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

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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 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 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, 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 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 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 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 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 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 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 $H^2(\Omega)\cap H^1_0(\Omega)$ 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[1]. Our evolution field approaches permit to extend this viewpoint to the topological shape optimization [2].

3.2.1. Shape differential equation

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: $< \mathcal{A}\varphi, \varphi > \geq |\varphi|^2_H$ 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 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 $t \to \infty$) 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 [3] [4] [5].

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

[2] 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

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

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

[5] 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

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 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 [6]. 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. [7]

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 and involving also EADS (Common Research Center) and Datamat (Italy).

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

[6] 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.

[7] 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

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 relates 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 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.

4.1.3. 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.

4.1.4. 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 air-foil 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 parametrisation 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 (Lizhe Wang).

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 multi-disciplinary code validation and verification in aeronautics. A demonstator of this platform is currently being designed in cooperation with CIMNE (Spain).

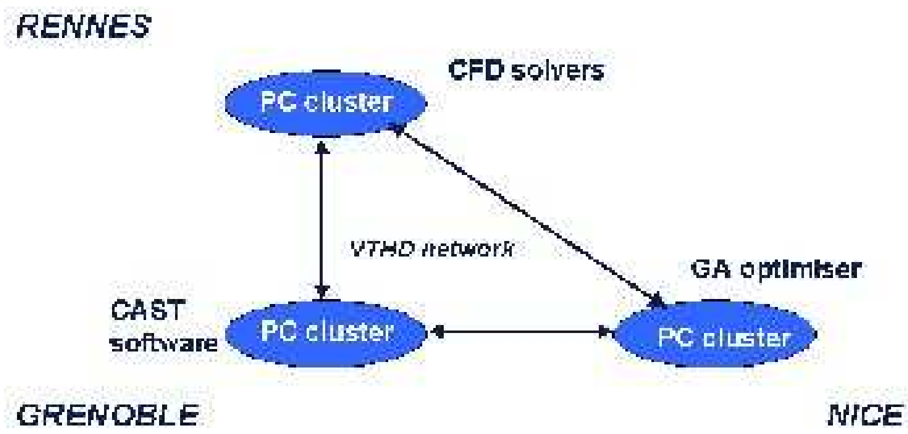

Figure 1. PC Cluster over the VTHD netwok

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, the Nelder-Mead simplex method and the multi-directional search algorithm from Torczon [57].
- modules allowing the use of a parallel architecture to instantiate the cost function evaluations (genetic algorithm and multi-directional search algorithm)

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], 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 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.

5.2.2. BZPARAM:

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

Participants: Michele Andreoli [former trainee], Aleš Janka [former Post Doctoral Student].

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. 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 [former trainee, simplex algorithm and validation], Yannick Berard [former trainee, hybridization in PIKAIA], Régis Duvigneau [Multi-directional search algorithm and validation, parallel implementation], Abderrahmane Habbal [hybridization in PIKAIA], Aleš Janka [former Post Doctoral Student, 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;
- the Nelder-Mead simplex algorithm;
- the Torczon multi-directional search 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 "real-coded" genetic algorithm PIKAIA (public domain software) employing a first-order gradient interpolation of fitness values on subsets (clusters) of the current population.

5.3. Numerical Modules for Gradient Computations in Electromagnetics

Participants: Claude Dedeban [France Télécom, La Turbie], Pierre Dubois, Jerôme Picard, 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 (6.4.10). This code is to be latter interfaced with the code for array antenna optimization (6.4.9).

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].

