Understanding and Solving Multiphysics Problems for Industry and Society with Large Scale Simulation", INRIA, Grenoble, 10-12 May, 2007 (J.-A. Désidéri).
- *Optimum-Shape Design in Aerodynamics and Coupled Disciplines: Multilevel Parametric Algorithms*, China-Europe Workshop, Integrated Computational and Experimental Multiphysics for New Challenges in Aeronautics, Nanjing, October 22-24, 2007 (J.-A. Désidéri).

- *Optimum-Shape Design in Aerodynamics and Coupled Disciplines: Split of Territories in Concurrent Engineering,* Nanjing University of Aeronautics and Astronautics, October 25, 2007 (J.-A. Désidéri).
- *Partage de territoire en optimisation concourante*, Workshop "Applications Nouvelles, Optimisation de Forme et Problèmes Inverses, EDP et Applications", Ecole Mohammadia, Rabat, Maroc, 7 Novembre 2007 (J.-A. Désidéri).
- *Same title*, Université de Montpellier II, 20 Novembre 2007 (J.-A. Désidéri).
- *Same title*, Institut des Sciences de l'Ingénieur de Toulon et du Var (ISITV), 29 Novembre 2007 (J.-A. Désidéri).
- *Nouvelles tendances en optimisation de structures dans un contexte multidisciplinaire* Université Technologique de Compiègne, march 2007 (A. Habbal).
- *Collaborative Platforms for Multiphysics Design Problems* Seminar FiDiPro DESIGN Project (University of Jyväskylä (Finland), 26 September 2007 (T. Nguyen).
- *Shape metrics and geodesics*, IFIP 23rd TC7 World Conference, Cracovia, Poland, July 2007 (J.-P. Zolésio, plenary lecture).
- *Variational modeling for incompressible Euler equations*, Numath, Graz, Austria, September 2007 (J.-P. Zolésio).
- *Hidden regularity in Maxwell equations*, CRM Montreal, Canada, October 2007 (J.-P. Zolésio).
- *Level sets by galerkin techniques*, Biological Modeling, Linz, November 2007 (J.-P. Zolésio).

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