

*Project-Team IDOPT**Systems optimization and identification in
physics and environment**Rhône-Alpes*

THEME 4B

Activity
Report

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1. Team

The IDOPT project is a joint project between the CNRS (SPM department), the Joseph Fourier University (Grenoble 1), the INPG and the INRIA Rhône-Alpes. This project is localized in the LMC-IMAG laboratory.

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2. Overall Objectives

In physics, mechanics and environmental sciences, many systems are modelled by partial differential equations with distributed parameters. These equations describe the behavior in space and/or in time of the system variables. From this general formulation two problems arise :

2.1.1. i) Identification :

Some parameters or some functions appearing in the model are unknown or only an estimation is available (e.g. diffusion coefficients in parabolic equation, source and sinks terms in fluids, initial and/or boundary conditions,...). Direct problems can solve the equations when all the information is available. Inverse problems are dedicated to the estimation of the unknown parameters using the information provided by experimental observations of the system. Solving inverse problems is useful for physicist: in many cases an approximation only of the unknown parameters is available, and these parameters cannot be measured by devices either because they are used to parameterize small scale phenomena (e.g. turbulence in fluids) or because the measurement is expensive (e.g. measurements inside the solid earth or in the deep ocean). This point of view is essential in many domains of physics.

2.1.2. ii) Optimization:

The physical systems described above may have some inputs (e.g. forcing terms) which can be controlled by an operator. A problem is : how to control the inputs in order to optimize the behavior of the system? The related mathematical problem is the estimation of these optimal inputs in open loop or closed loop (stabilizing feedback).

3. Scientific Foundations

3.1. Optimal control

Participants: Jacques Blum, Fran ois-Xavier Le Dimet.

For identification and optimization problems, we have to minimize a functional depending on the solution of a Partial Differential Equation (PDE). The identification problem can be formulated as the minimization of the quadratic difference between the experimental observation and the quantities calculated by the resolution of a system of equations. The control variables are, in this case, the parameters or the functions to be identified. The minimization of functionals depending on the solution of a PDE (e.g. through the initial conditions, the boundary conditions...) follows the optimal control theory [36].

3.2. Data Assimilation

Participants: Fran ois-Xavier Le Dimet, Victor Shutyaev, Yousuff Hussaini, David Furbish.

A mathematical model alone is not sufficient to predict the evolution of a geophysical flow. Neither are data alone. Being able to provide a forecast requires to retrieve the state of the flow at an initial moment, and that this retrieved field be in agreement with the physical properties of the flow (i.e. satisfy the governing equations). Data Assimilation covers the techniques dedicated to jointly use the mathematical information provided by the equations, the physical information obtained by observation, and the statistical information in order to retrieve at best the state of the flow. At the present time there exist two basic techniques: variational methods and filtering-type methods. Variational methods are based on the minimization of a function measuring the discrepancy between a solution of the model and the observation. Le Dimet (Le Dimet 1982, Le Dimet and

Talagrand 1986) has suggested to use optimal control techniques for this purpose. The inputs of the model are then used as control variables. The Euler Lagrange condition for optimality is found by the solution of the "Optimality System" (OS) that contains the adjoint model obtained by derivation and transposition of the direct model. It is important to point out that this OS contains all the available information : model, data and statistics. Therefore the OS can be considered as a generalized model.

The adjoint model is a very powerful tool permitting to carry out sensitivity studies, identification... Despite its high computational cost, this technique has been adopted by the main operational meteorological centers (MeteoFrance, European Center for Medium Range Weather Forecast —Reading UK—,...)

During these last years an important contribution of IDOPT has been the study of second order properties, and its application to sensitivity studies. As a matter of fact, a major problem in the forecast of the evolution of the physical environment is to estimate the quality of the prediction, or in other words the impact of model and data uncertainties on the prediction. A so called second order adjoint has been introduced, which allow to extract the second order properties of the OS (Le Dimet, Navon and Daescu, 2002). It is shown that predictability properties, i.e. the impact of errors both in the model and in observations, are linked to the properties of the Hessian of the cost-function.

Another way to take into account the model error is to add an extra term to the model and to control this term in order to reduce the discrepancy with the observation. Such a study was carried out in A. Vidard's Ph.D. and then in a more recent paper by Vidard, Piacentini and Le Dimet. Using the second-order adjoint it was also possible to follow the impact of uncertainties from its source to the prediction (Le Dimet, Shutyaev). The application to underwater propagation are described in a paper by Le Dimet, Shutyaev, Ngepieba, Mu Mu.

Finally, an important topic is the adequation of models and data. It has been demonstrated (Le Dimet, Hussaini, Ngnepieba) that for the same set of data the best prediction is not necessarily associated to the best model. Improving the quality of a model may damage the prediction. This direction of research is presently underway.

3.3. Statistical inverse problems

Participants: Anestis Antoniadis, Theofanis Sapatinas, Felix Abramovich, Jeremie Bigot.

This section contains an exposition of wavelet related completed work. Wavelets are mathematical building blocks that can be used to represent functions and data sets. They combine useful modeling features such as locality and varying degrees of smoothness. As modeling and analyzing tools they allow us to "zoom-in" on the problem at various scales and therefore are part of what is called "multiscale" and "multiresolution" analyses, a class of problems investigated within the IDOPT project. We had already realized during previous investigations that wavelets are a powerful tool for dealing with some inverse problems. Paper [10], originally drafted in 2002, and published in 2003, was jointly written with Theofanis Sapatinas from University of Cyprus. We consider there the prediction problem of a continuous-time stochastic process in terms of its recent past. We first discussed some known, as well as recent, methods to predict such a stochastic process on an entire time-interval. They are based on the notion of autoregressive Hilbert processes that represent a generalization of the classical autoregressive processes to random variables with values in a Hilbert space. A careful analysis revealed, in particular, that these methods are related to the theory of function estimation in linear ill-posed inverse problems. In the deterministic literature, such problems are usually solved by Tikhonov-Phillips regularization. We proposed three wavelet methods to efficiently address the aforementioned prediction problem. We presented wavelet regularization techniques for the sample paths of the stochastic process and obtained consistency results of the resulting prediction estimators. We have also illustrated the performance of the proposed wavelet methods in finite sample situations by means of two real data examples. The first example concerned with the prediction of tourist evolution in Granada over a year, while the second example concerned with the prediction of the entire annual cycle of climatological El Niño-Southern Oscillation time series one year ahead.

