Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique
European Center for Research and Advanced Training in Scientific Computing

CERFACS
Scientific Activity Report
Jan. 2000 – Dec. 2001

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Foreword

Welcome to this two-year issue of the CERFACS Scientific Activity Report. This issue does indeed cover both 2000 and 2001, as it appears that such a periodicity might be more suited to the pace of progression of scientific activities than the more usual yearly publication.

What have been the major scientific achievements of these past two years ? Reading through the report will hopefully provide the reader with very many answers to this question, but let me just select a few results for each team as an appetizer :

Parallel Algorithms
Many tools developed by team have found applications within simulation methods developed by other teams and/or partners (domain decomposition method for CFD and for Dassault-Aviation; preconditioning technique for electromagnetic solvers, both in-house and at EADS). Following a workshop organized in late 2000, a method for controlling the numerical quality of solvers with both internal and external iterations has been successfully validated with EDF.

Computational Fluid Dynamics
The NSMB solver developed cooperatively by the team is now in the production mode at AIRBUS and is used for the design of the A380. The future of aerodynamics simulation codes is also prepared, with, e.g., the agreement signed with ONERA to make CERFACS a full partner for the development of the new elsA software. The quality of the work has been recognized through the highly-competitive BMW prize which was awarded to B. CARUELLE, a then CERFACS Ph.D. student. Progress in the development of simulation methods for turbulent combustion has been very rapid, with also new applications in the field of two-phase flow and the AVBP code, now recognized as the main French code for unsteady combustion.

Computational Electromagnetism
A more efficient, two-level, method for use within the fast multipole code has been developed by the team, allowing one to address very large sized problems with more than 1,000,000 degrees of freedom. A successful application has been realized with the simulation of the interaction between a satellite and its antenna. Progress is still taking place simultaneously in the field of processing singular integrals within electromagnetism codes.

Climate Modelling and Global Change
It has been shown by the team that the structure of the surface temperature field in the north Atlantic ocean is a six-month precursor of the North-Atlantic Oscillation (NAO), a key factor for European climate. The prototype for the seasonal climate prediction system based on a coupled ocean-atmosphere model with full oceanic data assimilation is progressing again at a rapid pace, after full scientific documentation of the key role of variational data assimilation. The MERCATOR group successfully provided the MERCATOR project with a fully tested Atlantic ocean model at intermediate resolution, which is now used operationally every week for providing oceanic forecasting. The successor for this model, the so-called PAM model, is in its final stage of validation, before replacing the former one in the operational suite. The PALM tool, developed for allowing data assimilation methods to be easily implemented and upgraded, is included in a number of applications, including those for MERCATOR.

Signal and Image Processing
The team has developed a very powerful method for better GPS processing, based on a novel mathematical approach for the resolution of integer ambiguities. The development of the SMOS1 simulator is progressing rapidly, and should become an important building block for the ground segment of this satellite mission.

Technology Transfer
The so-called N'S'3 platform, including the package for collaborative working, is now fully tested and in the process of being commercialised.

Computing resources
Thanks to special funding, it has been possible to replace CERFACS' main computer, which provides 32 Gflop/s peak in 2001, with a 5-fold increase being planned for 2005.
CERFACS scientific production is still high:

- the number of high-standard publications, i.e. in internationally-refereed journals, is 65, a number close to the mean rate of 30 publications per year;
- CERFACS' researchers have produced yearly more than 120 technical reports, book chapters, papers in conference proceedings ;
- they are very active in training new researchers, with 13 Ph. D. theses being awarded over the period, and with 4 "Habilitations Diriger des Recherches" (HDR) over the same period.
- they have also very actively developed applied research, with a total of approximately 60 grants per year being held over the period, approximately 20 of them coming from the European Commission through its various programmes, and the rest, of the order of 40, being awarded by other funding agencies and, or industrial partners ;
- CERFACS web site is experiencing a very rapid development, with the number of monthly hits by external visitors increasing from 100,000 in early 2000 to 200,000 at the end of the period (see Fig.1), demonstrating CERFACS' steadily-improving attraction. Another interesting feature can be seen in Figs. 2 and 3, where the "Parallel Algorithms" team is the one with the largest number of accesses ;
- let us also finally mention that CERFACS wide-interest seminars have attracted high-level and well-known external scientists (see below).

At the end of 2001, the number of people working at CERFACS was 80 (full-time equivalent) scientists (see Tables ii to viii), with a global budget of 5.6 M.

I sincerely hope that you will have some time to read through the detailed activity reports of the teams, and that you will find there enough interest to pursue your collaboration with us, or to initiate some new ones.

Enjoy your reading.

Jean-Claude ANDRÉ
CERFACS Director

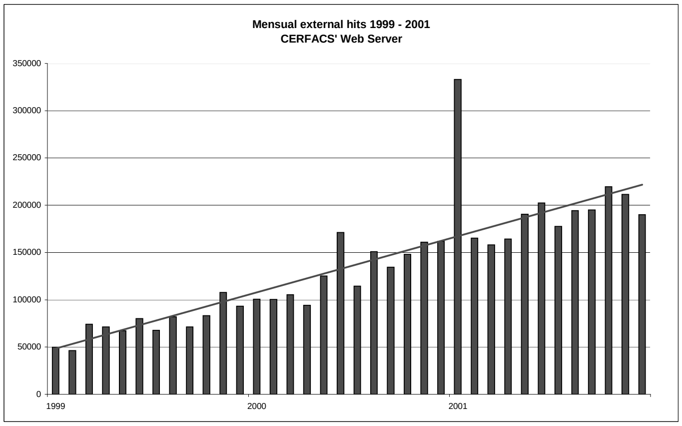


Figure 1: Mensual external hits on CERFACS' Web server during the period 2000-2001

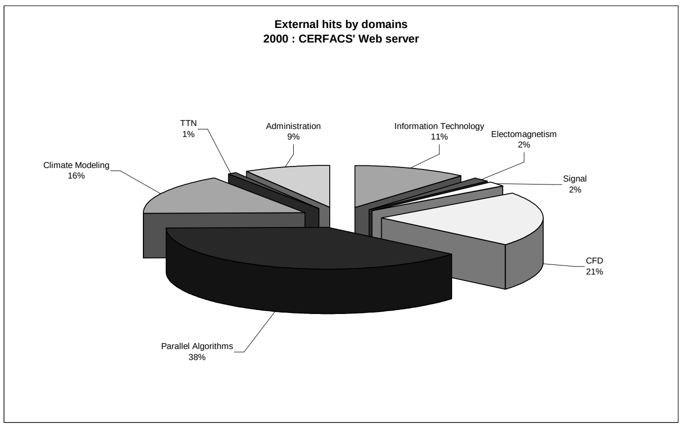


Figure 2: External hits by domain on CERFACS Web server during the year 2000

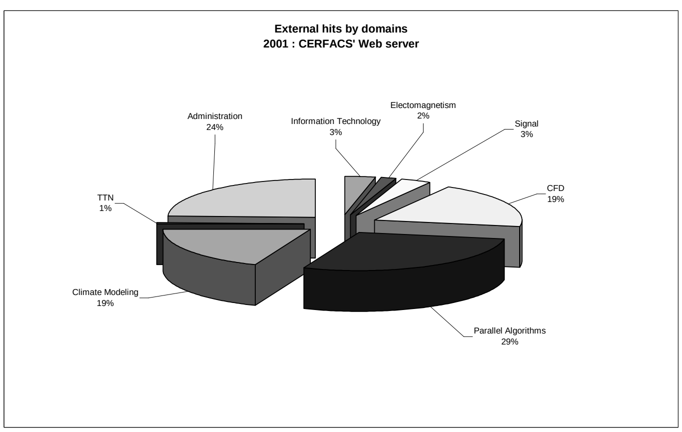


Figure 3: External hits by domain on CERFACS Web server during the year 2001

CERFACS Structure

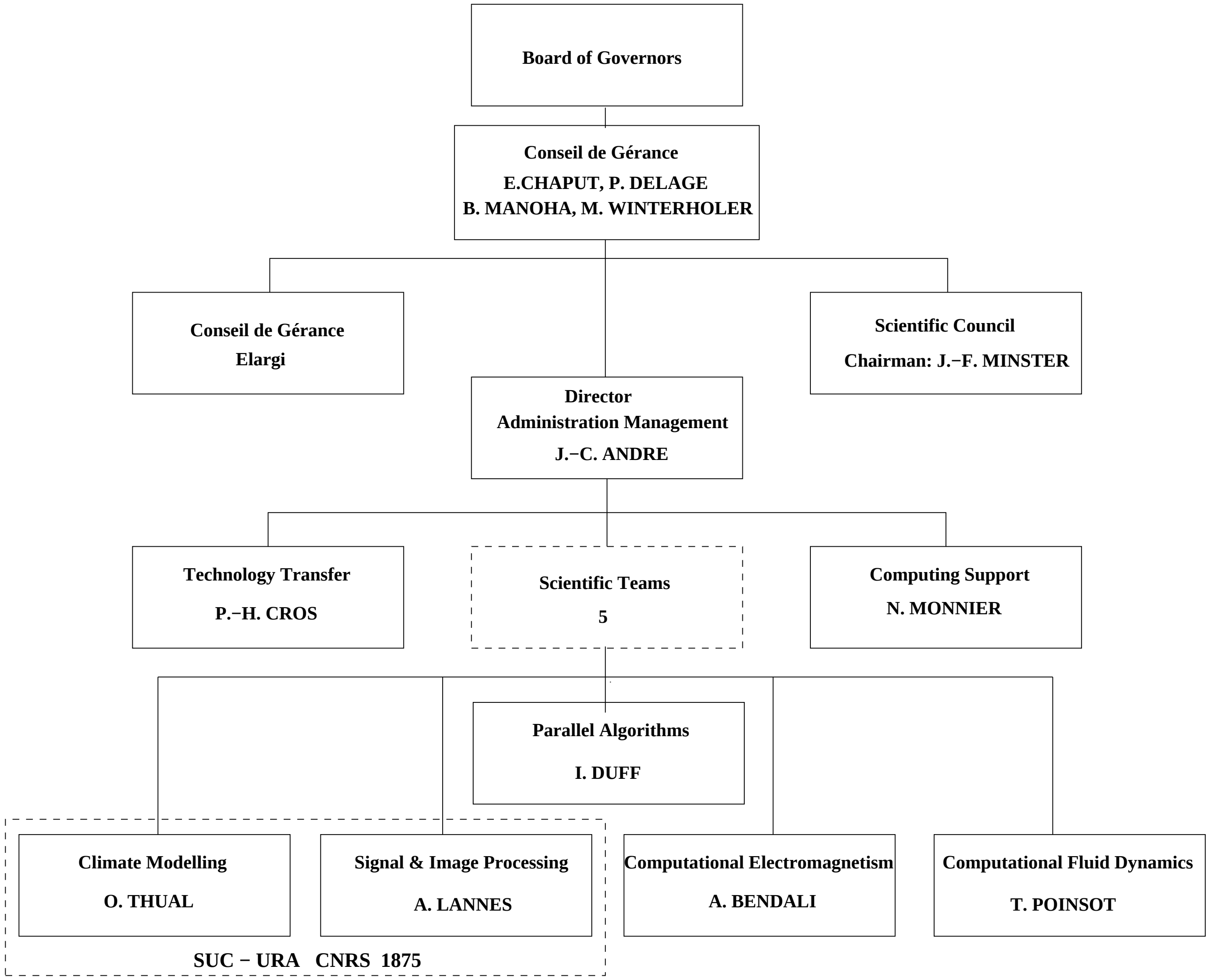
As a ”Société Civile” CERFACS is governed by two bodies. Firstly, the ”Conseil de Gérance”, composed of only 4 managers (in French, ”Gérants”) nominated by the 4 shareholders (see table i), follows quite closely the CERFACS activities and the financial aspects. It met 8 times during the period (18 April 2000, 11 July 2000, 8 September 2000, 5 December 2000, 6 February 2001, 29 June 2001, 18 September 2001 and 6 November 2001). Secondly the Board of Governors (in French ”Assemblée des Associés”), composed of representatives of CERFACS shareholders and of 3 invited personalities, including the Chairman of the Scientific Council. It met 4 times during the period (14 January 2000, 21 September 2000, 16 January 2001 and 28 September 2001).

CERFACS Scientific Council met for the fourth and fifth times, on 9 June 2000 and June 1st 2001, under the chairmanship of Prof. Jean-François MINSTER.

The general organization of CERFACS is depicted in the CERFACS chart, where the two support groups (Administration and Computing) are shown together with the other teams.

EUROPEAN AERONAUTIC DEFENCE AND SPACE COMPANY (EADS)	22 %
CENTRE NATIONAL D’ÉTUDES SPATIALES (CNES)	26 %
ÉLECTRICITÉ DE FRANCE (SYNERGIE, DÉVELOPPEMENT, SERVICES)	26 %
MÉTÉO-FRANCE	26 %

Table i: Table of Société Civile Shareholders.



CERFACS chart as of Dec. 31, 2001

CERFACS Staff

The staff of the scientific teams and of the computing support group, consisting of, on December 31, 2001, a total of 114 scientists and technical staff (8 project and group leaders, 19 senior researchers, 20 post-doctoral fellows, 35 PhD students, 22 engineers and 4 technicians, and 6 long-duration visitors of various origins) is shown in Tables ii to ix.

NAME	POSITION	PERIOD
DUFF	Project Leader	1988/11
CHATELIN	Group leader	1988/09
FRAYSSE	Senior	1994/11-2001/08
GIRAUD	Senior	1993/10
DALLAKYAN	Post Doc	1998/12-2000/09
LEGER	Post Doc	1999/03-2000/02
MESKAUSKAS	Post Doc	2000/03
PLANTIE	Post Doc	2000/04-2001/08
ROJAS	Post Doc	1999/11-2001/11
TRAVIESAS	Post Doc Ph.D student	2000/10 1997/10-2000/09
BOURAS	Ph.D student	2000/02-2000/09
CARPENTIERI	Ph.D student	1998/10-2001/12
LANGOU	Ph.D student	1999/10
MARTIN	Ph.D student	2001/10
ORBAN	Ph.D student	1997/10
RIOUAL	Ph.D student	1999/01
VOEMEL	Ph.D student	1999/10
ZAOUI	Ph.D student	1997/10-2000/10
BOUSQUET	Student	2001/05-2001/07
DANIEL	Student	2001/05-2001/08
LEBLOND	Student	2000/03-2000/08
MANDRY	Student	2001/05-2001/07
VALENTIN	Student	2001/06-2001/08
YOUAN	Student	2000/03-2000/08
TSHIMANGA	Visitor	2001/04-2001/08

Table ii: List of members of the PARALLEL ALGORITHMS project.

NAME	POSITION	PERIOD
LANNES	Project Leader	1994/01
PICARD	Ph.D student	2001/10
ANTERRIEU	CNRS	1993/07
RAMILLIEN	CNRS	2001/02

Table iii: List of members of the SIGNAL & IMAGE PROCESSING project.

NAME	POSITION	PERIOD
POINSOT	Project Leader	1992/09
CHEVALIER	Senior	1999/11
CUENOT	Senior	1996/10
DARRACQ	Senior	1999/04
DUCROS	Senior	1998/02-2001/07
JOUHAUD	Senior Post Doc	2001/10 2000/03-2001/08
KOURTA	Senior	1987/10-2001/06
MONTAGNAC	Senior Post Doc	2000/11 1999/11-2000/11
NICOUD	Senior	1995/11-2001/08
SCHONFELD	Senior	1993/12-2001/07
BENKENIDA	Post Doc	2000/01-2001/01
ESCRIVA	Post Doc	2001/11
GICQUEL	Post Doc	2001/05
GRONDIN	Post Doc	2000/03
JIMENEZ	Post Doc	1999/12-2001/04
MARQUEZ	Post Doc	1999/12-2000/11
PAOLI	Post Doc	2001/04
PUIGT	Post Doc	2001/10
STIRIBA	Post Doc	2000/10-2001/10
BENOIT	Ph.D student Student	2001/10 2001/03-2001/08
BOHBOT	Ph.D student	1998/09
CARUELLE	Ph.D student	1997/07-2000/09
CORMIER	Ph.D student	1998/09-2000/09
DABIREAU	Ph.D student	1999/09
DELBOVE	Ph.D student Student	2001/10 2001/02-2001/09

Table iv: List of members of the COMPUTATIONAL FLUID DYNAMICS project (1/2).

KAUFMANN	Ph.D student Student	2000/09 2000/03-2000/09
KOZUCH	Ph.D student	1998/09
LAPORTE	Ph.D student	1998/09-2001/12
LARTIGUE	Ph.D student Student	2000/10 2000/03-2000/06
LEGIER	Ph.D student	1999/01-2001/10
MASSOL	Ph.D student	2000/10
MOET	Ph.D student	1999/12
MOSSA	Ph.D student Student	2001/10 2001/03-2001/07
PRIERE	Ph.D student Student	2001/10 2001/03-2001/08
SCHLUTER	Ph.D student	1997/09-2000/09
SELLE	Ph.D student	2000/09
SOULERES	Ph.D student	1999/10
TRUFFIN	Ph.D student Student	2001/09 2001/02-2001/07
BUIS	Engineer	2000/08
CHAMPAGNEUX	Engineer Research	1997/11
JONVILLE	Engineer	2000/03-2000/09
MARTIN	Engineer	2000/10
PASCAL-JENNY	Engineer	2001/03
PIRAS	Engineer	2001/03
SOMMERER	Engineer	2000/10
STRUIJS	Engineer	1999/02-2000/08
BOHM	Student	2001/04-2001/08
CADENE	Student	2000/04-2000/07
COUSIN	Student	2001/02-2001/08
FIALA	Student	2001/02-2001/07
GARNIER	Student	2000/03-2000/08
LE SAINT	Student	2000/06-2000/08
PADEY	Student	2001/03-2001/08
PASUTO	Student	2001/03-2001/08
RAFFARD	Student	2001/03-2001/09
ROCHE	Student	2000/07-2000/09
SCHMITT	Student	2001/03-2001/07
WINTREBERG	Student	2000/03-2000/08
MULLER	Visitor	1997/11
NICOUD	Visitor	2001/10
RIZZI	Visitor	1987/10
RUDGYARD	Visitor	1995/04-2001/04

List of members of the COMPUTATIONAL FLUID DYNAMICS project (2/2).

NAME	POSITION	PERIOD
THUAL	Project Leader	1991/09
PIACENTINI	Research Engineer	1996/10
VALCKE	Research Engineer	1997/02
ROGEL	Senior	1998/10
TERRAY	Senior	1992/10
WEAVER	Senior	1999/11
DELON	Post Doc	2000/10
MACHU	Post Doc	2000/11
CASSOU	Ph.D student	1998/02-2001/06
CIBOT	Ph.D student	2001/08
DREVILLON	Ph.D student	1998/09
JOUZEAU	Ph.D student	2001/10
MASSART	Ph.D student	1999/11
RICCI	Ph.D student	2001/01
VIDARD	Ph.D student	1998/12-2001/11
DECLAT	Engineer Research Engineer	2001/08 1999/11-2001/04
GUEVARA	Engineer	2000/08-2001/07
LAGARDE	Engineer	2000/05-2000/06
MAISONNAVE	Engineer Research Engineer	2000/12 1999/02
MOREL	Engineer Research	2000/03
AUFFRAY	Student	2000/06-2000/08
BESSIERES	Student	2001/04-2001/07
CAILLEAU	Student	2000/02-2000/06
CAUBEL	Student	2001/03-2001/09
CREPIN	Student	2001/01-2001/06
CREVOISIER	Student	2001/07-2001/09
ESTIVALS	Student	2000/04-2000/09
KAMIL	Student	2001/03-2001/07
LACOSTE	Student	2000/06-2000/08
MONNERIE	Student	2001/02-2001/06
ROMAN	Student	2000/04-2000/06

Table v: List of members of the CLIMATE MODELLING & GLOBAL CHANGE project.

NAME	POSITION	PERIOD
MONNIER	Project Leader	1996/12
D’AST	Engineer	1996/10
LAPORTE	Engineer	1988/04
DEJEAN	Technician	1990/11
FLEURY	Technician	1999/10
PARISELLE	Student	2000/04-2000/06
RAYNAL	Student	2000/06-2000/09

Table vi: List of members of the COMPUTER SUPPORT group.

NAME	POSITION	PERIOD
FLEURY	Senior Post Doc	2001/03 1998/09-2000/08
SIEFRIDT	Senior	2000/01
TRANCHANT	Senior Post Doc	2001/07 1999/07-2001/07
LELLOUCHE	Post Doc	2000/09
REMY	Post Doc	2001/11
DRILLET	Engineer Research	1999/03
LOTRONG	Engineer	1999/04-2000/10
MAES	Engineer	2000/02-2000/06
PEREZ	Engineer	1999/07-2001/01
DOUAZAN	Student	2000/04-2000/06
GAUFFRE	Student	2001/04-2001/06
MARTIN	Student	2000/03-2000/09
GONDET	CNRS	2000/12

Table vii: List of members of the MERCATOR group.

NAME	POSITION	PERIOD
BENDALI	Project Leader	1996/01
FARES	Senior	1992/06
MILLOT	Senior	1995/11
BARTOLI	Engineer Research Ph.D student	2000/02 1997/12-2000/01
BOUBENDIR	Ph.D.student	1997/01
CANOUET	Student	2000/03-2000/07
LABOURDETTE	Student	2001/06-2001/08
LANGLOIS	Student	2001/06-2001/08
LIGNERES	Student	2000/06-2000/07
TAILLANDIER	Student	2001/05-2001/08
COLLINO	Visitor	1994/04

Table viii: List of members of the COMPUTATIONAL ELECTROMAGNETISM project.

NAME	POSITION	PERIOD
CROS	Project leader	1997/04
BAUBE	Charge mission	1998/09-2001/07
GRES	Charge mission	2000/09-2001/08
BARDY	Technician	2001/02-2001/09
BOUREBABA	Technician	2000/03-2001/12
JONVILLE	Engineer	2000/10
LE GOULVEN	Engineer Student	2001/09-2001/09 2001/04-2001/08
MOINAT	Engineer Research	2000/03

Table ix: List of members of the TECHNOLOGY TRANSFER group.

CERFACS Wide-Interest Seminars

Pierre Sagaut (ONERA, Châtillon) : *Unsteady simulation of turbulent flow: from LES to multiresolution algorithms.* (Feb. 3, 2000)

Charles Meneveau (Johns Hopkins University, Baltimore): *A scale-dependent dynamic model for LES of turbulence.* (Feb. 11, 2000)

Stéphane Lanteri (INRIA, Sophia-Antipolis): *Parallel multigrid algorithms on unstructured mesh and applications in CFD.* (Apr. 6, 2000)

C. Despre and J.L. Gobert (ONERA): *Flow active control activities at ONERA.* (May 4, 2000)

Alexis Coppalle (CORIA, Rouen): *Subgrid modelling of point source dispersion in the atmosphere.* (Jun. 8, 2000)

C. Roberto Mechoso (Department of Atmospheric Sciences, University of California, Los Angeles, USA): *The El Niño-Southern oscillation model simulations and exploration into the underlying coupled atmosphere-ocean processes* (Oct. 23, 2000)

G. Montseny (LAAS, Toulouse): *Diffusive representation: bases and applications.* (February 27, 2001)

John J.H. Miller (Mathematics Department, Trinity College, Dublin, Ireland): *Robust layer-resolving methods for the numerical solution of laminar problems in fluid mechanics.* (March 15, 2001)

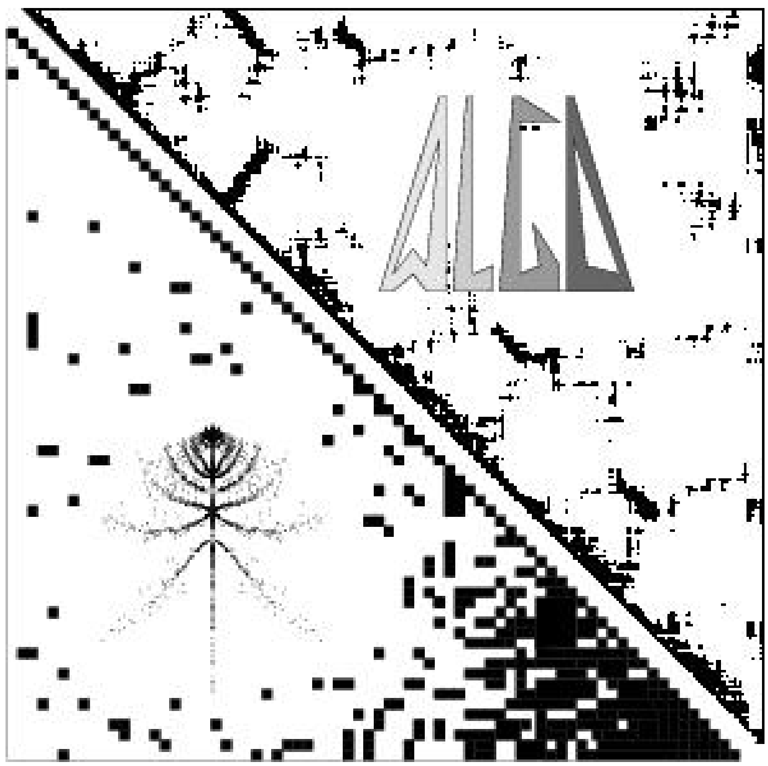
Patrick Gillieron (Direction de la Recherche, Renault SA): *The control of the flows in the car.* (April 26, 2001)

Marc Thiriet (Laboratoire d'analyse numérique, Université Pierre et Marie Curie et INRIA): *Biofluid mechanics and its role in physiology, in pathophysiology and in cybermedecine.* (May 31, 2001)

Thierry Georjon (Direction de la Recherche et de l'Innovation Automobile, PSA - Automobiles Peugeot Citroën): *CFD Computations for modern piston engines.* (November 21, 2001)

1

Parallel Algorithms Project



1 Introduction (I. S. Duff)

The research programme conducted by the Parallel Algorithms Project combines the excitement of basic research discoveries with their use in the solution of large-scale problems in science and engineering in academic research, commerce, and industry. We are concerned both with underlying mathematical and computational science research, the development of new techniques and algorithms, and their implementation on a range of high performance computing platforms.

The description of our activities is presented in several subsections, but this is only to give a structure to the report rather than to indicate any compartmentalization in the work of the Project. Indeed one of the strengths of the Parallel Algorithms Project is that members of the Team work very much in consultation with each other so that there is considerable overlap and cross-fertilization between the areas demarcated in the subsequent pages. This cross-fertilization extends to formal and informal collaboration with other teams at CERFACS, the shareholders of CERFACS, and research groups and end users elsewhere. In fact, it is very interesting to me how much the research directions of the Project are increasingly influenced by problems from the partners.

Members of the Team very much play their full part in the wider academic and research community. They are involved in Programme Committees for major conferences, are editors and referees for frontline journals, and are involved in research and evaluation committees. These activities both help CERFACS to contribute to the scientific life of France, Europe and the world while at the same time maintaining the visibility of CERFACS within these communities. Some measure of the visibility of CERFACS can be found from the statistics of accesses to the Algo Web pages at CERFACS where we have recorded more than 100,000 hits during the reporting period. On our publication pages alone, people have requested no fewer than 233 different reports in 2001.

Our main approach in the direct solution of sparse equations continues to be the multifrontal technique originally pioneered at Harwell in the early 1980s. During this last period we have further developed the MUMPS package in conjunction with our colleagues at ENSEEIHT and elsewhere. The code is now very robust and has been downloaded by over 150 researchers from the MUMPS website. Extensive comparisons, conducted with the support of funding from the France-Berkeley Fund have shown that the performance of MUMPS is on a par or better than any similar code from the United States. The MUMPS code has been used extensively within domain decomposition software both at CERFACS and in the DDM code at Parallab in Bergen. It has also been evaluated positively for use by Dassault-Aviation. As I write this, preparations are well underway for a significant new release that will include better integrated ordering options and more sophisticated scheduling strategies. Recent work has included an in-depth study of the MPI send/receive mechanism and investigation of techniques to make the MUMPS code robust in the presence of different implementations of MPI. We have also explored the dynamic scheduling strategy to avoid a severe overestimate of storage requirements. The MUMPS Project is also responsible for some secondary or spin-off research, an example being the work on incremental norm estimation which should prove to be very useful in the context of rank revealing factorizations.

At the level of international efforts for standards in numerical linear algebra, we have been very involved in the development of a new standard for the Basic Linear Algebra Subprograms (or BLAS) coordinated through the BLAST Technical Forum. The report on the standard will appear as a special issue of the journal “High Performance Computing Applications”. We have been the developer for the Fortran 95 instantiation of the Sparse BLAS from within this project, and the resulting software is available on the CERFACS web and has been downloaded nearly 150 times. We have submitted papers both on the Fortran 95 implementation of the sparse BLAS and on the design of the sparse BLAS to ACM Trans Math Softw.

Although iterative methods remove many of the bottlenecks of direct approaches, particularly regarding memory, it is now well established that they can only be used in the solution of really challenging problems if the system is preconditioned to create a new system more amenable to the iterative solver. During this last period we have continued our work on developing such preconditioners, including two-level schemes that have been used successfully in both dense electromagnetics applications and in domain decomposition methods for solving partial differential equations in device modelling. Work has continued on the use of the MUMPS direct solver as a preconditioner within a domain decomposition scheme and the resulting algorithm and code have been used with success in the solution of problems from drift diffusion in semiconductor device modelling in a joint collaboration with INRIA. On a more theoretical but very practical track, the loss of orthogonality when performing a QR factorization using modified Gram Schmidt has been extensively analysed. The GMRES and FGMRES codes that were discussed in a previous activity report are available through the CERFACS web and have attracted over 600 downloads, some from important establishments including partners of CERFACS. Our use of sparse preconditioning techniques within a fast multipole code from our partner EADS has resulted in the efficient solution of dense problems in over 1 million unknowns from highly challenging models of an Airbus aircraft.

The main area of interest for the Qualitative Computing Group concerns a deep understanding of the influence of finite-precision computation on complex scientific numerical applications. One of the major areas studied has been that of inner-outer iteration, two principal and important applications being the use of Krylov solvers (inner iteration) within an eigensystem calculation (outer iteration), and the use of an iterative solver on the Schur complement in a domain decomposition context (outer iteration) where, at each iteration, a subproblem or preconditioner might require a system solution (inner iteration). It was shown experimentally that, almost counter-intuitively, it is possible to relax the accuracy of the operator or inner iteration in a controlled way without affecting overall convergence. A project with our partner EDF has involved moving this work from a research environment to one of their major industrial codes. The Group has also collaborated closely with CNES in the context of the Jason project, principally studying the solution of integer least-squares problems. The second area of important research has been on Inexact Computing, which is based on the theory of homotopic perturbations. A global theory has been developed which allows one to understand why numerical artifacts occur when pseudospectra are computed in finite precision. Thirdly, on a more fundamental level, algorithms and theory have been developed for the use of hypercomplex numbers which can be a more natural way of representing actual physical processes. Other work includes more robust termination criteria for Arnoldi-based methods, the development of more robust eigensolvers using hybrid algorithms in a joint effort with INRIA, and work on the solution of Schrödinger equations and triple-deck boundary layer problems.

Current areas of research include major work on an approach for solving ill-posed problems where a regularized solution is obtained after the solution of a subsidiary eigenproblem. Recent work includes the development of efficient preconditioners for the eigenproblem and the use of the algorithm and software in medical tomography and image restoration applications. On the latter application, extensions which respect nonnegativity constraints are being developed. A major research kernel in optimization is the primal-dual trust-region interior point method. This has been extensively analysed and an approach defined that has componentwise fast asymptotic convergence. The work has been extended to the case of parametrized variants of Newton’s method. An important requirement of the international community in the development and use of optimization techniques is the existence of a versatile testing environment and set of test examples. Work has been conducted at CERFACS into the expansion and reorganization of the well known and respected CUTE package to produce the forthcoming CUTEr (r for revisited) package. The work on the use of large scale optimization and the use of state-of-the-art techniques in meteorological data assimilation, in conjunction with our shareholders from Météo-France, the PALM and MERCATOR Team has continued.

The Parallel Algorithms Project is heavily involved in the Advanced Training aspects of CERFACS' mission. We ran internal training courses for new recruits to all Projects at CERFACS to give them a basic understanding of high performance computing and numerical libraries. This course was also open to the shareholders of CERFACS. Following a specific request of CNES through its CCT "calcul scientifique" we organized a three day training course entitled "Outils de programmation efficace et robuste pour le logiciel scientifique" targeted at CNES engineers. We are also involved in training through the "stagiaire" system and feel that this is extremely useful to young scientists and engineers in both their training and their career choice. It can also help us to focus our research efforts and thus can benefit the work of the Team. A win-win situation. Members of the Team have assisted in many lecture courses at other centres, including ENSICA, INPT, Météo, Toulouse 1 and UPS. During this past year, both Valérie Frayssé and Luc Giraud successfully defended their habilitation theses (HDR). Valérie summed up her many activities under the umbrella of the power of backward error analysis and Luc described with great clarity his many contributions to the iterative solution of linear equations. Four other Team members successfully defended their PhD theses. These were Elisabeth Traviesas with a thesis on matrix spectra (and pseudo-spectra), Amina Bouras on the convergence of embedded Krylov solvers in eigensystem or linear system calculation and Ahmed Zaoui on his contributions to eigensolvers and hypercomplex computation, and Dominique Orban on "Interior-point methods for nonlinear programming", a cotutelle thesis between INPT and the University of Namur in Belgium.

We run a regular series of "internal seminars" that are primarily for Team members to learn about each other's work and are also a good forum for young researchers to hone their presentational skills. We run a series of seminars from external people who are visiting the Team that attract a wider audience and this has benefited greatly during this period through an extensive visitor programme. Indeed, our list of visitors is a veritable who's who of numerical analysts, including many distinguished scientists from Europe and the United States. We have included a list of the visitors at the end of this introduction. John Gilbert from Xerox Parc in California was one of our longer staying visitors 2001 and was involved in many interactions as witnessed in Section 2.10 of this report. As always, it was a pleasure to host Gene Golub for a week when he came for the Anniversary meeting. He is particularly helpful and inspiring to our younger researchers with his enthusiasm and interest.

The Parallel Algorithm Team hosted two significant international meetings during the reporting period. One was the Workshop on inner-outer iterations organized at the request of three of our shareholders and held at CERFACS in September 2000. Gene Golub gave the keynote address, and there were invited presentations from Andreas Griewank and Sven Hammarling. The program was completed by several contributions from CERFACS researchers and the shareholders' representatives. The Parallel Algorithm Project also organized and hosted a Sparse Day meeting held in June 2001. We were able to take advantage of our visitors to design a very interesting programme that attracted 38 participants from not only outside Toulouse but also outside France. Some researchers from the partners of CERFACS also participated. The speakers and programme are described further in Section 6.2 of this report. We were also strongly involved in the CERFACS Anniversary meeting in October 2001. Gene Golub from Stanford University and Gérard Meurant from CEA gave invited talks and two PhD students, Bruno Carpentieri and Jean-Christophe Rioual had the chance to present their work to a distinguished audience.

I am very pleased to report that, over the reporting period, we have continued our involvement in joint research projects with shareholders and other CERFACS' partners, and with other teams at CERFACS. We are involved in research committees such as the CCT of CNES. We have successfully completed a major project on orbitography with CNES. We have two projects with EADS on preconditioning techniques in electromagnetics and a sponsored PhD on the study of iterative solution techniques for multiple right-hand sides. We are involved in the training programme for the Mastere, organized by ENM at Météo-France. One of the two active collaborations with INRIA has been successfully finished by the defence of a PhD and the other on domain decomposition will hopefully yield another thesis in the spring of 2002. We are involved in a contract with EDF to utilize our findings on inner-outer iteration within their Aster code. We help the other Projects at CERFACS on almost a daily basis, for example in giving advice to CFD and TSI on OpenMP, but sometimes collaborate on a more substantial level as for instance in the PALM project or on the optimal use of our public domain linear solvers with EMC. The work on the performance evaluation on clusters was also of great interest for both other CERFACS Projects and shareholders (in particular CNES and Météo-France).

Visitors to Parallel Algorithm Project in 2000-2001

In alphabetical order, our visitors during the years 2000 and 2001 included: MARIO AHUES (St Etienne University), FILOMENA DIAS D'ALMEIDA (Porto University), NERSES ANANIKYAN (Armenia), NECULAI ANDREI (Research Institute for Informatics, Roumania), MARIO ARIOLI (RAL, UK), CHARLES AUDET (Rice University), ROBERT BEAUWENS (ULB, Brussels University), MATTHEUS BOLLHÖFER (Berlin), TONY CHAN (UCLA), EDMOND CHOW (Lawrence Livermore National Laboratory), JOHN DENNIS (Rice University, Houston, Texas), QUANG V. DINH (Dassault Aviation), JAQUELINE FLECKINGER (Toulouse I), MICHAEL FRIEDLANDER (Stanford University), ANDREAS FROMMER (Wuppertal University), JOHN GILBERT (Xerox Parc, California, USA), GENE GOLUB (Stanford University), NICK GOULD (Rutherford Appleton Laboratory), ANDREAS GRIEWANK (Dresden University), LAURA GRIGORI (INRIA-LORIA, Nancy), ANDREAS GROTHEY (Edinburgh University), GUNDOLF HAASE (Institute for Computational Mathematics, Austria), ELDAD HABER (University of British Columbia, Canada), SVEN HAMMARLING (NAG), PER CHRISTIAN HANSEN (Technical University of Denmark , Denmark), JOHN HAWS (Raleigh), GARY HOWELL (Florida Institute of Technology), ABDERRAZAK ILAHI (Tunisia), ERRICOS KONTOGHIORGHES (Neuchatel University), JACKO KOSTER (Parallab, Bergen), JEAN-YVES L'EXCELLENT (INRIA-ENSL, Lyon), MARTIN VAN GIJZEN (TNO, The Netherlands), ERRICOS KONTOGHIORGHES (University of Neuchatel, Switzerland), ALAIN LARGILLIER (St Etienne University), RASMUS LARSEN (Stanford University), SVEN LEYFFER (Dundee University), DANIEL LOGHIN (University of Oxford, UK), MARDOCHEE MAGOLU (ULB, Brussels University), LUIZ CARVALHO (IME-UERJ, Rio de Janeiro, Brazil), OSNI MARQUES (NERSC, Berkeley), EMERIC MARTIN (IRISA, Rennes), GÉRARD MEURANT (CEA), JOHN MILLER (Dublin University, Dublin), SHANE MULLIGAN (Dublin University, Dublin), JORGE NOCEDAL (Northwestern University), BERESFORD PARLETT (UC Berkeley), BERNARD PHILIPPE (IRISA, Rennes), MIRO ROZLOŽNÍK (Academy of Sciences of the Czech Republic, Prague), YOUSEF SAAD (Minneapolis University), ANNICK SARTENAER (FUNDP, Namur), JENNIFER SCOTT (RAL, UK), DAN SORENSEN (Rice University, Houston, USA), MASHA SOSONKINA (Minnesota University), PIERRE SPITÉRI (ENSEEIHT), TROND STEIHAUG (University of Bergen, Norway), GUILLAUME SYLVAND (INRIA-CERMICS, Nice), DANIEL SZYLD (Temple University), PATRICK LE TALLEC (Ecole polytechnique), PHILIPPE TOINT (FUNDP, Namur), JEAN TSHIMANGA (University of Namur, Belgium), MIROSLAV TŮMA (Academy of Sciences of the Czech Republic, Prague), and STEVE WRIGHT (Argonne National Laboratory, Illinois, USA).

2 Dense and Sparse Matrix Computations

2.1 Updates to the Rutherford-Boeing sparse matrix collection (I. S. Duff and D. Orban)

The Rutherford-Boeing sparse matrix collection [1] extends its predecessor, the Harwell-Boeing sparse matrix collection in a number of respects, including the representation of the problems in the Rutherford-Boeing sparse matrix format.

With asssistance from a stagiaire, Pierre Valentin, all the data from the Harwell-Boeing sparse matrix collection have been converted into Rutherford-Boeing format and are documenting this data and incorporating other relevant data. Ultimately, the collection will consist of a comprehensive archive of test matrices, stored in Rutherford-Boeing format, along with the relevant related data, such as right-hand sides, solution estimates, orderings, etc.

In order to leave as much latitude as possible and to allow older solvers to solve problems from the Rutherford-Boeing collection without modification, a number of conversion tools, to and from the Matrix Market format, the Matlab format and the Harwell-Boeing format, will also be provided. Tools to plot or view on the screen the sparsity pattern of the matrices have been designed.

[1] I. S. Duff, R. Grimes, and J. G. Lewis, (1997), The Rutherford-Boeing Sparse Matrix Collection, Technical Report RAL-TR-97-031, Rutherford Appleton Laboratory, Oxon OX11 0QX, UK.

2.2 Rank-revealing and incremental norm estimation (I. S. Duff and C. Vömel)

An incremental approach to 2-norm estimation for triangular matrices has been developed which is important for the detection of ill-conditioning, one of the basic problems arising in the numerical solution of linear systems. Applications of the scheme include the calculation of forward error bounds based on the condition number, robust pivot selection criteria and rank-revealing factorizations, in particular, when *inverse* factors arise in the factorization. In [ALG53], such a scheme is introduces, it is applicable for both dense and sparse matrices which can arise for example from a QR, a Cholesky or a LU factorization. If the explicit inverse of a triangular factor is available, as in the case of an implicit version of the LU factorization, this results can be related to incremental condition estimation (ICE) presented in [2]. Incremental norm estimation (INE) extends directly from the dense to the sparse case without needing the modifications that are necessary for the sparse version of ICE. INE can be applied to complement ICE, since the product of the two estimates gives an estimate for the matrix condition number. Furthermore, when applied to matrix inverses, INE can be used as the basis of a rank-revealing factorization. The quality of this results on standard test cases is consistently high and demonstrates the general reliability of the scheme. A revised version of [ALG53] which contains also a theoretical analysis of this scheme will appear in BIT.

[2] C. H. Bischof, (1990), Incremental Condition Estimation, **11**, 312–322.

2.3 The sparse BLAS (I. S. Duff, M. A. Heroux and R. Pozo)

The effort by the BLAS Technical Forum to produce an updated version of the Basic Linear Algebra Subprograms has continued for many years and it was with some relief that everything came to a conclusion in 2001. The standard itself [3] should be appearing as two parts in The International Journal of High Performance Computing Applications and an article on the standard [4] has been submitted to ACM Transactions on Mathematical Software. Major extensions to the earlier BLAS include added functionality, mixed precision BLAS, and sparse BLAS.