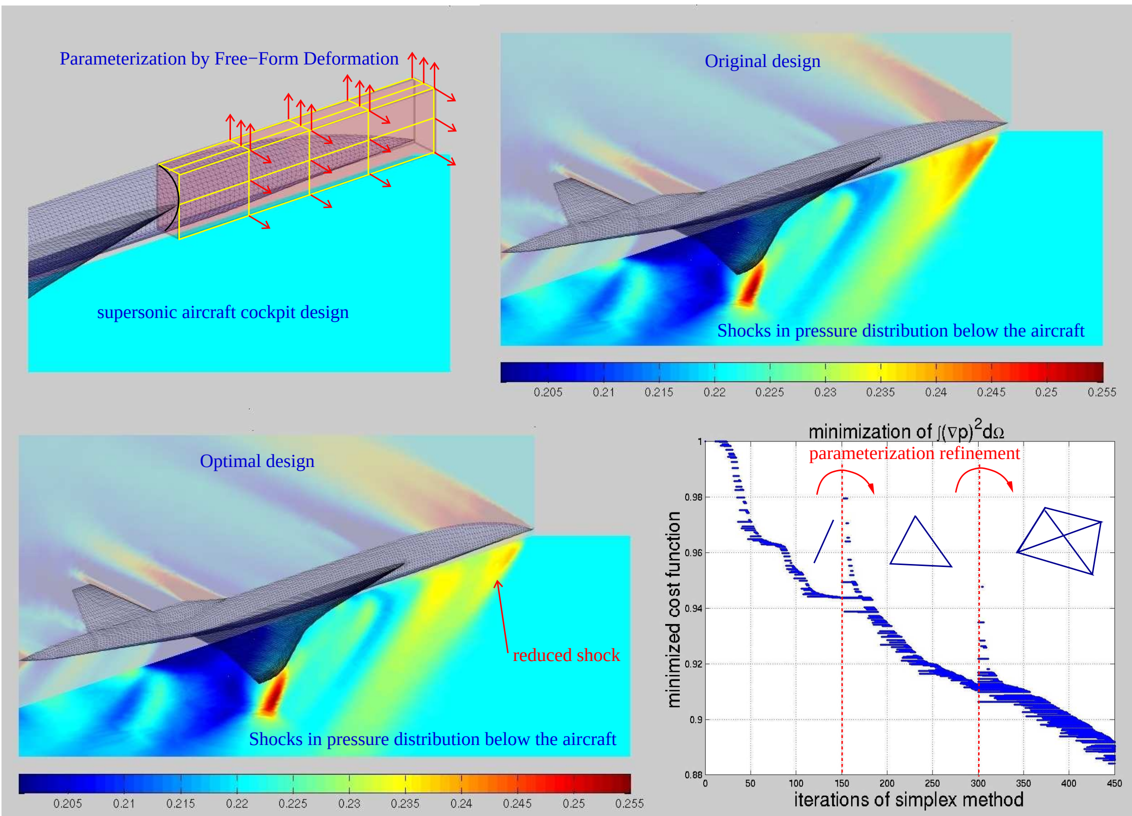

Figure 2. Shape optimization of a supersonic business-jet geometry for external noise reduction; Free-Form Deformation parameterization in the nose region of a generic geometry (courtesy of Dassault Aviation); initial supersonic flow (pressure field); optimized flow demonstrating reduced shock attached 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: $M_\infty = 1.8$, $\alpha = 1^o$; 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.

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 the long run, the simulation tool will be used in a control loop to prevent flood or reduce the damages it causes.

The proposed numerical approach consists in simulating the flow by solving the shallow-water equations, as it is customary in estuary-flow-type simulations, by an adequate finite-volume method. The present work has been initiated by a thorough literature review of the numerical enhancements proposed in recent years concerning such numerical formulations, with particular attention to the so-called *"equilibrium scheme"*. The next step will be to construct a realistic numerical terrain model, in cooperation with geographs; such a model could then serve to devise a mesh for the finite-volume simulation. Special boundary conditions will be implemented to account for the possibility of flood.

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 is very difficult for coupled models, and is 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), as well as algorithmic and software aspects (parallel and grid computing).

6.2.1. Shape parameterization, hierarchical (multilevel) algorithms, adaptivity and parallel computing

Participants: Badr Abou El Majd, Jean-Antoine Désidéri, Régis Duvigneau, Abderrahmane Habbal, Aleš Janka [Analysis and Scientific Computing Institute, EPFL, Lausanne].

We are concerned with the general problem of minimizing a functional of a state variable which is a vector field solution of a PDE subject to shape-dependent boundary conditions. The prototype 2D test problem is the optimization of an airfoil shape immersed in a two-dimensionnal 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* [58] 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) [42].

A quadratic conceptual model of shape reconstruction has been constructed to support a spectral analysis of a steepest-descent-type algorithm, identified to the classical point-Jacobi iteration applied in a particular linear setting. This model involves an integral operator whose kernel includes an explicit factor depending on the parameterization. As a result, parameterization-dependent eigenmodes have been identified, very similar to Fourier modes. Pursuing the analogy with multigrid, a form of *two-parameterization ideal algorithm* (analogous to the two-grid ideal method) has been proposed and is currently being incorporated in the more general FAMOSA method [43].

Besides, in the more particular framework in which the BFGS method [8] is used as the optimization relaxation method within a multilevel strategy, the question of the continuity of the Hessian estimate, or inverse-Hessian estimate through transfers by degree elevation or adaption, has been addressed. Enforcing this continuity results in significant improvements in convergence rate [35] [34].

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 [42] [40].

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 selects 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” had originally allowed us, 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.