Paper [46] originally drafted in 2002 and submitted for publication in 2003, is an important paper in the field. It is a joint work with Felix Abramovich, Theofanis Sapatinas, Brani Vidakovic. The paper considers the

testing problem in fixed-effects functional analysis of variance (FANOVA) models. We show how the existing optimal (in the minimax sense) testing procedures for testing a zero signal in a “signal+noise” model can be adapted for FANOVA and derive optimal procedures for testing the significance of the components of the FANOVA model. The resulting tests are based on the empirical wavelet coefficients of the data. We performed a simulation study to illustrate the behaviour of these tests and applied them also to a real-life data arising from physiological experiments.

The techniques developed in the above mentioned work were further applied by Jérémie Bigot, a PhD student at the LMC to address the problem of the alignment of multiple sets of curves and their comparison with FANOVA techniques. In paper [23], a non-parametric approach is proposed to estimate the zero-crossings lines of the continuous wavelet transform of a 1D signal observed with noise. A new tool, the “structural intensity”, is introduced to represent the locations of the significant landmarks of an unknown curve via a probability density function. This technique yields an automatic landmark-based registration method to synchronize a set of curves. Fixed-effects FANOVA model is then used to test the significance of main/interaction effects and to show the usefulness of curve alignment.

3.4. Kalman filtering

Participants: Jacques Blum, Alain Le Breton, Dinh Tuan Pham, Jacques Verron, Ibrahim Hoteit.

Filtering is the basic tool in the sequential approach to the problem of data assimilation into numerical models, especially in meteorology and in oceanography. This approach, of stochastic nature, is justified by the fact that the dynamical system studied is chaotic and thus behaves similarly to a stochastic system. Moreover, the initial state of the system, being unknown, can be conveniently modelled by a random vector, and further the deficiency of the dynamical model can be taken into account by introducing a random noise term. The goal of the filtering is to obtain a good approximation of the conditional expectation of the system state (and also of its error covariance matrix) given the observed data. These data appear as the realizations of a random process related to the system state and contaminated by an observation noise. In applications to meteorology and oceanography, the above filtering approach has encountered two major difficulties. The first one is the nonlinearity of the dynamical equations, which leads to the use of a sub optimal filter called extended Kalman filter, in which the above equations are linearized around the current estimate of the system state. Such filter however can be unstable and sometimes diverges completely. The second difficulty is the very large dimension of the system state vector. The application of the filter would lead to prohibitive calculations. Further this large size poses the problem of adequately specifying the statistical characteristic of the errors.

Our goal in this project is to investigate in depth the possibility of the above filtering approach to apply it to real data. To this end, we have developed a new filter of extended Kalman type, based on the use of a singular low rank filter error covariance matrix. The filter operates according to the principle of not making any correction along the direction of natural attenuation of the error. The corrections are made only along the directions belonging to a vector sub-space, which is constructed initially by the method of empirical orthogonal functions (EOF), but then evolves in time according to the model equations. This filter is thus called *Singular Evolutive Extended Kalman* [42][43]. It has been first tested in a reduced configuration based on a quasi-geostrophic ocean model, which yielded very satisfying results [42][43]. It has been then experimented with success to the altimetric data assimilation in a realistic framework of a primitive equation model of the tropical Pacific ocean [45][41]. Recently, we have worked towards the improvement of the filter, on the one hand to reinforce its robustness against the system nonlinearity [40] and on the other hand, to reduce further the computational cost without noticeable degradation of its performance.

On the first point, the idea is to drop the linearization in the extended Kalman filter in favor of the interpolation and the Monte-Carlo drawing. In this way, we have developed another filter called SEIK (*Singular Evolutive Interpolated Kalman*) [38][39][41], which appears more robust against the nonlinearity, with the advantage of being simpler to implement. Moreover, we have explored advanced stochastic filtering techniques to overcome the difficulties related to strong nonlinearities of the system [40].

On the second point, the idea is to enrich the correction basis by addition of some local correction basis vectors and to simplify the evolution of the basis by letting only the global basis vectors evolve. This way the correction basis can contain more vectors, which better captures the errors and yet requires less computation as it is only “semi-evolutive”. Such kind of filters have been experimented in various realistic ocean model settings, yielding quite satisfactory results [29][30] [11][5].

In addition to the activities centered on the stochastic approach to the data assimilation, other works of more theoretical nature have been performed, in the domain of filtering, of control and identification for stochastic systems with dynamical noise of fractional type [31], [33], [32], [35], [34]. These studies allow interesting perspectives in modelling as they permit to take into account the eventual phenomenon of long range dependence in the dynamics.

4. Application Domains

4.1. Identification and Optimization in Physics

Key words: *Capillarity, optimal control, cristallogenesis, electromagnetism, free surface, nuclear fusion, optimal design, plasma, inverse problem, microfluidics.*

The applications are the physics of plasma (nuclear fusion), cristallogenesis (Bridgman process for cristal formation) and the capillarity problem. In each of these topics, an optimization is performed in order to identify a physical quantity, to minimize an energy or to optimize a form or a free surface..

4.1.1. Plasma physics

Participants: Jacques Blum, Isabelle Charpentier.

Identification problem in plasma physics. A method of numerical identification of the plasma current density in a Tokamak fusion reactor from experimental measurements is proposed. This problem consists in the identification of a non-linearity in a semi-linear 2D elliptic equation from Cauchy boundary measurements, from integrals of the magnetic field over several chords and from measurements of magnetic field at specific points.

The problem is solved using fixed-point optimization algorithm based on the finite element method, followed by object-oriented C++ implementation aiming at real-time use as diagnostic at JET and other tokamaks.

4.1.2. Microfluidics and wetting hydrodynamics

Participants: Jérôme Monnier, Patrick Witomski.