We discuss the interface design for the Sparse Basic Linear Algebra Subprograms (BLAS), the kernels in the recent standard from the BLAS Technical Forum that are concerned with unstructured sparse matrices. The motivation for such a standard is to encourage portable programming while allowing for library-specific optimizations. In particular, this interface can shield one from concern over the specific storage scheme for the sparse matrix. This design makes it easy to add further functionality to the sparse BLAS in the future.

In the report [ALG56], the use of the Sparse BLAS with examples in the three supported programming languages, Fortran 95, Fortran 77, and C is illustrated. A Fortran 95 implementation of the sparse BLAS is described in the report [ALG55].

[3] BLAS Technical Forum Standard, *The International Journal of High Performance Computing Applications*, **15**, (2001).

[4] S. Blackford, J. Demmel, J. Dongarra, I. Duff, S. Hammarling, G. Henry, M. Heroux, L. Kaufman, A. Lumsdaine, A. Petitet, R. Pozo, K. Remington, and R. C. Whaley, (2002), An Updated Set of Basic Linear Algebra Subprograms (BLAS), *Submitted to TOMS*.

2.4 Development of kernels for sparse numerical linear algebra (I. S. Duff and C. Vömel)

The Basic Linear Algebra Subprograms for sparse matrices, the Sparse BLAS, are defined by the BLAS Technical Forum and consist of a set of kernels providing basic operations for sparse matrices and vectors. A principal goal of the Sparse BLAS standard is to aid in the development of iterative solvers for large sparse linear systems by specifying, on the one hand, interfaces for a high-level description of vector and matrix operations for the algorithm developer and, on the other hand, leaving enough freedom for vendors to provide the most efficient implementation of the underlying algorithms for their specific architectures.

The Sparse BLAS standard defines interfaces and bindings for the three target languages: C, Fortran 77 and Fortran 95. Our Fortran 95 implementation is intended as a reference model for the Sparse BLAS. The design is based on the idea of matrix handles so that the user need not be concerned with the details of the underlying storage schemes. It is envisaged that these kernels will be widely used in the solution of sparse equations by iterative methods. Our work is documented in [ALG54], [ALG55] and [ALG57]. The software together with its description [ALG55] has been sumbitted for publication as algorithm to ACM Trans. Math. Softw.

2.5 Analysis and comparison of distributed memory sparse solvers (P. R. Amestoy, I. S. Duff, J.-Y. L'Excellent and X. Li)

This work was awarded a grant from the France Berkeley fund for teams at ENSEEIHT-IRIT and CERFACS to collaborate with NERSC at Lawrence Berkeley National Laboratory on distributed sparse solvers. This grant started in January 1999 and was extended until May 2000, enabling Duff to visit Berkeley twice for discussions with Li and Amestoy (who was on sabbatical leave for the year).

The main result was an in depth analysis comparing the merits of a supernodal solver (SuperLU) [5] with MUMPS (see §2.9). This showed broadly that MUMPS generally outperformed SuperLU although the latter showed somewhat better scalability and was competitive on a large number of processors. Many ideas for improvements to both codes were generated during this investigation and both will be enhanced as a result.

The main report to the France-Berkeley Fund [ALG37] was accepted and a shorter version has been submitted to the ACM Transactions on Mathematical Software [ALG36]. The work has been presented at the SIAM Parallel Processing Conference in March 2001 [ALG38].

[5] J. W. Demmel, J. R. Gilbert, and X. S. Li, (1999), An asynchronous parallel supernodal algorithm for sparse Gaussian elimination, *SIAM J. Matrix Analysis and Applications*, **20**, 915–952.

2.6 Study of the effect of matrix orderings on MUMPS and a code from Argonne National Laboratory (I. S. Duff, S. Leblond and H. Tufo)

In this work, two different solvers for the direct solution of sparse equations on multiprocessor machines were examined. This investigation was conducted by a stagiaire Simon Leblond [ALG68], primarily under the guidance of Duff.

The first part of the investigation deals with the MUMPS multifrontal method for an LU factorization computation. The phases of this approach were described and results on a few large tests made on the supercomputer COMPAQ IXIA were analysed. The main study concerned the effect of the ordering algorithm on the analysis and the performance of the code when an ordering was input by the user. Some suggestions for future improvements to MUMPS are presented.

The second part concerned an approach using an $X^T X$ factorization developed by Tufo and used in a massively parallel environment to obtain factors of the inverse of a large sparse matrix [6]. The findings showed that the current version of the code was rather slow in the factorization phase but very quick for the backsolves. This had been the design intention of Tufo who, partly as a result of this study, is tuning the factorization part of his algorithm.

[6] H. M. Tufo and P. F. Fischer, (2001), Fast parallel direct solvers for coarse grid problems, *J. Parallel and Distributed Computing*, **61**, 151–177.

2.7 Use of orderings for large entries on the diagonal (I. S. Duff and J. Koster)

Although the original work of the author on this set of algorithms for permuting large entries to the diagonal was completed some time ago and the resulting code `MC64` was placed in the HSL mathematical software library in 2000, the most recent journal paper on this work appeared in 2001 [ALG14] and the algorithm and code has been used extensively over this past year by many people in the solution of large sparse systems of equations and in preconditioning techniques for sparse matrices.

In many cases, the routine can be very helpful when factorizing very unsymmetric systems as has been the experience with `MA41` and `MUMPS` [ALG2]. It has also proven almost a necessary preprocessor for algorithms that use static pivoting strategies as in `SuperLU` [9]. More recently, Gupta [8] has reaffirmed the importance of such a permutation in his work on sparse direct solvers and Benzi and his colleagues [7] have found that it is absolutely necessary to use `MC64` if preconditioning techniques are to be successful on highly indefinite and nonsymmetric matrices.

[7] M. Benzi, J. C. Haws, and M. Tůma, (2000), Preconditioning highly indefinite and nonsymmetric matrices, **22**, 1333–1353.

[8] A. Gupta, (2001), Improved symbolic and numerical factorization algorithms for unsymmetric sparse matrices, Tech. Rep. RC 22137 (99131), IBM T.J. Watson Research Center, Yorktown Heights, NY.

[9] X. S. Li and J. W. Demmel, (1999), A Scalable Sparse Direct Solver using static pivoting, In *Proceedings of the Ninth SIAM Conference on Parallel Processing for Scientific Computing*, San Antonio, Texas.

2.8 Candidate-based dynamic scheduling for a distributed direct linear solver (P. R. Amestoy, I. S. Duff and C. Vömel)

The asynchronous distributed memory multifrontal solver MUMPS ([ALG2, ALG37]) exploits three types of parallelism when a sparse matrix is factorized. A first natural source of parallelism is established by independent branches of the assembly tree. Furthermore, tree nodes with a large enough contribution block can be updated in parallel by splitting the update between several slaves of the master that is factorizing the block of fully summed variables. Finally, the root node can be treated in parallel if it is big enough.

While the *master* processor of each node in the tree (i.e. the one that is responsible for the factorization of the block of fully summed variables) is chosen during the analysis phase, the *slaves* for the parallel update of large contribution blocks are only chosen during the factorization phase. This dynamic task scheduling takes place in order to balance the work load of the processors at run-time. Problems arise from offering too much freedom to the dynamic scheduling. If every processor is a candidate for a slave then, on each processor, enough workspace has to be reserved during the analysis phase for the corresponding computational tasks. However, during the factorization, typically not all processors are actually needed as slaves (and, on a large number of processors, only a very few are needed), so the prediction of the required workspace will be overestimated. Thus the size of the problems that can be solved is reduced unnecessarily because of this difference between the prediction and allocation of memory in the analysis phase and the memory actually used during the factorization.

With the concept of *candidate processors* it is possible to address this issue. The concept originates in an algorithm presented in [10] and extends efficiently to MUMPS. For each node that requires slaves to be chosen dynamically during the factorization because of the size of its contribution block, a limited set of processors from which the slaves can be selected is introduced. While the master previously chose slaves from among all less loaded processors, the freedom of the dynamic scheduling can be reduced so that the slaves are only chosen from the candidates. This effectively allows one to exclude all non-candidates from the estimation of workspace during the analysis phase and leads to a more realistic prediction of workspace needed. Furthermore, the candidate concept allows one to better structure the computation since it is possible to explicitly restrict the choice of the slaves to a certain group of processors and enforce a 'subtree-to-subcube' mapping principle.

Preliminary tests with a prototype version have shown the benefits of the concept that is currently being integrated into a compact scheduling module for MUMPS. It unifies static and dynamic mapping while at the same time taking account of tree modifications by node amalgamation and splitting.

[10] A. Pothen and C. Sun, (1993), A Mapping Algorithm for Parallel Sparse Cholesky Factorization, **14(5)**, 1253–1257.

2.9 An analysis of MPI send/receive in the context of MUMPS (P. R. Amestoy, I. S. Duff, J. Y. L'Excellent and X. S. Li)

This work was developed from the research performed as part of the France-Berkeley project [ALG37] and is intimately associated with the tuning of the MUMPS and SuperLU sparse direct solvers on distributed memory computers using MPI for message passing.
The send and receive mechanisms of MPI are examined in detail and the question how to implement message passing robustly so that performance is not significantly affected by changes to the MPI system is addressed. The discussion of this is made within the context of two different parallel algorithms for sparse Gaussian elimination: a multifrontal solver (MUMPS), and a supernodal one (SuperLU). The performance of initial strategies based on simple MPI point-to-point communication primitives is very sensitive to the MPI system, particularly the way MPI buffers are used. Using more sophisticated non-blocking communication primitives improves the performance robustness and scalability, but at the cost of increased code complexity. The report [11] has been submitted to the journal Parallel Computing.

[11] P. R. Amestoy, I. S. Duff, J.-Y. L'Excellent, and X. S. Li, (2001), Impact of the Implementation of MPI Point-to-Point Communications on the Performance of Two General Sparse Solvers, Tech. Rep. RT/APO/01/4, ENSEEIHT-IRIT.

2.10 Structure prediction and symbolic factorization for partial pivoting (J. R. Gilbert, senior visitor)

The answers to several theoretical questions about nonzero structure and column dependencies in sparse LU factorization with partial pivoting could have consequences in the analysis phase of LU factorization codes. Laura Grigori, co-worker, is a graduate student at LORIA in Nancy.
A symbolic all-at-once lower bound for the structure of the column elimination tree has been recently described in a technical report [ALG59] submitted for publication. This lower bound applies to the case of so-called strong Hall matrices.
The proof of a symbolic lower bound result for the structure of L and U under partial pivoting for all nonsingular matrices has been given. This result was already known for the case of strong Hall matries. However, the general case is of interest because many nonsymmetric LU codes do not preprocess the matrix to block triangular form. The hope is that it will be possible to extend this work to get an exact lower bound; if this is done with an efficient way to implement it, it is planned to experiment it as an improvement to the current structure prediction in SuperLU.
An other goal is to extend the column tree result from a symbolic bound to an exact bound.

2.11 Weighted matching for symmetric indefinite factorization (J. R. Gilbert, senior visitor)

The objective here is to use weighted bipartite matching (as in Duff and Koster's MC64 code) to identify good static (or at least initial) pivoting orders for symmetric indefinite factorizations. Such orderings might also be useful for incomplete symmetric indefinite factorizations or for the iterative solution of symmetric indefinite systems.
A maximum weight matching may not be symmetric, even for a symmetric matrix. One may ask to what extent one can capture the elements of such a matching in small symmetric block pivots by permuting the matrix symmetrically. The answer turns out to depend on the cycle structure of the matching permutation.
The experiment started with the idea of first permuting the matrix symmetrically to have small diagonal blocks with large elements, then following this with another symmetric permutation that is chosen for

sparsity, then using this as input to `MA57`, a symmetric indefinite multifrontal factorization. The sparsity permutation, approximate minimum degree, is computed on the quotient graph by the diagonal blocks, in order not to break up the block pivots. It is planned to report on the results of these experiments during 2002.

2.12 Support theory for preconditioning (J. R. Gilbert, senior visitor)

Support graphs and support theory are a combinatorial approach to preconditioning sparse linear systems that date from the early 1990s but have recently seen some promising new developments. A survey lecture on the topic, covering both our work and others', was done at the Sparse Day at CERFACS in June, with the intention of getting more researchers interested in working on it. Trond Steihaug of the University of Bergen pointed out a connection to a spanning tree preconditioner for network problems that has been studied by Resende and others in the optimization community. The Sparse Day talk also led to a visit to Jean Roman's group at LABRI in Bordeaux: it is planned to collaborate on these and related ideas in the context of the block incomplete preconditioners that Roman's group is designing.

A workshop on combinatorial preconditioning, during which the sparse linear systems community can explore these and related problems, is on the way to be organised, perhaps at CERFACS.

2.13 Matlab toolboxes (J. R. Gilbert, senior visitor)

The Matlab mesh partitioning toolbox, which Shang-Hua Teng and Johm Gilbert wrote several years ago and which Tim Davis had most recently updated to run under version 5 of Matlab has been updated. The newly updated toolbox includes an interface to METIS and runs under Matlab 6. The updated toolbox is now available at http://www.cerfacs.fr/algor/Softs/MESHPART/index.html

With the collaboration of Gary Howell (of the Florida Institute of Technology, visiting CERFACS), successfull experiments with using f2c as an intermediary in connecting Fortran sparse matrix codes to Matlab has been made. A routine to read sparse matrices in Rutherford-Boeing format into Matlab has been developped. The routine is not yet comprehensive (it currently handles six of the R-B matrix types), but it demonstrates that using the new format with Matlab will be considerably simpler than using the older Harwell-Boeing format. Student Pierre Valentin helped a good deal with sample matrices from his summer work on the Rutherford-Boeing collection.

3 Iterative Methods and Preconditioning

3.1 Loss of orthogonality in the modified Gram-Schmidt algorithm (L. Giraud, S. Gratton and J. Langou)

During the past two years many efforts have been put on the study of the modified Gram-Schmidt algorithm. The modified Gram-Schmidt (MGS) algorithm is a well known orthogonalization method used in many linear algebra algorithms. For example, it is a fast way to compute a QR factorization. Although this method is widely used, some theoretical questions on its behaviour in finite precision arithmetic are still open.

On a computer, the modified Gram-Schmidt orthogonalization is applied to a matrix in finite-precision computation, this introduces errors that one wants to control. This subject has already been considered by Björck in 1963 [13], then continued by Björck and Paige in 1992 [12]. They give useful bounds on the orthogonality obtained in term of norms. Their results has been extended to provide bounds on singular values. The results obtained can be viewed in term of numerical rank. This fact enables to develop a reorthogonalization algorithm that gives impressive results in terms of speed. This algorithm is particulary efficient in an Arnoldi context. Experiments are still going on to control the quality of the obtained result in a more general framework.

It is well known that the set of computed vectors may lose orthogonality; however, it is experimentally observed that this set has full rank. In [ALG60], a theorem that gives a theoretical explanation of this phenomenon is given. This theorem applies to a large set of matrices. This is the set of not "too ill-conditioned" matrices. To complete this theorem, a 3×3 matrix, called *CERFACS*, is given, this matrix does not belong to this set but is indeed very close. On that matrix, MGS generates a numerically rank deficient set of vectors. This justifies the sharpness of the domain of validity of the theorem given. Finally, the combination of it with a well known result from Björck gives that two sweeps of MGS are indeed enough to get a matrix whose columns are orthogonal up to machine precision. We recover the famous sentence of W. Kahan [14] : "*twice is enough*."

[12] A. Björck and C. Paige, (January 1992), Loss and recapture of orthogonality in the modified Gram-Schmidt Algorithm, *SIAM J. Matrix Analysis and Applications*, **13**, 176–190.

[13] A. Björck, (1967), Solving linear least squares problems using Gram-Schmidt orthogonalization, *BIT*, **7**, 1–21.

[14] B. Parlett, (1980), *The symmetric eigenvalue problem*, Prentice Hall.

3.2 Robust preconditioning of dense problems from electromagnetics (B. Carpentieri, I. S. Duff and L. Giraud)

In recent years, there has been a significant amount of work done on the simulation of electromagnetic wave propagation phenomena, addressing various topics ranging from radar cross section to electromagnetic compatibility, to absorbing materials, and antenna design. To address these problems the Maxwell equations are often solved in the frequency domain leading to singular integral equations of the first kind. The discretization by the boundary element method (BEM) results in linear systems with dense complex matrices which are very challenging to solve. In this project new preconditioning strategies for the iterative solution of these systems are proposed. In a first study [ALG22] a comparison of different preconditioners of both implicit and explicit form in connection with Krylov methods is done. Particulat emphasis is put on sparse approximate inverse techniques based on Frobenius norm minimization that use a static nonzero pattern selection. The novelty of this approach comes from using a different nonzero pattern selection for the original matrix from that for the preconditioner, and from exploiting geometric or topological information from the underlying meshes instead of using methods based on the magnitude of the entries. An extract from this work has been accepted for publication in the Proceedings of the *Second Conference on Numerical Analysis and Applications* (Rousse, Bulgaria). The results of the numerical experiments suggest that the new strategies are viable approaches for the solution of large-scale electromagnetic problems using preconditioned Krylov methods. In particular, this strategie is applicable when fast multipole techniques are used for the matrix-vector product on parallel distributed memory computers. A paper [ALG5] related to this research has been accepted for publication. The numerical scalability of this preconditioner implemented in EADS' FMM code, is currently tested on large problems. In a second project [ALG43], implicit preconditioners based on incomplete factorization algorithms are used. Imaginary diagonal perturbations are incorporated, which significantly improves the performance. This project is still ongoing.

3.3 Sparse symmetric preconditioners for dense linear systems in electromagnetism (B. Carpentieri, I. S. Duff, L. Giraud and M. Magolu monga Made)

In order to further develop the study presented in [ALG5], reseach has been done on symmetric preconditioning strategies for the iterative solution of dense complex symmetric non-Hermitian systems arising in computational electromagnetics. In particular, numerical behaviour of the classical Incomplete Cholesky factorization as well as some of its recent variants are reported but well-known factorized approximate inverses are considered. This illustrates the difficulties that these techniques encounter on the linear systems under consideration and give some clues to explain their disappointing behaviour. The proposition consists in two symmetric preconditioners based on Frobenius-norm minimization that use a prescribed sparsity pattern. The numerical and computational efficiency of the proposed preconditioners are illustrated on a set of model problems arising both from academic and from industrial applications. More details on this work are available in [ALG43].

3.4 Combining fast multipole techniques and approximate inverse preconditioners for large calculations in electromagnetism (B. Carpentieri, I. S. Duff, L. Giraud and G. Sylvand)

For large electromagnetic calculations that involve several tens of thousands or a few million unknowns, the use of fast multipole techniques is mandatory to evaluate the matrix-vector product. For such simulations, an investigation of the numerical scalability of the approximate inverse preconditioner [ALG5] implemented in a parallel distributed code [15] has been done. Because the preconditioner naturally becomes more local when the size of the problem is increased, even though the Green functions decay rapidly, the observation is that the convergence rate deteriorates when the size of the linear system increases. To overcome this drawback and improve the numerical robustness of the linear solver an embedded scheme is applied; it consists of a FGMRES Krylov solver for the outer iterations and a preconditioned GMRES inner scheme. For this outer solver, an accurate fast multipole calculation for the matrix-vector evaluation, preconditioned by a few inner preconditioned GMRES iterations is used. For the inner GMRES scheme, a less accurate fast multipole calculation for the matrix-vector computation and the Frobenius norm minimization approach as preconditioner is used. The efficiency of this numerical scheme is demonstrated on large test problems. The benefit of the new scheme is highlighted in Table 3, where the number of outer and inner fast multipole matrix-vector products as well as the elapsed time to solve a problem with around one million unknowns arising from a simulation of an Airbus aircraft are diplayed. GMRES(30) and FGMRES(5)/GMRES(20) are considered because both use the same amount of memory. The target computer is a Compaq SC Alpha server.

Sphere with 1.0 10^6 degrees of freedoms				
GMRES(30)		FGMRES(5) + GMRES(20)		
# accurate FMM	Elapsed time	# accurate FMM	# less accurate FMM	Elapsed time
1196	11 hours	17	260	1 hour 30 mn
Airbus aicraft with 1.1 10^6 degrees of freedoms				
GMRES(30)		FGMRES(5) + GMRES(20)		
# accurate FMM	Elapsed time	# accurate FMM	# less accurate FMM	Elapsed time
no convergence	–	19	300	4 hour 20 mn

Table 3 : Numerical behaviour observed on a 16 processor Alpha Compaq Server.

[15] G. Sylvand, (2002), *Résolution Itérative de Formulation Intégrale pour Helmholtz 3D : Applications de la Méthode Multipôle à des Problèmes de Grande Taille*, PhD thesis, Ecole Nationale des Ponts et Chaussées.

3.5 Grid transfer operators for highly variable coefficient problems in two-level non-overlapping domain decomposition methods (L. Giraud, F. Guevara Vasquez and R. S. Tuminaro)

A robust interpolation scheme for non-overlapping two-level domain decomposition methods applied to two-dimensional elliptic problems with discontinuous coefficients is proposed. This interpolation is used to design a preconditioner closely related to the BPS scheme proposed in [16]. The definition of this interpolation is natural on structured meshes with uniform rectangular subdomains and a generalization to unstructured meshes is proposed. This generalization preserves the constant function while taking into account possible discontinuities. The unstructured grid interpolation was inspired by AMGe [17] and also by the fact that it reduces to the original operator dependent interpolation on uniform meshes. Through numerical experiments, it is shown on structured and unstructured finite-element problems that the new preconditioning scheme reduces to the BPS method on smooth problems but outperforms it on problems with discontinuous coefficients. In particular it maintains good scalable convergence behaviour even when the jumps in the coefficients are not aligned with subdomain interfaces. This work has been presented during the Preconditioning 2001 Conference, and was completed during a visit to Sandia National Laboratory, Livermore after the conference. Results related to this work are reported in [ALG62]

[16] J. H. Bramble, J. E. Pasciak, and A. H. Schatz, (1986), The Construction of Preconditioners for Elliptic Problems by Substructuring I., *Math. Comp.*, **47**, 103–134.

[17] M. Brezina, A. Cleary, R. Falgout, V. Henson, J. Jones, T. Manteuffel, S. McCormick, and J. Ruge, (2000), Algebraic Multigrid based on element interpolation (AMGe), *SIAM J. Sci. Comput.*, **22**, 1570–1592.

3.6 Domain decomposition methods in semiconductor device modelling (L. Giraud, J. Koster, J.-C. Rioual and A. Marrocco)

In the framework of a joint research project between INRIA (A. Marrocco), Parallab (J. Koster) and CERFACS (L. Giraud, J. C. Rioual), the authors are developing a parallel domain decomposition code

for the solution of the drift diffusion equation involved in semiconductor device modelling. A nonlinear time dependent problem has to be solved where each nonlinear iteration requires the solution of a linear mixed finite-element problem resulting in a large sparse linear system.
In order to solve these linear systems in a parallel distributed memory environment using message passing, direct and iterative substructuring techniques are investigated. These techniques imply the computation of the local Schur complement matrices associated with each subdomain. If a classical sparse direct solver is used, the computation of the local Schur complement matrices is usually costly in computation time. Some functionalities of the multifrontal parallel solver MUMPS [ALG2] are used to compute them efficiently. Having an explicit distributed formulation of the Schur complement it is possible to implement substructuring methods, direct or iterative. Direct substructuring is efficient and numerically stable. Iterative substructuring requires a good preconditioner for the Schur complement system. In collaboration with Parallab from Bergen University, the Parallab implementation [18] of a Balanced Neumann-Neumann preconditioner [18, 19] has been tested and compared with another two-level preconditioner designed at CERFACS [ALG6, ALG7]. Various scaling techniques on the Schur complement to improve the numerical stability of the method have also been investigated. The joint work with Parallab was partially funded by an Egide Aurora grant, that enabled J.-C. Rioual to visit Bergen and reciprocally J. Koster to come to CERFACS. This work was presented during the 13^{th} conference on Domain Decomposition Methods in Scientific Computing and more details are available in [ALG61, 20].

[18] P. E. Bjørstad, J. Koster, and P. Krzyżanowski, (2000), Domain decomposition solvers for large scale industrial finite element problems, In *PARA2000 Workshop on Applied Parallel Computing*, vol. 1947, Lecture Notes in Computer Science, Springer-Verlag, 373 – 383.

[19] J. Mandel, (1993), Balancing Domain Decomposition, *Comm. Numer. Meth. Engrg.*, **9**, 233–241.

[20] J.-C. Rioual, (2002), *Solving linear systems in semiconductor device modeling on parallel distributed computers*, PhD thesis.

3.7 Spectral two-level preconditioners (B. Carpentieri, I. S. Duff, L. Giraud and J.-C. Rioual)

When solving the left preconditioned linear system $M_1Ax = M_1b$ with a Krylov method, the smallest eigenvalues of M_1A often slow down the convergence. In the symmetric positive definite case this situation is well-understood and arguments exist for unsymmetric systems to explain the bad effect of the smallest eigenvalues on the rate of convergence of the unsymmetric Krylov solver. A class of spectral two-level preconditioners based on a low rank update is proposed. It aims at shifting these smallest eigenvalues of M_1A close to one. Consequently the resulting two-level preconditioner does not suffer anymore from the effect of those small eigenvalues. Our technique requires the explicit computation of a few eigenvalues that makes it independent from the Krylov solver being used. Symmetric and symmetric positive definite variants can be derived for symmetric and symmetric positive definite linear systems. In that latter situation, the resulting preconditioner is similar to those proposed in [ALG7] in the framework of domain decomposition for elliptic equations where the shape of the smallest eigenvectors might be *a priori* approximated. The effectiveness of the new preconditioners is demonstrated on symmetric non-Hermitian problems arising from electromagnetism [21] (similar problems to those considered in Section 3.3) and on symmetric positive definite and unsymmetric linear systems arising in domain decomposition for the simulation of semiconductor devices [22] (similar problems to those considered in Section 3.6). Although described for left preconditioners in this short section, this spectral two-level technique applies also for right preconditioners.

[21] B. Carpentieri, (2002), *Sparse preconditioners for dense linear systems in electromagnetic applications*, PhD thesis.

[22] J.-C. Rioual, (2002), *Solving linear systems in semiconductor device modeling on parallel distributed computers*, PhD thesis.

3.8 Real/complex Krylov solvers package for sequential and parallel computation (V. Frayssé, L. Giraud and J. Langou)

To complete the GMRES package developed in 1997 [23] (downloaded more than 280 times so far), and the Flexible-GMRES package developed in 1998 [24] (downloaded more than 61 times so far), a set of conjugate gradients solvers for Hermitian linear systems has been developed for both real and complex, single and double precision arithmetic suitable for serial, shared memory and distributed memory computers. For the sake of simplicity, flexibility and efficiency, the conjugate gradient solvers have been implemented in Fortran 77 using the reverse communication mechanism for the matrix-vector product, the preconditioning and the dot product computations. Finally the implemented stopping criterion is based on a normwise backward error.
The source codes and the user's guide [ALG58] can be accessed from the CERFACS Web server at the following URL address:

`http://www.cerfacs.fr/algor/`

This public domain software has received much interest. Amongst the downloaders, e.g. Bell-Lab, CRS4, EDF, INRIA and ONERA.
In some cases, some support upon request has been given to the downloaders, this has permitts to improve the robustness of the code and the clarity of the User's Guide.
The solution of dense complex non-Hermitian linear systems arises in computational electromagnetics. In this context, iterative methods are appealing but with several right-hand sides iterative methods may become less attractive than a single factorization (direct method). A solution is to adapt iterative methods for multiple right-hand sides.

A block GMRES solver and a seed GMRES solver have been developed and interfaced with the EADS code . To extend the range of applicability, they are based on reverse communication and are available in real and complex, single and double arithmetics.
Some promising preliminary experiments have been done on the test case CETAF with 5391 degrees of freedom and nine right-hand sides. Each of the right hand sides correspond to a different angle for the wave illuminating the object. In that experiment, the difference between two successive angles is one degree. The seed GMRES method converges in 226 iterations against 718 accumulated iterations for GMRES applied successively to each of the nine right-hand sides.

[23] V. Frayssé, L. Giraud, and S. Gratton, (1997), A Set of GMRES Routines for Real and Complex Arithmetics, Tech. Rep. TR/PA/97/49, CERFACS.

[24] V. Frayssé, L. Giraud, and S. Gratton, (1998), A Set of Flexible-GMRES Routines for Real and Complex Arithmetics, Tech. Rep. TR/PA/98/20, CERFACS, France.

3.9 Combining OpenMP and MPI on clusters of symmetric multiprocessors: some basic promising experiments (L. Giraud)

Some experiments on different clusters of SMPs have been done, where both distributed and shared memory parallel programming paradigms can be naturally combined. Although the platforms exhibit the same macroscopic memory organization, it appears that their individual overall performance is closely dependent on the ability of their hardware to efficiently exploit the local shared memory within the nodes. In that context, the cache blocking strategy appears to be very important not only to get good performance out of each individual processor but mainly to get good performance out of the overall computing node since sharing memory locally might become a severe bottleneck. A simple benchmark, representative for many large simulation codes, shows through numerical experiments that mixing the two programming models enables to get attractive speed ups that compete with a pure distributed memory approach. There are many possible fields of application for this embedded parallelism including the development of numerical librairies [25]. This can also be of central interest for large industrial codes that have been develloped for years on vector machines and are then ported, with a significant manpower effort, to parallel distributed vector computers using message passing. In many cases those codes are efficient only on a moderate number of processors as they were not initially designed for parallel computers. Using OpenMP to parallelize most of the vectorial loops, in combination with MPI, might be a viable opportunity for smoothly moving these codes onto the emerging and promising platforms for intensive scientific computing that are the clusters of SMPs. Another illustration is from numerical linear algebra where one can mention domain decomposition or more generally block preconditioning techniques for the solution of large sparse linear systems. For those techniques, the numerical scalability is often related to the number of blocks or subdomains. In classical parallel distributed implementations, one assigns one block per processor. Consequently increasing the number of processors for solving a given problem results in a less efficient numerical solver that does not fully take advantage of the computing power of all the processors. Combining the two programming models enables to efficiently exploit some parallelism at a block level, through the use of parallel direct solvers for shared memory for instance. In that context, the number of processors used to perform a given simulation can be increased without deteriorating the numerical property of the numerical algorithm since the number of blocks does not need to be increased. For more details on that work one may refer to [ALG63].

[25] J. J. Dongarra, S. Moore, and A. Trefethen, (2001), Numerical libraries and tools for scalable parallel cluster computing, *Int J. of High Performance Computing Applications*, **15**, 175–180.

4 Qualitative Computing

Group members: Françoise Chaitin-Chatelin, Amina Bouras, Sargis Dallakyan, Valérie Frayssé, Claire Mandry, Tadas Meškauskas, Laurent Plantié, Elisabeth Traviesas and Ahmed Zaoui.

The work of the Qualitative Computing Group is a collaborative effort to assess the validity of computer simulations. The central question is to give meaning to computer results which are seemingly wrong such as in chaotic computations. This goal can be reached by uncovering the laws of computation which govern finite precision computations in the neighbourhood of singularities.

Some of these laws are now well understood. For example, one can cite i) the role of the normwise backward error to assess the reliability of numerical software in finite precision, ii) the role of nonnormality which makes approximated singularities appear much closer than they are in exact arithmetic.

A number of new laws have emerged more recently, which have been the focus of the Group's attention in recent years. The new laws concern in particular:

a) *inexact computing* and the associated homotopic pseudospectrum and backward error as a fruitful framework to understand approximate numerical methods, in exact arithmetic,

b) the unreasonable robustness of Krylov-type methods to perturbations in the data,

c) the (underestimated) role of Geometry in Scientific Computing.

This research and understanding is vitally nourished by work on practical numerical software applications in Physics and Technology, which come from CERFACS partners. The work accomplished in the years 2000 and 2001 in several related areas is reviewed below.

In 2000 a particular focus was on embedded iterative solvers. A workshop on this topic (`http://www.cerfacs.fr/algor/iter2000.html`) was organised at CERFACS, September 11-12, 2000, with the support of SMAI, following a request of CERFACS shareholders EADS, EDF and CNES. This brought together several mature researchers in the area.

4.1 Inner-Outer iterations

It is well known that *asymptotic* methods, such as Newton-like methods for systems and the power method for eigenvalues, need to be performed with more and more accuracy as one gets closer to the solution.

On the contrary, *direct* methods such as Krylov-type methods exhibit a remarkable robustness to perturbations in the data. The only requirement is that, when the incomplete Krylov method is used *iteratively*, as in the *restarted* versions, the first steps in each new iteration loop are computed to full working accuracy, which can be later relaxed as the convergence proceeds inside the loop [ALG30, ALG31, ALG39, ALG40, ALG41, ALG42].

This amazing property results in substantial savings in the overall cost of running a 2 level-solver, when the *outer* iteration is of Krylov type: it was one of the highlights of the talks presented at the Workshop "Inner-Outer iterations" at CERFACS, 11-12 September 2000.

Although a theoretical proof is still lacking, more and more empirical evidence exists, they are confirmed by similar results from researchers worldwide.

In 2000, the concept of inexact Krylov method was used by V. Frayssé [ALG31, ALG39] in the context of a GMRES method with *inexact* matrix-vector products. It was applied to eigenvalue computation [ALG40] and to domain decomposition [ALG42]. Methods such as domain decomposition are used to solve discretized partial differential equations and consists in solving a condensed system whose matrix, the Schur complement, involves the local matrices associated with the subdomains. The Schur complement is positive definite when the matrix associated with the whole domain is positive definite. Then, the condensed system can be solved using the conjugate gradient method which is of Krylov type. However, inverse matrices appear in the Schur complement. Then, linear systems at each step of the conjugate gradient method have to be solved. The solution of these systems forms the inner loop and it is possible to apply the *relaxation strategy* exposed above. This work is described in [ALG42]. The numerical experiments show that a significant number of local matrix-vector products can be saved.

In 2001, T. Meškauskas has worked on inner-outer iterations for mode solvers in structural mechanics in research supported by EDF. He investigated an implicitly restarted Arnoldi method with shifts, coupled with a preconditioned conjugate gradient linear solver. This algorithm is applied to the generalized eigenvalue problem and fits into the general framework of inner-outer iterations when one iterative solver, referred to as the inner solver, is embedded into another one, referred to as the outer solver. In this case, each outer step of the eigensolver (an implicitly restarted Arnoldi method with shifts) requires the solution of a linear system, provided by an iterative linear solver (preconditioned conjugate gradient), which is the inner iteration. As expected, the accuracy of the inner iteration can be *relaxed* when the outer process comes closer to the solution [ALG44]. The *relaxation strategy* was implemented in the `Code_Aster` code and tested on large industrial problems.

[26] A. Ilahi, (1998), *Validation du calcul sur ordinateur: application de la théorie des singularités algébriques*, Ph.D. dissertation, Université Toulouse I. TH/PA/98/31.

[27] R. A. McCoy and V. Toumazou, (1997), PRECISE User's Guide - Version 1.0, Tech. Rep. TR/PA/97/38, CERFACS, Toulouse, France.

4.2 Arnoldi method and the happy breakdown

A convincing theory of the convergence of an iterative Arnoldi method is still a tantalizing goal for numerical analysts in Linear Algebra. This question is approached by considering the incomplete Arnoldi method on a matrix of order n as a *finite*, or *direct* (as opposed to iterative or asymptotic) method. In this approach, it is of prime importance to understand the relation between the starting vector v_1 and the happy breakdown at step $k_0 \ll n$. This requires, in particular, eliminating the conventional assumption that the matrix is non-derogatory. Because, if the matrix is non-derogatory, no early happy breakdown can occur unless the starting vector lies exactly in an invariant subspace in exact arithmetic.

In finite precision computations, it is well known that detecting the exact happy breakdown is difficult. Using the relation between v_1 and k_0, two different heuristic stopping criteria have been proposed [ALG26, ALG69]. The quality of the eigenvalues computed by the Arnoldi method has been a topic of study for more than four years in the Qualitative Computing Group [ALG51, ALG26, ALG69, ALG34]. These studies show that, for some initial vectors, it is not desirable to stop the Arnoldi algorithm in finite precision at the same time as in exact arithmetic. These particular initial vectors have certain components in the eigenvector basis which are too small to be considered in finite precision; only the components which are sufficiently large with respect to machine precision can be considered. So the notion of a neighbourhood of a happy breakdown is introduced.

A comparison between results from homotopic perturbations and results using the toolbox PRECISE [ALG24, 27] and [26] has been performed. The software PRECISE has also been updated in order to be compatible with MATLAB 6.

At the beginning of 2001, with S. Gratton from CNES, a condition number formula was established, which expresses the sensitivity to the initial vector for the Arnoldi process [29]. In collaboration with Prof. B. N. Parlett from Berkeley University, California (USA), an attempt to apply it to determine the number of distinct eigenvalues of a symmetric matrix using the Lanczos process has been done. Such a problem was posed by Prof. Lax (Courant Institute, New York).

[28] F. Chaitin-Chatelin and V. Frayssé, (1996), *Lectures on Finite Precision Computations*, SIAM, Philadelphia.

[29] F. Chaitin-Chatelin, E. Traviesas, and S. Gratton, (2001), Sensitivity from the initial vector for Krylov based methods. Work in progress.

4.3 Inexact Computing

Inexact Computing can be described as follows: given two matrices A and E such that $B = A + E$, the problem to is solve $(B - zI)u = y$. The rule of the game is that it is allowed only to use E and the resolvent field $z \rightarrow (A - zI)^{-1}$ to solve the system.

To play such a game, it is useful to introduce the homotopic family $A(t) = A + tE$, $t \in \mathbb{C}$, such that $A(0) = A$ and $A(1) = B$. This describes in its simplest form the homotopic perturbation theory which has been studied and put to use by F. Chaitin-Chatelin in various guises for more than 30 years [30, 31, 28].

The homotopic perturbation theory can also be interpreted from a purely *information theoretic* point of view. This allows one to:

i) interpret the computing activity in terms of knowledge acquisition,

ii) structure the field of singularities of $(A(t) - zI)^{-1}$ with two families of curves: the singular rays and the singular orbits,

iii) give a *global geometric view* of the resolvent field for the family $A(t) = A + tE$, when there is **no restriction** on E. In particular $\|E\|$ can be arbitrarily large. This is a big step forward since all previously known perturbation theories were local [30].

Such an analysis provides an efficient conceptual tool to understand how well separated eigenvalues can be grouped by the deviation matrix E induced by a numerical method, in exact arithmetic.

It also puts into fuller light the difference between E of rank 1 and E of rank greater than 1 [ALG34]. In the second case, eigenvalues can go out of phase in a striking manner [ALG52].

An early version of these ideas was presented in [ALG34], together with an important application to the happy breakdown of Arnoldi (see preceeding Section 4.2). This was published in [ALG10].

[30] F. Chaitin-Chatelin, (1983), *Spectral approximation of linear operators*, Academic Press, New York.

[31] F. Chaitin-Chatelin, (1988), *Valeurs propres de matrices*, Masson, Paris.

4.4 Geometric aspects of Computing

In conventional scientific computing the four arithmetic operations $(+, -, \times, /)$ are usually defined on scalars or real numbers, that is 1D vectors. Linear Algebra is performed on matrices and vectors of potentially very large dimension, but the numbers themselves are either real scalars (1 dimension) or complex scalars (2 dimensions). Hypercomplex scalars are usually not used in Numerical Linear Algebra. However, it is known since the days of Hamilton and Graves that one can multiply and divide real vectors of dimension 2^k, $k = 0, 1, 2, \ldots$, which define algebras of hypercomplex numbers. This requires introducing an additional geometric operation, the conjugation. These 5 operations define the arithmetic-geometric core of Nature's Computation. For example, the laws of Classical Mechanics and of Maxwell's electromagnetism can be written most efficiently by using products of quaternions, which are 4D vectors. The real component can be interpreted as Time and the 3 imaginary components as Space.

This suggests using a quaternion parameter t with 4 dimensions, rather than a complex one with only 2 dimensions, to extract meaning from the singularities of $A(t) = A + tE$. Such a line of thought, which complements the point of view developed in Section 4.3, is currently under development and is expected to be completed in 2002.

A similar approach can be taken with 8D-octonions. Preliminary discussions have taken place with the TTN Group (see Part 6), in order to use the potential of the Virtual Reality machine to visualize the dynamics of knowledge acquisition, when computation is analysed by means of a multidimensional parameter t with 4 or 8 D in which one dimension, the first, is "felt" but not seen, the next 3 dimensions are spatial, hence visible, and the remaining 4 are non visible. Several invited talks have been presented on this topic [32, 33, 34, 35, 36, 37].

The research in this area conducted in 2000 can be described as follows. The focus has been made on the principle of recursive construction of the hypercomplex algebras [ALG47]. This little known construction permits to recover $\mathbb{C}$ and the quaternion and octonion algebras from $\mathbb{R}$ but can be continued indefinitively yielding algebras of dimension 2^k. It provides more synthetic formulae than the classical ones and highlights the essential role of the geometrical notion of conjugation. This recursive construction principle is also applied to the binary algebras, the initial algebra being then $B_0 = \{0, 1\}$.

In connection with this first aspect, the quadratic iteration $x \to rx(1-x)$ have been explored over the quaternions and octonions in finite precision [ALG23, ALG35, ALG48]. Other aspects of the role of geometry in the computation of algebraic singularities are presented in [ALG8, ALG25].

[32] F. Chaitin-Chatelin, Calcul Qualitatif et Sens de la vie. Ecole d'Ingénieurs CPE, Lyon, 10 May 2001, talk.

[33] F. Chaitin-Chatelin, Computing Thoughts. Workshop on Numerical methods for evolutionary problems, Peschici, Italy, 17-21 Sept. 2001, talk.

[34] F. Chaitin-Chatelin, Hypercomplex Computation. IBM, New York, USA, 27 Dec. 2001, talk.

[35] F. Chaitin-Chatelin, Life Computation. The Institute of Ecotechnics Conference on Time: Metapatterns, The Present Moment and Evolution. Aix-en-Provence, 26-29 Oct. 2001, talk.

[36] F. Chaitin-Chatelin, Nature's Computation: a theory of Qualitative Computing. CERFACS, Toulouse, France, 30 March 2001, talk.

[37] F. Chaitin-Chatelin, Qualitative Computing. IFIP WG 2.5 Meeting, Amsterdam, the Netherlands, 26-27 May 2001, talk.

4.5 Eigenvalue computations - Collaboration with INRIA

This research concerns the study and the implementation of the software ISABeL: Itérations Simultanées et Arnoldi BLoc. The problem consists in computing the r closest eigenvalues to a given complex value. The projection methods of Krylov (Arnoldi) and of subspace iteration are used. The Arnoldi method is fast but might not yield all the desired eigenvalues. On the other hand, subspace iteration is reliable but slow. The software ISABeL couples both methods and combines their advantages. In this software, the Arnoldi method has a role of a "predictor". Moreover, a safety principle (computation of more than r eigenvalues) which enables to control the separation condition in the subspace iteration method is used.