Adaptivity is a key element to achieve higher convergence, that is better shape definitions for a given computational effort [33] [41]. This activity is currently being generalized to three-dimensional flow formulations by means of iterative regularization of the free-form deformation setting.

6.2.1.4. Parallel optimizers.

The multi-directional search by Torczon [57] has been used to replace the Nelder-Mead simplex method in the parallel-computing environment of a cluster of PC’s. In this method, the search in the solution space is realized by a sequence of simultaneous parallel instanciations of the analysis code, a number of times equal to the number of design parameters. For the three-dimensional Piaggio-wing-shape aerodynamic optimization test-problem, preliminary, but very successful results have been achieved, demonstrating that the parameterization could be enlarged for higher accuracy still maintaining the computational elapsed time [41]. Thus this method offers an alternate route to convergence enhancement.

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

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

[8] BFGS: the Broyden-Fletcher-Goldfarb-Shanno (BFGS) method is a method to solve an unconstrained nonlinear optimization problem; see http://en.wikipedia.org/wiki/BFGS_method

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:

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

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 [29]:

- Direct problem – The functions $x(t)$ and $\omega(t)$ being fixed:
  - for $\alpha \geq 2$, the functional is strictly convex;
  - there exists a critical α_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, although obviously less general, but in a design loop it realizes feasible trade-offs between criteria.

Current aspects of this research includes the following two topics [54]

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.

6.2.4. Hybrid optimization algorithms

Participants: Abderrahmane Habbal, L. Fourment [CEMEF], D.T. Tho [ENSMP].

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. First family contains *P*owell-like algorithms developed in the 60s. these methods can not pretend to perform global optimization. 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 approach 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, which is another innovative aspect of this work. The method has since been extended to a cluster-free formulation guaranteeing a smoother interpolation and demonstrating a superior performance in the optimization process[33].

6.2.5. Application of sensitivity analysis and optimization algorithms to complex problems in Computational Fluid Dynamics

Participants: Régis Duvigneau, Michel Visonneau [Laboratoire de Mécanique des Fluides CNRS UMR6598, Nantes], Dominique Pelletier [Ecole Polytechnique de Montréal].

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[37] and drag reduction for a bluff body[45].

Some improvements have also been reported in sensitivity analysis (Continuous Sensitivity Equation Method) by increasing the accuracy of the functional gradient for shape parameters when complex problems are considered, such as flows with mixed convection[39], [38].

6.2.6. Numerical Shape Optimization of Axisymmetric Radiating Structures

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

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

To initiate these developments, we have considered first the simplified approximation known as "Optical Physics" for which the fields are known explicitly for a given geometry. This approximation has been validated by comparison with the result of a 3D solver of the Maxwell equations provided by France Télécom R & D, in terms of radiating diagrams. The next step will be to test a free-form deformation approach to optimize the shape in a particular setting, and compare it with a basic gradient-based method.

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

6.3.1. Validation of mathematical models in wound healing

Participants: Abderrahmane Habbal, Olivier Duhamel, Nicolas 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 mono-layer 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. A survey article based on these results is in preparation.

6.3.2. Anti-angiogenesis for Solid Tumours

Participant: Abderrahmane Habbal.

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.

In our approach, the media is treated as porous and subject to a theoretical game in which the structural stiffness (computed by linear elasticity) competes with the ability of the tumour to develop a blood network (modeled by Fick's law). The problem was formulated as a static topology design with complete information, 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 extracellular 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.
This study is based however on simplified modeling and assumptions. Many improvements will be considered.

First, the dynamic growth of the tumor must be taken into account, and more generally a *dynamic* with incomplete information game is 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 agiogenesis factors.

From computational viewpoint, our next goal is to run realistic three dimensional calculations coupling porous media and elasticity models. In this view, MPI parallelization of the implemented program was achieved (Opale team of INRIA Grenoble).

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 *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 papers.

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. [56].

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. 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.

6.4.6. 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 $\mathcal{J}$ 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 (althrough the convergence process) w.r.t. quantitative and qualitative criteria[23]

6.4.7. 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.

6.4.8. 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.

6.4.9. Array Antennas Optimization

Participants: Louis Blanchard, Jean-Paul Zolésio.

We are developing a new approach for modeling array antennas optimization. The 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. Two publications are prepared for the IFIP conferences proceedings (R. Glowinski / I. Lasiecka eds.)

6.4.10. 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.