We study mathematical and numerical models treating of liquid droplets spreading on solid surfaces. The studies concern the two following problems: a droplet impact on a solid surface (and/or a tape plunging in a liquid) and a droplet spreading using an electrical field. These free surface flows are micrometric and the important phenomena are interfacial.

The first study concerns the dynamic contact line problem: the motion of an advancing liquid on a solid surface and displacing a gas. The final goal is to simulate numerically the motion. The physical phenomena of dynamical contact line appear in many industrial processes such as coating of solids by liquids and biotechnologies. The mechanical and mathematical modeling of the moving contact line is delicate. J. Monnier and P. Witomski study the Shikhmurzaev’s model arising from interfacial rheology. This kind of model leads to a coupling between surface equations of conservation with free surface flows. These studies are done in collaboration with the “Particules Interfaces Microfluidique” -PIM- project-team, LEGI, Grenoble.

The second study treats of the spreading of a droplet using an electric field. The experiments are done at “Laboratoire de Spectrométrie Physique”, Grenoble. It leads to an innovative process of an adaptative optical lens. In our project, we seek to model and compute numerically the physical phenomena using an inverse optimal design approach. Some physical aspects (e.g. the behavior of the curvature at very small scale) are still not well understood.

4.2. Data and Models in Environmental Sciences

Key words: *Data assimilation, High Performance Computing, Optimal Control, Domain Decomposition, Adaptive Meshing, Meteorology, Oceanography, Hydrology, Filtering, Prediction, Predictability, Inverse Problems.*

The use of numerical models for meteorological prediction has been proposed by Charney and Von Neuman in the '40s. This practice became operational in the '60s. Generally geophysical flows have several particularities requiring mathematical and algorithmic developments:

- Geophysical flows are nonlinear. Therefore there is an interaction between the different scales of the models. The small scale effects (smaller than the mesh size) will have to be estimated by some additional terms in the equations. These terms cannot be measured by a physical experiment. This is a typical inverse problem.
- Every geophysical episode is unique: a field experiment cannot be reproduced. Therefore the validation of the model has to be carried out with several situations, all different, and the role of the data in this process is crucial.
- The geophysical fluids are non closed i.e. there is always interaction between the components of the environment. The ocean interacts with the atmosphere, the atmosphere interacts with continental water interacting with the ocean. A consequence is that boundary terms, associated to the interactions, will have to be provided in a model dedicated to one component of the environment. The quantitative estimation and parameterization of this term is also a typical inverse problem.

Since a few years there is a strong societal demand for a precise prediction in meteorology, oceanography and hydrology. Following meteorology, an operational center for oceanic prediction (MERCATOR) and a center for flood prediction (SHARPI) have been recently opened in Toulouse. The development of numerical prediction rises many mathematical and algorithmic problems. The vocation of IDOPT is not to carry out numerical prediction but to be a support for the mathematical problems raised by this approach. In this sense the basic components of the water cycle modelling are studied in IDOPT. Worldwide very few research groups have this particularity.

4.2.1. Oceanography

Participants: Didier Auroux, Eric Blayo, Didier Bresch, Jacques Blum, Laurent Debreu, Veronika Fedorenko, Christine Kazantsev, Evgueni Kazantsev, François-Xavier Le Dimet, Véronique Martin, Maëlle Nodet, Dinh Tuan Pham, Céline Robert, Jacques Verron, Christophe Vouland.

Understanding and forecasting the ocean circulation is presently the subject of an intensive research effort from the international scientific community. This effort was primarily motivated by the crucial role of the ocean in the earth climate, in the perspective of global change. Moreover important recent research programs aim at developing operational oceanography, i.e. a near real-time forecasting of ocean circulation, with applications to shipping, fisheries, weather forecasting... Another related field is coastal oceanography, dealing for example with pollution, littoral planning, or management of ecosystems. Essential tools for such goals are modelling systems, which require the development of performant numerical models and data assimilation methods. In this context, the IDOPT project conducts efforts on the following topics :

- *Multiresolution approaches and coupling methods:* Many applications in coastal and operational oceanography require high resolution local models. These models can either be forced at their boundaries by some known data, or be dynamically coupled with a large-scale coarser resolution model. From a mathematical and numerical point of view, such model interactions demand specific studies on open boundary conditions, mesh refinement methods, and coupling algorithms.
- *Higher order numerical schemes:* Most ocean models make use of simple second order finite difference schemes. We are seeking for higher order schemes allowing both accuracy and good conservation properties.

- *Parameterization and modelling of boundary layers*: A striking feature of ocean dynamics is the existence of several types of boundary layers, either lateral (near the coastlines), or vertical (near the ocean surface and bottom). Despite their relatively small size, these layers have a very important role in the global dynamics, and must be accurately represented in the model. New modelling and numerical approaches to this problem are studied.
- *Data assimilation methods for ocean modelling systems*: As in atmospheric models, the main difficulties encountered when assimilating data in ocean models are the huge dimension of the model state vector (typically 10^6 - 10^7), the strongly nonlinear character of the dynamics, and our poor knowledge of model error statistics. In this context, we are developing reduced order sequential and variational data assimilation methods addressing the aforementioned difficulties. Moreover, we have started this year the study of two new specific problems: assimilation of lagrangian data, and design of data assimilation methods for multiresolution models.

Most of these studies are led in strong interaction with physicists, in particular from the Laboratoire des Ecoulements Géophysiques et Industriels (LEGI, Grenoble).

4.2.2. Control of flow

Participants: François-Xavier Le Dimet, Yousuff Hussaini.

A body in a fluid in motion produces drag. A way to reduce the drag is to use blowing and suction at the surface of the body. In (Daescu, Hussaini, Navon, Le Dimet) it has been shown how the tools of optimal control can be used to optimally reduce the drag. A possible extension, under works, coupled to data assimilation is to consider a closed loop system, the inputs being the measurements of sensors and the result a minimal drag.

4.2.3. Hydrology and river hydraulics

Participants: William Castaings, Marc Honnorat, François-Xavier Le Dimet, Cyril Mazauric, Jérôme Monnier.