This work forms the first part of the Ph. D thesis of A. Zaoui [ALG35], which ends a 3 year collaboration between CERFACS and INRIA: October 1997 – October 2000, see also [ALG29].

4.6 Integer ambiguities correction - Collaboration with CNES

An overview of carrier phase differential GPS has been conducted. The main obstacles for using this technique to achieve centimetre-levels of accuracy are the difficulties related to correct integer ambiguity estimation (see also Part 2). The LAMBDA method provides integer least-squares estimates for ambiguities which provides the best unbiased estimates. This method was the main subject of these investigations. Apart from a minor bug (noninteger result) which was fixed, the algorithm for the Z-transformation has been improved.

However, working with the test cases provided by CNES it was shown that the LAMBDA method is unable to find correct integer ambiguities in a reasonable time. To overcome this obstacle the search algorithm has been modified. Our modified search algorithm allows an *exponential speed-up* which is a considerable achievement [ALG46]. This modified search algorithm may be used for static/kinematic applications and may allow one to process the data from regional networks of GPS stations as well as the data from Low Earth Orbiting satellites for orbitographic purposes.

4.7 Other work

4.7.1 Analysis of the boundary layer problem of triple deck type

The canonical problem of the boundary layers of triple deck type is studied. This problem, introduced in 1969, is close to the classical Prandtl problem but the pressure is unknown. The physical data is the asymptote of the longitudinal velocity, which is a straight line of nonzero slope in these models, and the pressure cannot be deduced from it directly. In [ALG28], the associated Von Mises problem is analysed; the existence of a solution and study the asymptotic behaviours is proved. An original method based on a semi-discrete scheme is used. A non-uniqueness result observed in numerical simulations is presented. Details are given in [ALG73, ALG74].

4.7.2 Numerical analysis of Schrödinger problems

Numerical analysis of two different initial boundary-value problems for a derivative nonlinear Schrödinger equation was presented in [38, ALG70]. The boundary conditions were Dirichlet or generalized periodic ones. A two-step algorithm was proposed for the numerical solution of this problem. The method consists of Bäcklund type transformations and difference schemes. The convergence and stability in C and H^1 norms of Crank–Nicholson finite difference scheme for the transformed problem is proved. There are no restrictions between space and time grid steps. For the derivative nonlinear Schrödinger equation, the proposed numerical algorithm converges and is stable in the C^1 norm.

4.7.3 Electrocardiogram processing

A method, based on $1/f$ noise analysis, which measures slopes of spectral functions derived from electrocardiogram (ECG) has been proposed [ALG71]. Statistical tests show that spectral slopes are cardiac indicators, separating *normal* (NRM) subjects from these suffering *idiopathic dilated cardiomyopathy* (IDC).

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5 Nonlinear Systems and Optimization

5.1 High rates of convergence in primal-dual interior point algorithms for nonlinear programming (N. I. M. Gould, D. Orban, A. Sartenaer and Ph. L. Toint)

Local convergence properties of the primal-dual trust-region interior point method designed to minimize a nonlinear, possibly nonconvex, objective function subject to linear equality constraints and general inequalities by means of a log-barrier approach has been analysed. The analysis presented follows that of [39, 41, 42, 43]. Asymptotically, for each value of the barrier parameter, a single primal-dual linear system is solved, yielding a point that already matches the barrier subproblem stopping tolerances, and Q-superlinear convergence, which can be as close to quadratic as desired, is achieved. Moreover, this fast asymptotic convergence occurs componentwise. Since the inner minimization phase—used in [ALG12] to solve a barrier subproblem—is not required asymptotically, the conclusions drawn hold independently of the inner minimization procedure [ALG67]. This convergence rate is essentially as fast as that previously obtained for exterior penalty methods [42].

Going further, the question is how fast the rate of convergence may be when the aforementioned extrapolation step is followed by a number of further Newton steps. In two frameworks, it has been shown that a convergence rate that is as fast as desired may be obtained provided one is ready to compute sufficiently many Newton steps. The iterates converge at a Q-rate which can be chosen as close to 2^{q+1} as desired if q Newton steps are taken, and as before, this convergence occurs componentwise. The first framework is that in which the inner iteration is irrelevant in the asymptotics. The second is the trust-region framework of [ALG12]. This work resulted in the report [ALG66].

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5.2 SifDec: a lonesome SIF decoder (N. I. M. Gould, D. Orban and Ph. L. Toint)

The Constrained and Unconstrained Testing Environment (CUTE) [44], briefly described in Section 5.3, strongly relies on a device used to convert SIF-encoded optimization problems into a set of Fortran 77 subroutines, which can in turn be used by solvers to evaluate the objective function values, constraint functions values, compute their derivatives and so forth. This device—the SIF decoder—has been isolated and ported to a variety of popular platforms, for a variety of popular Fortran 77 and Fortran 90/95 compilers. The resulting package has been named SifDec.

Although the main usage of SifDec is presently in conjunction with CUTEr (see Section 5.3), the fact that it is now isolated opens new doors, such as the implementation of a converter from SIF input format to Ampl [45] input format.

The general SifDec documentation may be found in the report [46], the software is formally described in the report [ALG64] and the official SifDec website is located at http://cuter.rl.ac.uk/cuter-www/sifdec.

[44] I. Bongartz, A. R. Conn, N. I. M. Gould, and P. L. Toint, (1995), CUTE: Constrained and Unconstrained Testing Environment, *ACM Trans. Math. Softw.*, **21**, 123–160.

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5.3 CUTEr: a Constrained and Unconstrained Testing Environment revisited (N. I. M. Gould, D. Orban and Ph. L. Toint)

The Constrained and Unconstrained Testing Environment (CUTE) [47] is a versatile environment for testing small to large-scale nonlinear programming problems arising from both real practical applications and from academic circles. It provides Fortran tools for computing function values, gradients, Hessians, matrix-vector products and handles both dense and sparse problems. It has been designed with multi-platform environments in mind and the test problems are written using the SIF (Standard Input Format) description language, formerly used by LANCELOT [48]. CUTE also provides tools to help the users build their own interface to their optimization package, as well as ready-to-use interfaces to famous existing packages like MINOS and OSL.

The purpose of this research is to polish CUTEr, the new version of CUTE. CUTEr is available on a variety of popular platforms, including the quickly growing Linux platforms, for a variety of popular Fortran 77 and Fortran 90/95 compilers and is suited to heterogeneous local networks. Its installation phase, driven by *Imakefiles* make it portable across platforms, is faster, easier, more efficient and makes better use of disk space and memory as architecture-dependent parts have been carefully isolated. CUTEr provides more tools, with enhanced capabilities that implement recent developments in dense and sparse linear algebra and interfaces to more recent optimization packages like KNITRO and filterSQP. CUTEr relies on the SIF decoder, described in Section 5.2.

The general CUTEr documentation may be found in the report [49], the software is formally described in the report [ALG64] and the official CUTEr website is located at http://cuter.rl.ac.uk/cuter-www/.

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5.4 Componentwise fast convergence in the solution of full-rank systems of nonlinear equations (N. I. M. Gould, D. Orban, A. Sartenaer and Ph. L. Toint)

Following the good local convergence properties of primal-dual interior point methods for nonlinear programming [ALG67], the asymptotic convergence of parameterized variants of Newton's method for the solution of nonlinear systems of equations is considered. The original system is perturbed by a term involving the variables and a scalar parameter which is driven to zero as the iteration proceeds. The exact local solutions to the perturbed systems then form a differentiable path leading to a solution of the original system, the scalar parameter determining the progress along the path. A homotopy-type algorithm, which involves an inner iteration in which the perturbed systems are approximately solved, is outlined. It is shown that asymptotically a single linear system is solved per update of the scalar parameter.
It turns out that a *componentwise* Q-superlinear rate in the sequence of iterates may be attained under standard assumptions, and that this rate may be made arbitrarily close to quadratic. The theoretical results presented in the original report have been extended to show that the exact same convergence rate, which still applies componentwise, also occurs in the residuals. Numerical experiments have been added to illustrate the new results and the relationships that this method shares with interior methods in constrained optimization have been discussed. This work is in [ALG65].

5.5 Optimization techniques for the regularization of large-scale discrete forms of ill-posed problems (M. Rojas, D. C. Sorensen, T. Steihaug, D. Noll and G. Tanoh)

This project consists of using optimization techniques for the numerical treatment of ill-posed problems from inverse problems in different application areas. Two of the main features of this type of problem are the ill-posedness of the operators involved and the presence of noise in the data. Regularization methods try to recover useful information about the solution of these problems by solving a related problem with better conditioning where the effect of the noise in the data is minimized.
The regularization problem can be formulated in different ways. One of the most popular regularization approaches is the classical Tikhonov regularization which is equivalent to the problem of minimizing a quadratic subject to a quadratic constraint. The latter is known in optimization as the trust-region subproblem.
Methods for both the linear and nonlinear formulations of ill-posed problems as well as the application of those techniques to the solution of problems with field data are considered. At the core of this project is the method LSTRS for the large-scale trust-region subproblem presented in [50]. LSTRS is an iterative procedure that requires the solution of a large eigenvalue problem at each step. This gives rise to new problems in the area of large-scale eigenvalue computation and will be described later.
Linear Regularization. This subject deals with the solution of large-scale linear systems and linear least-squares problems where the coefficient matrix is highly ill-conditioned and the right-hand side is contaminated with noise. These problems arise in important areas such as seismic inversion, medical imaging and image restoration. Our work in this area includes:

- With Dan Sorensen from Rice University, Houston: solving seismic inversion problems such as those presented in [ALG75].
- With Trond Steihaug from the University of Bergen, Norway: developing a method for the problem of minimizing a quadratic function subject to quadratic and nonnegativity constraints in a large-scale and ill-posed setting [ALG76]. This kind of problem arises when solving inverse problems in image

restoration. Our technique is one of the very few methods available for the efficient computation of nonnegative restorations.

- Some work on image restoration problems without nonnegativity constraints has been done and the techniques developped has been tested for linear regularization on applications from magnetic field reconstruction.

Nonlinear Regularization. There have been few attempts to treat ill-posed problems as nonlinear problems, mostly limited to the nonlinear least squares formulation. This is mainly due to the fact that until now there were no efficient methods that could handle the high-degree singularities present in these problems. Very recently LSTRS has been presented, this is a method for the large-scale trust-region subproblem that is able to handle such singularities and has proven to be very efficient in practice [50]. This method can be used at the heart of an optimization method relying on the trust-region globalization strategy, and such an optimization method can be used in turn to treat nonlinear ill-posed problems.
Our work in this area consists of the development of a trust-region interior-point method using LSTRS [50] to solve the subproblems. Applications will be in the area of medical tomography. This work is in collaboration with Germain Tanoh and Dominique Noll from Université Paul Sabatier, Toulouse [51].
Preconditioning Large-Scale Eigenvalue Problems. As already mentioned, the main computation in LSTRS is a sequence of large-scale eigenvalue problems. Thus, the success of the trust-region method depends on how efficiently and accurately the eigenvalue problems are solved. This is especially relevant in the ill-posed case where the eigenvalues of interest tend to be very clustered and therefore, eigensolvers based on the Lanczos method, such as ARPACK, will exhibit slow convergence. One way to overcome this problem is to precondition the eigenvalue problems. With Dan Sorensen from Rice University in Houston, work is done on the design of efficient preconditioners for the eigenvalue problems arising in LSTRS. By taking advantage of the special structure of these problems it is possible to design efficient preconditioners, and some preliminary results for these new techniques are promising.

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5.6 Numerical optimization techniques for data assimilation (A. Piacentini, A. Sartenaer and A. Weaver)

Variational data assimilation methods (as used in meteorology or oceanography for instance) rely on optimization solvers. In collaboration with the Climate Modelling and Global Change team (more precisely the PALM project and the “ocean data assimilation” project, see Chapter 5 in Part 5), a framework whose goal is twofold has been started. The first is to select existing numerical optimization techniques (such as limited memory methods, conjugate gradient methods, etc) adapted to data assimilation, and to compare their numerical behaviour and performance when embedded in the PALM software. The second goal is to investigate the possibility to enrich these exisiting optimization techniques, knowing that important issues are for instance the development of good preconditioners to accelerate the conjugate gradient method, multi-level resolution techniques, and (weakly) non-quadratic formulations of the data assimilation problem.

6 Publications

6.1 Journal Publications

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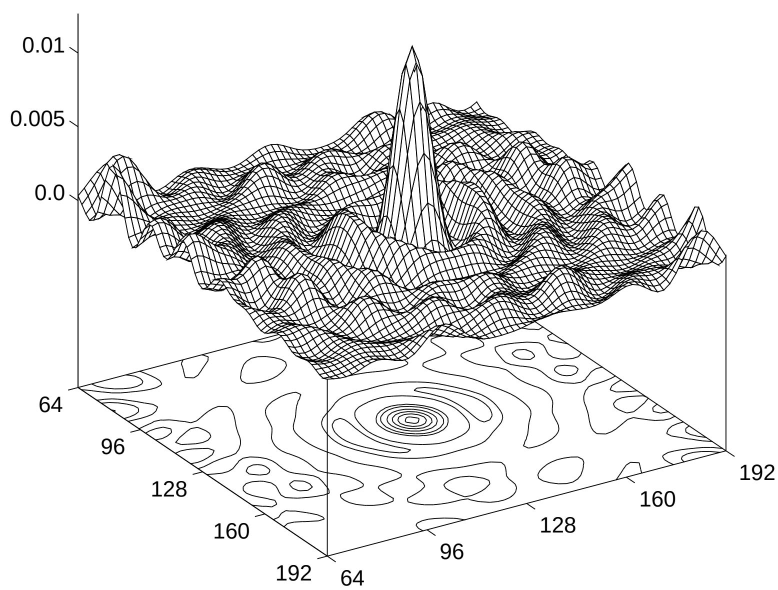
2

Signal and Image Processing



Introduction

A. Lannes

The Signal and Image Processing (SIP) team is now involved in two major projects at the European level:

(1) EGNOS (for European Geostationary Navigation Overlay Service);

(2) SMOS (for Soil Moisture and Ocean Salinity).

The international context of EGNOS is the following: The European Space Agency (ESA), the European Commission (EC) and the European Organisation for the Safety of Air Navigation (Eurocontrol) are cooperating on the development and implementation of the first generation civil navigation satellite service EGNOS. Several European civil aviation and other organisations also support the programme through the European and Infrastructure Group. By means of additional signals relayed by geostationary satellites, the military-based constellations GPS (Global Positioning System) and GLONAS will become usable for a number of safety-critical applications. EGNOS is being developed in the framework of the ESA ARTES-9 programme under a contract with a European/Canadian consortium led by Alcatel Space Industries.

SMOS is an ESA Earth explorer project whose main objective is to deliver a crucial variable of the land surface: soil moisture. This project will also yield sea surface salinity fields. At the related wavelengths ($\lambda \simeq 20$ cm), the measured signal is directly related to the brightness temperature of the surface (negligible atmospheric contribution), which in turn, through the emissivity, is directly linked to the dielectric constant of the target (i.e., moisture or salinity). Actually, the sensitivity of brightness temperature to soil moisture and salinity is optimum in the L band (1.4 GHz, 27 MHz). From an experimental standpoint, SMOS is the result of preliminary studies on MIRAS (Microwave Imaging Radiometer by Aperture Synthesis), a program in which the SIP team is involved since 1994.

The phase calibration problems arising in aperture synthesis [SIP1, SIP2], and in particular for the SMOS antenna [1], and those of integer ambiguity resolution in high-precision kinematic GPS, share a common feature [SIP3]: in both cases integer ambiguities have to be raised, the rational numbers in question being allocated to the cycles of a graph, an interferometric graph in the first case, and a GPS graph in the second. This surprising connection, which was discovered at CERFACS [SIP6, SIP3], is now under extensive development in the SIP group. The experience of the team in phase calibration can therefore be transmitted to the GPS community. The related approach to GPS integer ambiguity resolution proves to be very efficient in practice, especially when the rank of the integer ambiguity lattices to be considered is large, in other words when the number of satellites and receivers is large. The preconditioning methods developed by the team for the radio imaging arrays such as the VLBA (Very Long Baseline Array) and ALMA (Atacama Large Millimeter Array) can be transposed to the GPS context. In the SIP approach, the problem is solved in a global manner. As a result, several processors may tackle the same problem simultaneously. It was therefore quite normal that CERFACS be involved in the related research.

The phase calibration problem had been analysed so far in two extreme situations, the one of nonredundant arrays [SIP2], and the one of full-phase arrays [1] (the SMOS antenna is of this last type). The studies conducted by the SIP team in 2001 concerned the general case of partly-redundant interferometric graphs. They complete the results already obtained in this field. The corresponding theoretical framework is based on the Smith normal decomposition of the spectral phase closure matrix. Two integer ambiguity problems have then to be solved successively [2, 3].

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2 Integer ambiguity resolution on interferometric and GPS graphs

A. Lannes

The notion of integer ambiguity resolution is associated with the following general problem: given some $\mathbf{x}$ in $\mathbf{R}^p$, find the node $\mathbf{n}$ in $\mathbf{Z}^p$ closest to $\mathbf{x}$, the distance being the one induced by a given quadratic form. This classical problem of algebraic number theory is currently solved by using discrete search algorithms in which the notion of reduced basis plays a key role. These algorithms can of course be applied to the particular situations arising in in Aperture Synthesis and in GPS, but the statement of these particular problems also appeals to the notion of graph, and thereby to algebraic graph theory. The work of the team in this field was to show that powerful preconditioning methods can then be developed, and therefore, from a more conceptual point of view, that there exists a common theoretical framework which cannot be ignored.

The n vertices of an interferometric graph are the pupil elements of the aperture synthesis device: the antennas in radio imaging, the telescopes in optical interferometry. An interferometric graph is not necessarily complete: the number q of its edges, then called baselines, may be less than $n(n-1)/2$. The vertices of a GPS graph are the receivers and the satellites of the GPS device (see Fig. 2.1).

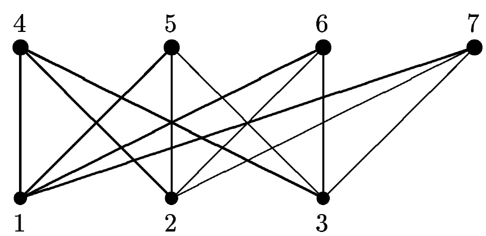

Figure 2.1: Example of GPS graph. Here, the number of vertices, $n = n_{\mathrm{r}} + n_{\mathrm{s}}$, is equal to 7; bottom: 3 receivers; top: 4 satellites. In most cases encountered in practice, the number of edges, q, is equal to $n_{\mathrm{r}}n_{\mathrm{s}}$. The thick lines correspond to a spanning tree of this graph. The related loops are characterized by the remaining edges. Here, we have 6 loops of order 4.

A spanning tree of a graph $(\mathcal{V}, \mathcal{E})$ ($\mathcal{V}$ for vertex, $\mathcal{E}$ for edge) is a subgraph of n vertices and $n-1$ edges without any cycle in it (see Fig. 2.1). Here, a cycle is said to be a loop, since the notion of wave cycle plays an important role in GPS. The number of loops defined through a given spanning tree of the interferometric graph $(\mathcal{V}, \mathcal{E})$, p, is therefore equal to $q-(n-1)$, the number of loop-entry edges. In most cases encountered in aperture synthesis, the loops are of order 3, whereas they are of order 4 in GPS (see Fig. 2.1).

Let $x(j,k)$ be an $\mathcal{E}$-function, i.e., a function that takes its values on the edges of graph $(\mathcal{V}, \mathcal{E})$. In the sense of Kirchhoff, the closure terms of x are the compilations of the values of x along the directed edges of the loops of $(\mathcal{V}, \mathcal{E})$. By definition, the closure operator provides a vector $\mathbf{x} \in \mathbf{R}^p$ whose components are the closure terms $x^{(i)}$.

The reference problem presented in Section 2.1 is exactly the one of phase calibration in aperture synthesis, but only an introduction to what is referred to as Differential GPS. The complete GPS transposition cannot be outlined here by lack of space.

2.1 Reference problem

Let B be the bias operator $(B\varphi)(j,k) \triangleq \varphi(j) - \varphi(k)$, and $\{t\}$ be the value of $t \in \mathbf{R}$ wrapped into the interval $(-1/2, 1/2]$:

$$\{t\} \triangleq t - \lfloor t \rceil, \qquad (\lfloor t \rceil\text{: nearest integer to } t).$$

On each edge $(j,k) \in \mathcal{E}$, the object-data relationship is then of the form:

$$x_{\rm e}(j,k) = \{x_{\rm o}(j,k) + \phi_{\rm e}(j,k) + \varepsilon_{\rm e}(j,k)\} \qquad \phi_{\rm e}(j,k) \triangleq (B\varphi_{\rm e})(j,k).$$

Clearly, $x_{\rm o}$ is the object $\mathcal{E}$-function, $x_{\rm e}$ is the data $\mathcal{E}$-function, $\phi_{\rm e}$ is the experimental bias, $\varphi_{\rm e}$ is an experimental $\mathcal{V}$-function, and $\varepsilon_{\rm e}$ is the error term. Given some approximation $x_{\rm m}$ to $x_{\rm o}$ (m for model), the reference problem is to specify how the data allow this model to be constrained.
As $\{(x_{\rm e} - \phi_{\rm e}) - x_{\rm m}\} = \varepsilon_{\rm em}$, in which the error term $\varepsilon_{\rm em}$ is a priori small on all the edges of the graph, one is led to search a bias term $\phi_\star$ (in the range of B) that minimizes the square of the norm of $\varepsilon \triangleq \{(x_{\rm e} - \phi) - x_{\rm m}\}$:

$$\|\varepsilon\|^2 \triangleq \sum_{(j,k)\in\mathcal{E}} \varepsilon^2(j,k)\, \varpi(j,k).$$

Here, ϖ is a weight function whose choice takes account of the size of the error term $\varepsilon_{\rm em}$. The quantity $\varepsilon_\star \triangleq \{(x_{\rm e} - \phi_\star) - x_{\rm m}\}$ is referred to as the optimal model shift. Indeed, the constrained model $x_{\rm m\star}$ is then equal to $x_{\rm m} + \varepsilon_\star$.
Let $\widehat{\mathbf{x}}$ be the vector whose components are the p closure terms of $x_{\rm e} - x_{\rm m}$ divided by 2π, and $[\Omega]$ be the variance covariance matrix of the closure terms. By considering the unwrapped version of the problem, it is easy to show that

$$\varepsilon_\star = \sum_{i=1}^{p} \big(n_\star^{(i)} - \widehat{x}^{\,(i)}\big),$$

in which $\mathbf{n}_\star$ is the integer ambiguity vector that minimizes the functional

$$f : \mathbf{Z}^p \to \mathbf{R}, \qquad f(\mathbf{n}) \triangleq [\mathbf{n} - \widehat{\mathbf{x}}\,]^{\rm tr}[\Omega]^{-1}[\mathbf{n} - \widehat{\mathbf{x}}\,].$$

2.2 Introduction to the SIP approach

The methods that are currently used for solving this problem do not benefit from a very nice property of the variance-covariance matrix of the closure terms. This property results from the fact that the problem is then to be analysed in the specific framework of algebraic graph theory. It can then be shown that the functional to be minimized can be written in the form

$$f(\mathbf{n}) = \inf_{\phi\in L} \Big\| \sum_{i=1}^{p} \big(n^{(i)} - \widehat{x}^{\,(i)}\big)\xi_i \;-\; \phi \;\Big\|^2.$$

Here, L is the range of B, and ξ_i is the characteristic function of the $i^{\rm th}$ loop-entry edge of the graph: ξ_i is equal to unity on this edge and vanishes on the others. The interest of the expression above is related to the fact that the ξ_i's are mutually orthogonal. The global preconditioning method developed in the team is based on a local alternate minimization in ϕ and $\mathbf{n}$. In the GPS context, the related method can be regarded as a relaxed bootstrapping technique: an error on the most reliable ambiguities can thus be corrected in global manner. Moreover, several processors may tackle the same problem conjointly. GPS integer ambiguity resolution can thus be achieved in real time [SIP3].

2.3 Phase calibration of partly-redundant interferometric graphs

In the general case of redundant interferometric graphs, two integer ambiguity problems P must be successively solved: P1 and P2 [2, 3]. A problem such as P is to find the point $\mathbf{k}_\star$ of $\mathbf{Z}^\nu$ closest to a point $\widehat{\mathbf{z}}$ of $\mathbf{R}^\nu$, the distance being the one induced by a given quadratic form q. One then says that ν is the number of degrees of freedom of P. In the situations where there exist several $\mathbf{k}$ such that $q(\mathbf{k} - \widehat{\mathbf{z}})$ is of the order of $q(\mathbf{k}_\star - \widehat{\mathbf{z}})$, the problem is intrinsically unstable. Phase calibration instabilities may then occur.
The number of degrees of freedom of P1 is equal to $p - m_1$, where m_1 is the difference between m, the dimension of the variational spectral phase space K, and m_0 , the one of the intersection of K with the bias phase space L. Note that m is the number of spectral phase components to be determined. The number of degrees of freedom of P2 is equal to m_1 .
In the case of full-phase arrays, m_1 is equal to m; P2 proves then to be trivial. In the case of nonredundant arrays, m_1 is equal to p, so that P1 disappears. With regard to P2, as already mentioned and specified in [SIP2, SIP3], there exists a particular initialization procedure for the search for the nearest lattice point. The related techniques can of course be applied as they are to weakly-redundant situations. The less redundant the array is, the more efficient this initialization procedure.

3 Apodization functions for SMOS

E. Anterrieu, B. Picard, G. Ramillien

3.1 Introduction

The SMOS (Soil Moisture and Ocean Salinity) space mission, currently undergoing a phase A study in the frame of the Earth Explorer Program of the European Space Agency, will be the first attempt to apply, to the remote sensing of the Earth surface, the concept of imaging interferometric radiometry by aperture synthesis, initially developed for radio astronomy. For such an instrument, the apodization function to be applied to the complex visibilities should be optimized for ensuring the best spatial resolution at ground level, according to criteria relevant for extended sources typical of Earth surface scenes.

3.2 Hexagonal periodic lattices

Interferometer measurements, also referred to as complex visibilities, are obtained by cross-correlating signals collected by two spatially separated antennas with overlapping fields of view. In the SMOS case, where the synthesized antenna consists of a planar Y-shaped structure with equi-spaced radiating elements, the visibility functions are sampled over an hexagonal grid inside a star-shaped area H in the Fourier domain, so that hexagonal processing is the natural way for performing Fourier synthesis operations [6].

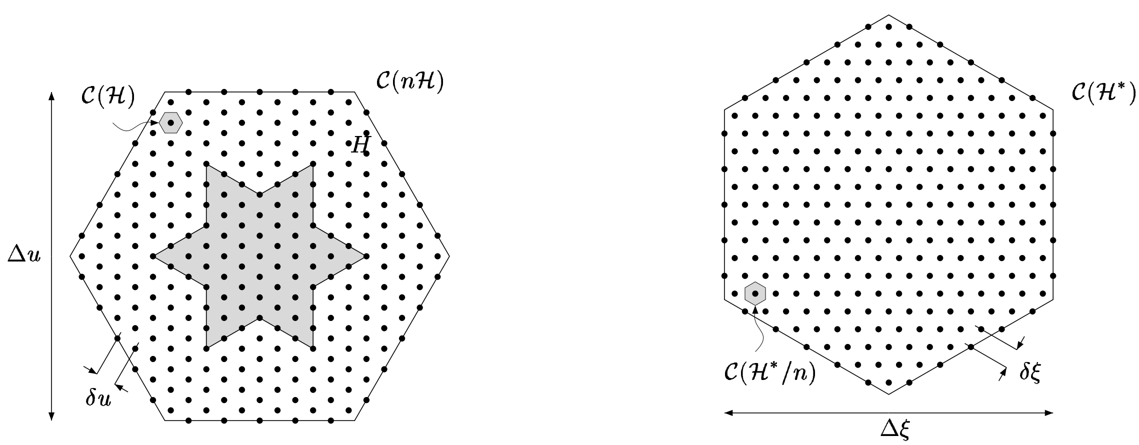

Figure 3.1: Elementary cells involved in the processing of hexagonaly sampled images: Fourier domain *(left)* and spatial domain *(right)*. The integer n is a power of 2 such that the star-shaped experimental frequency coverage H is contained in the elementary cell $\mathcal{C}(n\mathcal{H})$. According to a well known property of reciprocal lattices, the Fourier sampling interval δu, as well as the angular spectral bandwidth Δu, is related to the resolution scale $\delta\xi$ and to the field extension $\Delta\xi$.

By referring to Figure 3.1, it has been demonstrated that the hexagonal discrete Fourier transform operator could be implemented by re-using a standard FFT algorithm designed for Cartesian grids, thus making the development of an algorithm specific to hexagonal grids unnecessary [5].

3.3 Apodization functions

Apodization, sometimes also called tapering or windowing, is a mathematical technique used to reduce the Gibbs phenomenon which is produced by the truncation of the Fourier transform of a signal. In SMOS, this cut-off is due to the finite extent of the star-shaped experimental spatial frequency coverage H. Since there is no way of knowing the degree of discontinuity at the edges of H for any particular scene, the technique simply reduces the Fourier components at the boundaries in a gradual manner, so that no new discontinuities are produced. Each apodization function $\widehat{W}$ has its own specific transition from the central frequencies to the outer ones, and the result is a substantial reduction of the effects due to the sharp frequency cut-off. Nevertheless, this improvement comes at some cost. Indeed, as windowing is modifying the Fourier components, some reduction in the fidelity of the spatial representation is to be expected.

The traditional one-dimensional windowing functions can be adapted without any difficulty to the two-dimensional hexagonal case. Indeed, it is well known that hexagonal apodization functions may be expressed as functions of the radial variable $||\mathbf{u}||$ [5]. The natural region of support of such centro-symmetric windows is practically a disk. However, in the special case of SMOS, it will be truncated to the star-shaped experimental frequency coverage H. As a result, since H presents a twelve-fold symmetry, W will present the same order of symmetry. More than twenty windowing functions have been studied, some of them depend on a parameter leading to a family of apodization functions [4].

Among all the factors of merit used for characterizing the spatial properties of the Fourier transform W of a windowing function, three deserve attention because they have a physical meaning in the context of remote sensing: the full-width at half-maximum (FWHM) of the main lobe of the window intensity pattern, the highest sidelobe level (HSLL) of the window intensity pattern, and the beam efficiency at half-maximum (BEHM) which is the fraction of energy under the main lobe of the window power pattern within the FWHM. Shown on Figure 3.2 are the factors of merit of these apodization functions. It is worthy of note that the spatial properties of these traditional windows in the two-dimensional hexagonal context of SMOS do not necessarily reflect their qualities in a one-dimensional problem [4].

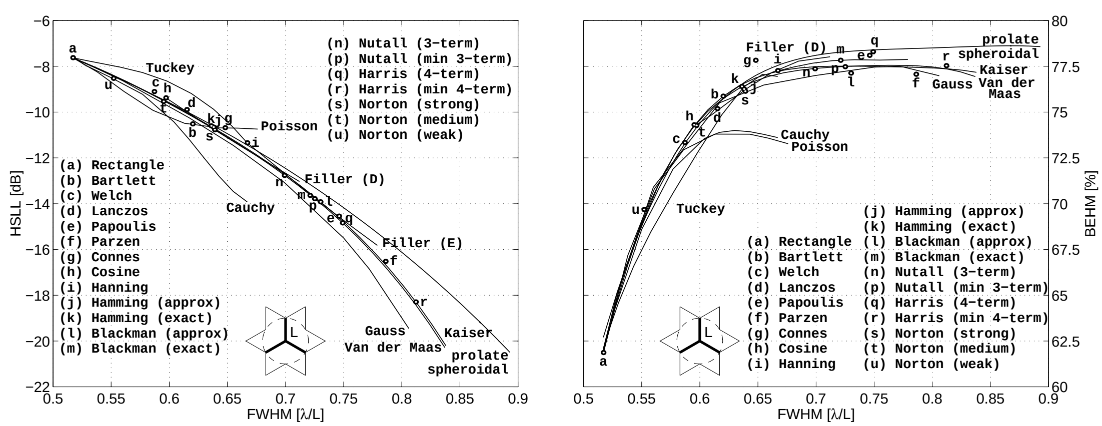

Figure 3.2: Traditional factors of merit: HSLL *vs* FWHM *(left)*, and BEHM *vs* FWHM *(right)*. The FWHM is expressed in units of λ/L, where L is the length of the arms of the array.

An additional factor of merit proves to be significant in the case where 2D scenes are likely to include a sharp discontinuity line (e.g. coastal line): the side area contribution radius (SACR). Assuming a straight line is drawn throughout the scene, this indicates the distance (away from the window's center) such that the relative energy contribution from regions beyond the line is smaller than a given percentage (as shown on Figure 3.3 this integrated relative contribution decreases from a maximum of 50% down to 0). Depending on the nature of the hypothetical scene discontinuity (forest versus grassland boundary, or coastline), the percentages to be considered range between 2% and 0.05%.

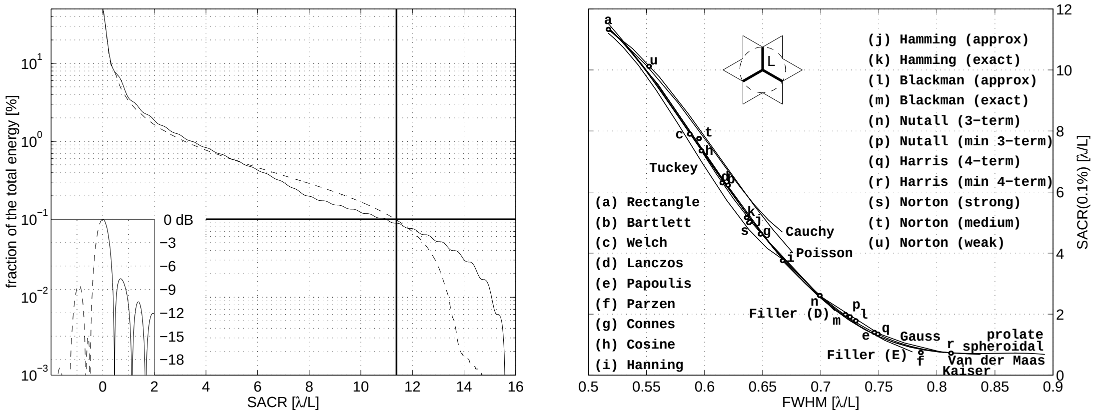

Figure 3.3: Energy fall-off as a function of the SACR for the rectangular window *(left)* and SACR (0.1%) *vs* FWHM *(right)*. Both FWHM and SACR are expressed in units of λ/L, where L is the length of the arms of the array.

3.4 Conclusion

This work can be viewed as a benchmark test for assessing the performances of apodization functions when looking at extended inhomogeneous targets. The performance of many apodization functions have been assessed: it proves to be possible to select, from a family of optimized functions, the best compromize between radiometric sensitivity and spatial resolution performances, accounting for criteria relevant for Earth's surface scenes. Future work is however needed to assess the respective influences of the scene structure, element spacing ratio and element antenna gain in recontruction errors, in order to be able to select optimal apodization functions.

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4 Publications

4.1 Journal Publications

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[SIP3] A. Lannes, (2001), Résolution d'ambiguïtés entières sur graphes interféromtériques et GPS, *C. R. Acad. Sci. Paris, Série I*, **t. 333**, 707–712.

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3

Computational Fluid Dynamics

Introduction

Thierry Poinsot

Year 2000 and 2001 have been very active for the three CFD sub-projects:

- *Modelling.* Developing advanced simulation codes requires a knowledge of the physics of the flows and of the models used to represent these flows. In 2000 and 2001, modelling at CERFACS has concentrated on unsteady flows, heat transfer, near-wall turbulence, combustion and two-phase flows.

- *Unsteady Flow Calculations on Unstructured Grids (AVBP).* AVBP has become the standard tool for LES of reacting flows at CERFACS but also for CERFACS partners. Laboratories (such as Ecole Centrale Paris, Institut Français du Pétrole, ONERA or Institut de Mécanique des Fluides de Toulouse) have used AVBP for their own research. Industrial partners (SNECMA, Turbomeca, Siemens) have renewed or intensified their collaboration with CERFACS to increase AVBP capabilities. New partners have established collaborations with CERFACS (Alstom Power or SNECMA DMF in Bordeaux for example).

- *Advanced Aerodynamics and Multiphysics.* CERFACS leads an intense research activity on structured multi-block codes, both in the classical Fortran framework (with NSMB which is now run routinely at EADS) and in the Object Oriented world (with elsA which is developed jointly with ONERA).

  Each sub-group has summarized its main achievements during the last two years in the next pages. General remarks are listed below:

  – Most European contracts (Framework programme, FP'5) accepted in 2000 have started in 2000 or 2001. These proposals include wake vortices studies (C Wake, S Wake, Wakenet 2), LES of combustion in gas turbines (Icleac, Preccinsta, Molecules), atmospheric pollution (Stopp), Direct Numerical Simulations of partially premixed flames in piston engines (G-level). Additional contracts (Fuelchief, Desire, Awiator) submitted and accepted in 2001 for the last calls of the FP'5 will start in 2002.

  – The size of the team continues to increase: it gathered 30 persons in January 2001 and more than 40 at the end of 2001. At the same time, many CFD group members have left: B. Caruelle and J.P. Légier have joined Airbus, B. Marquez and J. Cormier went to engineering companies, G. Jonville to the TTN team, O. Colin and A. Benkenida to Institut Français du Pétrole, J. Schluter to Stanford University. The quality of the research produced by CERFACS seniors was also recognized: Dr Nicoud moved to a professor position in Applied Maths in Montpellier, Dr Schonfeld to the AEA company and Dr Ducros to CEA. The departure of these three seniors has put some additional constraints on the team but confirms the high level of senior scientists trained at CERFACS.

  – New topics are also beginning as requested by CERFACS partners: for example, in the modelling group, two-phase flow studies have begun in 2000 for EDF in close collaboration with Institut de Mécanique des Fluides de Toulouse. In the field of aerodynamics, the collaboration with ONERA on elsA is growing rapidly: in 2001, six scientists will be working full time on elsA.

- In the field of reacting flows, AVBP has been now identified by EADS, SNECMA and Turbomeca as the main french code for unsteady combustion and the national program ‘PRC Combustion’ submitted to SPAE has been accepted (in collaboration with ONERA and the major french laboratories working in this field) to develop AVBP for two-phase flow LES applications in the next four years (starting in January 2002).
- The collaboration with laboratories continues: in the field of rotating flows, the PhD thesis of L. Kozuch with Ecole Centrale de Lyon will be completed in the first months of 2002 and the collaboration with ENSICA in the Ocmath regional project has also lead to many fruitful interactions. In the field of combustion, AVBP and NTMIX are now used at IMF Toulouse, Ecole Centrale Paris and Institut Français du Pétrole. The CRCT (‘Centre de Recherche sur la Combustion Turbulente’) is very active: CRCT meetings organized in December 2000 (at IFP) and 2001 (at ECP) gathered more than 40 scientists from IMFT, PSA, CERFACS, Ecole Centrale and IFP who collaborate directly or indirectly to CRCT. This collaboration with the academic community also appears through the high level of publications (25 papers in refereed journals in 2000 and 2001) and the presentation of two habilitation thesis in the team in 2000 (Dr F. Nicoud and Dr B. Cuenot). The quality of the formation work at CERFACS was also recognized through the Leopold Escande prize awarded by INP Toulouse to Olivier Colin for his PhD and the first BMW prize awarded to B. Caruelle for the best PhD in 2000 (world contest).
- Because of the multiple contracts proposed to the team, it has been decided to transfer studies which do not contain enough fundamental work to the TTN team of CERFACS. This was the case in 2000 for the ASICA project which is now handled by TTN. It also reflects the objective of the team to conserve a high academic level.

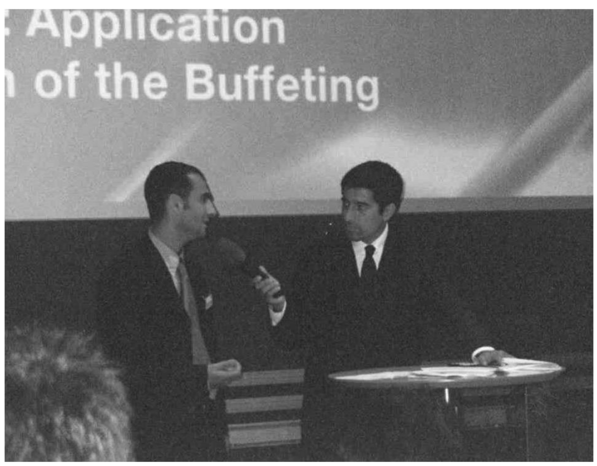

Figure 1.1: Dr B. Caruelle receiving his BMW award in Munich for the best PhD work of 2000.

2 Modelling

Turbulent flows need to be modelled in order to build truly predictive numerical codes for the design and understanding of many industrial flows such as those around aircrafts or propellers, in gas turbines, piston engines or burners. Most numerical tools used for practical calculations are based on the Reynolds Averaged Navier Stokes (RANS) formulation where the modelling problem is extremely difficult due to intermittency. Large Eddy Simulation (LES) avoids this problem since it computes the larger turbulent eddies and models only the smaller ones. In both approaches, one needs to model subgrid Reynolds stresses and heat fluxes as well as chemical source terms in the case of turbulent reacting flows. To address the modelling problem, it is often convenient to rely on reference data coming from accurate Direct Numerical Simulations (DNS). At CERFACS, the DNS expertise of the CFD group is used to propose new models for RANS and LES techniques for both reacting and non-reacting flows. These models are validated and used in the CERFACS codes presented in chapters 3 and 4. The section is divided in two main parts: reacting and non-reacting flows.