6.5. Virtual computing environments

Participants: Lizhe Wang, Vincent Bel, 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 for demanding applications that can now be deployed on thousands of connected processors and they can connect petabytes of data through 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 uncommonly available expertise in the computer science field [55]. Users have become in the last decade experts in the manipulation of Web browsers to access inter-continental mass of data and remotely execute 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 which is marketed currently by software vendors is "on demand computing" and "Utility computing". Other companies have developed niches where "virtual clusters", "user-centric virtual environments" and "virtual data-centers" can be rented and charged based on hourly and resource fees. These approaches are basically offering distributed and integrated data and compute centers to large customers. Resellers make grid and parallel compute centers available to the application users. This does not however solve two problems:

- the seamless access of large compute power to SMEs
- the easy and affordable design, deployment, execution and monitoring of complex applications to non experts

To solve these two problems, the approach that is currently 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 services implemented on top of existing grid middleware environments. The goal is to provide standardised services and the corresponding procedures to help the non-expert application developers specify the resources and computing infrastructure they need to run the complex multidisciplinary applications they want to execute. This implies the design of generic graphic problem solving interfaces, the implementation of enabling "upperware" and ad-hoc interfaces on top of existing grid middleware. An international consortium has been set up on this subject called HEAVEN, 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 the subject of Lizhe Wang doctoral thesis on Virtual Computing Environments. In this work, the heterogeneous nature of current grid middleware has to be taken into account. The CAST platform has therefore been interfaced with the UNICORE and GLOBUS middleware (GT3 and GT4, WSRF) , and also with the J2EE and standard Web service (WSDL) environments by Vincent Bel and Lizhe Wang. Ongoing work implies the deployment of this software enviroment and the implementation of parallel 3D airfoil optimisation testcases using hierachic multilevel parametrisation on the Grid5000 research network.

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. RNTL Network

Opale participates in the RNTL[9] Project "OMD" for multi-disciplinary optimization. This project was set-up by the CNRT Aéronautique. The involvement of Opale is to be finalized; it should include 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.

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.

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).

8.1.3. Action COLOR 2005 : Ab in vivo ad in silico

A. Habbal is responsible in the OPALE project for the Action COLOR *Ab in vivo ad in silico*. The other partners are the "Institut de Pharmacologie Moléculaire et Cellulaire" IPMC (CNRS and INSERM) and EPIDAURE project. The grant is 11 Keuros for one year.

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

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. 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 multidiciplinary 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 application 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).

8.2.2. European Network of Excellence MACSInet

The project has participated 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.

8.2.3. Support Action AEROCHINA

The OPALE project participates in the European project AEROCHINA which started in october 2005 and aims at developing the cooperation between European and Chinese industries and research institutions in multidisciplinary modeling, simulation and design in aeronautics. This is a large network of participants. It involves twelve major European companies and institutes (ONERA, DLR, Airbus, EADS, Dassault-Aviation, ...) and twelve major Chinese partners. The goal is to implement a reference framework for modeling and simulation for research and industry in the domain of multidisciplinary design in aeronautics.

The project's participation is to contribute jointly with CIMNE (Barcelona, Spain) and ACTRI (China) to develop software tools for data collection and cooperative work and to participate in the definition of numerical methods for multiphysics analysis and optimization. Cooperation will be developed particularly with the universities of Nanjing and Tsing-Hua in aerodynamic optimization.

The next event will be a meeting of European and Chinese experts to be held in Xian in april 2006.

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.

8.2.5. Collaboration with India

J. Périaux has participated in a French delegation of experts from the Universities of Paris VI and Toulouse, INRIA and aeronautical establishments (Airbus, SNECMA, ONERA) visiting India. The program included:

- SAROD International Conference (Hyderabad, December 8-9, 2005), a forum describing on-going Indian programs on the design of civilian, military and space vehicles;
- French-Indian Open Workshop (Bangalore, December 12-13, 2005), related to numercal simulation methods and tools for multicriterion/multidisciplinary optimization in Aeronautics;
- visit of the Aeronautical Development Agency (ADA, Bangalore, December 14, 2005).

A follow-up French-Indian Open Workshop is planned to be organized in December 2006 at INRIA Sophia Antipolis by the Opale Project jointly with A. Dervieux (Tropics Project).

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" (20 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, adaptative Optimization (J.-A. Désidéri).

9.1.2. Ecole Polytechnique Universitaire (EPU), Nice

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

- Numerical Engineering methods (first year, 50 hrs)
- Programming mathematics (first year, 16 hrs)
- Numerical Methods in Finance (third year, 18 hrs)

J.-A. Désidéri teaches the following courses ("Applied Mathematics and Modelling"):

- Introduction to numerical analysis (13hrs)

9.1.3. Ecole Centrale de Nantes

R. Duvigneau teaches the following courses in the Master's degree "Conputational Mechanics":

- Introduction to numerical optimization (12hrs)

9.2. Participation in International Courses

- Participation of Jean-Antoine Désidéri in a course on design optimization organized by the European Research Community on Flow, Turbulence and Combustion [42].