Floods prevention and prediction are critical issues. Flooding is the result of complex interactions of the water cycle between meteorology, hydrology and hydraulics. Mathematical and numerical modelling is becoming accepted as a standard engineering practice for both prevention and prediction of those catastrophic events. The models (shallow water equations 1D and 2D) and the industrial softwares (e.g. Telemac2D, Carima1D) are quite satisfying for some configurations. Nevertheless for practical applications, initial and boundary conditions (e.g. observed water level, discharge) are partial and difficult to prescribe and empirical parameters (land roughness) are calibrated manually using hydraulic expertise. Realistic and reliable forecasting of those catastrophic events requires a completely integrated approach with all components (models and data) integrated in a consistent manner into an hydro-meteorological prediction chain with affordable computational cost.

Data assimilation methods, that have shown their potential in other geosciences like meteorology and oceanography, are now in the forefront in hydrology. This prediction chain is far from being operational.

The problems adressed in IDOPT related to data assimilation for catchment scale hydrology and river hydraulics are part of the investigations to be carried out. The current research topic led in team-project IDOPT are the following.

Data assimilation and parameter identification as applied to 1D and 2D river hydraulics models. During his PhD, C. Mazauric achieved a prospective study on the application of optimal control techniques to river hydraulics. Data assimilation methods were developed for both 1D and 2D models and their potential was evaluated using appropriate test cases. First and second order sensitivity analysis were carried out in order to study the contribution of inputs (model input parameters and observation data) to the model response in a data assimilation framework.

Image Data assimilation. M. Honnorat began his PhD in October 2003, treating of image data assimilation for flood models. The two mathematical problems tackled are the reconstruction of the flow dynamic using

images type data and the high sensitivity of the water front with respect to data uncertainties (topography and land roughness). This study is funded by CNES and CNRS.

Sensitivity analysis for rainfall-runoff models. Flash flood events are usually generated by heavy convective precipitation over a relatively small area but catchment hydrology plays a major role in their occurrence. Important factors like initial soil moisture and infiltration parameters govern rainfall abstractions and therefore control the partition of rainwater between infiltration and runoff. Adjoint sensitivity analysis and data assimilation are investigated by W. Castaing for an event-based distributed flash flood model. This work is done in collaboration with Toulouse Fluid Mechanics Institute (IMFT) in the framework of PACTES project. All these studies are led in the framework of different projects with numerous collaborations.

- The european project ANFAS (1st Jan. 2000 - 31 March 2003) was dedicated to the design of a Decision Support System for flood prevention and protection. During this project, hydraulics models (1D/2D) were adapted to the Loire pilot site. -See partners in European collaboration section-.
- The national project PACTES (Prévention Anticipation des Crues au moyen des Techniques Spatiales) was initiated by the French Space Agency (CNES) and the French Ministry of Research, in order to improve the operational management of floods, through a joint approach involving the operational users, scientific laboratories and industry. Scoping interactions in terms of models and data with the continental water cycle, available gauged watersheds for evaluation and validation developed collaborations with the French hydro-meteorological community (Meteo France, CETP, LTHE).
- The regional project (Région Rhône-Alpes) “Numerical Prevention for Floods”, led by J. Monnier, conducts researches in data assimilation and parameter fitting methods, uncertainties propagation and use in real-time of numerical simulations. The participants are applied mathematicians and numericians (team-project IDOPT), hydrolicians (Cemagref Lyon), hydrologists (LTHE Grenoble) and research engineers (Sogreah Company).

5. Software

5.1. Numerical Computations in Microfluidics

Participants: Jérôme Monnier, Patrick Witomski.

MICRALEFE (MICROfluidics ALE Finite Element) is a C++ finite element software in 2D (axisymmetric or not). The current version of the software treats of plate wetting. It models the triple point Dynamics (liquid-gas-solid) and the contact angle dynamic, [37]. The model is based on the equations of the free surface Navier-Stokes equations with surface tension forces. The dynamic of the free surface is described using an ALE formulation (Arbitrary Lagrangian Eulerian). The code is based on the Rheolef C++ finite element library. In addition of the classical conditions, Micralefe capabilities include the dynamic of the contact angle, the triple point dynamic, variable surface tension coefficients, slip type boundary conditions, local Mangorini effects and automatic mesh refinement. The code modularity allows us to plan further developments such as modeling of droplet impacts and/or coupled models (Developments planned for 2004 and funded by AGFA Co).

SHAPELDROP (Shape Electrified Droplet) is a shape optimal design software written in C++. It models the spreading of a droplet using an electrical field. The experiments are done at LSP Grenoble. The model is based on an inverse approach: it performs the droplet shape such that it minimizes its energy (capillarity and electrostatic terms). The current version performs the droplet shape in accordance with the experimental results until a critical potential. In view to a better understanding of a locking phenomena observed, it remains to compute precisely the curvature at small scale in the vicinity of the triple point.

5.2. Wavelet Denoising MATLAB Toolbox

Participants: Anestis Antoniadis, Jeremie Bigot, Theofanis Sapatinas.

A wavelet toolbox and an accompanying paper “Gaussian Wavelet Denoising Matlab Toolbox” was jointly developed by A. Antoniadis, J. Bigot and T. Sapatinas, where various wavelet shrinkage and wavelet thresholding estimators in nonparametric regression appearing in the literature are discussed in detail and implemented. These estimators arise from a wide range of classical and empirical Bayes methods treating either individual or blocks of wavelet coefficients. See <http://www.jstatsoft.org/v06/i06>.

5.3. Adaptive Grid Refinement

Participants: Eric Blayo, Laurent Debreu, Christophe Vouland.