2.1 Reacting Flows

2.1.1 DNS for Turbulent combustion (B. Cuenot, C. Jimenez, A. de Lataillade, T. Poinsot)

In 2000 two FP'5 European projects have started, and continued in 2001: Glevel and STOPP.
Related to the topic of turbulent stratified combustion, the project Glevel is now focusing on Direct Numerical Simulations of octane/air stratified flames (see Fig. 2.1). Performing such DNS with complex chemistry schemes is one of the unique capacities found in the CFD team ([CFD43]). The octane chemical kinetic scheme has been provided by RWTH Aachen, partner of the project. Diagnostics are performed to analyse the effect of a non-homogeneous reactant mixture on the primary flame front and on the secondary or post-flame. The complexity of chemical kinetics makes it difficult to identify simple structures in the secondary flame, and a particular effort in modeling this reaction zone has to be done. In parallel work is still going on with Prof. Dan Haworth (Penn State University) on propane stratified combustion (2000 CTR Summer Program).
These two projects provide a unique data base of the processes involved in stratified combustion. The next step is to develop models, which is the coming part of Glevel. Such modeling is already in progress in collaboration with PSA and University of Southern California (Pr. Egolfopoulos) who studied stratified combustion in Direct Injection engines [CFD14]. The team is still involved in the american ITR/ACS project, first submitted to NFS, later to AFOSR, coordinated by D.Haworth and involving Dr. S. Pope (Cornell) and Dr. J. Chen (Sandia). The aim of this project is to implement the ISAT technique in our DNS code, to compute complex chemistry at a reduced cost.

The Research Training Network STOPP, coordinated by CERFACS, is also fully operational. Seven young researchers have been hired up to now in the Network, and at least two other persons should join in the coming months. The scientific objective of the project is a better understanding of pollution processes:

pollutant emissions by industrial systems as well as dispersion and reaction in the atmosphere are studied. The contribution of CERFACS in this project is to study LES of turbulent combustion, and a PhD thesis (A. Kaufmann), has started in September 2000 to work on this topic.

The PRIDE project (FP'4) has been terminated in March 2000. Direct Numerical Simulations of turbulent diffusion flames with NOx formation have been achieved and used for assessment of turbulent combustion models. This project has also given the opportunity to develop the chemistry reduction procedure ICC, now coupled to the AVBP code for an operational use in complex configurations computations.

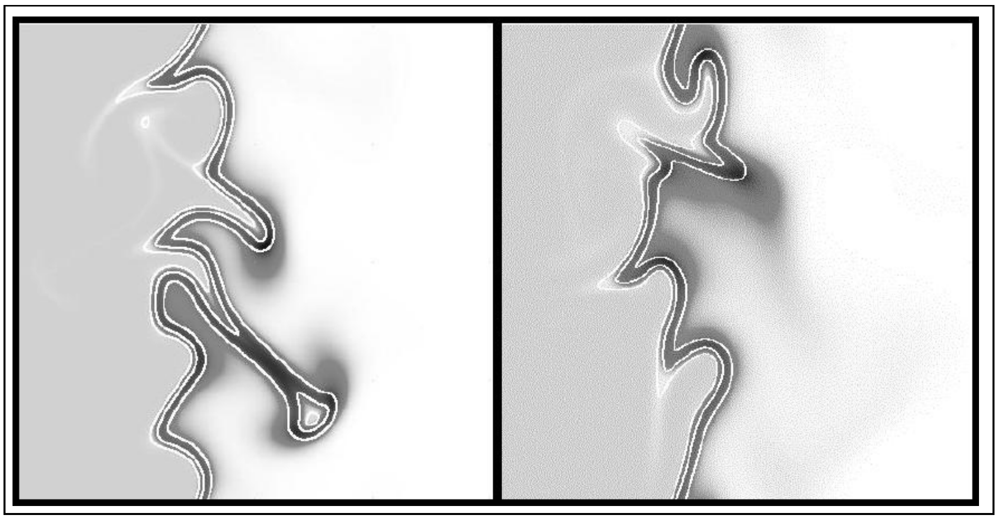

Figure 2.1: DNS of stratified octane/air combustion: heat release. Left: homogeneous mixture, right: stratified mixture.

2.1.2 LES of turbulent combustion (J-P. Légier, G. Lartigue, L. Selle, K. Truffin, C. Prière, L. Gicquel, B. Cuenot, C. Jimenez, F. Ducros, F. Nicoud, T. Poinsot)

The thickened flame model for LES of turbulent combustion developed in collaboration with Ecole Centrale Paris [CFD4] is now routinely used in AVBP calculations [CFD127, CFD134]. However its assessment and validation still need some work, which will be mainly based on DNS. An example is the work done on the problem of the subgrid scale variance and dissipation of a scalar field [CFD41]. Another example is the study of diffusion flames stabilisation processes in a turbulent environment [CFD46].
To incorporate more realistic chemistry into AVBP [CFD102], multi-reaction schemes are needed in order to reproduce not only the pollutants formation but also the flame temperature (see Fig. 2.2). To this end, a new collaboration with IFP (A. Torres, G. Gauthier) has started in early 2000. A prototype multispecies version of AVBP, suitable for the implementation of multi-reaction kinetics, is now available at CERFACS.
In the field of LES, flame transfer functions have been computed for various geometries. This information is the key data needed in global acoustic models for predicting the stability map of the combustion. Transfer functions obtained from AVBP calculations are being compared to measurements performed on both academic (ICLEAC european project and SNECMA CIFRE thesis, experiment done at EM2C) and more industry oriented burners (Siemens KWU, experiment done at Univ. of Karlsruhe).

CERFACS is also involved with Ecole Centrale de Paris (Laboratoire E.M2.C.) and CORIA in a project supported by the COS (Comité d'Orientation Supersonique) program, to study new combustion technologies for supersonic flight. CERFACS and CORIA develop models and Ecole Centrale performs an experimental investigation to validate LES models.

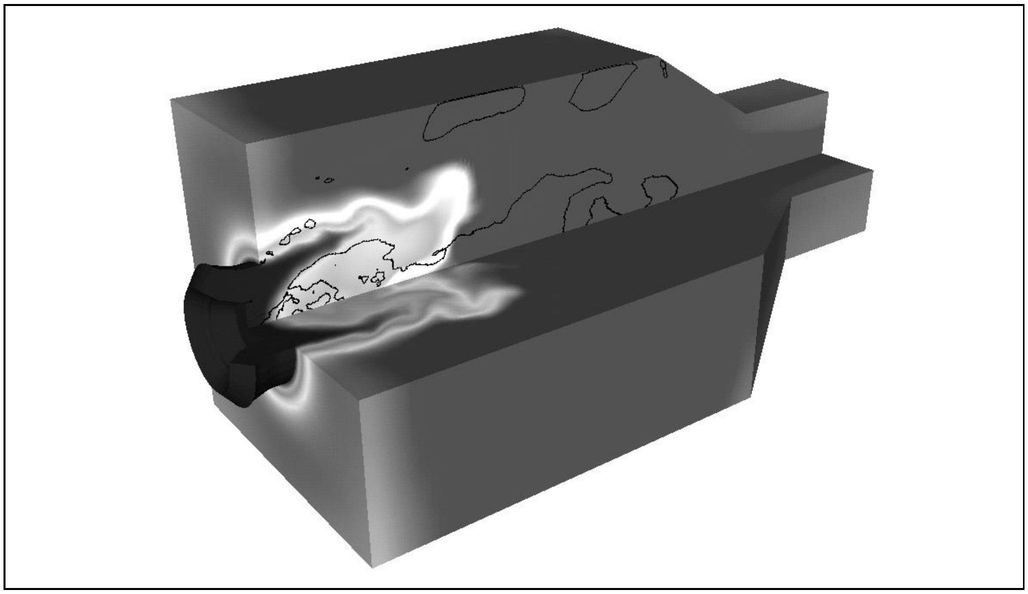

Figure 2.2: LES of combustion in a gas turbine (temperature field).

2.1.3 Reduced kinetics for LES of combustion (K. Truffin, G. Lartigue)

Being able to include more complex kinetics into LES is a necessary condition for the future. CERFACS has investigated various reduced schemes to reach this goal, first for methane / air combustion, starting from two steps schemes up to four steps. Results obtained with the classical Jones Linstedt scheme have proved to be interesting since they provide correct flame structures at a reasonable cost (Fig. 2.3). These schemes will be implemented into AVBP in 2002.

2.1.4 Flame/acoustics interactions (A. Kaufmann, L. Selle, F. Nicoud)

In practice, it is possible to introduce acoustic perturbations in many different ways in a stable calculation. Not all these techniques lead to reliable results in terms of flame transfer function. Both analytical and numerical work have been done in order to study the way a flame should be excited in a LES [CFD98].

2.1.5 Flame/wall interaction (F. Dabireau, A. de Lataillade, B. Cuenot, T. Poinsot)

CERFACS has developed a strong expertise in the field of flame/wall interaction since 1995, both for piston engines and rocket engines applications. These studies have addressed the case of premixed flames interacting with cold walls. Since 2000, a new project has been started, supported by CNES and SNECMA/DMF, to perform DNS's of H2/O2 flames interacting with an isothermal wall. This mechanism is essential for the design of nozzles in rocket engines.

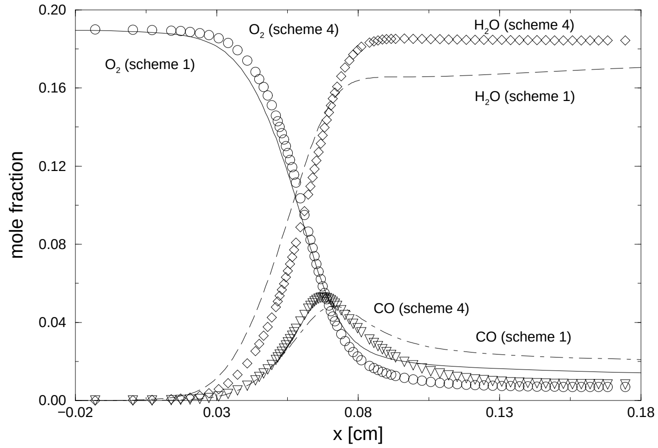

Figure 2.3: Premixed flame structure for a methane / air flame computed with a full chemical scheme (1) and with a four step scheme (4).

2.1.6 Atmospheric pollution (B. Cuenot, R. Paoli, F. Laporte, F. Cousin)

Two projects support the activity related to atmospheric pollution. One is a regional project PREPA (coordinated by Météo-France, CNRM Toulouse), started in january 2000. Work has been performed on the problem of the subgrid scale segregation of reactive species [CFD77]. This work is now continuing at CNRM and Laboratoire d'Aérologie through a PhD thesis (supported by CNRS and ADEME).
The other project is supported in the framework of the Comité d'Orientation Supersonique (COS). CERFACS is involved to perform reactive simulations of airplane wake, as started in April 2001.

2.2 Non-Reacting Flows

2.2.1 DNS of two phase flow modelling (A. Massol, F. Ducros)

The modelling activity in the field of two phase flow has started through the collaboration with EDF and IMFT (O. Simonin). The issue is to measure the transfer coefficients (momentum and passive scalar) between the flow and an array of particles. The analysis is conducted through DNS performed with AVBP (Fig. v in the appendix). The underlying motivation is to improve the heuristic laws generally used for such transfers for both the Lagragian/Eulerian and the Eulerian/Eulerian modellings. The first step has been to estimate the validity of existing drag laws for fluidized beds, in order to propose new and improved correlations.

2.2.2 Assessment of U-RANS and related V-LES techniques: (B. Caruelle, F. Ducros)

The main results here show a comparison between LES, U-RANS using the Spalart-Allmaras model and the Detached Eddy Simulation (DES) approaches on various test cases from attached boundary layer to full transonic 2,5 airfoil profile. The DES is shown to behave better than other investigated modellings for buffeting (under restrictions that have been determined and discussed [CFD60]). As already said in the introduction, the PhD thesis of B. Caruelle received the first BMW scientific award contest.

2.2.3 LES modelling fundamentals: (C. Jimenez, B. Cuenot, F. Ducros, F. Nicoud)

Theoretical work on LES modelling has continued in order to propose and/or improve new formalisms with high potential.

- a former work related to the filtered standard models based on resolved turbulents scales has come to an end with the assessment of a clear formalism ([CFD66]). This kind of model is routinely used in AVBP (on the filtered Smagorinsky form) for many contracts (see Fig. i in the appendix).
- a generalized relaxation procedure has been set up in order to stabilize and control the variation of the constant coming along with the standard dynamic procedure. This produces a new family of dynamic models, strictly local in space and stable enough to be used without clipping or averaging procedures ([CFD10]).

  These two works have been done in collaboration with ONERA Chatillon.
- The previous model for the subgrid scale (SGS) variance has been checked against a-priori tests ([CFD41]). Moreover it has been extended to take into account the numerical dissipation brought up by the scheme as a source term in the SGS variance transport equation ([CFD37]).
- The DES technique proposed by Spalart (Boeing) some times ago has been assessed as a mean of treating the wall problem in LES. This fundamental collaborative work [CFD18] underlined some of the resolution requirements of this technique and helped to understand some results of Caruelle's thesis (see above).
- The fundamental work started in collaboration with the Center for Turbulence Research (Stanford University) about the design of optimal law-of-the-wall for LES [CFD116] has been continued during the 2000 Summer program [CFD26], leading to a better understanding of the limitations of law-of-the-walls for LES's.

2.2.4 Heat transfer calculation in RANS formulation (F. Dabireau, F. Nicoud)

The task of deriving law-of-the-wall is much easier for steady RANS than for LES. However, almost all the previous studies available in the literature assume that density is constant in the process of deriving the relationship between the velocity field and the wall shear stress. Two formulations accounting for the thermophysical variations [CFD17, CFD82] have been tested against DNS data for subsonic [CFD115, CFD15] and supersonic flows. These law-of-the-wall formulations have been implemented in AVBP and in N3S-NATUR, and performances have been compared.

3 Unsteady Flow Calculations on Hybrid Grids – The AVBP Project

This project covers the unsteady flow activities of the CFD team on unstructured and hybrid grids. These studies are mainly based on the CERFACS in-house solver AVBP, which is a parallel finite-volume CFD solver of the compressible Navier-Stokes equations. Structured, unstructured or hybrid grids are handled for 2-D, 3-D and axi-symmetric configurations. AVBP is primarily used to solve problems in the fields of unsteady turbulence and combustion. Through these activities the AVBP project is strongly interlinked to the “Modeling” project of the CFD-group. Since the modelling aspects of many of these projects have already been described in the “Modeling” section 2, this part focuses on numerical issues.

The success of the AVBP project was confirmed in 2000 and 2001 by several facts of both academical and more applied nature resulting in several publications in CFD journals [CFD4, CFD3, CFD22] and the PhD-thesis defenses of O. Colin [CFD61], J. Schlüter [CFD66] and J.P. Légier [CFD64]. The participation of CERFACS with AVBP to the turbulence summer program at Stanford University represents a second major scientifical event [CFD46].

On the industrial side the current contract with Siemens KWU has ended in 2000 to an overall satisfaction of both partners, which has resulted in a follow-on project of similar size in 2001. Discussions with SNECMA and Turbomeca have lead to the selection of AVBP as the main LES code in the PRC Combustion, a national program funded by DGA. This confirms the interest in AVBP expressed by French gas turbine manufacturers to perform LES. Similar discussions are underway with Institut Francais du Pétrole and PSA to use AVBP for LES in piston engines.

Two-phase flows are now becoming one of the essential research topics for AVBP. CERFACS shareholder EDF has manifested his interest through a PhD thesis conducted in the field of two-phase flows. The new PRC combustion discussed above also focuses on LES for two-phase flows. On a more political level, a decision was made at ONERA to evaluate the capabilities of AVBP and to collaborate on two-phase flows: the code was delivered and installed in Toulouse and Chatillon in 2000. Finally, preliminary activities in the challenging domain of bio-medical blood flow simulations (conducted in collaboration with Toulouse University Hospital) has broadened the application spectrum of the AVBP solver.

Current bilateral links to industry have been pursued with EADS Missiles Division, SNECMA, SEP and Siemens KWU in Germany, while contacts with Alstom Power in Switzerland have resulted in a PhD thesis started in 2001 and two additional PhD in the framework of the EC project Fuelchief accepted in 2001. Therefore, the AVBP solver is now employed in multiple ongoing FP’5 European Programmes. Finally, the code is proposed as module of the hands-on training course for final year master students in fluid mechanics at ENSEEIHT engineering school in Toulouse.

These increasing activities have resulted in the beginning of four new PhD students at CERFACS in 2000 and six in 2001 together with the opening of a first software support engineering position. In 2001, more than 25 people were working full-time on AVBP, amongst them 15 PhD theses at CERFACS, Institut Français du Pétrole, IMFT and Ecole Centrale Paris. The overall code management and integration tasks are centralized at CERFACS.

3.1 Code Engineering (Y. Sommerer)

The rising importance of code engineering aspects was expressed in 2000 through the opening of an engineer position, reflecting the need to provide a complex software tool, that is reliable and fast, robust and user-friendly (where all conditions have to be seen in the context of a research code). Although in 2001 a preliminary prototype version of a two-phase flow module in AVBP was written, no spectacular modifications were incorporated into the releases of AVBP 4.4, 4.5, 4.6 and 4.7. Both two-phase flow capabilities (AVBP TFP) and also multiple-species features (AVBP 5.0) constitute the next major release scheduled in 2002.

The “QPF - Quality Program” for the verification and validation of AVBP has been pursued. This enables to continuously ensure the solution quality of the solver. The numerical methods and physical models are validated on academic test cases before their application to complex geometries.

The current version of AVBP is still built upon the parallel library COUPL which was developed initially in collaboration with the Oxford University Computing Laboratory (OUCL). This generic library of subroutines aims to free the non-specialist user from the need to consider aspects of high performance computing such as data partitioning or message passing.

3.1.1 Pre- and postprocessing tool and documentation (A. Kaufmann, T. Schönfeld, Y. Sommerer)

In 2000 an important action was initiated to further improve and harmonize the pre- and postprocessing tools around AVBP. These tools are essential for the exploitation of time-dependent flows and allow to post-processes the solution files: statistics of unsteady turbulence (LES), recording and flow tracing at selected points, evaluation of integral mass flux values across in- and outlet boundaries, etc. The toolbox has been partially rewritten in Fortran90 language, which renders the routines independent from the COUPL library and significantly increases their portability.

The documentation has followed the general trend away from paper support towards Internet help menus: the previous “AVBP User’s Manual” has become on-line and the resulting “AVBP Help Desk” contains a summary of various help menus, bug reports, news infos, FAQs and a flow chart. In addition, the “AVBP HandBook”, that represents a collection of individual technical notes, has been updated and is available in classical paper form which can be downloaded as pdf-File.

3.2 Numerical Methods and Grids

3.2.1 Numerical schemes and boundary conditions (O. Colin, F. Nicoud)

A set of several new boundary conditions has been implemented into AVBP [CFD15], in order to satisfy the various aspects related to unsteady flow simulations in internal geometries: pulsating inlet conditions, relaxation of all three velocity components and the temperature towards target values (while preserving a non-reflecting behavior), swirled flows conditions, etc. A novel integral formulation allows to impose integral values for the mass flux at inlet and outlet boundaries. The main area of application for this new boundary condition are combustion instabilities, where often only integral values of the experimental data are available at inlet sections.

Another development was tested to increase the computation speed for low velocity flows by rescaling the sound velocity: it enabled significant CPU reduction for these cases [CFD6].

3.2.2 Computational grids (J.-D. Müller, T. Schönfeld)

One of the main characteristics of AVBP is the capability to handle cells of different types within the frame of the same mesh. With the use of these hybrid grids, one aims to combine advantages of structured and unstructured grid methodologies. One of the clear benefits of using hybrid meshes is the ability to minimize the number of grid points and to optimize their position in the global grid.

Most grid related aspects (like grid adaptation or the extrusion of 2-D grid towards 3-D grids) are handled by the grid manipulation tool 'hip', developed by J.-D. Müller (now at Belfast University). New features are implemented frequently into hip, such as new file formats but also routines that allow for generic 1-D cuts in an unstructured grid or the interpolation between two arbitrary grids.

In a feasibility study, conducted in 2000, the existing adaptive local grid refinement tool for steady state external flows has been extended to time dependent cases [CFD51]. The method has been applied to unsteady flows through the usage of a C-shell script that couples the grid refinement module of hip with the CFD flow solver AVBP. Fig. 3.1 shows the locally refined domains of the computational grid for the reactive flow in a combustion chamber. The grid is adapted on the gradient of the temperature and nicely captures the steep gradients across the flame front. The work has evidenced certain limitations of the local grid refinement method when applied to unsteady flows. Most importantly, the very small cells can result in unrealistically small time steps. Further, in the context of rapidly moving flow features (like a flame front) de-refinement capabilities and frequent adaptation steps are crucial, but slow down the overall computing times. The entire procedure must be developed in a parallel framework. This work will be intensified in collaboration with IFP: an ALE formulation is now available in AVBP to compute flow in moving meshes and the strategy to handle variable meshes now becomes critical; it will be the topic of a PhD thesis at CERFACS starting in 2002 with the support of IFP.

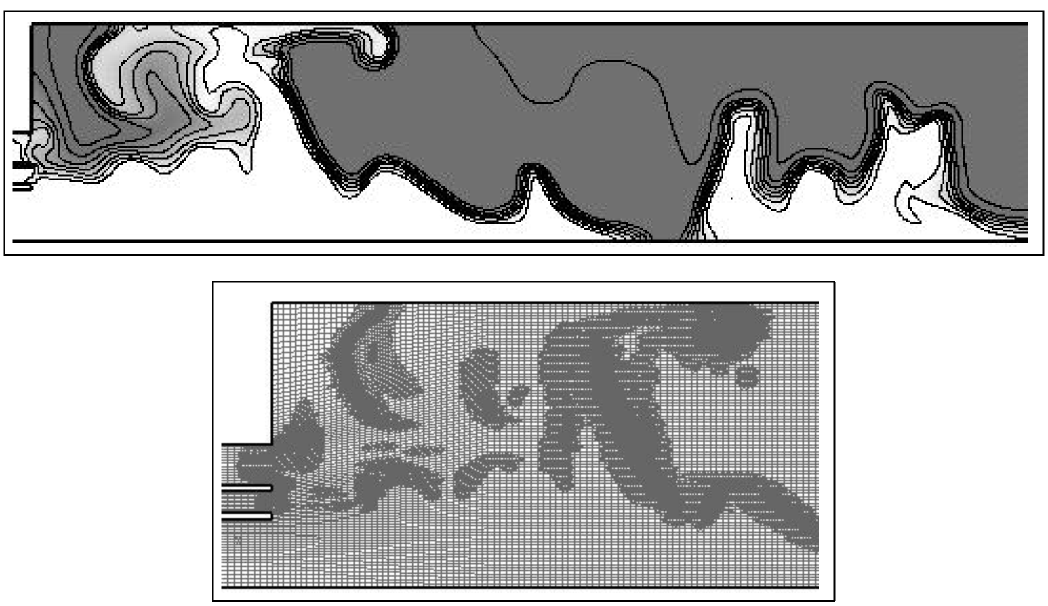

Figure 3.1: Global view of temperature field and final adapted grid (zoom of inlet section).

3.3 Selected Applications

Many projects performed with AVBP have already been described in the "Modelling" chapter 2. The present section only presents some additional specific examples involving issues related to numerical techniques and AVBP.

3.3.1 Bio-medical blood flow simulations (JB. Mossa, F. Nicoud, T. Schönfeld)

Flow simulations in the field of bio-medical applications represent a new activity explored in 2000 [CFD53]. The new integral boundary conditions presented above, have been successfully applied for the blood flow simulations in cardio-vascular systems such as the thorax aorta shown in Fig. 3.2.

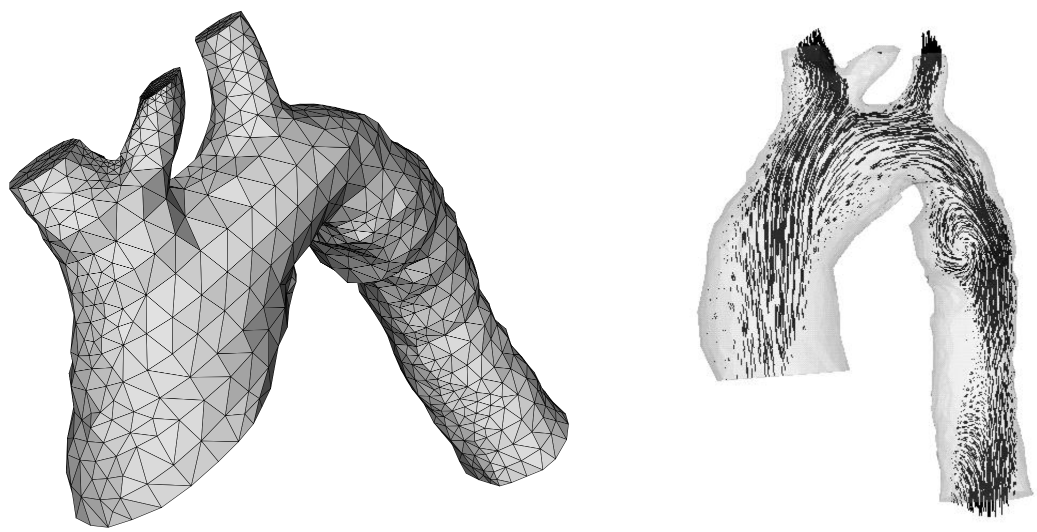

Figure 3.2: Surface grid of thorax aorta (left) and velocity vectors indicating a recirculation zone.

3.3.2 Development of a two-phase flow Euler / Euler LES solver (A. Kaufmann, JB. Mossa, F. Ducros, B. Cuenot)

The capacities of AVBP for gaseous reacting flows are now sufficiently clear to recognize that a step must be taken to move to two-phase flows. The choice of CERFACS has been to address this problem from a novel point of view: instead of using a Lagrangian formulation for droplets and coupling it to the gas equations, it was decided to write a full Euler Euler code. This involves first a number of numerical challenges linked to the coupld resolution of the two phase set of equations. A beta-version of the code resolving the basic Eulerian/Eulerian compressible transport equations for particles laden flows has been written in AVBP and tested in 2001, mainly to check numerical stability issues. Many points have been discussed with O. Simonin (IMFT/EDF). A more elaborated implementation has been started motivated by an enhanced interest expressed by industry. The related work will be the basis of the PRC combustion in collaboration with ONERA-Toulouse: during this program, both Euler / Lagrange (at ONERA) and Euler / Euler formulations (at CERFACS) will be tested for LES in AVBP. This will also allow comparisons between both approaches.

3.3.3 LESFOIL – Unsteady computations over an airfoil (F. Ducros)

The European LESFOIL project has ended in 2000. During this project many problems have been investigated: numerical stability for complex geometry simulation, cross comparisons between wall-resolved and wall-functions for LES and between structured and unstructured solvers. Most of the results confirm pioneering results previously obtained at CERFACS [CFD25]. In particular, it is shown that the use of wall-functions (developed in both the AVBP and NSMB solvers) yields acceptable results concerning flow separation, but reveals strong difficulties to deal with transition near the leading edge.

4 Advanced Aerodynamics and Multiphysics

In the field of aerodynamics and modeling for fluid dynamics the objectives of the CFD Team are 1) the development of reliable, efficient and accurate predictive CFD softwares for their use in industrial environment, 2) the numerical investigation of complex flow physics making use of high-performance computing.

The CFD Team develops physical models to study flow fields in and around complex geometries. These models must be implemented in efficient solvers to be tested and used. Two numerical tools are used and developed at CERFACS for aerodynamics: 1) NSMB has been the main code for aerodynamics since 1993 and now is the production tool for Navier-Stokes computations at Airbus France, 2) for the future, a significant step in code technology has been taken with the introduction of *elsA* at CERFACS during last quarter 1999. With the help of advanced meshing techniques, convergence acceleration strategies, numerical algorithms and vectorization/parallelism implementation, NSMB has reached today a sufficient level of robustness, accuracy and efficiency for steady state aerodynamics around complex industrial geometries. In particular with the use of advanced meshing techniques (General Patched Grid, Automatic Mesh Refinement AMR) developed at CERFACS, structured grids around complex geometries can be strongly optimized. An engineer has been recruited in 2001 to improve the integration and versioning processes at CERFACS. To benefit from new expertise on high-order schemes and turbulence modelling two new members, proposed by CERFACS, have joined the NSMB consortium: ENSAM-Paris (2000) and IMF-Toulouse (2001). Nevertheless, for such large codes as NSMB, the Fortran 77 language suffers from a lack of readability and of modularity. Amongst other, for this reason, ONERA and Airbus France have launched the *elsA* project which is a CFD code written in C++. Since 2000 CERFACS has been involved in the development of *elsA*.

The year 2000 was the beginning of the involvement of CERFACS in the CFD software platform *elsA* with just two person working in *elsA*. That work was done under a contract between Airbus France, ONERA and CERFACS dubbed '*elsA*/NSMB tighthening'. The aim of that contractual activity was to

1. enable eventually the possibility to swap production calculations from NSMB to *elsA* without the usual "learning curve" coming with the use of new software tools. This could be done by ensuring the commonality of the methods and of their results in NSMB and in *elsA*;

2. create in the CERFACS an *elsA* development team with the NSMB background and experience;

3. establish an efficient working relation with the original *elsA* developers in ONERA;

4. transfer development activities from NSMB to *elsA* progressively;

5. in the near future, transfer of the applications/modeling activities from NSMB to *elsA*.

During that 2000-01 period the *elsA* team in CERFACS has grown from two to six people :

- during the year 2001, two staff members have joined to help with the development activities on the *elsA*/NSMB "tightening project": the adaptation of ONERA's "Local Multigrid" (aka AMR) for Euler flows to 3D turbulent flows on the one hand, and preliminary development work on Multigrid on the other hand.
- the transition from development-only team to modeling and new application has begun: modification to the turbulent transport equation schemes to ensure robustness of the Spalart-Almaras model, turbulence models with the development of the Durbin ($k, \varepsilon, v'^2 - f$) Model.

One have to point out the structuring effect of the 'NSMB/*elsA* tightening' contract to the organisation and methods for collaborative development of CFD codes. For the ease of complex development at different locations with people from different organisation, the ONERA/DSNA has setup a web site *http://elsA.onera.fr* where information and documentation is shared.
The willingness of the ONERA and CERFACS to work together has motivated the signature (march 5, 2001) of an ONERA / CERFACS cooperation agrement on *elsA*.

The year 2000 has been a transition year for several reasons:

i. The end of WAVENC (19 Jan.) and MFLAME (15 Mar.) of the FP'4;

ii. The kick-off of S-WAKE (20 Jan.) and C-WAKE (21 Jan.) of the FP'5, CERFACS is Work Package manager of all activities related to numerical simulations and modelling. The kick-off of OCMATH Regional Program (26 May);

iii. The launch and development of the hypersonics activity in close relation with EADS Launch Vehicles and CNES;

iv. The growing involvement of the team in the *elsA* project;

v. The arrival of several new researchers in the team related to the development of these new activities.

4.1 Numerical Aerodynamics

4.1.1 Wake vortex characterisation of high-lift aircraft (A. Benkenida, G. Jonville, G. Puigt, D. Darracq)

In the frame of the C-Wake program, inviscid simulations of the lift-induced wake around full high-lift aircraft grid systems have been deeply investigated with NSMB. Parametric studies have also been carried out. It has been demonstrated by CERFACS that, if the numerical dissipation is carefully controlled, the wake vortex system could be predicted even in the extented near field (13 and 6.5 wingspans for, respectively, the NLR-SWIM generic model [CFD29] and the DLR-F11 realistic model [CFD28]). It should be noted that other European CFD codes involved in C-Wake used by INTA (Spain), CIRA (Italy), DLR-EA (Germany), BAe Systems (United Kingdom) and CFD-N (norway) can only resolve the wake vortices until 1-2 wingspans.

4.1.2 Wake vortex dynamics (F. Laporte, H. Moet, D. Darracq)

Wake vortex instabilities are a promising way of reducing the trailing edge wake vortex hazard on a following aircraft during approach or take-off phases at an airport. With the support of the EC (C-Wake, S-Wake, WakeNet) and of the aeronautical industry (Airbus), CERFACS has developed a strong expertise on this topic. By the means of LES, CERFACS has provided numerous analysis of the effect of the turbulence on a vortex sytem: decay, short-wavelength and long-wavelength instabilities. CERFACS is investigating this domain by use of numerical methods through a close collaboration with CNRS-IRPHE and Airbus France, leading to a patented device. NSMB has been improved to handle such flows in the following manner:

1. automatic adaptative time step selection based on error evaluation;
2. injection of turbulence by the means of a characteristic boundary condition;
3. extrapolation from numerical/experimental inlet plane.

This activity is still strongly supported by Airbus and EC.

4.1.3 Flight Dynamic Coefficients (J. Cormier, S. Champagneux, P. Guillo)

The CERFACS was involved in this field of research since 1998 [CFD34]. This work was initialized both by EADS Missiles and Airbus France for the evaluation of missiles and aircraft stability. Its results are useful for areas such as flight dynamics or systems. The final aspects consisted for the largest part of the validation and the evaluation of the method previously implemented in the CFD code NSMB for steady configurations [CFD75]. It has been compared to traditionally employed semi-empirical methods (ESDU) and has permitted to assess the field of relevancy of each method. The swept-back ONERA M6 wing has been considered in a wide range of flying conditions [CFD93]. Now, the numerical method provided to Airbus France has reached the level of a design tool within the framework of "steady" coefficients for pitching, rolling and yawing movements. The computation of "unsteady" coefficients, which is very close to aeroelastic studies in terms of numerical ingredients to implement and validate, is the next step to be considered.
In the frame of the European Project AWIATOR starting in June 2002, CERFACS will produce the analysis of the damping derivatives coefficient of a full aircraft equipped with large winglets by means of RANS simulations.

4.1.4 Turbomachinery Flows (L. Kozuch, R. Struijs, C. Martin, A. Fiala, D. Darracq)

The NSMB team has started turbomachinery activity at the end of 1998, in the frame of a regional contract (OCMATH) involving Liebherr-Aerospace Toulouse (LTS), Technofan and Ratier-Figeac as industrial partners. Specifically, LTS is interested in the noise generated by the fans they produce and CERFACS is to perform an unsteady calculation accounting for inlet distortion. The aerodynamic results will be used as input for the acoustic code used by LTS. At the present time, steady computations have been performed using Baldwin-Lomax turbulence modeling. The turbomachinery use of NSMB has been validated by comparing both aerodynamic and acoustic results with those obtained with an industrial turbomachinery code (BToB3D), using the same mesh. NSMB is also being validated on a turbofan test case, by comparison with experimental data. With the phase-lag technique, a major step towards the unsteady simulation has been made by developing a boundary condition allowing to compute a single blade-to-blade passage in the case of periodic flow. An inlet distortion has been simulated with this technique.
In the frame of the development of the analysis of the acoustics generated by turbomachines, CERFACS has fulfilled a contract of collaboration with the laboratory of Ecole Centrale de Lyon.

4.1.5 Propeller aerodynamics (G. Grondin, X. Escriva, D. Darracq)

Within the frame of the OCMATH region contract, the CFD team has started propeller activity in 2000. Ratier-Figeac is particurlarly interested in the prediction of aerodynamics around advanced high-speed propellers for aeroelastic analysis. CERFACS has developed parallel meshing techniques aiming at

performing steady and unsteady calculations around rotating propellers.
At the end 2001, a collaboration started with Airbus France on the A400M military aircraft project to provide CFD tools for aerodynamics 1) rotor-stator interaction making use of sliding-mesh technique, 2) damping derivatives of a propeller modelled by an actuartor disk (see Figure ii in the appendix).

4.1.6 Axial fan optimization (C. Martin, B. Marquez)

In the OCMATH project framework, a set of axial fan computations has been achieved in order to provide the TECHNOFAN society (SNECMA) with the most reliable settings of its CFD solver. These settings, guidelines and results can be consulted respectively in [CFD107] and [CFD108]. Through a collaboration contract with the laboratory of ENSICA, CERFACS is now involved in a an axial fan optimal design process so as to evaluate its efficiency in the TECHNOFAN fan design process.

4.1.6.1 Perfect gas computations of high speed flows (S. Champagneux, B. Marquez, G. Grondin)

The objective was to prove that the CFD code NSMB possesses the necessary numerical features to compute the flow around complex 3D geometries in hypersonic flight conditions assuming the gas to be perfect. The final test case, the flow around a re-entry capsule called ARD (see Fig.4.1) at a Mach number of 15, has been successfully computed with the restrictive assumption of dealing with a perfect gas. Numerical schemes, physical modeling of turbulence and computational strategies have been widely investigated to provide EADS Launch Vehicles an efficient way to compute such configurations. The CFD code NSMB has been delivered to EADS Launch Vehicles and is now used for various applications.

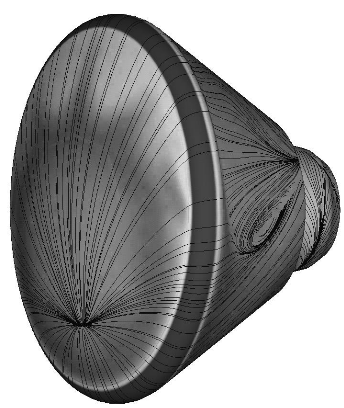

Figure 4.1: Perfect gas hypersonic viscous flow around the ARD: skin friction lines.

4.1.6.2 Real gas computations of high speed flows (Y. Stiriba, M. Duloué, G. Grondin, D. Darracq)

The NSMB code has also been extended and adapted to predict flows at chemical and thermal equilibrium using the upwind AUSM+ scheme in space, and the implicit LU-SGS (Lower-Upper Symmetric Gauss Seidel) in time. Air was modelled as a mixture of five species: O, N, NO, O_2 and N_2, with three chemical reactions. Thermodynamic properties were computed using Park's model. Validation of the new code was obtained for hypersonic flows around two different blunt bodies. Initially, the first order methods combined with the MUSCL reconstruction have been tested for a $2D$ hypersonic viscous flow with $M = 18$ around a cylinder. The second test was the $3D$ viscous flow around the ARD reentry vehicle with flight conditions provided by EADS Launch Vehicles.

4.1.7 Numerical Simulations of Crosswind Inlet Flows at Low Mach Numbers (S. Champagneux)

Work on this topic has been completed this year within the context of a contract with Airbus [CFD72]. Numerical tools developed during this study have been included in the official version of the CFD code NSMB. Cross-functionalities have been extended and verified (implicit, multigrid, central and upwind schemes) leading to an efficient and precise tool for solving inviscid, laminar and turbulent flows at all mach numbers with this compressible CFD code. The final study conducted at CERFACS consisted in the evaluation of the total pressure distortion that occurs in the fan plane of a nacelle in crosswind with its engine running when the aircraft is stopped at the ground just before taking off. This application has been applied on a generic shape of nacelle. Now, this tool is used by designers for realistic configurations at Airbus.

Finally, Ralf Heinrich from DLR-EA spent a three month period at CERFACS to implement this kind of method in the DLR Tau code.

4.2 Numerical Methods and Software Engineering

4.2.1 Finite Element Method in Unstructured Meshes (G. Chevalier, F. Ducros, B. Marquez)

The work on that field has followed three axis.

- first a work on the Domain Decomposition and preconditioning, with firstly the implementation of the ILDU method in an official version of AETHER, and secondly other improvements such as introduction of explicit Runge-Kutta scheme, variables interpolation, LES modeling. All these developments have been directly delivered to Dassault Aviation in an official version of AETHER;
- second a work concerning the modeling relative to the LES of complex unsteady flows. This work has involved the development and validation of two formulations of wall functions, validated on standard periodized channel flow. CERFACS has also collaborated with Dassault Aviation through the LESFOIL EC program, sharing expertise and data on the subject ([CFD89]);
- following the work on the preconditioning, a study has been conducted on the influence of the node numbering on the robustness and efficiency of the preconditioning. This was done on different types of preconditioning.

4.2.2 Meshing techniques (J. Bohbot, J.-Ch. Jouhaud, M. Montagnac, D. Darracq)

Grid generation is a crucial problem for the computation of complex aircraft configurations using a body fitted structured code. Furthermore, due to the data management of structured grids, the local refinements around the CAD (boundary layers, stagnation lines, wakes) will be propagated through the whole grid even in zones where gradients are expected to be low. This can lead to very large grids, especially for complex geometries. Two approaches permit to reduce this drawback: i) conservative patched grid, ii) automatic mesh refinement.
CERFACS is developing these techniques in order to help Airbus France in reducing the turnaround time and in enhancing the flow accuracy on a given grid size. These two meshing techniques have been implemented and validated in NSMB.

4.2.2.1 Conservative Patched Grid (CPG) (M. Montagnac)

The purpose is to develop an efficient way to simplify the grid generation and to deal with complex configurations using moderately sized grids. The approach has been chosen to use NSMB on meshes having no coincident interfaces. For this kind of meshes, blocks must have common interfaces but do not need the same location of grid nodes. This approach avoids mesh propagation from a block to another block. The flexibility of this kind of mesh allows mesh refinement and makes it easier to cluster grid points. A 3-D conservative patched grid algorithm using Jameson centered scheme has been implemented in NSMB. The Multigrid acceleration convergence technique has been extended when using patched grids strategy. The parallel programming has been implemented to maintain the CPU performance of the NSMB code. The efficiency of the method has been demonstrated on complex geometry. The wake vortices behind a civil aircraft (DLR-F11) have been calculated on ten processors using a grid containing 3 millions nodes with non-coincident interfaces (Fig.4.2).

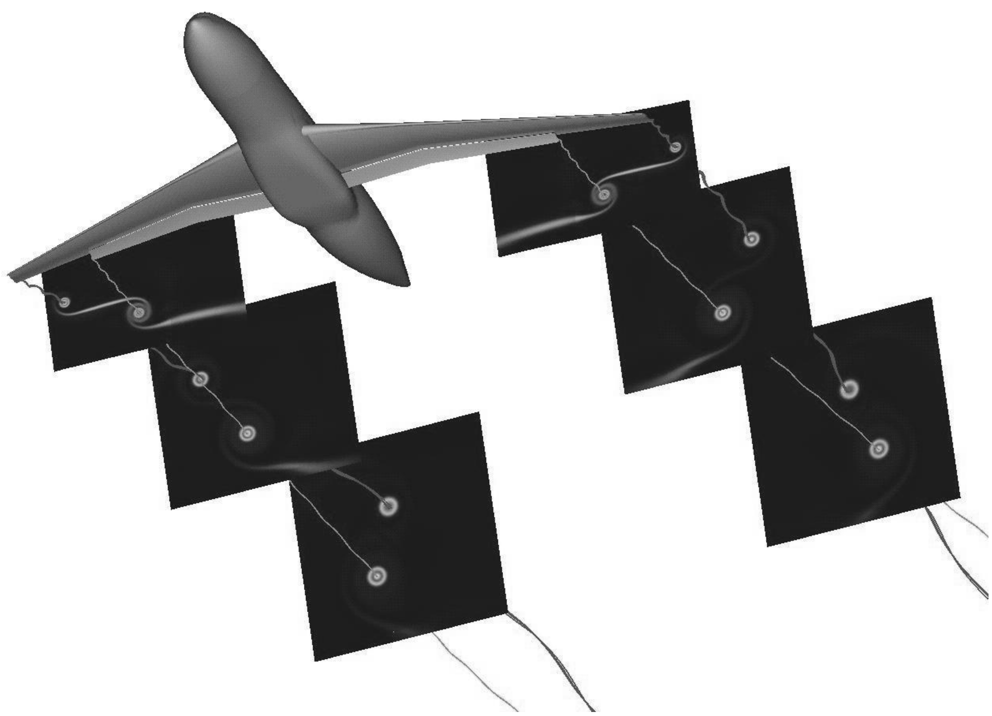

Figure 4.2: Flow simulation behind a civil aircraft during the landing configuration. Application of the AMR technique.