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.

Vincent Bel, University P. Mendes France, Grenoble; topic: interface of the CAST software with the UNICORE middleware (April-June, 2005); deployment and port of this iterface on the PC cluster at INRIA Rhone-Alpes and INRIA Sophia-Antipolis.

Abdou Wahidi Bello, University of Cotonou.

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.

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

Olivier Duhamel, University Paul Sabatier;

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

9.4. Organization of Scientific Events

As chairman of Working Group IFIP 7.2 *System Modelling and Optimization*, J.P. Zolesio organizes two conferences :

- Conference on System Modeling and Optimization: "Shape Analysis and Optimization", Turin, Italy, July 18-22, 2005.
- UCLA, IFIP 7.2: "Boundary Value Problems: Computation and Control" september 2005.

9.5. 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.-A. Désidéri has been nominated *Delegate for International Affairs* for the Sophia-Antipolis Research Unit. This responsability involves representing the center when hosting international delegations and delivering corresponding presentations. (The following delegations were hosted: Nippon Information Institute (NII); Italian Committee for Bio-Security and Bio-Technologies; Sup Com, Tunis, Tunisia; Chinese Deciders.)
- A. Habbal is member of the specialists board for sections 25-26-27 in IUFM of Nice.
- T. Nguyen is member of the Advisory Board of the French-Finnish Association for Scientific Research.
- J.P. Zolésio is chairman of Working Group IFIP 7.2 *System Modelling and Optimization*.

9.6. Invited or keynote lectures

- *Shape optimisation algorithms in aerodynamics: parameterisation issues*, European Research Community On Flow, Turbulence And Combustion (ERCOFTAC) Introductory Course on Design Optimisation, University of Manchester of Science and Technology (UMIST), UK, April 6-8, 2005. (J.-A. Désidéri)
- Optimal Control of Coupled Systems of PDE, Oberwolfach, Germany, April 17-23, 2005. (J.P. Zolesio)
- *Mathématiques du Vivant*, TAM-TAM : Trends in Applied Mathematics, Tunisia-Algeria-Morroco, Tunis, Tunisia, april 2005. (A. Habbal)
- Mini invasive procedures in medecine and surgery: mathematical and numerical challenges, Montreal, Canada, may 23-27, 2005. (J.P. Zolesio)
- *Tumoral anti-angiogenesis solved as a Nash game*, WCSMO-6 : Sixth World Congress on Structural and Multidisciplinary Optimization, Rio de Janeiro, Brazil, may 2005. (A. Habbal)
- 22nd IFIP TC7 Conference on System Modeling and Optimization, Torino, Italy, july 18-22,2005. (J.P. Zolesio)
- *Tumoral angiogenesis modeled as a Nash game* , Optimization in Medicine: CIM Thematic Term on Optimization, Coimbra, Portugal, july 2005. (A. Habbal)
- *Multilevel Strategies and Hybrid Methods for Shape Optimization and Applications to Aerodynamics and Metal Forming*, Evolutionary and Deterministic Methods for Design, Optimisation and Control with Applications to Industrial and Societal Problems Conference, EUROGEN 2005, Munich, Germany, September 12-14, 2005. (J.-A. Désidéri)
- Level set methods for direct and inverse problems Linz, Germany, september 14-16, 2005. (J.P. Zolesio)

- *Two-Parameterization Ideal Algorithm for Shape Optimization*, International Conference on Advances in Numerical Mathematics, Moscow, Russia, September 16-17, 2005. (J.-A. Désidéri)
- *Boundary value problems: computation and Control* IFIP UCLA, Los Angeles, USA, september 19-23, 2005. (J.P. Zolesio)
- *Multilevel Strategies for Shape Optimization in Aerodynamics*, Numerical Analysis and Scientific Computing for PDE's and their Challenging Applications Conference, CSC, Helsinki, Finland, October 6-7, 2005. (J.-A. Désidéri)
- *Static and Dynamic models for Tumoral anti-angiogenesis.*, IUTAM : International Union of Theoretical and Applied Mechanics, Symposium "Topological design optimization of structures, machines and materials - - status and perspectives", Rungstedgaard, Denmark, October 26 - 29, 2005. (A. Habbal)
- *Self-adaptive multilevel algorithms for shape optimization with application to Aerodynamics*, MEGADESIGN Workshop, German Aerospace Center (DLR), Braunschweig, Germany, November 29-30, 2005. (J.-A. Désidéri)

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