AGRIF (Adaptive Grid Refinement In Fortran, [27], [26]) is a Fortran 90 package for the integration of full adaptive mesh refinement (AMR) features within a multidimensional finite difference model written in Fortran. Its main objective is to simplify the integration of AMR potentialities within an existing model with minimal changes. Capabilities of this package include the management of an arbitrary number of grids, horizontal and/or vertical refinements, dynamic regridding, parallelization of the grids interactions on distributed memory computers. AGRIF requires the model to be discretized on a structured grid, like is typically done in ocean or atmosphere modelling. As an example, AGRIF is currently used in the following ocean models: MARS (a coastal model developed at IFREMER-France), ROMS (a regional model developed jointly at Rutgers and UCLA universities, [7]) and OPA (a general circulation model developed in the LODYC-France lab and by the French community). AGRIF is licensed under a GNU (GPL) license and can be downloaded at its web site (<http://www-lmc.imag.fr/IDOPT/AGRIF>), since August 2003.

6. New Results

6.1. Microfluidics and wetting hydrodynamics

Participants: Jérôme Monnier, Patrick Witomski.

We keep studying the model established by Y. D. Shikhmurzaev in ([44], [25]). We derived a new model coupling the dynamic of the triple line and the angle (surface and mesoscopic model) and the bulk fluid motion (Navier-Stokes with free surface and surface tension terms -macroscopic scale-). The mathematical and numerical analysis are done. Some partial 2D numerical results show the flow in the very local area near the triple point (caterpillar motion, [28]). A paper presenting this first study has been accepted [37].

In addition, a pre-doctoral student developed the full coupling between the surface and the bulk models. Future developments are required to finish the full resolution.

In other respects, this last work led to a new collaboration with the PIM project-team, Laboratory LEGI, Grenoble.

A postdoc funded by AGFA Co. will start next year on this topic (droplet impact on a substrat).

A pre-doctoral student developed the C++ optimal design software performing the numerical simulation of the experiment. This first stage allows us to focus now on the computation of the curvature at small scale ie very close to the triple point. As a matter of fact, this last aspect is probably the main cause of the “spread locking phenomena” observed and still not understood by the physicians.

Some future developments are required in order to continue the collaboration with C. Quillet and the PhD student M. Bienia leading the experimental aspects at Laboratory LSP, Grenoble.

6.2. High-order schemes for the shallow-water model

Participants: Eric Blayo, Christine Kazantsev, Eugène Kazantsev.

One of the major challenges in ocean modeling is the necessity to resolve explicitly eddy scales down to Rossby radius. This leads to a very large number of discretisation points, prohibiting any model implementation even on the most performant computers.

One obvious way to reduce the number of discretisation points and to reproduce the impact of small scales on the large scale processes is using improved numerical techniques, and namely high order schemes. This kind of schemes is widely used in atmospheric modeling. In particular, compact schemes of fourth, fifth and higher order have shown their great ability to reproduce complex physical phenomena in models at relatively low resolution.

However, the main difficulty in using high-order schemes in ocean modeling lies in the presence of boundary conditions. In fact, periodical boundaries in atmospheric models greatly simplify the implementation of high-order compact schemes.

High order schemes are also known to work well for the simplest ocean models in academic cases. One can cite the fourth order scheme of Arakawa for the Jacobian discretisation in quasi-geostrophic and barotropic model formulations.

But, when the model physics becomes more complicated, high-order schemes become much more difficult to use.

In the study of the shallow-water model on the C-grid (following the classification of Arakawa) we found that

- the total mass can be conserved by a fourth order scheme using a particular approximation of the boundary conditions;
- the energy cannot be conserved by a fourth order scheme on the C-grid;
- the group velocity of the Rossby waves may have locally a false direction that lead to deformation of the model solution.

These restrictions do not allow to use high-order schemes in their present form in ocean models. One can only apply high-order technique when the β -effect is weak [24].

6.3. Multiresolution approaches and coupling methods

Participants: Eric Blayo, Antoine Bouquet, Laurent Debreu, Veronika Fedorenko, Véronique Martin, Christophe Vouland.

The implementation of high-resolution local models can be performed in several ways. An usual way consists in designing a local model, and in using some external data to force it at its open boundaries. These data can be either climatological or issued from previous simulations of a large-scale coarser resolution model. The main difficulty in that case is to specify relevant open boundary conditions (OBCs). By performing a critical review of previous related works either in oceanography or applied mathematics, we have shown that such relevant OBCs must be based on the incoming characteristic variables (in the hyperbolic sense) of the model equations, and that the external data must be used in a way satisfying a consistency relationship. Numerical experiments are presently underway to implement these ideas in realistic ocean models, in collaboration with IFREMER and IRD (Brest).

Another way of designing such local models is to locally increase the resolution of a large-scale model. The design of local mesh refinement methods requires appropriate boundary conditions at the boundaries between coarse and fine mesh. Main difficulties rely on the treatment of distinct discrete boundary (e.g. due to different topography in ocean modelling) and the preservation of conservation properties. Topographic related issues have been treated specifically during the training period of Antoine Bouquet. When the refinement is adaptive, the initialization procedure is also of tremendous importance ([27]). Last the computer implementation of efficient local mesh refinement involves dynamic memory management, use of structured types and can be even harder when operated on parallel computers. The AGRIF software, presented in section 5.3, has been developed in the IDOPT project and is increasingly used in realistic ocean models.

An interest of the local refinement approach is the two-way interaction between local and global models. However a limitation is that the physics remains (at least nearly) unchanged from the global to the local scale, while it is well-known that large scale physics may be inadequate for representing local phenomena.

Therefore a more general approach consists in coupling different models, with possibly different resolutions, numerics, and even physics. We can then use the framework of domain decomposition methods to derive efficient algorithms with relevant interface conditions.

Our approach is twofold : on one hand, we conduct rigorous mathematical studies on simplified models, in collaboration with applied mathematicians from LAGA - Paris 13 (L. Halpern, C. Japhet, V. Martin). Exact and approximate absorbing interface conditions have been computed for tracer equations and for the 2-D linearized shallow-water system. Corresponding numerical experiments have also been performed.

On the other hand, a realistic configuration for coupling experiments has been realized in collaboration with oceanographers from LEGI - Grenoble (B. Barnier, S. Cailleau). It consists in the coupling of a regional high resolution model of the bay of Biscay with a coarser resolution model of the north Atlantic. Several numerical simulations, with different coupling algorithms, have been realized or are presently underway. Their performances will be analyzed and compared.