These CPG techniques were also developped in *elsA* as a product of the NSMB/*elsA* tightening. Full totally non-coicident patched grid techniques for 3D turbulent flows were implemented in the *elsA* code. Special care was also taken to ensure the use of these techniques when computing on parallel computers. An example is shown in the Fig.iii in the appendix for a 2D turbulent application : the RAE 2822 test case.

4.2.2.2 Adaptive Mesh Refinement (AMR) (J.-Ch. Jouhaud, M. Montagnac)

Another approach is to enrich the mesh with a hierarchical grid structure, that is to say using an Adaptive Mesh Refinement Strategy (AMR). It consists in splitting a cluster of grid cells in a characteristics regions (shocks, boundary layers, wake vortices, ...) and to automatically join these cells in new blocks. The activity on AMR has increased over the period with a new algorithm to improve the method. In particular, a parallel implementation has been realized. In the next phase, extension to viscous flows is planned.
The efficiency of the method has been demonstrated on a complex geometry. The wake vortices behind a civil aircraft (F11) have been calculated on ten processors using a grid containing 1.5 millions nodes with two levels of refinement.

The most recent investigations were realized within the *elsA* tool. Two major objectives were reached. Firstly, the extension of the AMR method to turbulent transonic flows. Secondly, the addtion of local time increment prolongations, as in standard multigrid strategies, in order to increase the convergence rate. The RAE airfoil and the AS28 wing test cases have shown the efficiency of this new AMR extension (Fig. iv in the appendix).

4.2.3 Spalart-Allmaras (H. Pascal-Jenny)

In the framework of '*elsA*-NSMB' convergence activities, the update of the one equation turbulence model functionnalities for a production-level use has been addressed during year 2001. This topic follows the work previously realized for the algebraic turbulence model of Baldwin-Lomax. The LU-SSOR implicit algorithm extension to the well-known Spalart-Allmaras (SA) turbulence model has been transfered from the NSMB code to the *elsA* software. Specific treatments (unknown's positivity monitoring, parallelism, ...) have also been implemented leading to a robust and efficient solver for the computation of turbulent flows over full aircraft configurations. The extension of the multigrid algorithm to the SA model is in progress and will be finalized during the beginning of year 2002. These activities are part of a contract with Airbus France with the goal of providing the same level of efficiency with both softwares in order to switch from one to the other in a transparent way inside the design process.

4.2.4 MAEVA (H. Pascal-Jenny)

During year 2001, CERFACS has seen a growing involvement in the developpement of the *elsA* software through the MAEVA project (Modelisations Aerothermiques des Ecoulements en Ventilation Avion) between Airbus France and ONERA. Indeed, CERFACS has been in charge of implementing a new turbulence model dedicated to strongly thermaly coupled flows (impinging jets for instance), namely the $(k, \varepsilon, v'^2, f)$ model of Durbin. This model is described by 3 additionals transport equations (k, ε, v'^2) and another one for f which is elliptic. An explicit version of the model has been implemented in the *elsA* software this year and validations are in progress. Extensions are scheduled for the year 2002.

4.2.5 Development and implementation of a wake vortex model in flight simulators (H. Moet, G. Grondin, D. Darracq)

In the framework of the S-Wake program, the CERFACS is involved in the safety aspects of aircraft wake vortices. An engineering wake vortex behaviour model (called VORTEX) developed with the purpose to do probabilistic investigations has been improved by integrating several decay models which govern the decay of circulation due to turbulence, stratification, viscosity and crosswind. The effect of crosswind on wake vortices has been investigated in order to incorporate the effect properly in the VORTEX model. A new decay model accounting for aircraft parameters and atmospheric turbulence characteristics has been developed at CERFACS [CFD49]. An analytical model has been developed which is integrated in industrial (Airbus Deustschland) and research (TU-Berlin, NLR, TU-Braunschweig) flight simulator environments to perform parametric studies for wake vortex encounters. These parametric studies (including variation of vortex parameters) have the purpose to obtain the safety hazard for an encounter, to obtain handling criteria and to determine the influence of cockpit motion on piloted simulations. Furthermore, a numerical model is developed which uses a more realistic vortex velocity distribution is used for the same purposes as the analytical model and to simulate a more realistic wake vortex encounter and to investigate the effects of ’low-vortex’- designs of future very large transport aircraft.

4.2.6 Software engineering (J. Bohbot, S. Champagneux, J.-Ch. Jouhaud, Ph. Piras)

Dealing with the CFD code NSMB, the CERFACS is more than ever considered as the official provider as much from the Airbus France point of view as the one of EADS Launch Vehicles . Integration, management and validation processes have consequently been improved in order to face this responsibility in a reliable way (control versioning with both CVS (integration) and SCCS (development), testing over a wide range a representative test cases). Transferring, optimizing and benchmarking the CFD code NSMB on various parallel platforms have also been carried out and continued, motivated by both Airbus France as well as EADS Launch Vehicles for the renewal of their own computing facilities. Algorithm performance improvements and various optimizations have been realized leading to an increased efficiency of the code both on vector and RISC architectures. Finally, the harmonization between computational tools coming from CERFACS and Airbus France has been continued with the delivery and the use of new software (JEDM, GAME, LAMA3D) so that developers at CERFACS can work within an industrial environment in order to reduce the cost of the know how transfer when a development is completed.

4.2.7 Object Oriented CFD with *elsA* (M. Montagnac, G. Chevalier, S. Champagneux, J.-Ch. Jouhaud)

In the year 2000 the collaboration with ONERA has started on the object-oriented code named *elsA ensemble logiciel de simulation Aérodynamique*. The *elsA* software comes along with procedures to enhance productivity in a multi-user and multi-platform environment: validation database, unitary test cases, cvs management tools, software quality program. This work takes fully part of the framework wanted by Airbus France for the harmonization between NSMB and *elsA*.

The CERFACS *elsA* team was in charge of the conception and the development of the implicit time-integration LU-SSOR method as well as of the Baldwin-Lomax algebraic turbulence model with generalized distances. It has also contributed to write the specification and the user guide manuals. Some validation and unitary tests have been integrated in the corresponding databases too.

All developments have been tested on usual cases as 2D-3D multi-blocks sequential or parallel square nozzle, flat plates, NACA and RAE profiles. These developments were integrated in the official version of *elsA*.

The code has been installed on FUJITSU VPP700 and VPP5000 vector machines to run the S3CH configuration (see Fig.4.3) for Airbus France.

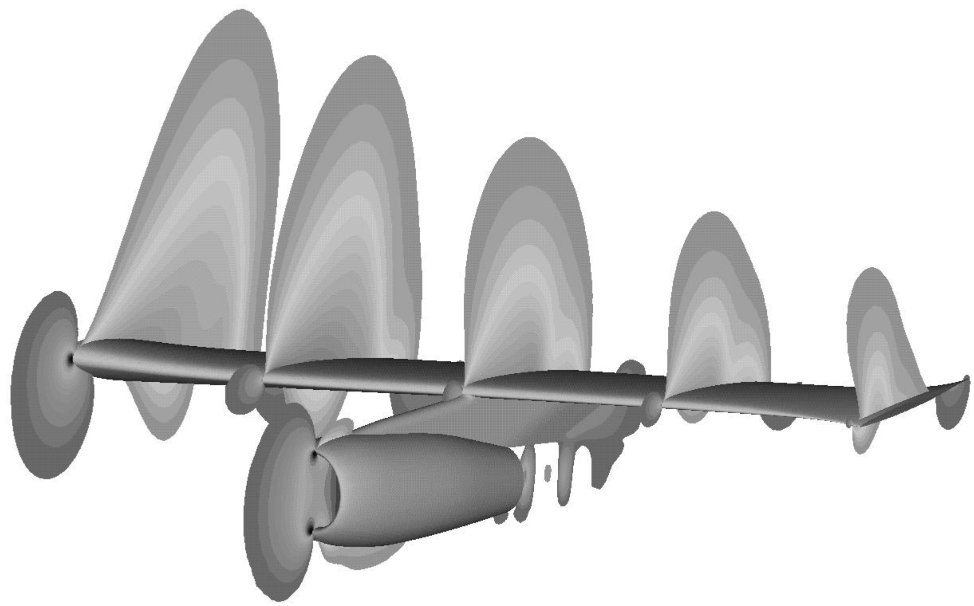

Figure 4.3: Cp distribution around the S3CH (wing+pylon+nacelle) configuration

4.2.8 CFD Team Support (S. Champagneux, M. Labadens, F. Dabireau, V. Roche)

This year, the CFD Team was involved in improving its communication by redesigning its website [CFD123] (*http://www.cerfacs.fr/cfd*). The most important work consisted in updating information about the team that now fit its current structure. A wide modernization has been conducted to make it more attractive, simpler to navigate and easier to maintain. A specific effort has been made to rationalize the management of the CFD Team bibliography that now consists of more than 600 references from year 1986 to 2001 from which some are available on-line.

5 Publications

5.1 Journal Publications

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4

Computational Electromagnetism

1 Overall presentation

A. Bendali

The team has carried on with its strategy of developing new methods and codes to address the difficulties involved in solving industrial and engineering problems related to propagation and scattering of electromagnetic waves. These difficulties result mostly from the very large size of the final system, due to the industrial requests to consider problems at higher and higher frequencies. The increase in size can also result from the consideration of small parameters related to the description of various objects: small details in the structure, a thin dielectric coating or substrate, a small distance separating two metallic sheets like those involved in patch antennas, etc.

The most important steps reached during the last two years can be described as follows:

- *General code:* Implementation of a high precision scheme for the computation of hypersingular integrals, implementation and parallelization of the so-called Combined Field Integral Equation, implementation of the extension of the code for the case of absorbing materials, studies related to simple and more accurate models for the feeding of a patch antenna, implementation of an `out-of-core` solver tailored for high performance parallel plateforms, treatment of the case of a metallic wire crossing the interface separating two different materials, test of some specific strategies to deal with deep cavities.
- *Fast multipole method:* Writing a new version of the multipole code in FORTRAN 90, implementation of the Combined Field Integral Equation, implementation of a novel way permitting to reduce the number of matrix multipole evaluations from four to two. The expertise accumulated in dealing with this intricate but powerfull technique has also been used to devise a novel and accurate way to perform the reconstruction of the electromagnetic field in the near zone of an antenna from the measurements of its far field patterns. Fully validated and implemented, this technique will provide a useful tool for CNES in the design of satellite antennas.
- *Prospective studies:* Robust effective impedance boundary conditions for scattering by metals coated by thin dielectric layers, deep theoretical study of the Després' integral equations, robust methods for domain decomposition solutions of scattering problems in the frame of an integral equation solution. N. Bartoli has defended her Ph. D. thesis which has consisted in a thorough study on the first two topics. At the time of writing, Y. Boubendir's Ph. D. thesis is close of being defended.

The overall policy of the team has been rewarded during the last two years by an important increase in the demand of collaboration coming from the industry. Joint studies with EADS on designing specific methods to efficiently deal with problems related to the scattering by a deep cavity have been followed this year by a closer collaboration on the multipole method. Meanwhile, the team has been approached for collaboration by several academic and industrial partners:

- KTH (Stockholm) for expertise in implementing boundary integral equations methods.
- ENAC (Toulouse) for a collaboration on boundary integral equations methods for micro-waves problems.

- DGA (French Ministry of Defense) for studies concerning some improvements in the multipole method relatively to the total cost of a matrix-vector product and its accuracy.
- CNES for numerical models of some special antennas and for a study of the influence of the environment of a antenna upon its radiation characteristics.
- CEA-CESTA (Bordeaux) for validation of electromagnetic codes for general problems and numerical models for a thin metallic wire crossing an interface separating two dielectric layers.

All these demands match the main axes of development of the team, which are still to develop an expertise in the treatment of large size problems through specific procedures and methods and to develop an as general as possible solver capable of solving microwaves problems.
The activities are detailed in the next parts. The scientific production of the team has resulted in the publication of two articles in internationally-reviewed journals and in several communications to international meetings. In 2000, two research lectures to specialists have been delivered by a member of the team at the invitation of KTH (Sweden) and INRIA (Sophia-Antipolis). In 2001, two members of the team have been invited to respectively deliver a plenary conference at the international workshop ”Grands systèmes linéaires” which has been held at INSA of Toulouse from 2 to 8 march 2001 and a minisymposium conference at the major international congress ”Computational Fluid Dynamic Conference” which has been held at Swensea, Englend, during august 2001.
Finally, let us mention that the researchers of the team are being asked to deliver high-level courses in academic institutions of Toulouse. N. Bartoli has indeed coauthored a book on stochastic algorithms [CEM1] last year.

2 Boundary Integral Equation Methods

2.1 The code CESC

M. Fares, A. Bendali, F. Collino

Much of the effort has been directed towards extending the capabilities of the code in terms of increasing the variety of problems which can be handled and the reliability of the results which are delivered. In this respect, the general solver code `CESC` has been extended in various directions:

- **Absorbing materials.** The code can now deal with absorbing materials. Dielectrics can be dissipative or present an absorbing magnetic permeability. This part of the code has been carefully validated through a comparison with similar codes developed by KTH.

- **Implementation of the CFIE.** The Combined Field Integral Equation is given in terms of a combination of the Electric Field integral Equation and the Magnetic Field Integral Equation. The MFIE requires the computation of singular integrals in the form

  $$\int_\Gamma \int_\Gamma \mathbf{n}_y \times \nabla_y \frac{\exp\left(ik\left|x-y\right|\right)}{4\pi\left|x-y\right|} \mathbf{J}(y)\cdot\mathbf{J}'(x)\, d\Gamma(y) d\Gamma(x)$$

  which were not available in the previous version of the code. Along with the implementation of the computation of these new integrals, a new version of the code improving the previous one has been written. As for the former parts of the code, the CFIE implementation has been parallelized to deal with large size problems. As a result, it has been used to validate the solution of the CFIE with the multipole method.

- **Accurate schemes for the computation of hypersingular integrals.** For problems involving a thin coating or a thin dielectric substrate, the singular integrals, having a singular part in $1/|x-y|^2$, include a kind of Dirac function when the domain of integration is a pairing of two parallel triangles separated by a very thin distance. Usual approaches fail to give accurate values for these integrals: a powerful procedure based on a recursive decomposition of the two triangles into small ones has been developed to obtain a correct approximation of these integrals, as well as of a case where the limiting value for an integral of this kind can be obtained exactly for its radiation.

  Figure 2.1 illustrates the improvement which results from the new procedure when the distance separating the two triangles goes to zero. Figure 2.2 shows that the accurate computation of these integrals are essential to prevent from meaningless results.

- **Patch antennas.** Patch antennas are commonly used as devices which can be conformed to the structure with powerful properties of emitting and receiving energy. Direct numerical modeling is important to predict their behavior. However, it gives rise to serious difficulties. CEA-CESTA has submitted a case where the determination of the gain of the antenna is decreased by a loss of accuracy near the resonance frequency. A simple scheme has been tried, which improves somewhat the calculation of the gain, although more progress has to be done in this direction. Also in connection with the patch antennas, accurate models of feeding the antennas are being implemented, specially by a coaxial feed.

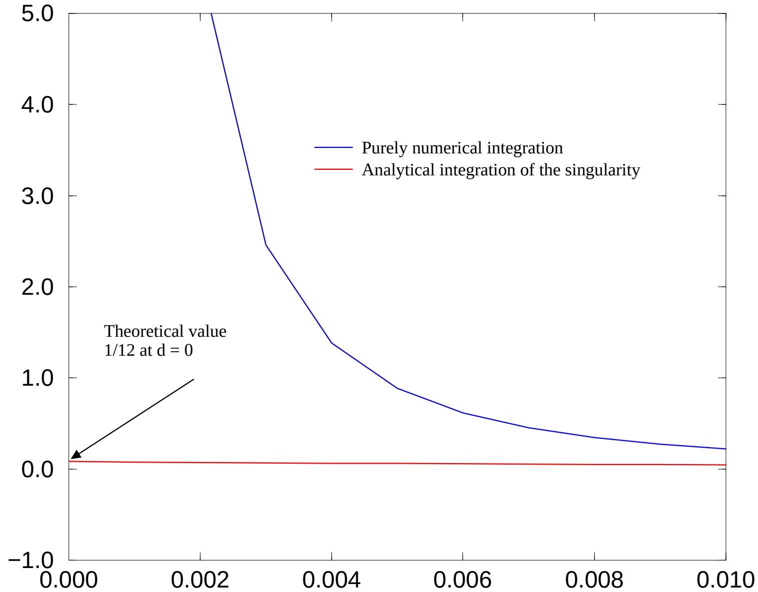

Figure 2.1: Plain numerical and analytical integration of the singularity

- **Validation of Electromagnetic Solver Codes.** For the last two years, the team has been involved in studies related to the validation of other Electromagnetic Solver Codes, mainly to deal with some extremely severe cases. Some parts of the solver code of KTH have then been validated, particularly for the test case proposed by Maci et all. [1] as a severe test to validate numerical codes and methods. In this context, a study related to a comparison of code `CESC` of CERFACS and code `ARLENE` of CEA-CESTA has also been conducted. The comparisons between the two concerned the computation of the RCS of a metal scatterer coated by a thin dielectric layer and the accuracy of the computation of singular integrals in some non standard situations. The results are reported in [CEM25].

- **Numerical models for wires crossing an interface between two media.** The possibility to deal with wires inside any dielectric medium has been added to the code `CESC`. This functionnality was previously limited to only the exterior infinite medium. The case where the wire is crossing the interface separating two dielectric media does not seem to have been dealt with, and requires a special treatment. Such a study has been conducted and has resulted in an accurate procedure. Figure 2.4 and Figure 2.3 depict an example of such a case and illustrates the accuracy wich has been reached by using the usual 1D model for the wire.

- **Out-of-core Solver.** An `out-of-core` functionnality has been added to code `CESC`. All the performances reached by the `in-core` version of the code, particularly in terms of taking advantage from parallel plateforms, remain inchanged. Presently, this solver can deal with problems involving up to 75 000 degrees of freedom on the COMPAQ machine of CERFACS. The strategy adopted to designe this solver is described in [CEM26].

2.2 Large size cavity problems

M. Fares, A. Bendali

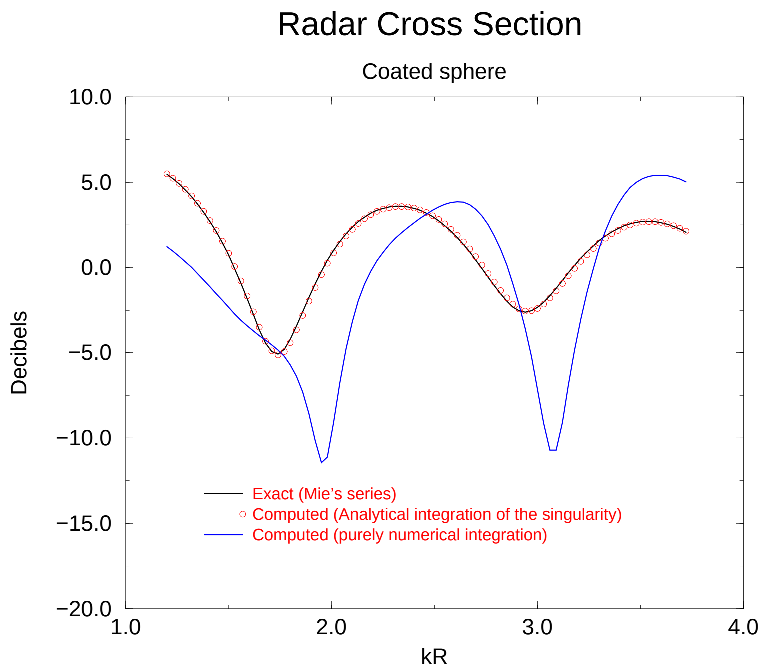

Figure 2.2: Monostatic Radar Cross Section of a coated sphere

The study conducted in 1999 on the JINA test case n^0 10, Waggon cavity, had brought out the need to clearly define the parameters involved in the models: light speed, degree of accuracy of the numerical computation of the integrals, etc [CEM10].
A preliminary study on the JINA test-case, cavity COBRA, has shown that the finite element procedure `INLET`, particularly suited to deal with deep cavities, can be used in the context of a Integral Equations solution. The use of the latter procedure has in principle the advantage that the solution are much more less dispersive than finite element procedures. Figure 2.5 constitutes a first step toward the validation of this approach.

[1] S. Maci et al., (1996), Analysis of surface-wave excitation and radiation mechanism of a monopole on circular grounded dielectric slab, *IEEE Proc.-Microw. Antennas Prop.*, **143**, 335–340.

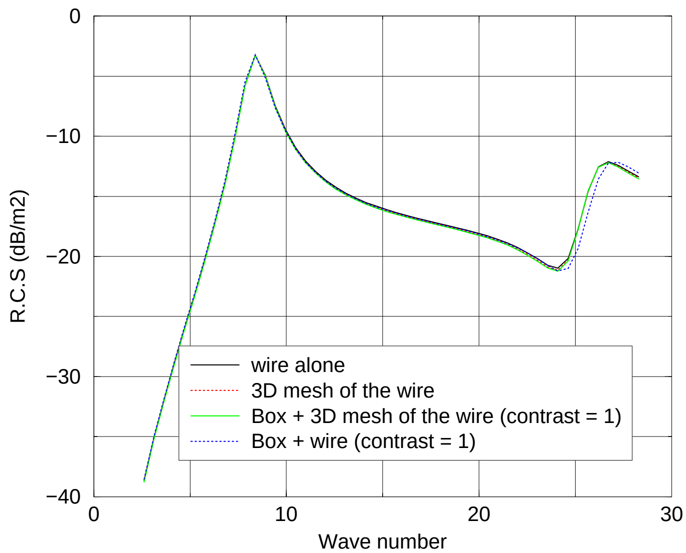

Figure 2.3: Validation of the numerical model of a wire crossing an interface between two dielectrics

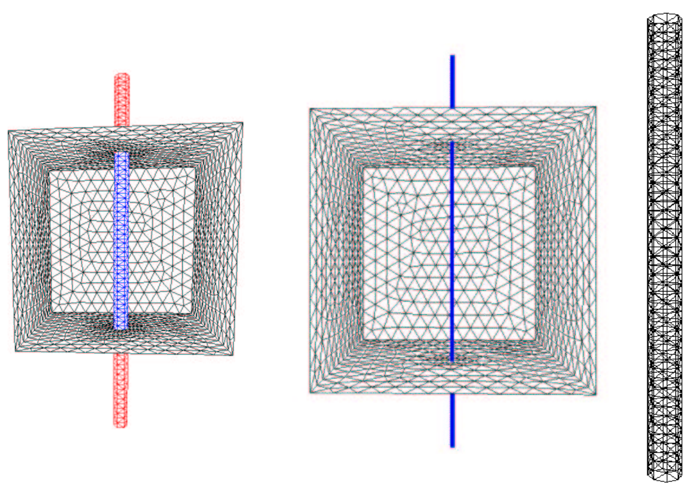

Figure 2.4: Various meshes used for the validation of the model

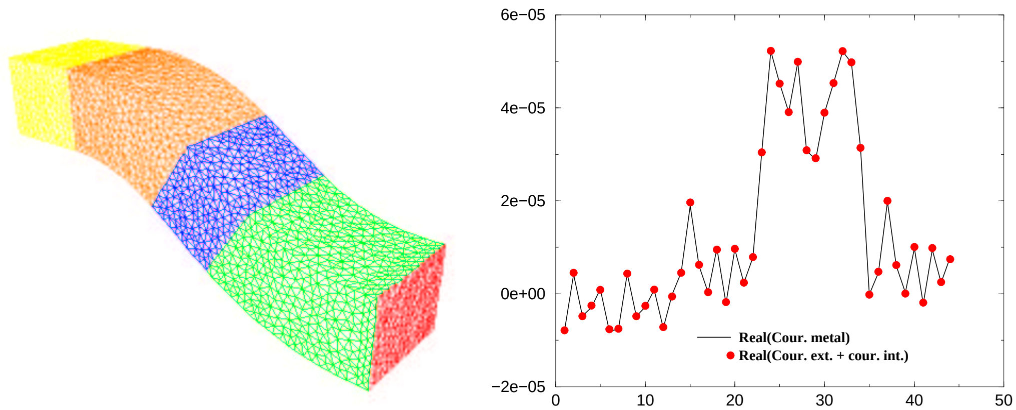

Figure 2.5: Direct and subdomain computation

3 Fast Multipole Method

3.1 Fast Multipole Method in electromagnetic calculations

F. Millot, F. Collino, N. Bartoli

Electromagnetic scattering solutions by integral equations methods lead to dense systems of linear equations. When the characteristic size of the obstacle is about six times the wavelength, the solutions can be computed by direct methods with high performance and massively parallel codes. However, if the size of the obstacle increases, the solutions can only be obtained by means of some iterative methods. The computation of the matrix-vector product then becomes the basic part of the iterative algorithm. It can be done efficiently by means of the Multilevel Fast Multipole Method (MFMM).

- **Computer implementation aspects have included:**
  - Rewriting a completely new version of the code `CESC Multipoles`, with `FORTRAN 90 and GNUMAKE`;
  - Implementing and runing the code on at least three distinct plate-forms;
  - Using extensively the capabilities of `FORTRAN 90` (derived types, dynamic allocation of memory, etc.), allowing for example easy coupling of this code with various iterative solvers;
  - Implementing and validating an out-of-core version of the code [CEM27], allowing to solve large scale diffraction problems (for example in the case of two conducting spheres with one million of unknowns);
  - Validating the code for an academic test case (scattering by a perfectly conducting sphere for which an exact solution is available in terms of a Mie's series expansion) and an industrial case (JINA test case n^0 10 *Waggon Cavity*);
  - Optimizing the computation of the transfert functions. Tranfert functions are defined on the unit sphere. They transform a far field of the charges included into a given box into a near field. After a shift and a numerical integration, this gives the corresponding potential at points contained into another box. The optimization uses the invariance of the transfert functions under various symmetries of the discrete unit sphere. This study has been supported by a contract with Dassault Aviation.

- **Theoretical aspects have concerned:**
  - **A comprehensive presentation of the method.** A general comprehensive presentation of the MFMM has been written at the demand of EADS [CEM21].
  - **An introduction of some new approaches.** Standard application of the MFMM to scattering problems in electromagnetism classically requires at least three scalar multipole calculations for each matrix-vector product, one for each component of the current, and in most cases four, another one for the charge. A new approach has been designed, implemented and validated. At the prize of a slight increase in the cost of each scalar multipole calculation, the complete multipole matrix-vector product is obtained with only two of such scalar calculations. This work has been supported by Dassault-Aviation [CEM23] [CEM9].

- **A Christiansen's Preconditionner for the EFIE.** Recently, Christiansen and Nedélec have proposed a new preconditionner for the Electric Field Integral Equation (EFIE). EFIE is the most popular equation for solving the diffraction of an electromagnetic wave on a conducting body. It leads to solve a linear system whose condition number is not very good, especially when open cavity geometries are occuring. Christiansen and Nédelec's idea consists in using one of the Calderon's identity to transform the EFIE into an equation involving a linear operator in the form "Identity + compact". The main difficulty is then to deal correctly with the $n(x)\wedge$ operator in the discrete setting. One has analysed this method and, in particular, fully understood the lack of inversibility of this new preconditionner. A first implementation has been carried out and some results on an academic case have been obtained. Some additional work remain to be done to have a clear understanding of the potentiality of this preconditionner.
- **A theoretical estimate of the accuracy of MFMM for very high frequencies.** The number of multipoles at a given level is a crucial parameter for the accuracy of the method. Some semi-empirical formulae have been proposed in previous studies. By means of theoretical estimates, some new formulae have been designed and validated, in collaboration with Q. Carayol (Dassault-Aviation).

- **Test cases and validation of the code CESC Multipole**

  - The MFMM utilizes several parameters which have to be brought under control. A method which calibrates these parameters according to the case to be dealt with has been designed and implemented. The main technique consists in computing, by an exact assembly process over two triangles, one column of the matrix and comparing the result with a multipole calculation. A crude search of the degree of freedom giving the largest error is performed. A few calculations give an indication for adjusting the parameters. The results indicate that the error strongly depends on the case being considered. The design of a more general strategy for choosing the parameters seems to be a difficult task.
  - The FMM code has been compared with other industrial codes using also the FMM method. In particular, results have been compared with those obtained at EADS and Dassault-Aviation. Good agreement has been observed. A technical report is under progress.
  - The method has been used to solve industrial test-cases, as, e.g., a non-academic case provided by Dassault (the "*CETAF*" benchmark) . Good results have been obtained. The difficult JINA test case n^0 10 *Waggon Cavity* has also been successfully performed, with convergence of the iterative process being reached. However this test has clearly indicated the difficulties met by the method for this type of problem. A report on the treatment of this test case by the direct solver as well as by the multipole code is available [CEM19].

3.2 Far to near field transformation using the multipole method

F. Collino, N. Bartoli

The radiating properties of a complicated antenna can often be documented by measurements only. Further, these measurements can be done only in the far zone. Many industrial studies, as those related to the determination of the coupling of a satellite and a radiating antenna, submitted by CNES, require the reconstruction of the electromagnetic field in the near zone from measurements of the far filed patterns.
Based on the machinery of the multipol method, a powerful approximation process has been designed to deal with this reconstruction. It yields accurate values for the field at a distance of only one quarter of the wavelength. This is largely beyond the capabilities of standard methods based simply on the addition of

a multiplicative factor $\exp(ikr)/r$. Table 3.1, giving a comparison of the field and of the currents on the satellite, obtained by a direct computation using code `CESC`, and that resulting from the knowledge of the dipole far field pattern only, demonstrates the efficiency of the approach. Note that the simple `exp` model completely fails in this case. Figure vi in the appendix gives an idea of the currents and of the far field which are computed.

Field	
`direct CESC`	0.0021%
`antenna2sat FMM`	0.9620%
`exp model`	56.7720%

Table 3.1: Error for the field on the satellite, antenna dipole is placed at a distance of $\lambda/4$.

One of the key points of the method lies on a correct interpolation of the far field pattern using spherical harmonics. This part has been validated on data obtained both experimentally by CNES and by simulation. Figure 3.1 respectively depictes the accuracy which has been reached [CEM17].

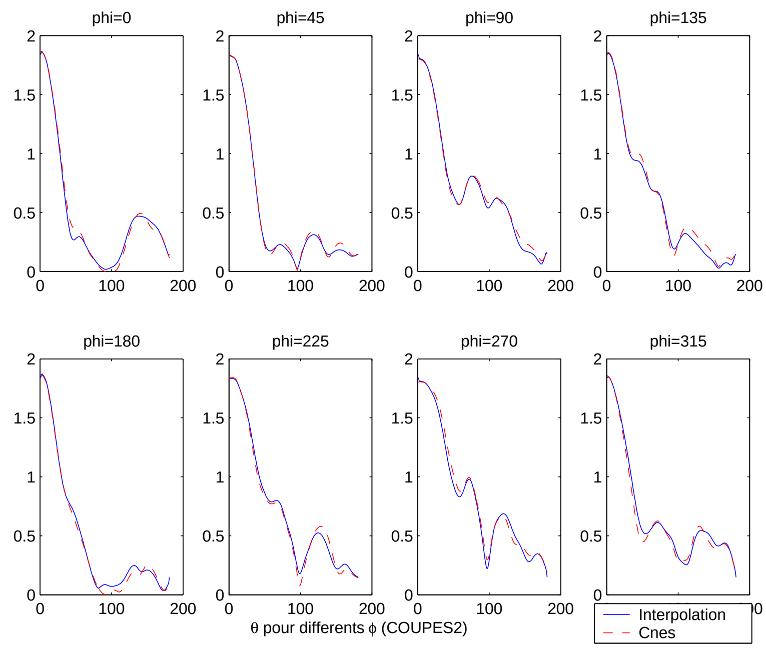

Figure 3.1: Modulus of $E_{\infty,x}$ for fixed ϕ computed from CNES measurements.

4 Prospective studies

4.1 High order impedance boundary conditions

N. Bartoli, A. Bendali, F. Collino

The objective is to investigate the scattering of a perfectly conducting obstacle coated by a thin dielectric layer. Solving the direct problem gives rise to some numerical instabilities when the shell thickness is too small. For this main reason the effects of the thin shell are classically taken into account by using some impedance boundary conditions. A process to build and to analyze these conditions has been devised. It yields numerical schemes totally free from the usual numerical instabilities. Appropriate impedance boundary conditions have been constructed for the case where the order of the approximation must be high enough to characterize the effects of curvature and to get more accuracy for the high frequencies. The third order impedance boundary conditions are then considered for arbitrary geometries. It then requires the use of pseudo differential operators, i.e., a combination of differential and inverse of differential operator. The theoretical aspects have been studied and a convergence theorem with an estimation error has been developed. Numerical applications have been performed to validate the approximation. This studies point out that pseudo differential operators are more stable and robust than classical differential one. This property becomes particularly robust when the problem involves some overmeshing requirement [CEM16], [CEM18].

4.2 Després Integral Equations

N. Bartoli, F. Collino

Investigation on the integral formulation of Bruno Després has been pursued. This formulation is based on a minimization of a quadratic functional. The resulting linear system involves only real and symmetric matrices. In contrast, the classical integral equations based on an EFIE (Electric Field Integral Equations) formulation yields a symmetric system but with a non-hermitian matrix. Furthermore, only direct methods are usually used in connection with classical formulations, while Després' formulation is specially appropriate for solving through iterative procedures. The basic properties of the method have been clearly exhibited and general theorems insuring the convergence of its solution by an iterative process have been established. Note that such a convergence is not guaranteed for the classical formulations. Many numerical examples are performed to investigate the potentialities of the method. For instance, for convex geometries (ellipse, square, ...) a good behavior is observed when the frequency increases or when the mesh becomes irregular. For a non convex geometry like a perfectly conducting cavity, the convergence is more difficult to obtain with the Jacobi algorithm. The GMRES algorithm is suitable to cope with this particular geometry. In addition, the system is particularly appropriate to solve scattering problems with impedance boundary conditions. Indeed, the right-hand side of the system depends on the impedance operator only. A last application concerns the domain decomposition techniques. Some algebraic properties of the system of Després proved to be of interest for the coupling with the domain decomposition. The first numerical results of this approach are promising [CEM6], [CEM4], [CEM5], [CEM12].

4.3 Domain Decomposition Method

Y. Boubendir, A. Bendali, F. Collino

The preliminary (1999) heuristic way to improve the domain decomposition method, initiated by B. Després, was aimed at allowing its use in the context of an Integral Equation solution. Particularly, this improvement gave rise to an efficient tool to couple a Finite Element Method and a Boundary Integral Equation. Much of the efforts for the two last years have been devoted to fully understand why the heuristic procedure works well, in order to develop confidence that it can be implemented within a general solver.
When studying special geometries, for which the waves can be separated in a propagative and an evanescent part, it has been shown that the previous procedures introduced by Deprés's damp strongly the propagative part but only very moderately the evanescent one. In the context of the numerical implementation of the domain decomposition method, inherent errors due to the scheme can lead to an increase in the level of the evanescent modes which, in the end, completely damage the solution. The new procedure, even if it is not optimal for propagative modes, introduces a strong damping of the evanescent ones. Figure 4.1 clearly illustrates this feature. Figure 4.2 presents a severe case of a cavity problem for which, despite a

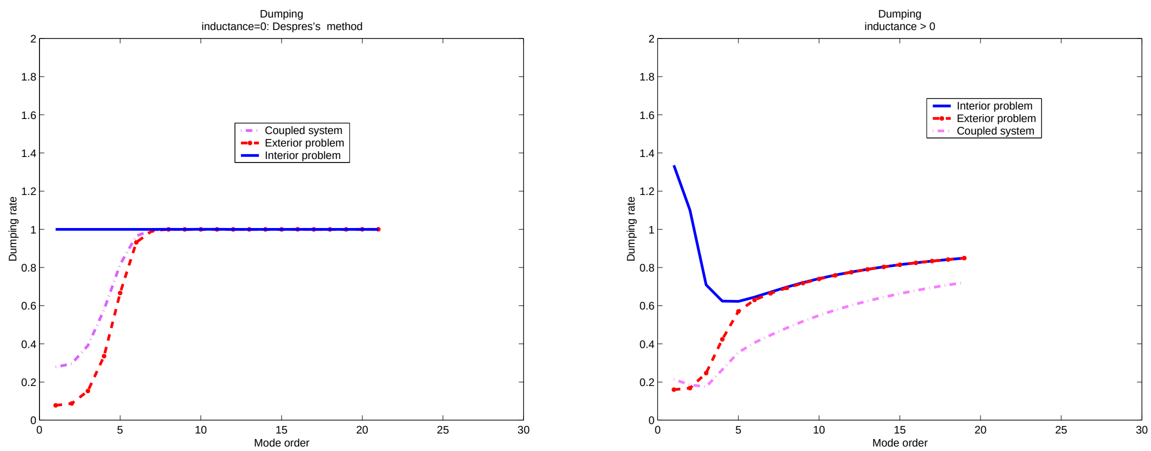

Figure 4.1: Previous and new procedure

strong coupling of the propagative and the evanescent modes, the residual during the iterations continues to exhibit a very nice behavior.
It has also been observed that domain decomposition methods bypass the difficulties related to ill-conditioning of the linear systems coming from direct formulations, in case of the presence of a dielectric. Figure 4.3 shows indeed that the distribution of the moduli of eigenvalues of interior and exterior problems is much more suitable for an iterative solution than the global problem resulting from a direct formulation.
A novel domain decomposition procedure has also been tested [CEM20]. The method is based on the numerical determination of the impedance matrix to take account for a part of the domain which afterwards is removed from the formulation. The benefit of this method lies in the fact that it does not resort to an iterative process, and that it becomes very attractive when the same geometrical object is repeated. However, the results require some further studies to validate or dismiss this approach.
The domain decomposition technique has been also extended to efficiently couple two different methods of solution, each one being adapted to the form of the problem in a related zone. The technique has been used to couple a nodal finite element solution, to deal with a non homogeneous dielectric material, with an integral equation, more appropriate to deal whith the propagation in the infinite exterior medium [CEM8].

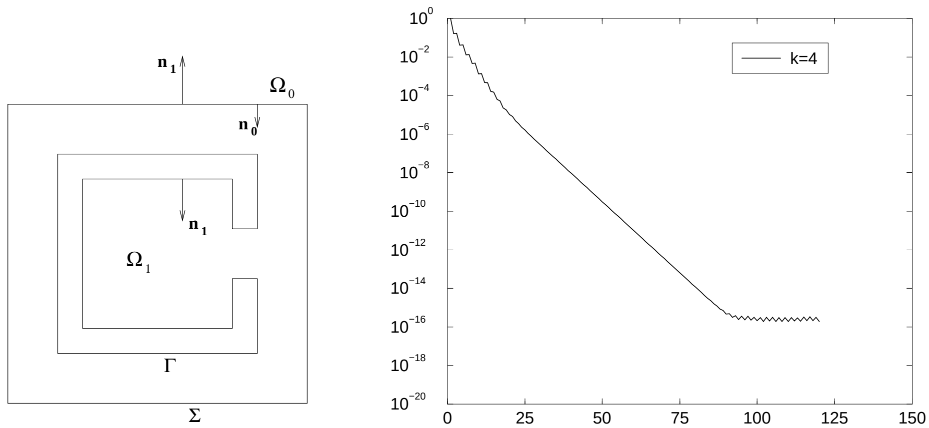

Figure 4.2: Behavior of the residual for a cavity problem

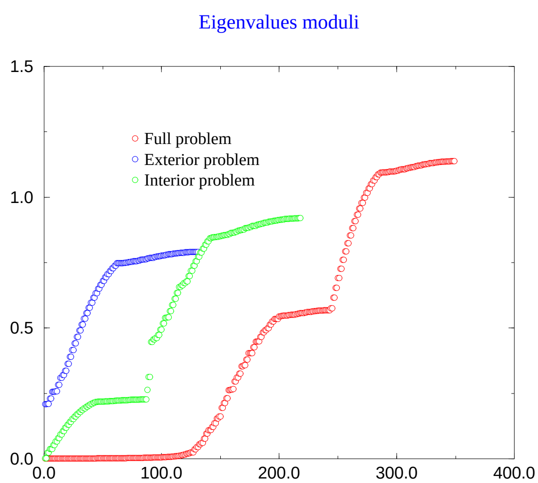

Figure 4.3: Eigenvalues moduli

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5.5 Technical Reports

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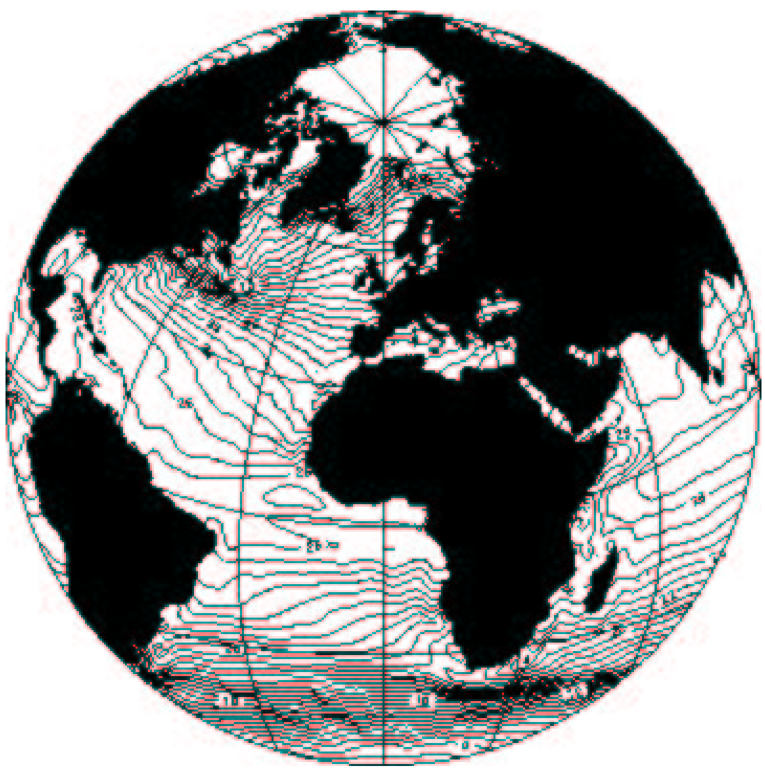
5

Climate Modelling & Global Change



1 Introduction

Olivier Thual

1.1 General overview

Six projects are described in this report. The first three are research oriented and can been sketched with the following titles:

- Climate variability,
- Seasonal prediction,
- Ocean data assimilation.