This work is granted by the national MERCATOR program.

6.4. Data assimilation methods for ocean models

Participants: Didier Auroux, Eric Blayo, Jacques Blum, Laurent Debreu, Yann De Visme, François-Xavier Le Dimet, Maëlle Nodet, Dinh Tuan Pham, Céline Robert, Jacques Verron.

Synthesis of reduced-order methods. Following several studies led these last years in the IDOPT project on sequential and variational reduced order data assimilation methods, a current PhD thesis (C. Robert) consists in drawing some synthesis of these methods. We aim at making for the first time a comparison of their applicability and performances in a realistic oceanic context (assimilation of in situ temperature data in a 3-D model of the tropical Pacific). Then we intend to try to design hybrid methods, making use of the best aspects of each method.

A number of experiments have been performed with variational reduced-order methods. A remaining difficulty was the choice of a relevant low-rank basis leading to an efficient assimilation in the case of real data (i.e. with an imperfect model). We have now designed a strategy to build such basis, which is a new result. Additional methods investigating the complementarity between low-rank and full-rank approaches are presently under development.

New data assimilation methods. The aim of this work is to investigate several new data assimilation techniques. Numerical experiments have been performed to test different possible applications of the nudging technique to ocean models like the barotropic quasigeostrophic model. The quasi-reversibility method was also tested for the identification of the initial state. Finally, a new class of algorithms generalizing the dual algorithm 4D-PSAS has been developed. This dual approach naturally allows to take into account the model error. Numerical tests carried out in the context of twin experiments with a baroclinic quasigeostrophic model show that the dual methods make it possible to obtain more quickly better results and to reduce the influence of an error term in the model equations. This work corresponds to D. Auroux's PhD thesis.

Assimilation of lagrangian data. This work is motivated by the Argo program, which aims at deploying a network of 3000 profiling floats over the world ocean. Argo is part of the international GODAE experiment (Global Ocean Data Assimilation Experiment). These profilers drift at a typical depth of 1500m, and perform a vertical profile of temperature and salinity every ten days. Their position is known every ten days, which gives a set of lagrangian data. We presently develop a variational method in order to assimilate such data. Twin experiments are performed with the OPAVAR model, in an idealized configuration. This work is the subject of the PhD Thesis of Maëlle Nodet, and is granted by the national project Mercator.

Assimilation in multiresolution systems. The objectives are to study the mathematical formulation of data assimilation methods for embedded grids (multiresolution systems) and to conduct numerical experiments for validation. This study is divided into two parts: the selection of the assimilated observations as a function of the grid resolution (definition of criteria and sensitivity analysis), and integration of the grid interactions in the assimilation system (the assimilation scheme should allow new types of grid interactions by taking advantage

of the iterative minimization procedure to add additional constraints at the coarse/fine grid interfaces). This work is granted by the national PATOM program.

6.5. Data Assimilation in Agronomy

Participants: François-Xavier Le Dimet, Wu Lin, Claire Lauvernet.

Laws governing biological systems are complex. Equations of conservation are not sufficient to predict the evolution of a single plant or a cultivated area. Nevertheless the growth of plants fulfills some empirical laws. This means that these laws contain some parameters that cannot be directly measured. Furthermore it is possible to act, to some extent, on the growth of plants by controlling water, insulation,... In cooperation with IRD, CNES, INRA, some applications of data assimilation have been carried out, one at the level of a single plant and the other to a more global level.

GreenLab - a plant functional-structural model. Started in Beijing in 1998, the GreenLab project aims at a mathematical description of plant growth, especially for the plant functional-structural characteristics. Many efforts have contributed to this modelling approach, i.e. double-scale automaton, substructure, stochastic modelling, and model-based optimization. The project is supported by CASIA/LIAMA, UJF/LMC in the frame of IDOPT, CIRAD and INRIA Rocquencourt.

Optimization based on plant functional-structural characteristics. Optimization is an important application of GreenLab. The basic formula of GreenLab is

$$Q(n) = \frac{E(n)}{R(n)}$$

where $Q(n)$ is the fresh biomass produced in growth cycle n , $E(n)$ is the fresh biomass production potential depending on the environment, and $R(n)$ is the plant resistance which is calculated according to the plant architectural and geometrical information and depends on the plant genetic parameters, i.e. organ sink strength, sink variation, leaf resistance, leaf lifespan, etc. We classify the optimization applications into two catalogues - genetic parameters optimization problems and environmental factor optimization problems.

The genetic parameters optimization in essence is to analyze the plant functional-structural characteristics, say the feedback of architectural information on plant growth. We take maize as an example. The source-sink relationships are optimized to achieve an optimal biomass partitioning for maize fruit yield. We catalogue this problem as a bound-constrained optimization problem with fruit yield as the cost function and with the fruit sink strength value as the optimization control variable. The optimization results help define a sink strength spectrum to evaluate the maize in the field according to their calibration fruit sink strength values, and possible instruction for hybridization can also be drawn.

With environmental factor optimization we introduce optimal control to plant growth. The sunflower water supply problem is defined as such an example. Let us suppose the biomass production potential $E(n)$ is proportional to the soil water content which complies with some soil moisture budget differential equation according to the water supply into soil at each growth cycle. The optimization problem is to find the optimal water supply strategy of certain amount of water for maximal sunflower fruit yield. We catalogue this problem as a mixed integer nonlinear problem. The optimization results show that the optimal sunflower can have a shorter height but a heavier fruit weight compared with non-optimal ones.

We formulate the fresh biomass production potential as a function of environmental light, temperature, and soil water content data as follows

$$E = E_0 \cdot x_T^{\alpha-1} (1 - x_T)^{\beta-1} \cdot a(1 - \exp(-bL)) \cdot x_W^{K1-1} (1 - x_W)^{K2-1}$$

where E_0 is the production potential under potential growth conditions, x_T, x_W are relative temperature and soil water content data, and L is the environment light intensity, $\alpha, \beta, K1, K2, a, b$ are environmental factor parameters.

Future work. Thanks to the interaction with light and temperature, a greenhouse energy control problem can be defined to maximize the tomato yield and to minimize the energy cost in greenhouse.

Calibration is needed for both genetic parameters and environmental factor parameters. Another problem is to retrieve environmental data according to plant measurement, which is an inverse problem.

Data Assimilation for Vegetation. The ADAM project (CNES-INRA, Assimilation des Données par Agro - Modélisation : <http://medias.obs-mip.fr/adam/>) is devoted to the use of tele-detection observations in a model of vegetation. The goal is to determine the parameters of the soil and those of the culture. The model used in this study is STICS developed at INRA by Brisson et al.. A major difficulty comes from the fact that the model is not differentiable, some processes involved in the model having thresholds. From the formal point of view it is possible to generate an adjoint model, but the results of the integration of this adjoint model will produce sub-gradients. The first step was to understand the application of variational models to a complex agronomical model. This was done with a simplified model simulating only biomass and leaf index. To achieve this goal it has been necessary to inverse a radiative transfer model (SAIL-PROSPECT). Therefore it was possible to estimate the reflectance of the vegetation from its optical properties. The software TAPENADE developed at INRIA Sophia-Antipolis is used for the derivation of the models.

6.6. Hydrology

Participants: William Castaings, Marc Honnorat, François-Xavier Le Dimet, Cyril Mazauric, Jérôme Monnier.

Cyril Mazauric defended his PhD in December 2003. The aim of this work is to present and test some methods based on the control theory which allow to use optimally every available information. Some applications of these methods will be treated, like parameter estimation, sensitivity analysis and model coupling.

The work of these last months has been focused on the parallelization of model coupling. The examples treated are based on the decomposition of a river. On each subdomain, the flux is computed on an independant processor and, thanks to data assimilation methods, the initial condition and boundary conditions are estimated simultaneously. Parallelization is limited to the communication of the boundary values to the neighbouring models.

Future work will be to test those methods on different domain and to couple models coming from oceanography and hydrology.

Marc Honnorat carried out some bibliographic work in the scope of a Master thesis concerning the analysis of numerical methods for the resolution of the Shallow Water equations. Time-discretization schemes, finite elements schemes and the characteristics method for the treatment of the advection terms have been considered. Moreover, the algorithmics of Telemac2D (a finite elements software for 2D shallow water flows, EDF-Sogreah Co.) has been studied. In the scope of the PhD, an additional bibliographic work has been done concerning data assimilation methods both from a theoretical point of view and for the application to river hydraulics.

Using a code developed by D. Froehlich (DaveF), our group adapted this model to the Loire pilot site, participated in the development and deployment of a parallel version, conducted model integration to the ANFAS system by specifying features and interfaces. At the end of the ANFAS project, 2D modelling of river/floodplain flood propagation and fuse plug spillway erosion was achieved for a set of scenarios for the Loire river pilot site and fully integrated to demonstrate the facilities provided by the ANFAS decision support system.

W. Castaing began his PhD in spring 03. It concerns sensitivity analysis and data assimilation applied to rainfall-runoff models. Flash flood events are usually generated by heavy convective precipitation over a relatively small area but catchment hydrology plays a major role in their occurrence. An event based flash flood model was developed by IMFT but the prescription of consistent initial conditions and calibrated parameters is a challenging task. In fact, important factors like initial soil moisture and infiltration parameters govern rainfall abstractions and therefore control the partition of rainwater between infiltration and runoff. Since the model is devoted to be integrated to an hydrometeorological prediction chain, its interaction in terms of models and data

was scoped and the direct model slightly modified. After a review of the application of data assimilation to hydrology, adjoint sensitivity analysis and variational data assimilation was initiated.

7. Contracts and Grants with Industry

7.1. National contracts

- A collaboration exists with the "Département de Recherche sur la Fusion Contrôlée" of the "Centre d'Études Nucléaires" at Cadarache on the problems of identification and control in plasma physics. A new contract is signed with the CEA (Cadarache) the current density in TORE SUPRA.
- A contract with IFREMER on the thematic "Modélisation côtière Sud-Bretagne" has been signed.
- A contract with MERCATOR on the thematic "Couplage de modèles océaniques" has been signed.

7.2. International contracts

Participants: François-Xavier Le Dimet, Cyril Mazauric, William Castaing.

IDOPT is a partner of the ANFAS project (<http://www.ercim.org/anfas>). The other participating institutes are:

- Bureau de Recherches Géologiques et Minières (France).
- CLRC - Council for the Central Laboratory of the Research Councils, Information Technology Department, Rutherford Appleton Laboratory (United Kingdom)
- ERCIM - The European Research Consortium for Informatics and Mathematics (France)
- FORTH - IACM Foundation for Research and Technology-Hellas (Greece)
- Matra Systemes & Information (France)
- Slovak Academy of Sciences, Institute of Informatics (Slovakia)
- University of Reading (United Kingdom)
- Chinese Academy of Sciences, Institute of Automation (China)
- Chinese Academy of Sciences, Institute of Remote Sensing Applications (China)
- Chinese Academy of Sciences, Institute of Atmospheric Physics (China)

The involved end-users are:

- Equipe Pluridisciplinaire du Plan Loire Grandeur Nature (France)
- Wuhan University, Department of River Engineering, School of water Resources and Hydropower P.R. (China)
- River Research Department, Yangtze River Scientific Research Institute (YRSRI), Jiuwanfang, Zhaojiatiao, Hankou district P.R. (China)

The overall objective of the ANFAS is to develop a Decision Support System for flood prevention and protection, integrating the most advanced techniques in data processing and management. INRIA/IDOPT was responsible of Workpackage 3:

- Models adaptation to pilot sites (Vah, Loire, Yangtsé)
- Modelling and data assimilation for flood prediction
- Parallel algorithms for computational hydraulics

Participants: François-Xavier Le Dimet, Eugène Kazantsev.

IDOPT participates to the joint project with the Numerical Mathematics Institut of the sciences academica of Russians "Etude de la réponse de la circulation atmosphérique aux petites perturbations extérieures" supported by EGIDE.