These climate modelling activities combine significant scientific contributions in several specialities (such as the study of the North Atlantic Oscillation) with the development of complex computing systems (such as a seasonal forecast chain with variationnal oceanic data assimilation). The two following projects of the "Climate Modelling & Global Change" team are based on the development of two softwares:

- The PALM software for data assimilation in models,
- The OASIS coupler for ocean-atmosphere models.

Theses two projects combine advanced scientific computing developments with deep implications in scientific applications, leading to high quality research on different topics (from applied mathematics to atmospheric pollution). The last project corresponds to development activities which are directly included in the MERCATOR project (aiming toward operational oceanography and gathering the contributions of several institutions). This CERFACS contribution is entitled as follows:

- The MERCATOR prototype

1.2 Significant achievements

The team is composed of 4 researchers, 2 post-docs, 5 PhDStudents and 7 research engineers. Since the last scientific report (2 years ago), 15 journal publications have been published, 15 contributions to conference proceeding have been recorded and 49 technical reports have been registered. Three PhD Thesis have been granted.

In parallel, 3 prototypes has been released: a validated prototype of a seasonal prediction chain, a ready-to-use (and used) version of the PALM prototype and the Atlantic and Mediterranean prototype in agreement with the MERCATOR working plan. The developement of the prototype for the variationnal assimilation chain for the global oceanic model has been also undertaken during this period.

Four European projects have started during this period under Framework Program 5 (PREDICATE, DEMETER, ENACT and PRISM) and have led to the hiring of one senior scientist, two new post-doc and one research engineer. Two research projects have been funded by the CNRS/PNEDC (National Program for Climate Dynamics Studies) and one by the CNRS/GMMC (Scientific research program for MERCATOR). Several collaborations with national, european or international laboratories have been active. Further details are contained in the following sections.

2 Climate variability over the North Atlantic-European region at inter-annual to decadal time-scales

2.1 Influence of sea surface temperature anomalies on low frequency atmospheric variability over the North Atlantic European sector (C. Cassou, M. Drévillon, L. Terray, S. Valcke)

The climate of the North Atlantic-European (NAE) sector exhibits considerable variability on a wide range of time scales. Improved understanding of this variability is essential to assess the likely range of future climate fluctuations and the extent to which these fluctuations are predictable. For instance, detailed knowledge of the so-called natural variability is a necessary prerequisite to assess the potential impact of climate change due to anthropogenic forcing [GLO14].

A large part of the climate variability over the NAE region is associated with a dominant mode of atmospheric circulation variability called the North Atlantic Oscillation (NAO). The NAO refers to a meridional oscillation in atmospheric mass with centers of action near Iceland and over the eastern part of the sub-tropical Atlantic (Azores). In its positive phase, low pressure anomalies over the Icelandic region are associated with high-pressure anomalies across the sub-tropical Atlantic. The NAO is a natural mode of variability of the atmosphere which emerges when atmospheric general circulation models (AGCMs) are forced with climatological annual cycles of insolation and Sea Surface Temperatures (SSTs) as well as fixed trace-gas concentrations.
There are clear indications that the North Atlantic ocean covaries with the overlying atmosphere. For instance, it has been shown that the SSTs are responding to the atmospheric forcing on monthly to seasonal time scales. On the other hand, observations show that SSTs have low frequency variations which could imprint themselves back onto the atmosphere. The question then becomes: do the ocean surface conditions play an active role in shaping mid-latitude atmospheric variability at low frequency ?

To answer this question, the strategy relies upon a dual approach which combines statistical methods applied onto observed or re-analysis data and numerical modelling with general circulation models. For instance, using reanalysis datasets from NCEP, the relationships between the low frequency variability of the zonal wind jet at 200 hPa (U200) over the North Atlantic-Europe domain and the geographical distribution of the SST anomalies have been documented. In contrast with other studies, non linear techniques such as cluster analysis have been used as this class of methods does not require any constraint regarding the symmetry and orthogonality of the variability modes. For the winter months over the 1958-1997 period, the signature of the two phases of the NAO is captured and is associated with the North Atlantic SST tripole. The classification also extracts a “La Niña mode” related to a strong ridge off Europe and reduced jet over the Azores.

By analysing the data coming from two ensembles of multi-decadal integrations performed with the ARPEGE model, a systematic assessment of the effect of Atlantic SSTs on low-frequency atmospheric variability over the North Atlantic-Europe region has been performed. In the first ensemble (GOGA) [GLO14], the observed SSTs and sea ice extents (SIE) from the GISST data set are prescribed globally while they are restricted to the Atlantic ocean in the second ensemble (AOGA). A signal-to-noise maximising EOF analysis is used to isolate the dominant forced response from the internal atmospheric variability. The method is applied to North Atlantic low-pass-filtered seasonal mean Mean Sea Level Pressure (MSLP) anomalies and the analysis is made for both the winter (DJF) and spring (MAM) seasons over the 1948-1998 period. The principal findings of this study are the following:

- The leading response in the GOGA simulations can be attributed to oceanic changes related to the El Niño-Southern Oscillation(ENSO). The spatial pattern of the leading forced mode in winter exhibits a primary center of action located slightly north of the Azores archipelago and a secondary maximum off the Florida coast. The time series of the forced response is strongly correlated to the Niño 3 index;

- In order to find out whether the local Atlantic SSTs do exert any influence on atmospheric variability over the NAE sector, two different approaches were used and compared. The ENSO influence was removed from the GOGA simulations with a simple linear regression of the MSLP data with the Niño 3 index and the EOF algorithm was applied to the residual part of the data. The EOF algorithm was also applied to the AOGA ensemble. A common detectable response is found in winter and to a lesser extent in spring. In fact, while the forced spring response from the AOGA ensemble is close to the common (GOGA and AOGA) winter signal, the forced spring GOGA response does not exhibit a large-scale coherent pattern. The characteristic temporal evolution of the winter response is also obtained from the application of the same algorithm to other atmospheric variables such as the AOGA 500hPa height field (Z500) and the 200hPa zonal wind (U200). This temporal evolution shows quasi-decadal variability (with a period between 6 to 8 years) superimposed on a lower frequency fluctuation. It is also well correlated with fluctuations in a tripole pattern of SST anomalies in the North Atlantic;

- The spatial structure of the leading forced response in winter is dominated by a large-scale dipole in MSLP, resembling the NAO structure but with a stronger mid-latitude center of action. Applying the signal-to-noise maximizing EOF algorithm to other variables (Z500 and U200) shows a very coherent signal with a quasi-barotropic signature close to that of the NAO. The low-frequency changes between the first part of the period ($1950 - 1970$) and the second part can be explained in terms of changes in the frequency of occurrence of a natural regime of atmospheric intraseasonal-interannual variability with a spatial structure very similar to that of the positive phase of the NAO;

- The leading forced atmospheric response is induced primarily by the tropical part of the SST tripole as shown by the strong correlation between the tropical North Atlantic SST index and the characteristic temporal evolution of the forced response. To further confirm this finding, two 30-year additional integrations were carried out with idealized SST anomalies representing the positive (TAP) and negative (TAN) phases of the tropical part of the SST tripole. Similarity between the difference $(TAP - TAN)$ fields and the leading forced responses from the AOGA integrations demonstrate that the tropical North Atlantic SST anomalies can lead to changes that tend to re-enforce the geopotential structure of the simulated NAO;

- The physical mechanism involves related changes in tropical convection, Hadley circulation and the modulation of the stationary planetary-scale waves by the low-frequency variability in subtropical winds induced by the persistent tropical circulation anomalies. Enhanced baroclinicity and related changes in planetary-scale transient eddies in the western subtropical North Atlantic may have a catalytic role in forcing and sustaining the anomalous stationary wave activity.

2.2 Study of the observed covariations of the Atlantic sea surface temperature and mid-tropospheric flow signatures over the extra-tropical North Atlantic (M. Drévillon, C. Cassou, P. Rogel, L. Terray, S. Valcke)

While there is statistical-cum-observational evidence of significant atmospheric forcing of the underlying SST at monthly-to-seasonal time scales, atmospheric model simulations have also shown possible influence of SST patterns upon the mid-latitude tropospheric flow and its associated storm-tracks. However, there is a large scatter in the responses of atmospheric models to SST anomalies, depending on the model physics and resolution, the basic mean state or the structure of the SST anomalous patterns. Thus, it is of great interest to assess directly from observed and reanalysis data the possible linkages between the SST and various atmospheric variables.

To address this question, the interactions between the SST, the Storm Track Activity (STA) and the time mean atmospheric circulation in the North Atlantic Europe region [GLO7] have been investigated. Lead-lag Maximum Covariance Analysis (MCA) between seasonal 500 hPa geopotential height (Z500) and SST over the NAE region captures a significant covariance between the previous summer SST anomaly and a winter NAO structure. The same analysis, but restricting the atmospheric zone to Europe, points out a strong anticyclonic (cyclonic) anomaly over Europe related to cold (warm) oceanic conditions off Newfoundland, this SST structure being independant on the considered atmospheric region. This summer SST anomaly is found to persist enough until winter through surface heat fluxes exchanges, when it can finally have an impact on the atmospheric circulation. Composite analysis (drawn from the MCA expansion coefficient) is applied to the winter STA and different transient and stationary eddies diagnostics associated with the extreme positive and negative events of the SST anomaly. These diagnostics suggest that the SST anomaly induces in winter an anomalous stationary wave, creating an initially small anomaly over Europe. Anomalous transient eddies located over northern Europe then strengthen this anomaly and maintain it during winter, thus acting as a positive feedback.

The sensitivity of the ARPEGE model to these observed summer SST anomalies is then assessed in a set of ensemble forced experiments. These simulations allow to better describe and understand this ocean-atmosphere interaction and to further study asymmetries and nonlinearities with respect to the sign of the SST forcing. As there are also evidences of autumn SST forcing of the North Atlantic Europe atmospheric winter circulation from the tropics, a complementary set of simulations is performed in order to investigate the possible mechanisms responsible for this remote tropical forcing prescribed in the model. Additional experiments with ARPEGE coupled with a simple oceanic mixed layer in the mid-latitudes are also carried out.

The fall tropical SST forcing induces in October-November-December (OND) a strong wave-like response both in the forced and mixed-layer-coupled experiments. This Rossby wave signal is due to the modification of the local Hadley cell branch over Amazonia/Carribean Sea affecting in fine the momentum convergence around the subtropical jet entrance, the latter exporting the signal to higher latitude. The occurrence of the winter weather regimes is affected in agreement with the significant spatial correlation of the midlatitude part of the wave response with the NAO pattern. We show that the thermal coupling between the ocean and the atmosphere allows a better representation of the midlatitude part of the response, which is further reinforced due to transient eddy feedbacks.

2.3 Asymmetries between the two phases of the NAO and their related SST structures. Implications for seasonal predictability (C. Cassou, M. Drévillon, L. Terray, S. Valcke, E. Maisonnave)

A detailed study of the asymmetry between the two phases of the NAO is carried out based on the climate regimes paradigm described in section 2.1 and applied on different observed (or reconstructed) datasets of MSLP, SST and precipitation. Among the 4 preferred winter atmospheric states extracted by the classification algorithms, two correspond to the negative and positive phases of the NAO. Departing from the traditionnal linear picture, the positive NAO regime shows a significant eastward shift of the Azores centre (about 30°) by comparison to the offshore meridional dipole aligned with the Icelandic Low for the negative NAO one. Ulbrich and Christoph [1] attributed the observed eastward shift of the NAO centres of action to the global warming induced by the greenhouse gases forcing. The regime approach modulates this statement as the eastward shift seems to be intrinsically related to the positive phase of the NAO (it is also present when analyses are limited over the 1900-1970 period), the latter being presumably favored in an anthropogenic perturbed climate.

The simultaneous SST anomalies related to the 2 NAO regimes exhibit a rather symetrical tripole structure between the 2 phases, over the North Atlantic basin. This oceanic signature is primarily due to the anomalous atmospheric surface conditions which imprints their shape through latent and sensible heat fluxes (as described in section 2.3). However, lagged relationships between winter regimes and previous summer SSTs anomalies reveal asymmetrical features according to the phase of the NAO. The negative one is associated with the summer oceanic mode extracted by linear techniques and described in section 2.2 (Horseshoe mode). The positive phase is related to a reinforced meridional SST dipole between the Labrador Sea and the Gulf Stream area. Both are also linked to a confined equatorial signal in the tropical Atlantic. The existence of the two midlatitude modes are investigated. Composites analyses show that these are linked to the previous winter SST tripole and to the simultaneous summer atmospheric forcing. The asymmetry between the two phases is thus explained by the difference in the persistence of the winter to winter oceanic tripole structure. A stronger SST gradient in winter (positive NAO phase) is likely to persist more than a reduced one (negative NAO phase) due to the nonlinearities of the oceanic mixed layer stability. As explained in section 2.2, the persistence of these 2 modes is high enough to further impact the atmosphere at the early beginning of the following winter when the climatological background is more favorable. The oceanic anomalies then affects the strength and the path of the synoptic storms leading to a modification and the maintain of anomalous stationary waves. The influence of the equatorial SST anomalies is set via the 2 local Hadley cells over South America and over the african continent. The local modification of the Walker cell between Africa and South America associated with the equatorial SST anomalies is indeed linked to the existence of locally modified Hadley circulation affecting the strength of the jet-streams both over Florida and over North Africa. The persistence of the modified tropical dynamics is persistent from summer to winter, the extension of the climatological stationary waves at early winter being responsible for the "junction between the jet anomalies" consistently with the establishment of the winter NAO phase.

This asymmetrical perspective links tropical and midlatitude forcings, both playing a role in the midlatitude atmospheric circulation variability. Based on the persistence of the oceanic modes and knowing the mechanisms at work, seasonal predictability is thus considered and presently under investigation (see fig. viii in the appendix). It is shown in this study that it is essential to have a global picture of the climate variability over the NAE region, being influenced by ENSO, the tropical Atlantic and the midlatitude oceanic conditions. It is also crucial to take into account the asymmetry of the ocean-atmosphere interactions.

[1] U. Ulbrich and M. Christoph, (1999), A shift of the NAO and increasing storm track activity over Europe due to anthropogenic greenhouse gas forcing, *Clim. Dyn.*, **15**.

3 Seasonal Prediction

The aim of the Seasonal Prediction project is to study how inter-annual climate anomalies can be forecasted some seasons in advance. Since a large part of the memory of the climate system at those time scales lies in the upper ocean, this requires the use of a coupled ocean-atmosphere model as realistic as possible, and the determination of accurate initial conditions, in particular for the ocean. This activity is then strongly linked to the global ocean data assimilation activity (see chapter 4).
After the completion of the DUACS European project early 2000, activities have focused on further exploitation of the existing experiments in preparation to the DEMETER program. This included the development of specific diagnostics described in the next subsection. Their applications to the numerical experiments are presented in the second subsection with emphasis on the Northern Hemisphere and Europe. The DUACS experiments have been further used to study the predictability of ENSO through an analysis of the temperature anomaly growth modes, described in the third subsection.
The upgrade of the coupled prediction system for DEMETER, described in the last subsection, began at the end of 2000, and constituted most of the work in 2001. Its exploitation began at the end of 2001.

3.1 Technical aspects of seasonal forecasting (E. Maisonnave, P. Rogel)

Since 1999, a series of ensemble forecast experiments has been done within the context of DUACS European project [GLO74]. These runs (using the coupled GCM OPA-8/ARPEGE-3-18f-cycle) were concluded in January 2000, producing a complete set of seasonal forecast ensembles, throught the years 1995 to 1999, (see Section 3.2).

Along this period, the tools developed in the framework of DUACS for preparation, launching, and control of seasonal experiments on Météo-France and ECMWF Fujitsu machines were not substantially modified, except for a better management of the successive launching of ensemble members. This was needed on the VPP5000 which power enables to run several members during one night or one week end. Those tools are documented in [GLO63].

Technical developments mainly consisted in creating a framework in which seasonal prediction experiments can easily be analyzed. Data are stored locally at CERFACS, which takes full benefit of the storage capacity and of its access from the SGI-Origin 2000 for postprocessing purpose. Those diagnostics, based on a series of scripts and Fortran programs, allow to handle hundreds of overlapping short coupled experiments that constitute a set of seasonal prediction ensembles. Among others, it is easy to compute and draw for each variable:

- ensemble means, spreads, deviations;
- mean climate drift, with respect to observations or analyses, and to remove it variable by variable;
- predicted anomalies, either ensemble means or individual forecasts;
- comparison with observed anomalies, or with analyses;

- prediction scores such as Anomaly Correlation Coefficients, or Root Mean Square errors, either globally or for selected regions;
- predicted probability of occurrence of selected events;
- probabilistic scores (see next section) for selected regions...

In order to visualize models outputs over geographical crucial areas, and considering the importance of processed data, new automatization tools were developed (Xmgr/Vairmer graphical software parameterization scripts, format converters . . .)
Finally, efforts were made on documentation tasks, concerning coupling strategy [GLO62] and [GLO64], seasonal forecast peculiar analysis tools [GLO63] and VPP700-VPP5000 porting procedures [GLO61].

This work made easier upgrading the forecast chain used on Demeter project (coupled GCM ORCA-2/Arpege-3-22a-cycle), see Section 3.3. The ORCA ocean model has been run first on the Cerfacs SGI-Origin 2000, and fully takes advantage of the Compaq server. The forced model begins to be used on new data assimilation experiments. Lots of technical tasks have been handled to take into account the new data storage format used by ORCA (NETCDF). A large set of diagnostics are now taken into account from the STATPACK software developed at LODyC (provided by P. Terray) that replace some functionalities of Vairmer, and visualised through IDL and FERRET. This analysis and visualisation library is to become a standard tool for most activities dealing with model outputs in the team.

3.2 Seasonal predictability studies in Northern Hemisphere and Europe (Ph. Rogel)

In preparation for the DEMETER project, whose main focus is to study atmospheric seasonal predictability in the European region, the DUACS coupled integrations were extended to the March 1993 - June 1999 period, and to 9 members (instead of 5). This ensemble size is the minimum needed to sample enough atmospheric variability in the regions of interest, in order to have reliable results on the predictive capability of the coupled model.
Classical scores (ACC, RMSSS) have been applied. The results have also been analyzed over the Northern Hemisphere and Europe using some scores studied in the PROVOST project. Those diagnostics are based on the choice of one "event" (e.g. temperature lower than climatology) for which seasonal prediction system forecasts the probability of occurrence. This probability can of course be estimated only from an ensemble of deterministic predictions. Brier Scores, ROC Curves and Economic Value scores (see [GLO53]) were thus used to evaluate the model prediction capability.

- The Brier score measures the difference between the event predicted probability from the coupled system and the one from a "perfect" system (100% if the event actually occurs, 0% if not). This score is illustrated in "reliability diagrams" (see figure 3.1) which plots for each forecast probability the ratio between forecasted cases that actually occurred and total forecasted cases;
- For a given event, a specific user of the forecast could consider that above a certain probability threshold, the event is to be considered as forecasted. The Relative Operating Characteristics (ROC) measures the relative variations of "Hit rate" (good forecasts) and "False alarm rate" (event erroneously forecasted) when this probability threshold varies. This score is illustrated in figure 3.2. The area under the ROC curve should be higher than the diagonal for forecasting system that is more predictive than climatological forecast;

- Economic value is linked to ROC, but weights the “Hit rate” and “False alarm rate” to compute mean user expenses, deduced from a simple economic system where a lost L is caused by an unforecasted event, and a cost C is spent to prevent this lost if the event is forecasted. For each C/L ratio and each probability threshold, figure 3.2 measures the relative gain of using coupled forecast versus climatological forecast. This allows to determine an optimal threshold for each application characterized by its C/L ratio.

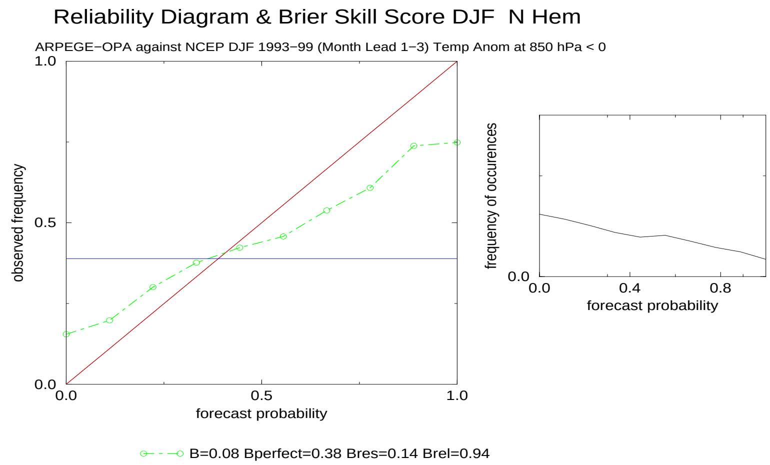


Figure 3.1: Reliability Diagram and Brier Score

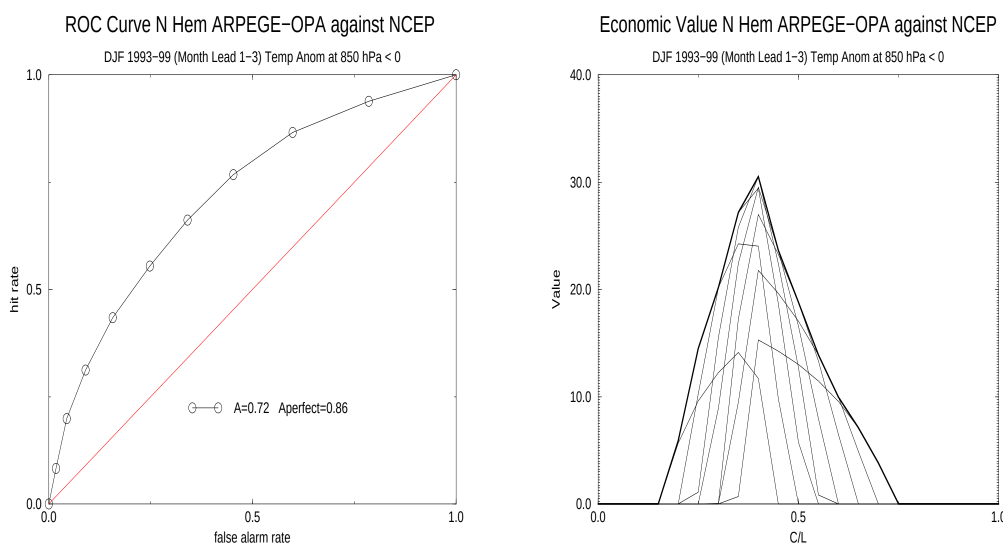


Figure 3.2: Relative Operating Characteristics and Economic Value

The event used to produce scores in figures 3.1 and 3.2 is “temperature at 850hPa lower than climatology”, and the verification is the NCEP re-analysis. Data over Northern Hemisphere have been considered. Scores found here, and on other events and regions, are comparable to results shown on ECMWF web site. They show that our coupled system has a prediction capability significantly higher than climatological probability. The effect of using altimeter data assimilation degrades the results, as expected from our previous results on ENSO prediction. However, over Europe, they are improved, maybe due to a sampling effect, but more probably to the fact that less intense ENSO event predicted with assimilation reduces the (erroneous) PNA extension over the North Atlantic.

3.3 Ocean anomaly and error growth in the ocean from seasonal prediction experiments (Ph. Rogel, H. Kamil, E. Machu)

In order to better understand predictability, and more especially in the ocean, we have developed a tool based on [2] study of the growth of SST anomalies. This tool is based on a statistical evaluation of oscillatory modes that are either damped or exponential. Since the system is stable, it is found that all modes are damped. The growth of ocean anomalies thus can only be explained by some constructive interference of those modes at some periods. It is possible to construct how the modes should interfere, what are the structure initially and how they evolve.

The initial study was done with historical SST anomalies, and the same analysis was reproduced on the coupled model SST issued from the DUACS experiments. Results (Fig. 3.3) show that the optimal growth structure of the model and its evolution over 6 months is very similar to that from real observations, which means that the model inherently has the capacity to produce realistic seasonal and interannual variability [GLO59].

This tool is currently used to extend the study to other ocean variables and the corresponding atmosphere forcing as it appears in the coupled model. In the framework of the perfect model, it also paves the way to a better understanding of the ENSO predictability, in allowing the description of the structures that produce more or less spread inside ensembles of coupled integrations. This work will be carried in 2002.

[2] C. Penland and P. D. Sardeshmukh, (1995), The optimal growth of tropical sea surface temperature anomalies, *J. Climate*, **8**, 1999–2024.

3.4 Description and early results of the DEMETER seasonal prediction system (Ph. Rogel, E. Maisonnave, E. Machu)

The beginning of the DEMETER European project has induced several changes in the way seasonal hindcasts are currently produced. Besides the evolution of the data assimilation system (see section 4.4), both ocean and atmosphere components have been upgraded, OASIS coupler (2.4 release, see section 6) and the method to produce forecast ensembles.

A new version of the OPA global ocean configuration (ORCA2) has been used since the end of the year. It was used in collaboration with LODyC, run on the CERFACS SGI-Origin2000, and ported on ECMWF VPP700, which will be the machine dedicated to DEMETER hindcast production. The physics of the version is close to the older one, but has a new grid configuration, and implements a free surface scheme which allows easier comparison with altimetry (and is a good thing for assimilation). A five-year forced experiment (1986-90) with ERA15 winds and fluxes was initially produced, and the construction of ERA40 forcing is being done currently, following the reanalysis production. This version is being coupled with the latest version of ARPEGE-Climat, as used at CNRM. Strategy to use ERA40 winds and fluxes was defined in collaboration with CNRM and LODyC, and we are in charge of the production of the unassimilated restarts both for LODyC and ourselves, so that a thorough comparison with their results will be possible at the end of the project.

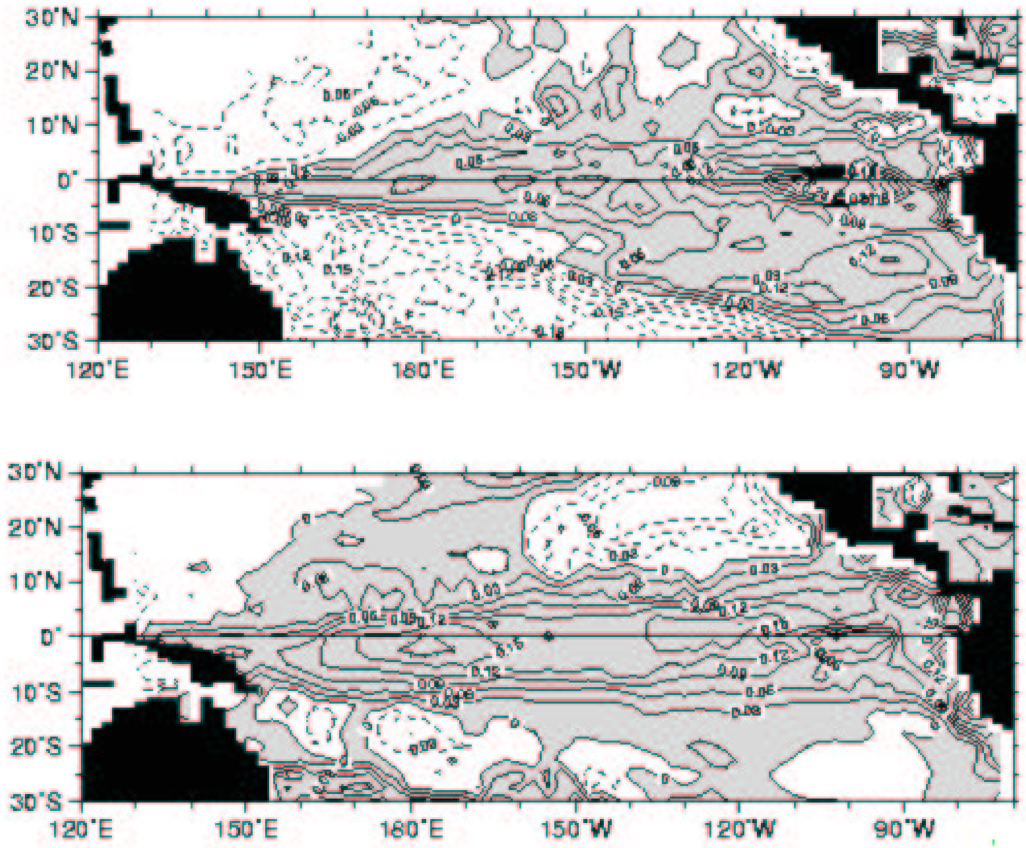


Figure 3.3: Sea surface temperature initial structure leading to the optimal anomaly gowth in the tropical Pacific (top) and its maximum evolution four months later (bottom).

In the framework of PROVOST and DUACS, the ensemble construction strategy was based on initialising the coupled model with atmospheric initial conditions from consecutive day analyses. For DEMETER, this strategy was changed to the use of forcing perturbations (wind, fluxes and SST). Practically, a set of daily wind perturbations, provided by ECMWF based on differences between two atmosphere analysis systems, and four sets of SST perturbations similarly built. This introduces initial anomalies in the ocean, thus more persisting than atmospheric anomalies. Perturbed initial conditions are also provided to LODyC. This ensembling technique is also used for data assimilation purpose in order to assess some assumptions about background error modelling (see section 4.4).

Early results show that the model has a warm bias in the tropics (thus of the opposite sign as for DUACS). A few hindcast experiments have been produced so far during the 1987-88 ENSO-La Nina period (Fig. vii in the appendix) It shows that the model is able to pick up the shift from warm to cold conditions. The amplitude is weaker for warm conditions, but as it corresponds to the very beginning of the period, it may be due to the fact that the ocean forced model is still in spin-up mode.

4 Ocean Data Assimilation

4.1 Three- and four-dimensional variational assimilation for the tropical Pacific Ocean (A. Weaver, S. Ricci, E. Machu, P. Rogel)

Three- and four-dimensional variational assimilation (3D- and 4D-Var) systems have been developed and extensively validated for a rigid-lid, tropical Pacific version of the OPA OGCM. This work has been done in close collaboration with the ocean modelling group at LODyC and the seasonal forecasting group at ECMWF. The tropical Pacific system serves as an important test-bed for developments to the global ocean assimilation system (section 4.4). An important design feature of the assimilation system has been to provide a clear development path from 3D- to 4D-Var. The systems have been developed following the incremental approach. The control variable of the variational minimization problem is an increment to the background estimate of the model initial conditions at the beginning of each assimilation window. The fundamental difference between the 3D- and 4D-Var formulations lies in the level of sophistication of the linear model used to transport the increment between observation times. In 3D-Var, a simple persistence model is used, whereas in 4D-Var a dynamical model derived from the tangent-linear (TL) of OPA is used. The incremental formulation of 3D-Var (also known as 3D-FGAT for First-Guess at Appropriate Time) can be viewed as a limiting case of incremental 4D-Var in which the TL operator is replaced by the identity matrix. In both systems, observations are assimilated at their appropriate times since they are compared directly to the background state which is propagated in time using the OGCM.

The assimilated observations consist of a quality controlled set of *in situ* temperature measurements from the Global Temperature and Salinity Pilot Programme (GTSPP). This data-set includes measurements primarily from the TAO array and XBT network. The systems have been cycled for the period 1993-98 using a 10-day assimilation window in 3D-Var and a 30-day window in 4D-Var. The reference experiment (the control) is an integration of the ocean model without data assimilation; i.e., using the past-history of the surface forcing as the only source of information. A meridional-vertical section of the 1993-96 average temperature at 140°W is shown in Fig. 4.1 for 4D-Var, 3D-Var and the control. The thermocline structure in the control experiment is too diffuse compared to observations. To compensate for this problem, the assimilation of *in situ* temperature data, in both 3D- and 4D-Var, produces a large mean correction to the thermal field, which results in a colder thermocline with increased stratification. The tilt of the isotherms in the North-Equatorial Counter Current (NECC) region between 5°N and 10°N is considerably reinforced in both data assimilation experiments. The thermocline tightness and tilt is stronger in 4D-Var than in 3D-Var (cf. Figs. 4.1 a and b, near 7°N). This steepening of the meridional temperature gradient results in a more intense NECC which is closer to observed climatology.

The assimilation improves not only the thermal mean state but also variability on interannual down to daily time-scales. For example, Fig. 4.2 shows the daily depth of the 20°C isotherm (D20) at 140°W, 5°N from TAO data and from the 3D-Var, 4D-Var and control experiments. The large oscillations (up to 60m from peak to trough) at a 30- to 40-day time-scale correspond to tropical instability waves (TIWs). There is no TIW activity during the April-to-June period. The control and 3D-Var do not exhibit clear TIW variability.

In 4D-Var, however, the TIWs are reproduced with the correct phase and amplitude. This is an impressive example of the ability of 4D-Var to fit variability in the data having a time-scale comparable to or shorter than the 30-day assimilation window.

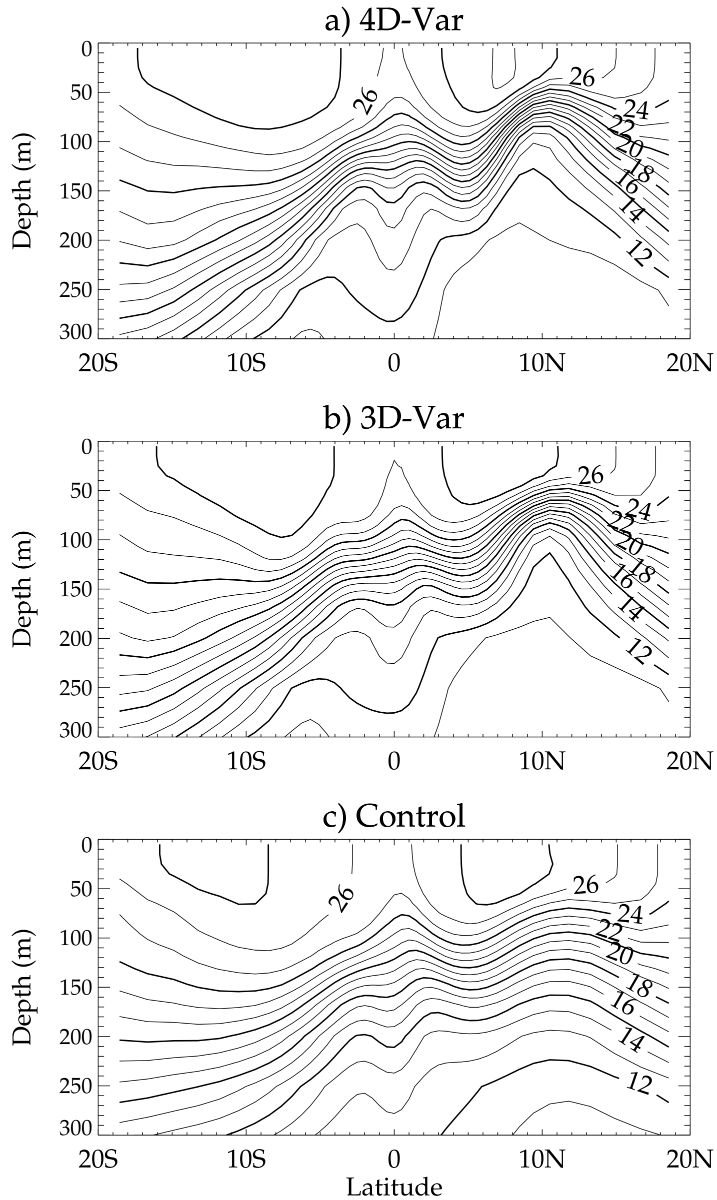


Figure 4.1: Meridional section along 140°W of the 1993-96 average temperature in a) 4D-Var, b) 3D-Var, and c) control. The contour interval is 1°C.

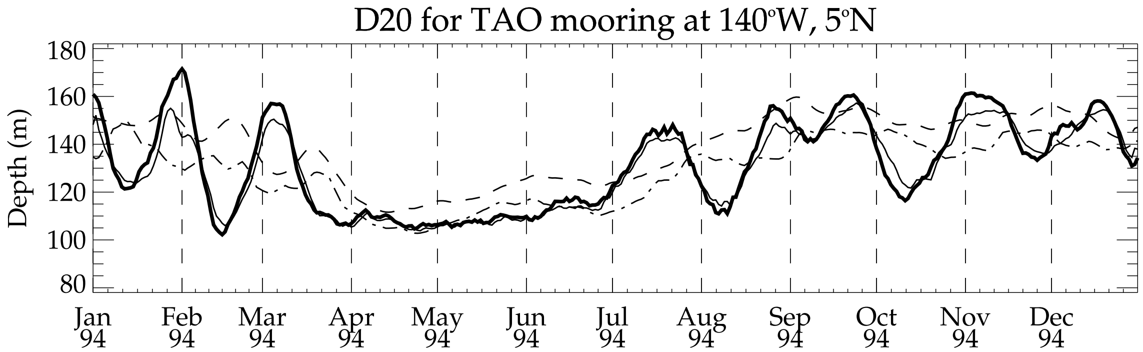


Figure 4.2: Time-series of the daily averaged D20 during 1994 at 140°W, 5°N. The thick solid curve corresponds to the (assimilated) TAO *in situ* data, the solid curve to 4D-Var, the dashed-dotted curve to 3D-Var, and the dashed curve to the control.

4.2 Background-error covariance modelling (A. Weaver, S. Ricci, E. Machu, A. Piacentini, P. Rogel, L. Bessières)

An important element of the data assimilation system is the statistical model used to represent the background-error covariances. In a variational assimilation system, the statistical model is embedded within a covariance operator that is applied in a preconditioning transformation on each iteration of the minimization algorithm. The numerical efficiency of the covariance operator is critical, especially for data assimilation problems involving large state vectors (typically greater than 10^6 components for global ocean applications). The operator should also be flexible enough to capture the main characteristics of the available estimates of the background-error covariances.

An error-covariance operator may be split into two main components: a univariate component and a multivariate component. The univariate component accounts for the auto-covariances of errors in the individual state variables, while the multivariate component accounts for the cross-covariances between errors of different state variables. For modelling the univariate component, a general correlation operator has been developed using an algorithm based on a numerical integration of a generalized diffusion equation [GLO16].

The model is sufficiently flexible to account for a variety of desirable features in a correlation model: functions with a wide range of shapes and spectral characteristics (Fig. 4.3); 2D and 3D anisotropy, geographically varying length scales, and flow dependence (Fig. 4.4). Moreover, it is particularly well suited for application in domains with complex boundaries, such as ocean basins. The (generalized) diffusion algorithm is currently solved using an explicit forward-differencing scheme. An implicit scheme is also being implemented to extend the range of functional forms permitted by the correlation model and to reduce its numerical cost. This work is being done in close collaboration with the Parallel Algorithms group at CERFACS, using software from the Harwell Subroutine Library (HSL).

The multivariate component of the covariance model is being developed using a powerful technique that involves separating the model state variables into balanced and unbalanced components. The balanced components of the state vector are defined through a set of linear transformations. A number of balance

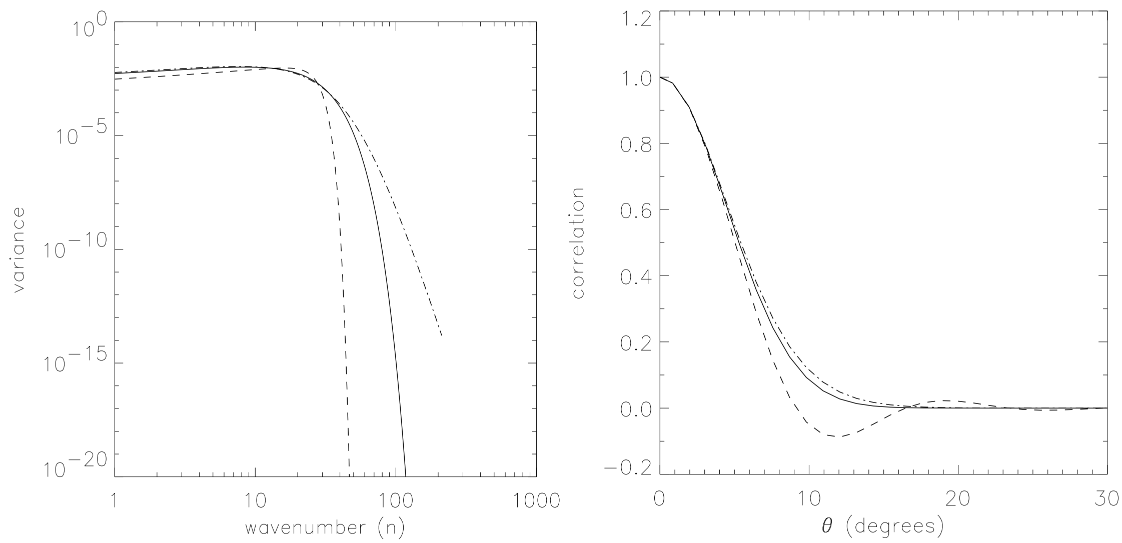


Figure 4.3: An example of three different correlation functions that can be generated using the generalized diffusion equation. The left panel shows their variance power spectrum; the right panel their grid-point values. The solid curve corresponds to a Gaussian. Important features of the functions are that they can be oscillatory in grid-point space (dashed curve, right panel) and can have a wide range of spectral decay rates (dotted and dashed curves, left panel).

transformations have been developed and are currently being tested in the tropical Pacific model. Figure 4.5 shows an example of a salinity increment generated from a temperature increment using a linearized T-S relation in the covariance model. Multivariate constraints between the mass and velocity errors are also being tested using hydrostatic and geostrophic balance relationships (with a high-order geostrophic relation applied near the equator).

The free parameters of the error-covariance model (correlation length scales, variances, regression coefficients in the balance transformations) are being tuned using time-averaged statistics of differences between members of an ensemble integration. Each member of the ensemble has been generated by forcing the ocean model with slightly different surface fluxes. Such an ensemble is designed to sample typical uncertainty (background errors) in ocean simulations. A similar approach is being used for ensemble seasonal forecasting in the DEMETER project.

4.3 Model error estimation in four-dimensional variational assimilation (P. Vidard, A. Piacentini, A. Weaver)

In formulating the 4D-Var, it is common to assume that the numerical model is perfect. For example, this assumption has been made in the OPA 4D-Var described in section 4.1. The reason for this assumption is primarily practical, but is difficult to justify since ocean models are known to have numerous deficiencies (e.g., systematic errors). These errors can lead to significant biases in the analyses produced by 4D-Var. New methods aimed at relaxing the perfect-model assumption in 4D-Var have been investigated. In particular, a new formulation of the 4D-Var has been proposed that accounts explicitly for systematic model

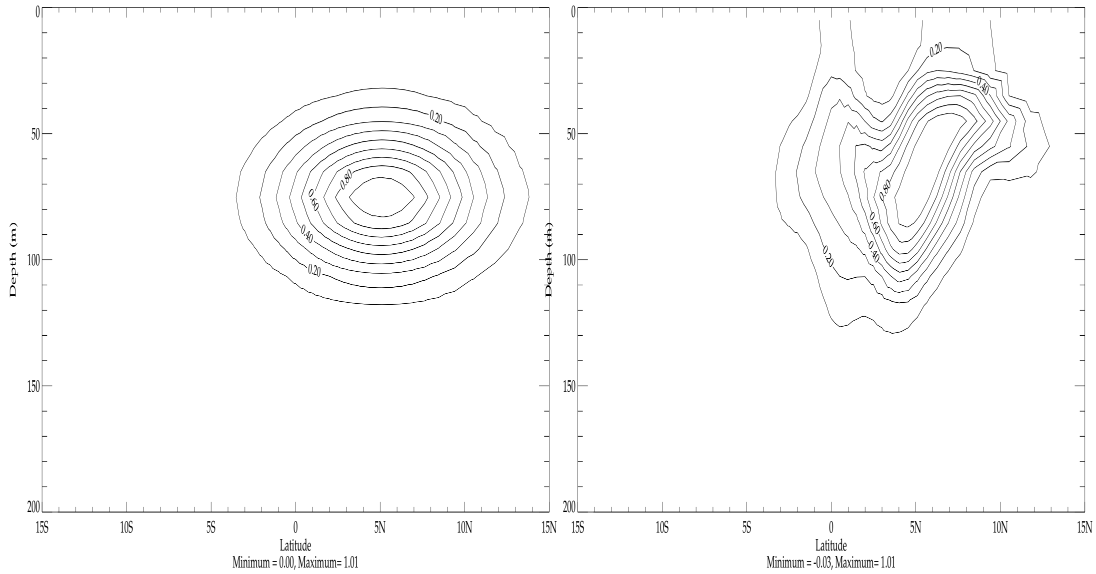


Figure 4.4: An illustration of different correlation structures that can be generated from the diffusion-based correlation model. The vertical axis is depth; the horizontal axis is latitude. The left panel illustrates an auto-correlation field defined in a geopotential coordinate system. The right panel shows the auto-correlation field defined in an isopycnal coordinate system (cf. with the meridional section of the thermal field at 8° N in Fig.4.1a).

error, resulting from, for example, missing model physics. This is done by including a bias correction term in the model equations to compensate for the missing physics. The time-evolution of the bias is specified by a deterministic bias model. The initial condition of the bias model is assumed to be unknown, however. The initial condition of both the bias and the model state vector are then estimated together in the 4D-Var minimization problem. (In the classical formulation of 4D-Var, it is only the initial state vector that is estimated).

Identical-twin experiments have been performed using a shallow-water model in which simulated (altimeter) observations of sea-surface height are assimilated in a model contaminated with systematic error, the latter being imposed by incorrectly specifying the windstress forcing and mixing coefficients relative to those used in the model run to generate the "observations". Figure 4.6 (left panel) shows how the analysis from 4D-Var with a bias correction term (modelled here as a time-independent bias) can lead to a significant improvement over a 4D-Var without bias correction. A particularly intriguing question is what to do with the model correction term in an ensuing forecast. Figure 4.6 (right panel) suggests that there may be substantial benefit to forecast quality if this term is persisted into the forecast step.

The 4D-Var with model bias correction has also been implemented in OPA and tested using the same configuration described in 4.1. Experiments show that 4D-Var with bias correction is able to alleviate some of the deficiencies in the original system in which initial conditions are taken as control variables; e.g., by reducing the size of the "jumps" between analysis steps, and by correcting a salinity drift.

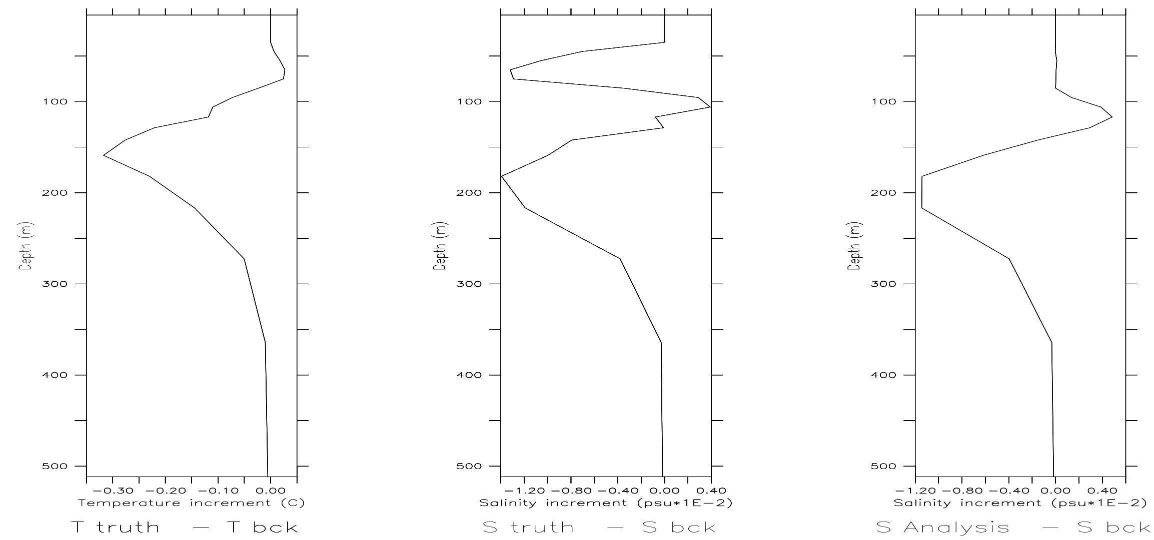


Figure 4.5: An example of how the linear T-S balance can be used to reconstruct a salinity perturbation. The temperature and salinity perturbations (δT and δS) have been generated from wind-perturbation experiments performed with the global (ORCA) model. The left panel shows a δT profile at the equator in the central Pacific, and the right panel the corresponding reconstructed δS profile. The middle panel shows the "true" δS profile. Note that the reconstructed profile is very close to that of the true profile except in the mixed-layer where T-S conservation breaks down.

4.4 Development of three- and four-dimensional variational assimilation for the global ocean (A. Weaver, P. Rogel, A. Piacentini, E. Machu, S. Ricci)

The present 3D- and 4D-Var systems have been extensively validated in the tropical Pacific basin. Global versions are being developed for the free-surface ORCA-version of OPA. ORCA is the ocean component of two coupled models (ORCA2-ARPEGE and ORCA2-IFS) being used for seasonal forecasting and data assimilation in the EC-FP5 projects DEMETER and ENACT. ORCA is also the prototype global configuration for MERCATOR.

One of the main reasons for developing the global assimilation systems is to provide improved ocean analyses for seasonal forecasting (DEMETER, ENACT). The 3D- and 4D-Var systems are being developed together since, apart from the TL and adjoint models, they share all other components. 3D-Var is computationally much less expensive than 4D-Var and hence is potentially more practical for high-resolution applications. It also provides a natural reference for evaluating (the more costly) 4D-Var. The important developments that have been made specifically for the global systems include:

- extending the control vector to include an initial condition increment for sea-surface height (SSH);
- related extensions to the background-error covariance matrix to include a diffusion-based correlation model for SSH;
- a general 2D interpolation (observation) operator, and its adjoint, for use with the distorted horizontal grid of ORCA;

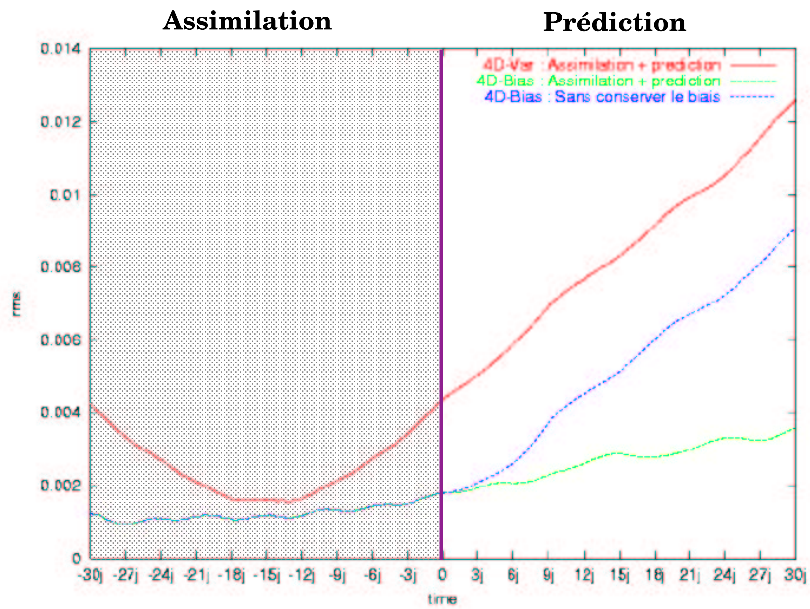


Figure 4.6: RMS error in the sea-surface height as a function of time (negative days correspond to the assimilation time-window, positive days correspond to the forecast) for 4D-Var without bias estimation (solid curve), for 4D-Var with bias estimation but with the correction term dropped during the forecast (dashed curve), and 4D-Var with bias correction and with the correction term persisted into the forecast (dotted curve).

- a 1D spline interpolation (observation) operator, and its adjoint, for the vertical grid;
- the TL and adjoint of the free-surface module of ORCA;
- a simplified TL and adjoint of isopycnal and eddy-induced diffusion parametrisations.

Validation of the systems is currently in progress.

5 The PALM software for data assimilation applications

5.1 Implementation of the PALM prototype (F. Guevara, T. Morel, D. Déclat, C. Martin, S. Buis, E. Gondet, A. Piacentini)

The design of the PALM software prototype was defined in the previous phases of the MERCATOR project. The coding has started in 1999 and the first applications with the earliest versions of the prototype date back to the second semester of 1999. The experience obtained with these applications and the increase of the manpower allocated to the PALM project have permitted a thorough rewriting of the PALM prototype in 2000 and 2001.

While keeping the three main characteristics of the old version (Fortran 90 programming, SPMD - Single Program Multiple Data paradigm, MPI1 message passing library), the rewritten prototype presents many new features which make it closer to what the final implementation of PALM will be. In particular, the internal modularity of the code has been greatly improved, making neater the role of each component of PALM. The PALM driver has been enhanced in order to correctly handle race conditions between units on separate branches. The internal storage has been entirely redefined: it is now more compact and the access and update time of the information handled by the driver are largely improved. The communication functions are safer and the problem of the temporary storage of large data between posting and reception has been fixed. The graphical interface has been completely rewritten. Its ergonomics is greatly enhanced, the coherency checks have been improved, the first functions for the execution post-mortem analysis have been implemented and the issue of the algorithm description through the graphical interface has been addressed. A thorough study on the implementation of the parallel communications and of the algebraic solvers has been carried on [GLO65]. The definition of the functionalities to be implemented in the algebra toolbox is summarized in [GLO40]. The implementation of the algebraic kernel has started at the end of the year.

At the overall level, the code is ported on SGI 02000, on Fujitsu VPP700 and VPP5000, on Compaq SC232 and on NEC SX5 and it has been optimized to take advantage of vector architectures.

The sources of the PALM prototype and of the graphical interface PrePALM_PROTO are handled with CVS.

The latest document on the state of play on the PALM prototype is [GLO67].

5.2 Documentation and Training for the PALM prototype (A. Piacentini, T. Morel, S. Buis)

The PALM prototype has been delivered at the end of 2001. Its use is free for research purposes and is encouraged for the MERCATOR related assimilation activities. That makes a good documentation a necessary “*atout*” for the diffusion of the software.

The PALM project is thoroughly presented on the web site: `http://www.cerfacs.fr/~globc`

The software is provided with an installation guide and a user guide. The user guide includes a tutorial to go progressively through all the features of the PALM prototype and of its graphical interface PrePALM.

A three day training session can be provided if necessary. One training was given in december 2001 to part of the MERCATOR staff and a second session is planned for january 2002.
The PALM team provides a constant user support for the PALM products. The mail address `palmhelp@cerfacs.fr` can be used by all users to contact the PALM team.

5.3 Development of a PALM breadboard (A. Piacentini, P. Vidard, V. Auffray)

The prototyping activity is naturally accompanied by an extensive testing of the new code. With the aim of testing the flexibility, the performances and the portability of the PALM prototype and of its interface PrePALM_PROTO, a bench case has been designed. It is based on a 2D Shallow Water nonlinear model and it makes use of its linear tangent and adjoint versions. The models have been developed and set into the PALM formalism (see section 4.3).
These models have been used to implement a 3D-Var and a 4D-Var assimilation scheme [GLO35]. Starting from these assimilation schemes, the bench case has been improved and it includes now twelve different cases implementing the 3D-Var, the 3D-FGAT, the 3D-PSAS, the 4D-Var, the incremental 4D-Var methods with different minimizers.
This bench case is the base of the development of an advanced tutorial for the PALM prototype applications in data assimilation.

5.4 Investigation of minimization algorithms and software (A. Piacentini, A. Sartenaer, S. Buis, J. Tshimanga)

PALM provides an algebraic toolbox to handle the most common operations in data assimilation. A very important element in variational data assimilation is the minimizer: variational assimilation is posed as a non-quadratic, very large scale optimization problem.
In order to choose the most suitable algorithms and the most performing implementations, we explore the existing software, using the Shallow Water breadbord as bench case.
This topic is treated in collaboration with the Parallel Algorithm team at CERFACS and with the Mathematics Department of the University of Namur (Belgium).

5.5 Design and implementation of the final version (D. Déclat, E. Gondet, T. Morel, F. Guevara, S. Buis, A. Piacentini)

The final version of PALM will be provided to the MERCATOR project by the end of the first semester of 2003. Starting from the experience obtained with the PALM prototype, the PALM group has designed and defined the MPMD (Multiple Programs Multiple Data) version of PALM. This version is identified as PALM_MP. The technical solutions to be retained for this version strictly depend on what the computer constructors and the software providers will provide for the next generations of supercomputers. For this reason a close contact with the main constructors is an important issue during the phase of design. A special collaboration have been established with the FECIT team of Fujitsu Europe.
The specifications for the internal structure of PALM_MP are summarized in [GLO66]. This is the starting point of the subdivision of the development of the code components among the members of the PALM team. A strict management of the teamwork is necessary to follow the development calendar imposed by the MERCATOR planning.

The implementation of the first lines of the final version has begun at the end of the year 2000 [GLO46]. By the end of 2001 the PALM prototype version has been frozen (but for maintenance) and all the manpower has been switched to the PALM_MP implementation.

5.6 Applications of PALM (B. Tranchant, J.M. Lellouche, Th. Lagarde, S. Massart)

5.6.1 Application to the MERCATOR prototype

The PALM prototype is used to implement the data assimilation suite in PSY1, the first prototype of the operational ocean forecasting system of the MERCATOR project. Satellite data are assimilated in a primitive equation model of the North Atlantic with a horizontal resolution of 1/3° (MNATL). The assimilation scheme is the sub-optimal interpolation method from SOFA3.
During 2001 the second MERCATOR prototype PSY2 has been implemented. Satellite data are assimilated in a primitive equation model of the North Atlantic and Mediterranean with a horizontal resolution of 1/15° (PAM). The assimilation scheme is the sub-optimal interpolation method from SOFA3.

5.6.2 Investigation of saddle point type algorithms

In [GLO33], a new class of variational data assimilation methods has been introduced based on the formulation of the optimization problems as a saddle point search. This class of method can be considered as a continuum between the well known primal and dual formulations of the variational assimilation. These new methods have been tested and compared with the classical formulations on a simple model. The implementation takes advantage of PALM modularity and parallelism concepts.

5.6.3 Model error estimation in four-dimensional variational assimilation

In [GLO34], the PALM prototype has been used for the first time to realise a full size data assimilation application with PALM. Further details on this work are given in the previous section.

5.6.4 Data assimilation for atmospheric chemistry

The aim of this work is the extensive comparisons of data assimilation methods methods for new applications. Simplified models for atmospheric chemistry have been used in order to compare different variational formulations and filters [GLO18]. This work is the object of a collaboration with EDF/DER.
The comparison of data assimilation methods for simple pollution models is also the object of the collaboration with INRIA/IDOPT and ENPC/CEREVE in the framework of the 'Action de Recherche Collaborative' COMODE.

5.6.5 Application to Numerical Weather Prediction

The PALM group is involved in a scientific and technical collaboration with SMC (Service météorologique du Canada) aimed to set the basis for the use of PALM in the next operational forecast/assimilation suite. As a counterpart, SMC will take part in some specific development of the final versions of PALM and will insure the porting to the supercomputers installed at SMC.

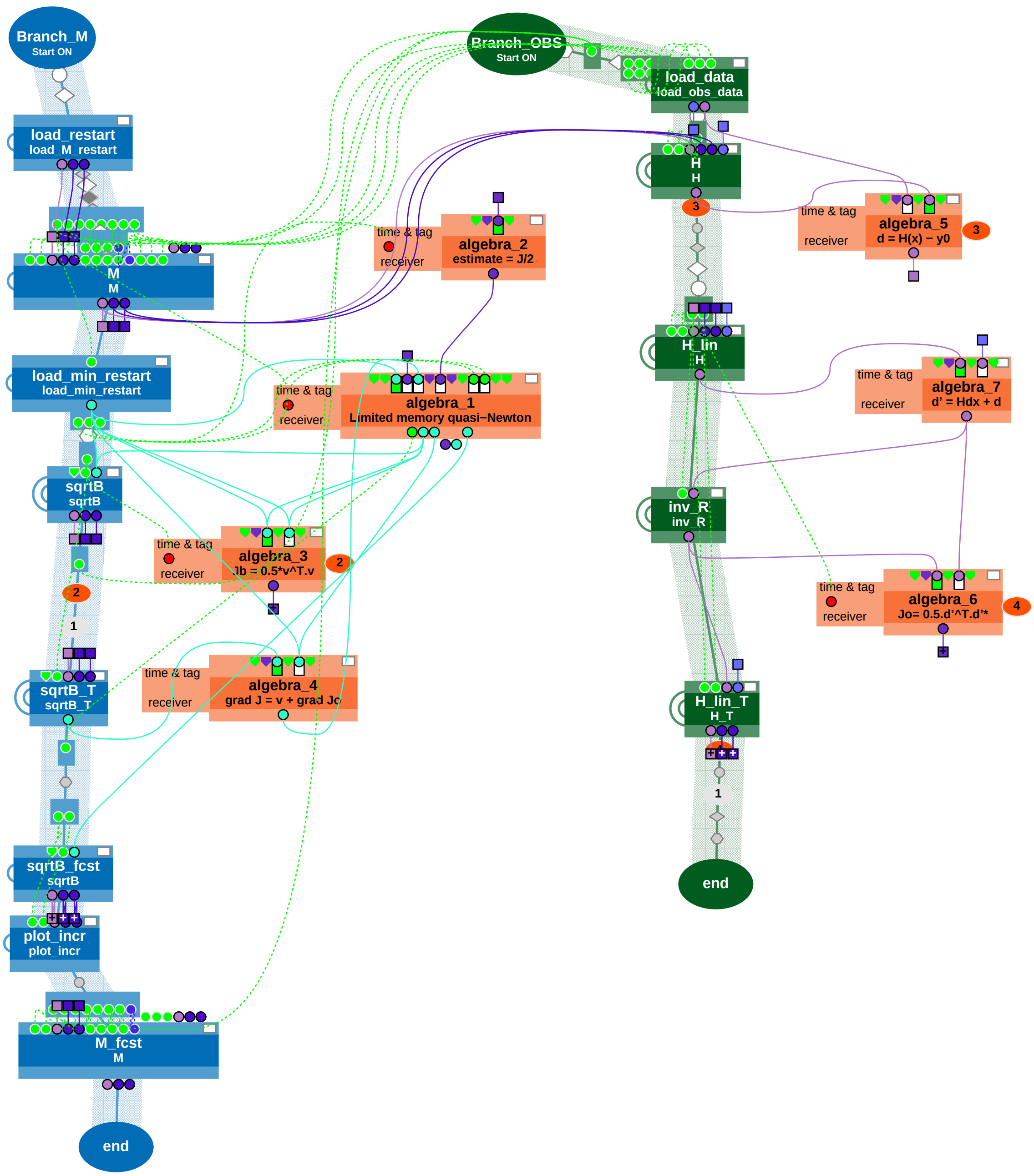


Figure 5.1: The 3D-FGAT method as seen through the PrePALM_PROTO interface

6 The OASIS coupler and applications

6.1 Development of the OASIS coupler and the PRISM project (S. Valcke, L. Terray, A. Piacentini)

Constantly improving the OASIS software, a new version OASIS 2.4 was released in June 2000. The main addition in this new version is the possibility of using the emerging standard MPI2 as message passing library within the CLIM communication technique. This improvement was realized in collaboration with J. Latour from Fujitsu/FECIT. Another important improvement was the new possibility of using the GMEM technique -introduced in OASIS 2.3- to couple a MPI parallel model.

Confirming the CERFACS as a central actor in the coupled climate modelling community, an international workshop on the "Technical Aspects of Future Sea-Ice-Ocean-Atmosphere-Biosphere Coupling" gathering about 70 scientists and engineers was organized jointly by CERFACS and FUJITSU in Toulouse in October 2000. The objective of the workshop was to assess the future needs in sea-ice-ocean-atmosphere-biosphere coupling. The workshop was very successful thanks to the active participation of all people present. The conclusions of this workshop helped the OASIS team to identify the preferred long-term OASIS development axes:

- design a generic interface to be used in the models allowing a standard, and possibly parallel, communication with OASIS;
- improve and develop the interpolation functionalities of OASIS;
- parallelize and optimize OASIS internal functionalities.

All these aspects will in fact be developed in the framework of the PRISM project funded by the European Community under Framework Program 5, that started on December 1st 2001. The objective of PRISM is to realize a flexible infrastructure which will facilitate the assembling, execution and post-processing of global coupled models for climate modelling. The PRISM System will be based on component models existing in different European institutions that will be modified to incorporate standard interfaces. The coupler will be based on OASIS; CERFACS is therefore leading the workpackage on the coupler development that will bring an additional resource of 88 person-months for the OASIS development. The work on the OASIS/PRISM coupler already started with a workpackage pre-project meeting in Toulouse in October 2001.

6.2 OASIS applications (L. Terray, S. Valcke, P. Rogel, E. Maisonnave)

The OPA-OASIS-ARPEGE coupled model assembled in the framework of our seasonal forecasting activities effectively produced hundreds of short coupled run that were scientifically analyzed (see section 3).

A control simulation and a scenario experiment based on another version of the OPA-OASIS-ARPEGE coupled model, were also realized at the Centre National de Recherches Météorologiques (CNRM) of Météo-France. This scenario takes into account the anthropogenic increase in greenhouse gases and their potential effect on the ozone photo-chemistry considering homogeneous and heterogeneous chemistry. The scientific assessment of the control run simulated climatology has already started, especially the characterization of the North Atlantic Oscillation variability.

Finally, a new CGCM using the model and coupler latest versions (OPA/ORCA2, ARPEGE V3, and OASIS 2.4) was assembled and is now running. This CGCM is being used in the PREDICATE project to perform a long 150-year simulation to study the natural variability of the current climate (see section 2).

7 The MERCATOR Prototypes

Laure Siefridt and Laurence Fleury

The Mercator project develops several ocean circulation modelling and assimilation systems to both serve the international Global Ocean Data Assimilation Experiment (GODAE) and the future French ‘Centre d’Océanographie Opérationnelle’. Two research axis have been selected. The ‘Prototype Atlantique et Méditerranée’ (PAM) is designed to investigate very high resolution forecasting feasability over a region that has already been widely studied. The ‘Prototype Océan Global’ (POG) addresses the global objective of *GODAE* and benefits from the previous PAM implementation.

7.1 The North Atlantic and Mediterranean Prototype: PAM (L. Siefridt)

The Atlantic and Mediterranean Mercator prototype is a very high resolution (5 to 7 km) forecasting system that includes many features of the global ocean Mercator system and that will run in an operational mode in 2002.
Its implementation is based on the OPA8.1 ocean general circulation model developed at LODyC (Paris) and benefited from the experience gained with the lower resolution (1/3°) MNATL configuration. This model has been inherited from the French multi-laboratory CLIPPER research project [8] aiming at simulating the Atlantic basin circulation. It is used as a handy research and development tool. Moreover it is part of the first Mercator operational system which is used for real time analysis and forecasts since January 17^{th} 2001.
The PAM model configuration was designed in 1998, implemented and tuned in 1999 and 2000. Sensitivity tests have been conducted during the years 2000 and 2001. They have led to the achievement of a 11-year simulation experiment in a spin-up mode and of a 1998 to 2000 interannual simulation. The interannual simulation shows very promising results and is actually under evaluation.

Along side, the implementation of the Mercator Assimilation System (SAM) has been performed. The first system is based on the SOFA3 optimal interpolation scheme [7] and on the PALM [GLO67] software which enables the coupling between the model and the assimilation scheme. It is designed to evolve by adopting more and more complex assimilation algorithms.

Activities during 2000 and 2001 have consisted in:

- performing MNATL 1/3° simulations to assess the relevance of the PAM strategy;
- processing and evaluating the forcing fluxes;
- performing some sensitivity experiments with the PAM model;
- designing, performing and validating multiannual PAM model simulations;
- designing the first SAM system (SAM-1) and implementing it in the MNATL 1/3° model;

- testing the multiprocessor approach of SAM-1 before its implementation in the PAM system;
- fully coupling the SAM-1 system to the PAM model;
- studying the implementation of a SEEK assimilation scheme for the SAM-2 version.

Next steps will concern the implementation in the ocean model of numerical schemes and parameterisations validated in the research community: the Beckmann and Döscher Bottom Boundary Layer method [3], the KPP [5] mixing scheme and the TVD [4] or MUSCL [6] advection scheme. The southern boundary will be further investigated. The introduction of temporal variability will first be tested in the actual buffer zone. As an alternative representation of the PAM southern limit, an open boundary is being introduced at 9°N. The objective is to make the model more realistic and prepare it to comunicate with the global prototype. On the other hand, the SAM-1 scheme will be upgraded with multivariate assimilation. A reanalysis will be performed from 1993 to 2001 with the PAM/SAM-1 system. *A posteriori* diagnostics of the analysis and the assimilation scheme are furthermore being implemented in the system following the methodology of O. Talagrand [9].

[3] A. Beckmann and R. Dörscher, (1997), A method for improved representation of dense water spreading over topography in geopotential-coordinate models., *J. Phys. Oceanogr.*, **27**, 581–591.

[4] I. James, (1996), Advection schemes for shelf sea ocean models, *J. Mar. Sys.*

[5] W. Large, (1998), Modeling and parameterization ocean planetary boundary layers, *E.P. Chassignet and J. Verron (Eds), Ocean Modeling and Parameterization, Kluwer Academic Publishers*.

[6] M. Levy, A. Estubier, and G. Madec, (2001), Choice of an advection scheme for biogeochemical models, *GRL*.

[7] P. De Mey and M. Benkiran, (2000), A multivariate reduced-order optimal interpolation method and its application to the Mediterranean basin -scale circulation, *Ocean Forecasting: Conceptual basis and applications, N. Pinardi, Springer-Verlag, in press.*

[8] Projet Clipper, (2001), Modélisation à haute résolution de la circulation dans l'océan Atlantique forcée et couplée océan–atmosphère – Rapport Final d'Activité Scientifique et Technique, Tech. Rep. CLIPPER-R1-2001.

[9] O. Talagrand, (1998), A posteriori evaluation and verification of analysis and assimilation algorithms, *proceedings of Workshop on Diagnosis of Data Assimilation Systems, Reading, England, 2-4 November 1998*.

7.1.1 The MNATL 1/3° studies

7.1.1.1 The southern buffer zone definition (L. Fleury)

The PAM domain extends from 9 to 70° N. The southern boundary location may be questionable because it excludes the tropical variability and may defavour the southern feeding of the Gulf Stream. To assess the influence of selecting the precise location of the southern boundary, we compared the results of two 10-year simulations performed using the MNATL 1/3° model over two different domains, the first one extending from 20° S to 70° N and the second one from 9°N to 70°N. The time-mean circulation as well as the eddy kinetic energy present similar patterns and intensities along the two simulations.
The design of the southern buffer zone has then been tested in the 1/3° model. The Caribbean Sea is free from any relaxation and the restoring coefficients profile follows a trilinear shape and corresponds to 3 days at the southern limit, to 3.3 days at 10.5°N, to 30 days at 15°N and 100 days at 17°N.

7.1.1.2 The CE98 forcing assessment (R. Bourdallé-Badie, L. Fleury)

Two 10-year spin up have been designed following the twin experiment methodology. They only differ by the surface forcing applied as a perpetual year. In one simulation, the model is forced by climatological

fluxes, which are the long-term average of the 1979-93 ECMWF reanalysis fluxes. In the second simulation it is forced by the operational ECMWF forecasts from March 1998 to February 1999 (CE98).
The aim of the study is to assess the so-called CE98 atmospheric forcing and its impact on the ocean simulation, as it forces the PAM model in its spin-up simulation.
At the basin scale, the two different forcing sets as well as the simulated ocean circulations present comparable features. However, a large difference is exhibited concerning the convection in the northern Atlantic which is partly inhibited in the simulation forced by CE98. As a consequence, a decrease of 2 Sverdrup is observed in the meridional overturning streamfunction.
Moreover, differences are observed in the Caribbean basin where the CE98 winds are relatively weak. Despite a different pattern of the circulation in the Carribean Sea and in the Gulf of Mexico, the Gulf Stream has a similar intensity in the two simulations.

7.1.1.3 The lateral friction scheme (R. Bourdallé-Badie)

The lateral boundary condition in the PAM high resolution model has been chosen to be a free slip condition. A no slip condition has been tested in PAM and led to less satisfying results: the transports through the major straits are decreased and a large and static eddy appeared at the separation of the Gulf Stream.
A new parameterisation of the lateral friction called ‘no slip accurate’ is introduced in the last OPA code version. Furthermore, a ‘hybrid condition’ that geographically discriminates the application of a classic ‘no slip’ condition and a ‘free slip’ condition has been designed.
Sensitivity tests have been performed with the MNATL configuration and have focused more specifically on the Caribbean basin and Gulf Stream separation.
The Gulf Stream separation from the coast, and more precisely the turbulent structures that are generated there, are very sensitive to the lateral condition. Using the ‘no slip accurate’ parameterisation does not improve the separation of the jet that exhibits again a static eddy. The ‘hybrid condition’, with the ‘free slip’ condition applied over identified small regions of the Caribbean basin and the ‘no slip’ condition everywhere else, has shown very encouraging results. The transports through the Caribbean straits are even increased.
This study will be pursued. Some parameters of the ‘no slip accurate’ condition need to be further investigated. On the other hand, an automatic discrimination of the strait locations should be implemented for the ‘hybrid condition’.

7.1.2 Evaluation of the forcing fluxes (L. Siefridt, H. Perez)

A global and regional evaluation of the ECMWF operational fluxes has been performed over the CE98 (March 1998 to February 1999) period. While a first investigation indicates that the net heat flux entering the ocean is globally balanced, very strong regional biases are identified with the introduction of the TL319 ECMWF new truncation grid. In particular, an irrealistic cloud cover is present at the Equator, just south of the southern boundary of the PAM model. Moreover, the clear sky atmosphere is too transparent to the solar incoming radiations leading to too much incoming energy at northern mid latitudes and overestimated gradients in the net heat flux. Then, while biases in evaporation and precipitation compensate over warm boundary currents, the overall net freshwater flux exhibits too much freshwater income.
In other respects, the Mediterranean fluxes are found consistent since the introduction of the new grid truncation because of the better representation of the orography.

A comparison between 6-hour and 36-hour ECMWF forecasts has been undertaken. The purpose was to evaluate the impact of the meteorological model spin-up phase (12 h) on daily surface forcing terms in order to possibly recommend the use of specific meteorological time forecasts to force ocean models. As expected, the imbalances, and especially the freshwater one, are reduced with the length of the forecast. However, since the introduction of the 4D-Var at ECMWF at the end of 1997, the impact has been drastically reduced in relation with the better handling of the meteorological spin-up phase. As the 6-hour wind are known reliable, and moreover, as the temporal coherence is crucial to the ocean model, there is no more strong motivation to use an other forecast length to derive daily forcing fluxes. It is found preferable to apply a .85 reducting coefficient to the precipitation and keep using the 6-hour forecasts.

7.1.3 The Atlantic and Mediterranean Prototype experiments

7.1.3.1 Tuning experiments (Y. Drillet)

Sensitivity tests to different parameterizations and calibration experiments have been performed before the achievement of the spin-up simulation. The principal tests concerned the lateral boundary condition, the viscosity and diffusivity coefficients, the southern buffer zone and the wind field. Objective criterions chosen to assess the 'best' simulation were based on the transport through the principal straits (Florida, Gibraltar, Denmark, ...) and on the principal current strength and position (Gulf Stream, Subpolar Gyre, North Atlantic Current, Azores current).
The spin up experiment, called PAM-05, has been performed. It is a 11-year simulation forced by the CE98 ECMWF atmospheric fluxes. The realisation of the simulation has required over 2000 CPU hours on the VPP5000 and has generated 1 100 Go of output files.

7.1.3.2 Evaluation of the PAM spin-up simulation (Y. Drillet, R. Bourdallé-Badie, L. Fleury, H. Perez, L. Siefridt)

The analysis of the simulation benefited from the experience of the CLIPPER and MERCATOR community, and also from the direct involvment of K. Béranger at LODyC concerning the Mediterranean basin and S. Theetten then C. Talandier at LPO concerning the east Atlantic.

The analysis has focused on the representation of the Gulf Stream and especially its separation at cape Hatteras, the other major currents like the North Atlantic Current or the Azores front, the Mediterranean outflow, the Caribbean Sea circulation and the meridional overturning streamfunction. The PAM simulation was first compared to lower resolution results, especially to the MNATL 1/3° simulation, designed as close as possible to the PAM simulation, and also to the Clipper 1/6° results. Secondly, it was confronted to equivalent resolution models, in particular to the american MICOM 1/12° [10] and POP 1/10° [11] simulations.

The first ensemble of comparisons allows to discriminate the benefit of the high resolution from the biases of the model and the physical parameterisations. Although the resolution does not solve problems such as the too northern separation of the Gulf Stream, the sinking of the Mediterranean waters at a non-realistic depth and the salinisation and warming of the Labrador waters, it induces interesting and realistic characteristics such as modal Madeira waters, African coastal upwelling, Meddies and turbulent activity up to the Gulf of Biscay. Moreover, we note that the residual eddy present at the separation of the Gulf Stream in the 1/6° CLIPPER simulation does not appear any more at PAM resolution.
An atlas of the simulation [GLO52] has been edited, following the format of the 1/6° CLIPPER one.

Some weaknesses of the simulation were further looked at with subsequent sensitivity tests. In particular, the meridional overturning streamfunction was found quite weak, so was the North Atlantic Current.

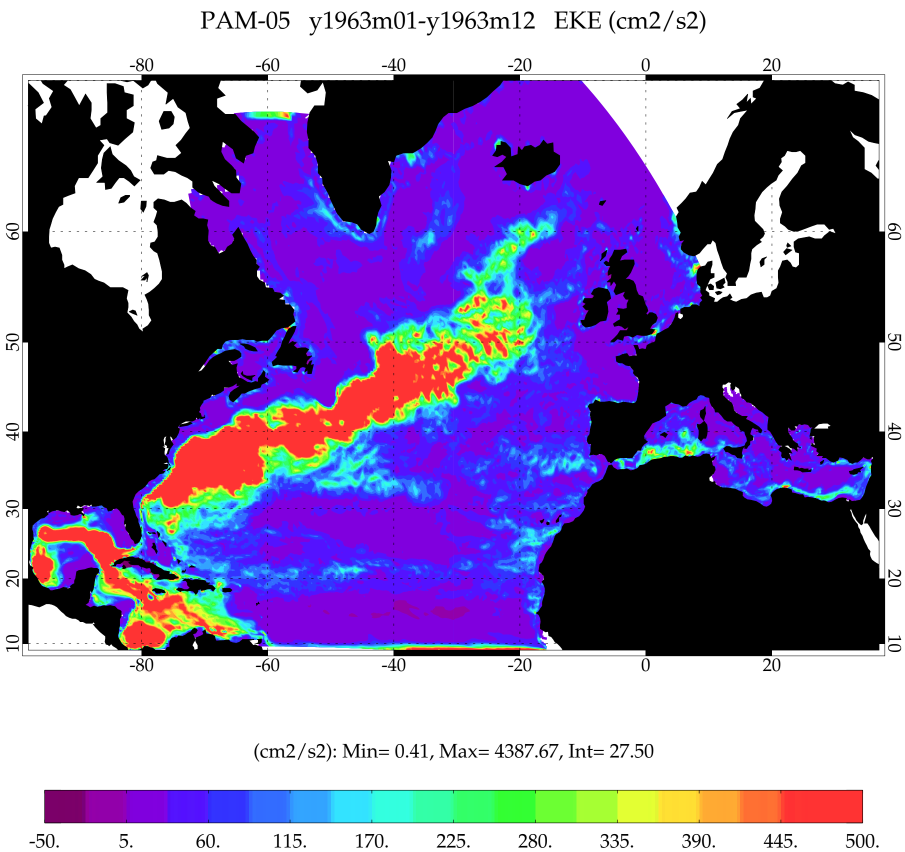


Figure 7.1: Annually averaged eddy kinetic energy (cm^2/s^2) as calculated by the spin-up simulation over the 3^{rd} year.

The second ensemble of comparisons allowed to confront different models and domain configurations at a comparable resolution. The PAM model behaves quite well, despite the limitations previously mentioned. The eddy kinetic energy levels are realistic according to satellite data, the first order circulation is good. The pathway of the Gulf Stream, after its separation at Cape Hatteras, is realistic and intermediate between the POP simulation that would locate it too much south and the one of the MICOM simulation.

[10] A. M. Paiva, E. P. Chassignet, and A. J. Mariano, (2000), Numerical simulations of the North Atlantic subtropical gyre: Sensitivity to boundary conditions and horizontal resolution, *Dyn. Atmos. Oceans*, **32**.

[11] R. D. Smith, M. E. Maltrud, F. O. Bryan, and M. W. Hecht, (2000), Numerical Simulation of the North Atlantic Ocean at 1/10, *J. Phys.Oceanogr.*, **30**.

7.1.3.3 Sensitivity experiments (Y. Drillet, R. Bourdallé-Badie)

A 2-year simulation experiment showed that a slight smoothing of the bathymetry (3 successive Shapiro filters) with a careful check of key topographic features such as the Florida strait is really improving the results. The transport through the strait of Florida is increased by 2 sverdrups, and the eddy kinetic energy field exhibits a northern penetration of the North Atlantic Current, which hardly existed in the spin-up simulation.

On the other hand, the CE98 year used to force the model in the spin-up simulation was found quite specific. The use of a 3-year averaged (1998 to 2000) forcing set allows to simulate a 'more standard' atmospheric state, and increases again the transport through the Strait of Florida by 1 sverdrup.

Moreover, several 6-month experiments have been performed to test and tune the introduction of a deep relaxation zone in the gulf of Cadiz in order to relocate the Mediterranean waters at a realistic depth. The relaxation zone is a 3 degree wide circle centered at 8°W. Temperature and salinity fields are relaxed to the Reynaud climatology with a coefficient linearly increasing from 500m to 1000m and constant downward. The maximum relaxation corresponds to 25 days at the center of the circle and at 1000m. The upper Mediterranean waters that are present in the spin up but not in the climatology are simulated again, and the lower waters are now represented with the right properties. Furthermore, the intrinsic ocean variability does not suffer so far from the introduction of the relaxation zone.

7.1.3.4 The interannual experiment (Y. Drillet, R. Bourdallé-Badie, L. Siefridt)

The interannual experiment benefited from the introduction of the upgrades previously mentioned (smoothing of the bathymetry, relaxation zone in the Gulf of Cadiz, new surface forcing). It also benefited from the correction of the Mediterranean initialisation fields that had been found instable. The surface relaxation to the climatological Reynaud salinity and to the Reynolds temperature has been decreased by a factor of 2.

The experiment consists in a 16-month spin-up simulation forced with the 1998 to 2000 3-year averaged ECMWF fluxes followed by a 3-year interannual simulation from 1998 to 2000.

This simulation is under evaluation. First results are very promising as highlighted by the eddy kinetic energy field displayed in figures 7.1 and ix in the appendix. Moreover the meridional overturning streamfunction exhibits an increased and quite realistic intensity.

7.1.4 Implementation of the assimilation (B. Tranchant, J.M. Lellouche)

7.1.4.1 The first Mercator assimilation system SAM-1

The OPA ocean circulation model and the SOFA3 assimilation code have been coupled with the PALM software (see chapter 5). The resulting SAM-1 system has been successfully implemented in the 1/3° resolution ocean model MNATL in a quasi operational mode. Since January 17^{th} 2001, Mercator bulletins have been available on line to observe and predict changing ocean conditions continuously.

SAM-1 is based on an optimal interpolation scheme (SOFA3 code) for which experience in assimilating satellite altimetry has been gained in different operational systems like SOPRANE and MFSPP. Only the SLA (Sea Level Anomaly) is assimilated with a univariate mode in the SAM-1 first version. The model initialisation is mainly based on the lifting-lowering method [12] used in the GANES project.

7.1.4.2 Implementation of SAM-1 in the PAM configuration

The assimilation scheme SAM-1 has been implemented in its actual version in the PAM configuration and should be operational in 2002.
Figure x in the appendix shows an example of SSH (Sea Surface Height) initial conditions calculated by the actual SAM-1/PAM system.

Due to the PAM size and the PAM grid complexity, two important modifications of SAM-1 were required:
- development of a multiprocessor version of SAM-1 where both ocean model and assimilation scheme are distributed over several processors. The sequential assimilation scheme has then been parallelized (model integration and analysis are distributed on the same processors). Therefore, a particular processing of parallel communications has been set up.
- adaptation of the data selection. In particular, a 'canvas' grid (2D irregular grid) has been introduced, so that model grid points and analysis grid points are located on the same reference coordinates, without needing an additional interpolation. Consequently, data points are easily selected which is an advantage for the calcul of the innovation vector.