Participants: Anestis Antoniadis, Gerard Grégoire.

Anestis Antoniadis is the coordinator of the French part of a research European network of the type "Interuniversity Attractions Poles", from 2002-2005, including 5 Belgian Universities (UCL, KUL, ULB, LUC, FUNP(NAMUR),), the UJF (LMC) and a German University (Aachen) on the theme "Statistical techniques and modeling for complex substantive questions with complex data".

8. Other Grants and Activities

8.1. Regional action

Collaborations with various regional research teams:

- MEOM (Modélisation des Écoulements Océaniques et des Marées) team from Laboratoire d'Écoulements Géophysiques et Industriels (Grenoble) : oceanography.
- Laboratoire de Transferts en Hydrologie et Environnement (Grenoble): inverse problems in hydrology.
- Département d'études des matériaux, section d'études de la solidification : CENG (Centre d'Études Nucléaires de Grenoble).
- Institut Laue-Langevin, Institut de Biologie Structurale du CENG et ESRF (Synchrotron) : stochastic methods for inverse problems.
- Pechiney : Centre de recherche de Voreppe.
- Cemagref Lyon, Department Hydrology and Hydraulics.
- LEGI, PIM project-team (Particules Interfaces Microfluidique).
- Regional project "prévention numérique de crues", (responsible: J. Monnier).

8.2. National actions

Interactions with other INRIA projects or actions:

- PARA PROJECT: Operational inverse mode.
- ESTIME PROJECT: Optimisation algorithm, operational inverse mode.
- TROPICS ACTION: Ajoint code automatic derivation (ODYSSÉE), operational inverse mode.
- SINUS PROJECT : Operational inverse mode.

Collaborations with other research teams in France :

- Participation to the national research programm MERCATOR (oceanography).
- Laboratory "Analyse, Géométrie et Applications" (Paris 13): Domain decomposition and coupling model.
- IFREMER Brest.
- IRD Brest.
- "Laboratoire de Météorologie Dynamique" in the ENS (Paris): data assimilation for environment.
- CEA Cadarache.

- Centre National de Recherche Météorologique, Météo-France (Toulouse): Data assimilation for atmospheric models.

Participation to national research groupements (GdR) CNRS :

- GdR SPARCH (simulation de faisceaux de particules chargées);
- GdR Optimal design;
- GdR Fluids in interaction;
- GdR EAPQ (Equations d'Amplitudes et Propriétés Qualitatives);

8.3. European actions

8.3.1. Western Europe

Collaboration of A. Antoniadis and G. Grégoire with the professors I. Gijbels and A. Kneip of the Institut de Statistique de Louvain-La-Neuve. Collaboration of A. Antoniadis with Dr. Umberto Amato of CNR Italien (Naples). Collaboration of A. Antoniadis with Dr. Sylvain Sardy (École Polytechnique Fédérale de Lausanne). F.-X. Le Dimet participates to the European project ECRASE (modelization in hydrology) and to the European project PIONEER (coastal oceanography). He is member of the ECMI Educational Board (European Consortium for Mathematics in Industry).

8.4. International actions

On the thematic “physique des plasmas” : collaboration with M. Vogelius (Rutgers university).

On the thematic “environnement” : IDOPT in in charge of the associated group "SEMINOLE" devoted to promote co-operative research between the Department of Computational Sciences and Information Technology at Florida State University and IDOPT. Several stays both in Grenoble and Tallahassee were carried out in the framework of the agreement. The theme of the agreement is "Data and models for geophysical flows".

A strong collaboration also exists between the Institute of Numerical Mathematics of the Russian Academy of Science, the Institute of Atmospheric Physics of the Chinese Academy of Sciences and IDOPT. Exchanges of scientists have been done in 2003.

9. Dissemination

9.1. Scientific community dissemination

A. Antoniadis is a member of the Editorial board of the *ISUP* journal since 1992.

A. Antoniadis is associate editor of the Journal of the French Statistical Society since 1998.

A. Antoniadis is Editor in Chief of the journal *ESAIM: Probability & Statistics* since 2001.

A. Antoniadis is associate editor of the Journal “Statistics and Computing” since 2002.

J. Blum is editor in chief in the electronic journal *ESAIM: COCV (Control, Optimization and Calculus of Variations)*.

A. Antoniadis has organized and presided the international conference “Wavelets and Statistics: watering the seed”, partially supported by INRIA, held in Villard de Lans from the 4 to 7 September 2003. J. Blum is member of the scientific committee of PSMN (Pôle de Simulation et de Modélisation Numérique) de l'ENS Lyon.

D. T. Pham is editor in chief of the journal *Journal of Time Series Analysis* since 1992.

F.-X. Le Dimet is member of the scientific committee of the european project GIR ECOFOR.

F.-X. Le Dimet is member of the Educational Board of ECMI

F.-X. Le Dimet is member of the scientific committee of UJF.

9.2. Teaching

There exists a strong link with the DEA in applied mathematics of the Joseph Fourier University and the Institut National Polytechnique de Grenoble (ENSIMAG). Most of the staff of the project give lectures in this formation, and our DEA and PhD students come from this formation. Among all the lectures given by the staff of the project, we can cite:

- Models and data for geophysical flows (E. Blayo, L. Debreu, F.-X. Le Dimet);
- Domain decomposition methods for PDE (E. Blayo);
- Problèmes inverses en imagerie médicale (A. Antoniadis);
- Control and optimization of systems governed by PDE (J. Blum, DEA de l'Université de Nice)
- "Numerical Models and PDEs" (J. Monnier, ENSIMAG);
- "Wetting hydrodynamics. Numerical Modeling aspects". Ecole CEA Grenoble "Interfaces and Microfluidics" (J. Monnier);
- "Numerical modeling dynamics of fluid-fluid interfaces: ALE and Level Set methods". Ecole CEA Grenoble "Interfaces and Microfluidics" (J. Monnier)

9.3. conferences, workshops

The members of the team have participated to various conferences and workshops. See the bibliography.

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