7.1.4.3 The second SAM system (SAM-2)

A collaboration has been initiated with the LEGI laboratory to implement a new Mercator assimilation system, named SAM-2, based on the SEEK (Singular Evolutive Extended Kalman) algorithm developped at Grenoble [13].
The SEEK algorithm is a Reduced Order Kalman Filter designed to assimilate altimeter and surface temperature data. The intrinsic advantage of the evolutive Kalman filter is the possibility of updating the state error covariance matrix with the dynamics of the model.
The SAM-2 prototype will have the same framework than SAM-1, and the transition is made simpler through the use of the PALM coupler. The Optimal Interpolation PALM unit will simply be replaced by a SEEK PALM unit. In this configuration, the assimilation PALM coupler will be used to drive both the ocean model and the SEEK filter which is implemented with the SESAM software.

[12] M. Cooper and K. Haines, (1996), Data assimilation with water property conservation, *J. Geophys. Res., 101, p.*, **101**, 1059–1077.

[13] C.-E. Testut, (2000), *Assimilation de données satellitales avec un filtre de Kalman de rang réduit dans un modèle aux Equations Primitives de l'océan Atlantique*, PhD thesis, Université Joseph Fourier (Grenoble I).

7.2 The Global Ocean Prototype: POG (L. Fleury)

The POG group has been initiated at PREVIMAR, a Meteo-France department, in 2000 and relocated at CERFACS in March 2001 as a team of two persons. Two other members joined in November 2001.
The group is in charge of the development of the 1/4º global ocean MERCATOR prototype, which will run in a pre-operational mode during the GODAE (Global Ocean Data Assimilation Experiment) period (2003-2005). In order to test different modelling and assimilation choices and to assess the system, a lower resolution (2º) prototype is developed as well and will be operated in near real time mid-2002.
The group is at the early beginning of the work and the next paragraphs will present mostly its perspectives.

7.2.1 The 2° prototype (N. Ferry, C. Derval, L. Fleury)

The prototype is based on the ORCA2 model, which is the standard configuration of the OPA code developed at LODyC (Paris) and is used in different European research laboratories. The ORCA-type grid for the global ocean proposes an original treatment of the North Pole singularity: two poles are present in the Northern hemisphere located over the Canada and the Russia. The latitude circles, which are regular from the southern limit of the grid to 20º North, become more and more elliptic from 20º to 90º North. The ORCA2 grid counts 181 $\times$ 149 points and 31 levels. It is as isotropic as it might be, except in the equatorial belt where the meridional resolution is diminished down to 0.5º.

Different questions have already been solved. First, the processing of the atmospheric forcing has been set up. The chain used for the already operational MERCATOR system has been modified in order to address the global domain (east-west periodicity and northern condition) and to write the forcing fields in the NetCDF format, using the IO-IPSL software. The new processing has been documented [GLO48].

The ORCA2 model has been installed on the Météo-France VPP5000. A four-year simulation has been performed, using a climatological forcing during the two first years and an interannual forcing afterwards. All the tools (pre-processing, model, post-processing) necessary to perform free simulations have then been tested.

An assimilation scheme is now being implemented in the model. The optimal interpolation scheme SOFA3 [7] is used and coupled to the model with the PALM software (see section 5).

7.2.2 The 1/4° POG prototype (L. Fleury, C. Derval, E. Remy)

The 1/4º global ocean configuration has been defined in collaboration with the French ocean modeling community. The model is based on the OPA8.2 primitive equation z-level model. The chosen parameterisations include a free surface condition, TKE vertical mixing, harmonic isopycnal tracers diffusion and biharmonic dynamics diffusion. The LLN (Louvain-la-Neuve) ice model already coupled with OPA for climate studies will be used.

An ORCA-type grid has been set up. It has 1442 $\times$ 1021 points and 42 vertical levels. The vertical spacing increases from 6 meters at the surface to 60 meters at 400 meter depth and 300 meters at the bottom. The bathymetry has been processed from the Smith and Sandwell dataset between 72º South and 72º North, the BedMap dataset south of 72º South and the IBCAO dataset north of 72º North. The bathymetry is now being checked ans tested through numerical simulation. The atmospheric forcing processing has been adapted to the 1/4º configuration.

The model routines have been set up. They originate mostly from the standard 2001 OPA8.2 sources, but also include diagnostics which have been used in the PAM model. New options have been added like the possibility of writing results in the NetCDF format while performing multiprocessor simulations. Some checking of the sources is still under process.

First simulations are expected to be performed in the first half of 2002. After validating the results, the optimal interpolation scheme SOFA3 will be coupled to the model with the PALM software.

8 Publications

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6

Technology Transfer Group

1 Introduction

Pierre-Henri Cros

The Technology Transfer Group's (TT Group) main duty is to take advantage of CERFACS results for developing new activities towards new customers, given that:

- each CERFACS' team work programme is agreed with CERFACS shareholders, which are the main beneficiaries of this research,
- each CERFACS team is managing its own work as far as diffusion of its results is concerned.

In this context, where technology transfer is part of every team's work, it is necessary for the TT Group to be innovative in order to offer a complementary approach, fully compatible with the other activities.

As CERFACS is mainly working with large companies, it has been decided that the TT Group would address SME's (Small and Medium Enterprises). To be innovative the TT group has implemented its work as follows :

- characterise CERFACS' offering from a generic point of view,
- develop a good understanding of user's needs, given that target enterprises did not previously work with CERFACS nor have familiarity with computer studies,
- establish an innovative approach,
- test it,
- and finally deploy the corresponding activity with the customer.

2 CERFACS offering

Susanne CHANSSARD, **Pierre-Henri CROS**

For the scientific community as well as for large companies, CERFACS' competencies are now well known for each application domain, for example., Computational Fluid Dynamics. They obviously understand that computer simulations have to be used to document different configurations.

To serve users who are not so familiar with computer possibilities, it was necessary to find a wording which would be both understandable by everyone and summarize correctly CERFACS' offering. It was finally chosen to present it as a ”Numerical Simulation offering”, a wording quite frequently used by different information means making it easier to contact target users even if they do not have a clear idea of what immediate advantage they can get from it.

3 Target user needs

Gilles BAUBE (since September 1999), Susanne CHANSSARD (until august 1999), Pierre-Henri CROS, Stphane GRES (since September 2000)

Thanks to the EC HPCN-TTN (High Performance Computing and Networking - Technology Transfer Nodes) programme, TT Group received support, in 1997, to meet such potential new users.

This programme involved 20 other European groups coming from important research centres who were willing to diffuse their numerical simulation know-how to SME's.

The three-year work included :

- studies to establish at which level of the process numerical simulation could offer improvements and to adapt one of CERFACS' numerical tool to one of the needs,
- organisation or participation in events promoting the use of numerical simulation.

The work programme was organised in large sectors, the TT Group leading the Aerospace Sector Group. During these three years, the TT Group worked closely with approximately 200 SME's, mainly in France but also in the rest of Europe.

Most SME's which have been contacted were designing their own products or were put in charge by big customers of designing more or less important parts of their product.

All SME's declared themselves as being interested by numerical simulation possibilities, and assessed that this technology could help them to meet their general challenges :

- shorten product design cycles,
- improve the product quality,
- be more reactive.

It has been necessary to understand why these companies apparently interested in numerical simulation, were finally not ready to use this technology. In order to introduce numerical simulation in their process the requirements are:

- hardware
- software
- expertise, for both maintaining and fully taking profit of the above means.

These three resources are difficult to get simultaneously, mainly because the associated costs must be charged against different projects, and because follow-on projects requesting similar resources are not always available in such SMEs.

Further to this analysis, it appeared that these companies could be interested in an offering consisting of access to a set of resources. This offering was described as a way to get all the missing means required for the duration of the project. It was further necessary to make SMEs feel this complementary to their own tools, and to favour better interactions with the TT Group's experts.

As a result the TT Group defined a so-called ”Service Platform”, that can be characterized in the figure 3.1.

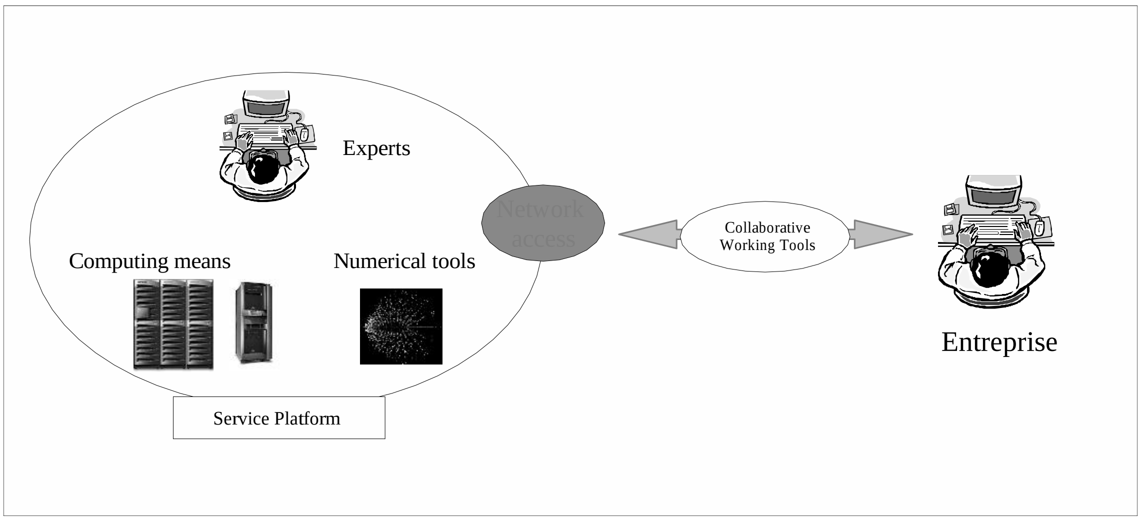


Figure 3.1: Service Platform

It is a complete service offering, based on collaborative working tools enabling the SME to remotely access the expertise, numerical tools and computing means requested to perform its numerical simulations.

4 Test the solution

Gilles BAUBE (until July 2001), Christophe BARDY (from March 2001 to September 2001), Reda BOUREBABA (from March 2000 to December 2001), Pierre-Henri CROS, Lars FRENZEL (from April 2001 to June 2001), Stphane GRES (from September 2000 to July 2001), Erwan LEGOULVEN (from March 2001 to September 2001), Gabriel JONVILLE (since October 2000), Philippe MOINAT (since March 2000)

Through a Ten-Telecom EC programme, the TT Group received a grant in 2000 to implement with two other research centres (University of Stuttgart-RUS, PDC-KTH-Stockholm), and four technology providers (Alcatel Space, Silicon Graphics, StorageTek and VirCinity), a two-year project enabling :

- implementing a prototype of this platform,
- testing in industrial scenarios,
- assessing the economic relevance of this service approach.

This project was called : European Numerical Simulation Services for SME's (ENScube).

As far as CERFACS is concerned, the setting up of the ENScube service platform prototype has relied on the CFD and CSG teams (see corresponding chapters) and on the possible access to the O-2000 computer. Furthermore, the following steps were identified as requiring interactive exchanges during numerical simulation project :

- specifications,
- parametrization,
- analysis of the results,
- validation of the results.

To enable participants of such projects to meet easily and every time that it was necessary, without having to travel, it has been necessary to develop a product for working remotely, called "ENScube Work package" characterized in the figure 4.1.

It is based on three displays having each a specific function :

- Display 1 is used to share documents. Each participant can take control to underline a particular point, to change words sentences or pictures. The document remains the property of whosever proposed it. This means that the modifications can only be accepted or declined by the owner, himself,
- Display 2 gathers all monitoring buttons (for allowing the control, for opening documents to be shared, for launching the co-visualization), audio and video functionalities, chat facilities and a shared whiteboard,

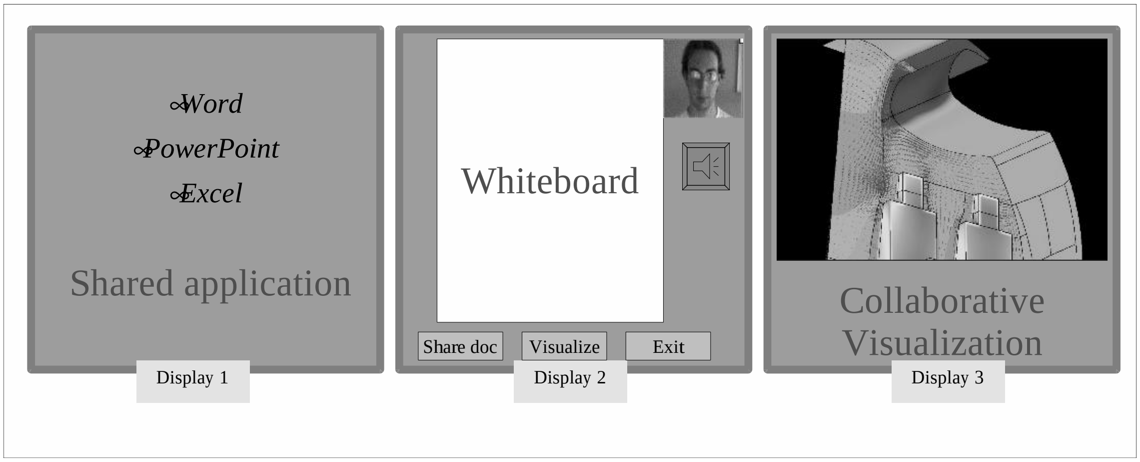


Figure 4.1: ENScube Work package

- Display 3 offers a functionality enabling participants to share and to manipulate interactively computing results.

Displays 1 and 2 are run by a Window PC and display 3 by an UNIX workstation.

Two types of scenarios have been implemented with 7 companies of different sizes (AIRBUS, EDF, Liebherr Aerospace, L'Hotelier, GNS gmbH, High Tech Engineering, Svenska Rotormaskiner).

Scenario 1
For this scenario (see figure 4.2), the work is performed between the Service Platform and the company, which was linked by ISDN facilities to CERFACS, thanks to the ENScube Work package.

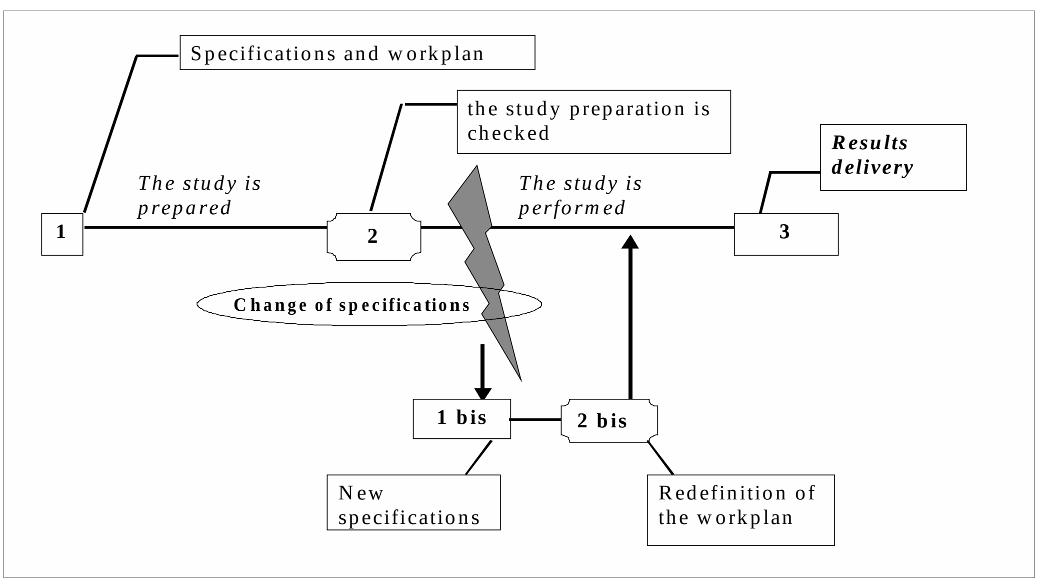


Figure 4.2: Scenario 1

Scenario 2

For this scenario (see figure 4.3), the work involves three sites having different skills, and linked by ISDN facilities thanks to the ENScube Work package.

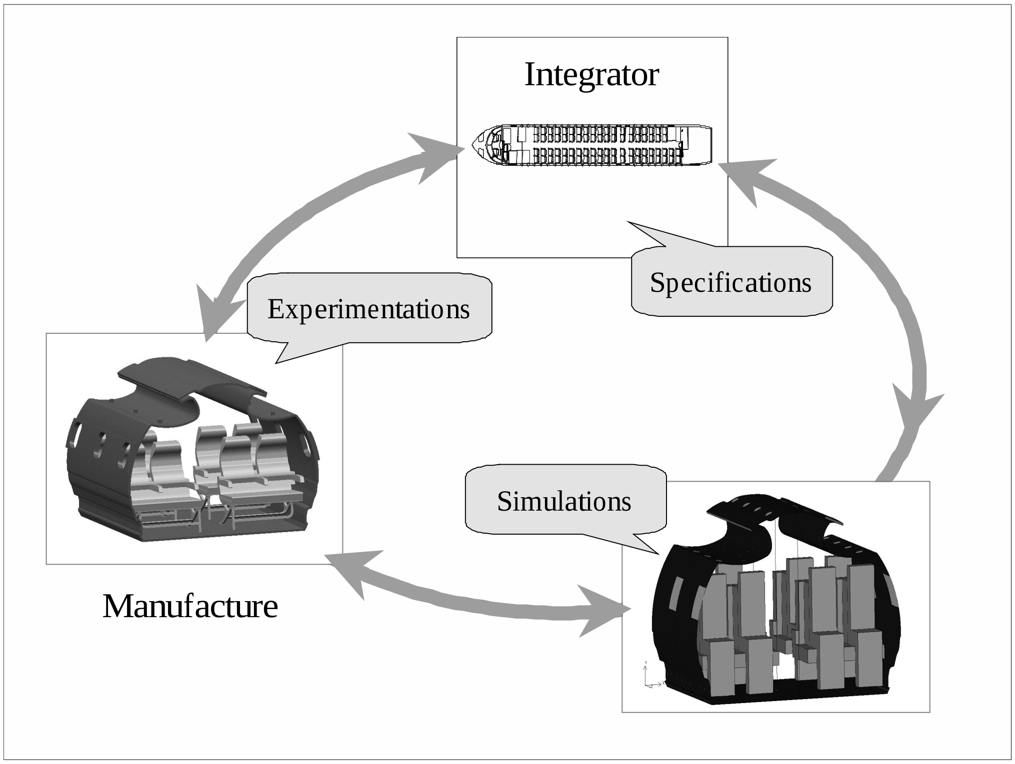


Figure 4.3: Scenario 2

The objectives of these two scenarios were to assess that working with this service platform thanks to the ENScube work package was :

- easy,
- allowed an easy use of distant means,
- met company requirements easily, and in real time, made them understandable,
- favoured the appropriation of the final results by the company.

To reach these objectives the workflow appeared as a critical step. One started the analysis from the work flow of a classical numerical simulation project (see Figure 4.4).

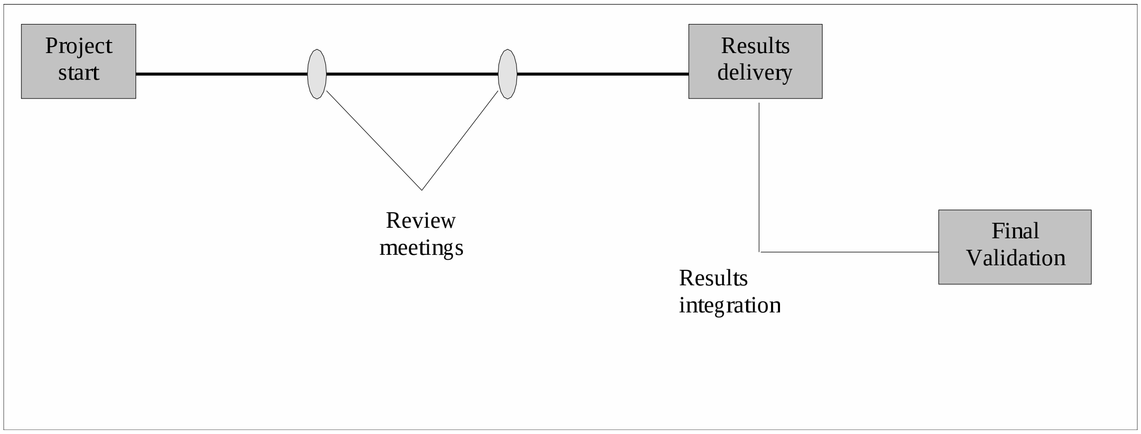


Figure 4.4: Workflow of a classical numerical simulation project

The review meetings are usually organized on a regular basis within the duration of the project, with an agenda such as:

- progress report,
- discussion of the problems encountered,
- decisions for corrective actions,
- future work plan

Consequently the validation of the final results is made quite often only after having being integrated in the company process. If it does not correspond exactly to what was expected, the only solution for the company is then to ask for another complementary study. To avoid this difficulty and to achieve a more interactive process we decided to:

- change the purpose of review meetings, which are now organised to better undertake the next steps,
- pay more attention at each step so that the delivery of the final product matches with the final validation.

This resulted in the following general concept (see Figure 4.5) and in implementing the work flow shown in the figure 4.6.

The objective is to determine at which moment it is necessary to meet, based on the type of work to be undertaken at a particular step. The schedule of remote meetings is however not definitive, and everybody has the possibility to call for an additional meeting if needed.

To reach the final objective, the company is asked to define at each validation step the type of skills which will be concerned when the final results will be used in the production phase.

The meetings organized at the end of each scenario study have been very interesting for the companies. Most of them are now working on new scenarios, which they would fund from their own resources.

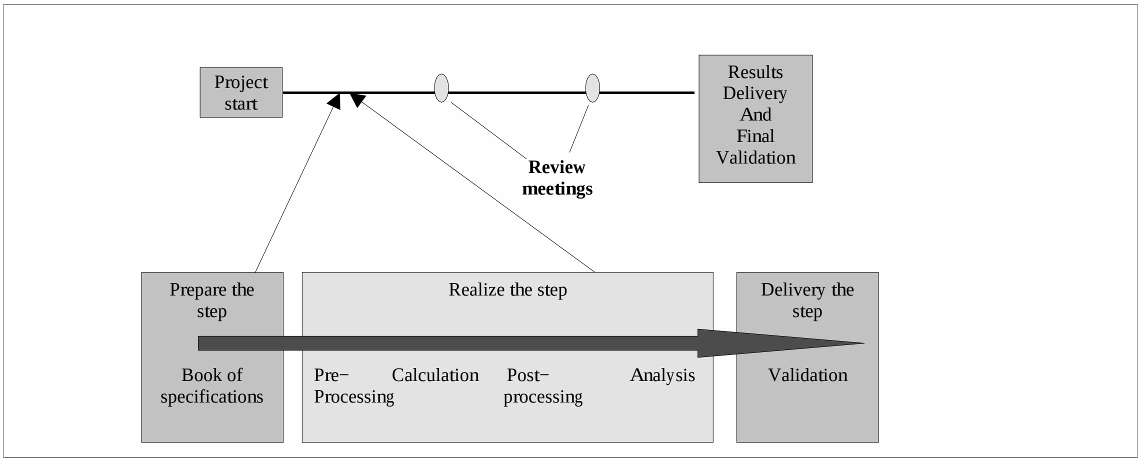


Figure 4.5: General Concept

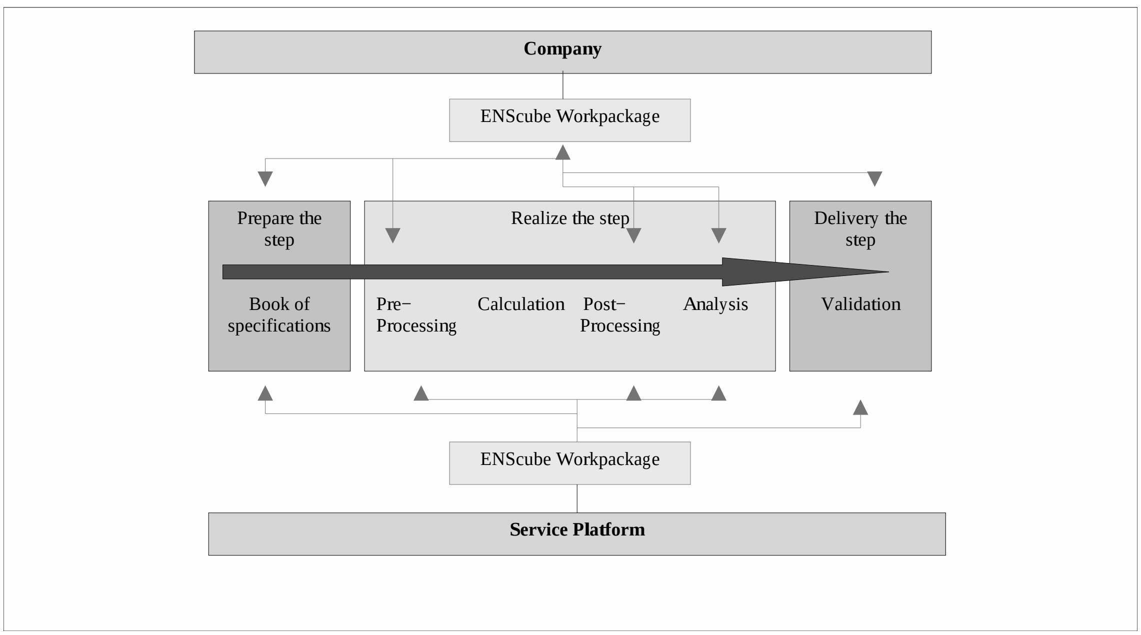


Figure 4.6: Revised workflow

5 Deploy the activity

Pierre-Henri CROS, Christian GARRIGUE (since October 2001), Gabriel JONVILLE (since October 2000), Philippe MOINAT (since March 2000)

Always with the help of the ENScube EC grant, and in parallel to the above tests, a market analysis has been undertaken. It shows that companies have to focus on their core business and form alliances with partners with complementary skills in order to improve their competitiveness when faced with increasing economic constraints.

The on-going restructuring of the aerospace and automotive sectors shows that their subcontractors/suppliers and more particularly the SMEs, are now facing this situation: they are asked more and more to be responsible for a subsystem, instead of being just suppliers of components compatible with given specifications.

This requires them to adapt their work flow to these new challenges and, for most of them, to increase the use of numerical simulation techniques for design and/or improvement of their products.

This leads then to join the concept of "**extended enterprise**":

The extended enterprise is the network made of one single enterprise with its partners within the framework of a common project and/or program. Its objective is to share information between those partners who, at a given time, on a given topic, share the same common interest. It implies new methods in program management and thus, new organizational structures.

and of "**concurrent engineering**" one,

This concept is based on taking into account, at the right time, the needs of all the product life cycle participants. Its objective is to design and manufacture the product right at the first attempt (design to cost). Concurrent engineering implementation is mainly based on forming multidisciplinary teams, made of representatives of all those entities involved.

This altogether means that these companies should have to adapt to the guidelines of the major industry and to adopt the same tools and standards.

The market analysis that has been undertaken has underlined that European SMEs in the manufacturing industry expressing a need for numerical simulation and for collaborative work and/or visualization tools are the first target. It has also underscored that potential new users of numerical simulation could also be companies already involved in CAD/CAM and supplying sub-components to larger contractors and integrators.

The promising results of the scenario campaign, analysed together with the results of the market analysis confirms that there is an emergent and large business to address.

6 Publications

Pierre-Henri CROS, Gilles BAUBES, Tomas MELIN (KTH),
E-business: Issues, Application and Developments IOS Press, 2000 : ENScube, Enhanced European Numerical Simulation Services for Small and medium sized enterprises (p.967).

Gilles BAUBE and Stéphane GRES.
7th International Conference on Concurrent Enterprising 2001 proceedings : Engineering the Knowledge Economy through Co-operation. ENS3 - Numerical Simulation at Hand (p 377).

7

Computer Support Group

1 Introduction

Nicolas Monnier

1.1 Key responsibilities

Key responsibilities of CERFACS' "Computer Support Group" are :

- To define CERFACS' Computer and Network architectures and perspectives for their upgrade and evolution;
- To provide, integrate and maintain all necessary and selected CERFACS' hardware and software solutions;
- To address CERFACS teams' needs with integrated solutions and services;
- To assist researchers providing them technical and application expertise including assistance with programming and optimisation;
- To spread all necessary practical information advising CERFACS' users in their main areas of interest.

This strong support activity is the responsability of a five people team.

1.2 General strategy

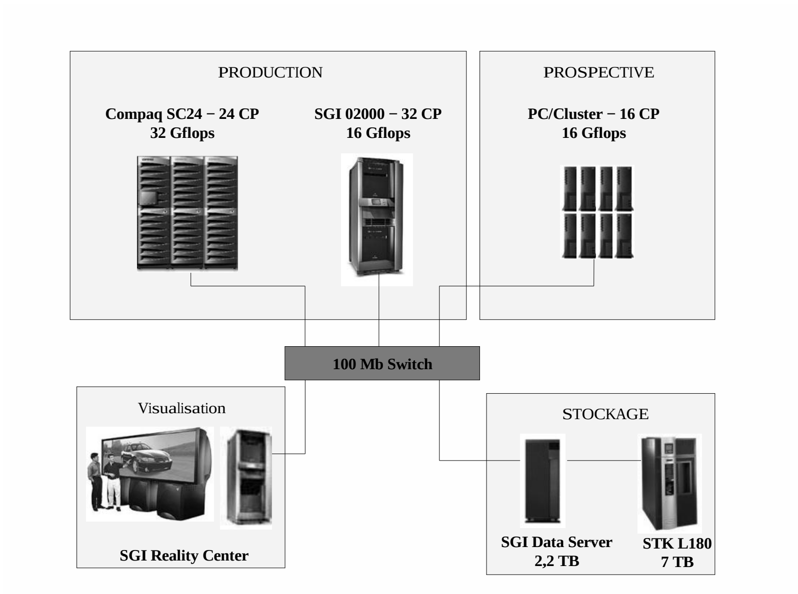
General strategy is :

- Listening to the users' needs, federating them to benefit from scaling factors;
- With the help of HPCN suppliers, allow CERFACS' researchers to work in an up-to-date software and hardware HPCN environment (Storage capacities, Computing power, Post-processing and Networking);
- Ensure developments portability through the access to a wide range of architectures;
- Establish partnership for accessibility to high-end configurations.

2 Architecture and Actions. Jan. 00 - Dec. 01.

Isabelle d'Ast, Gerard Dejean, Fabrice Fleury, Patrick Laporte

2.1 CERFACS' computing resources (As of Dec 01).



During this period (2000-2001) CERFACS computer resources have seen four main improvements :

- Data storage capacity : a new file server managing 2.2 TB of fiber channel disks (200 GB in 99);
- Computing power : a Compaq Alpha-Server (tripling in-doors GFlops peak performance);
- New visualisation resources : a SGI Reality Center integration;
- New prospective hardware : a PC-cluster configuration.

2.2 Software environment and Support.

CERFACS' software environment covers three domains :

- Scientific development tools : CERFACS' users need a whole array of tools which allow them to create, test, debug and exploit their computational simulations. In this frame, one looks for availability of a wide range of scientific tools (compilers, profilers, debuggers, scientifical libraries, and parallelization tools) and their associated documentation. The availability of several Operating Systems associated with their scientifical development environment guarantes portability of developments on a wide range of Unix machines;
- Job and data management tools : giving users a complete set of tools is not enough. One has to provide a job management environment on the central computers, including batch queues, rules of usage and accounting means to optimise global throughput of CERFACS' computers (NQS, LSF and PBS batch systems are currently in use). On the other hand, the "Computer Support Group" provides data backup / restore (Time Navigator);
- Dedicated applications servers : in addition to development and management tools, several dedicated application servers are essential to complete a high-level software environment. These application servers are either an extension of computing facilities (Visualization servers, Data Management Server, MatLab servers) or an integral part of CERFACS' infrastructure (Web servers, Mail server, printer server, NIS, ...).

2.3 Support to N'S3 project

The "Computer Support Group" has been quite extensively involved over the period with N'S3 project. It supported architecture definition, software and tools identification, tests and relations with vendors.

SGI Reality Center installation, usable by each CERFACS' researcher, was one of the spin-offs of this project.

2.4 PC cluster prospective

The main results of this study are :

- Recommendations for PC Cluster architecture and software, results concerning behaviour and stability of CERFACS' PC's cluster in a multi-user parallel and scientific environment;
- Evaluation of price/performance ratio in CERFACS' environment, and comparison with more classical solutions,
- Results sharing with CERFACS' partners (meetings with CNES and METEO-FRANCE, presentation at CEA Simulation and PFlops meeting),
- Porting of main CERFACS' codes on the cluster, for present exploitation in production mode.

Next year prospective studies will be launched concerning the new Intel 64 bits product line.

Appendix
Color illustrations

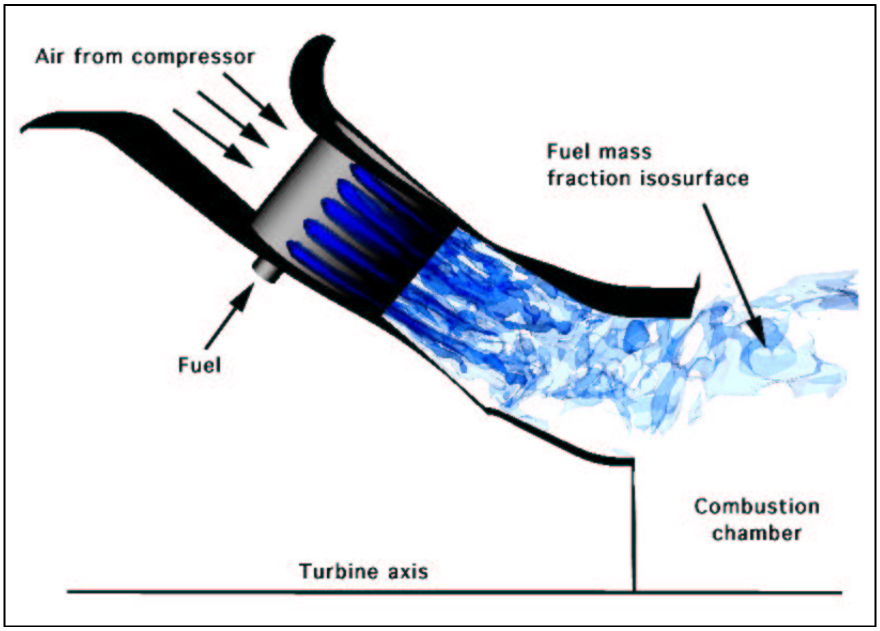


Figure i: LES of mixing in a gas turbine.

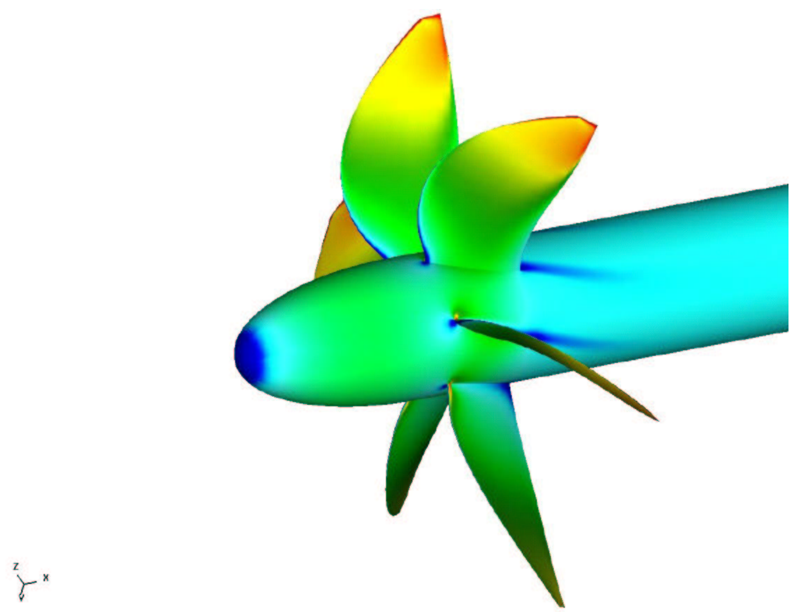


Figure ii: Euler flow simulation around the HSP propeller, $M = 0.7$.

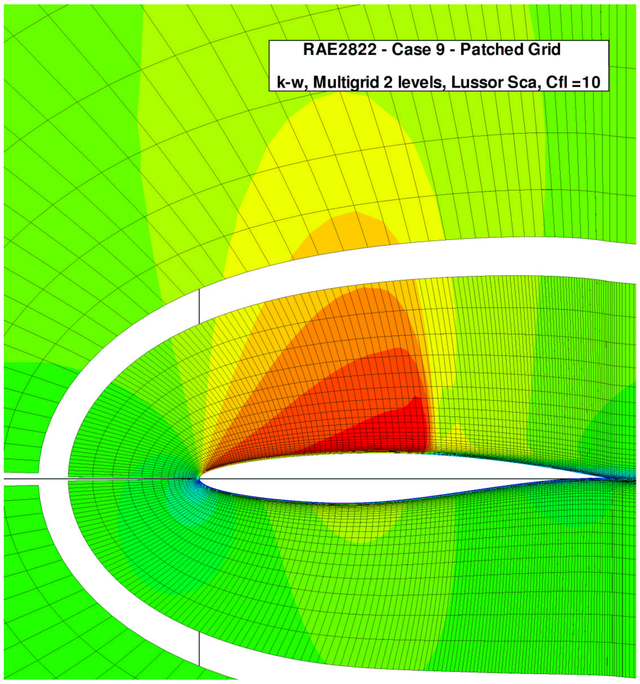


Figure iii: *elsA*/Patched grid technique applied to the RAE2822 test case

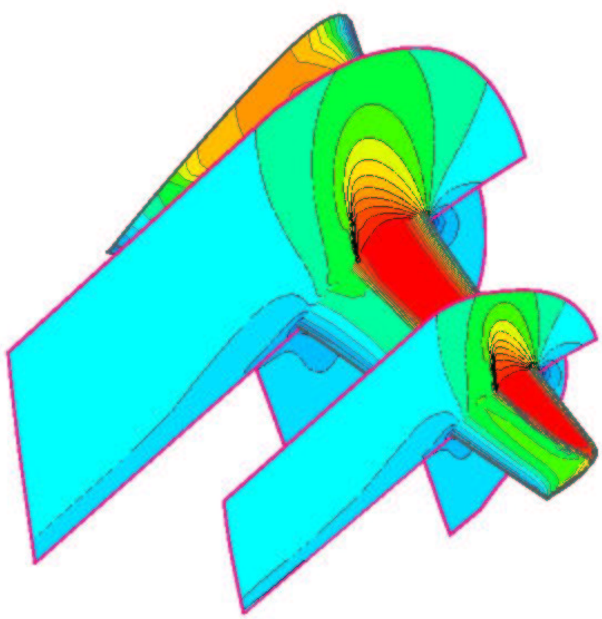


Figure iv: *elsA*/AMR technique applied to the AS28G airfoil

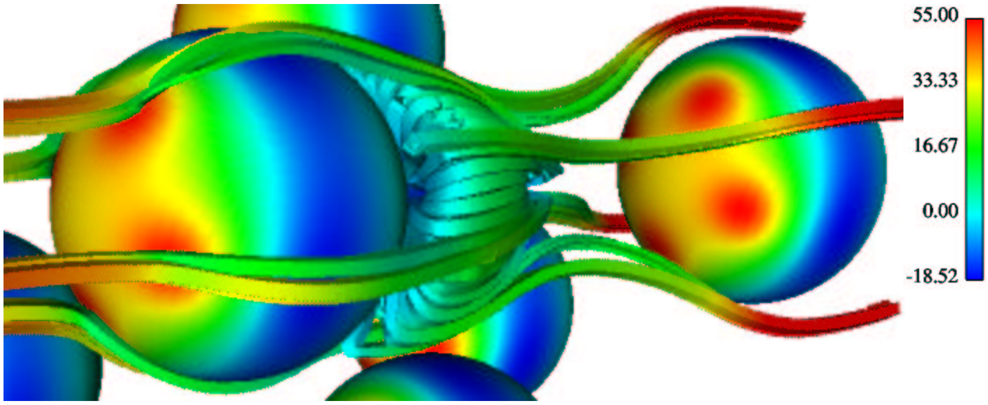


Figure v: Gas trajectories behind a particle. Trajectories are colored by the U-component of velocity, and particles are colored by the pressure coefficient. α_d = 0.15, Re=300.

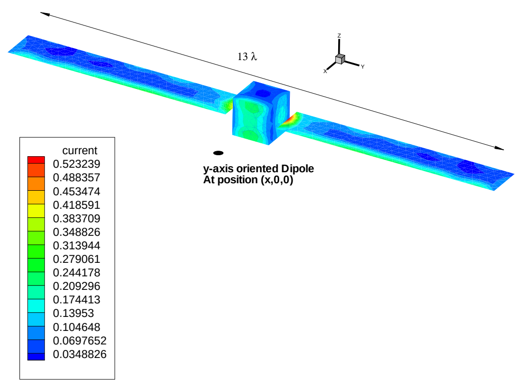


Figure vi: Currents on the satellite.

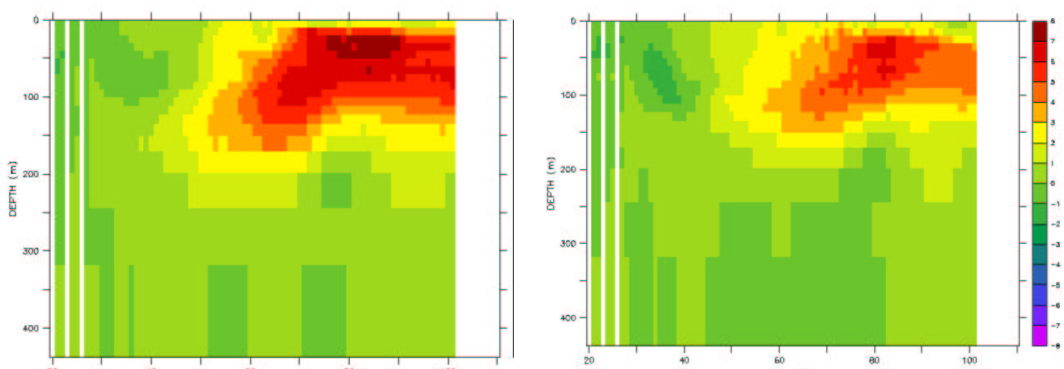


Figure vii: March difference of temperature along the equator between 1987 (El Nino) and 1988 (La Nina): as analysed (left) and coupled predicted (right).

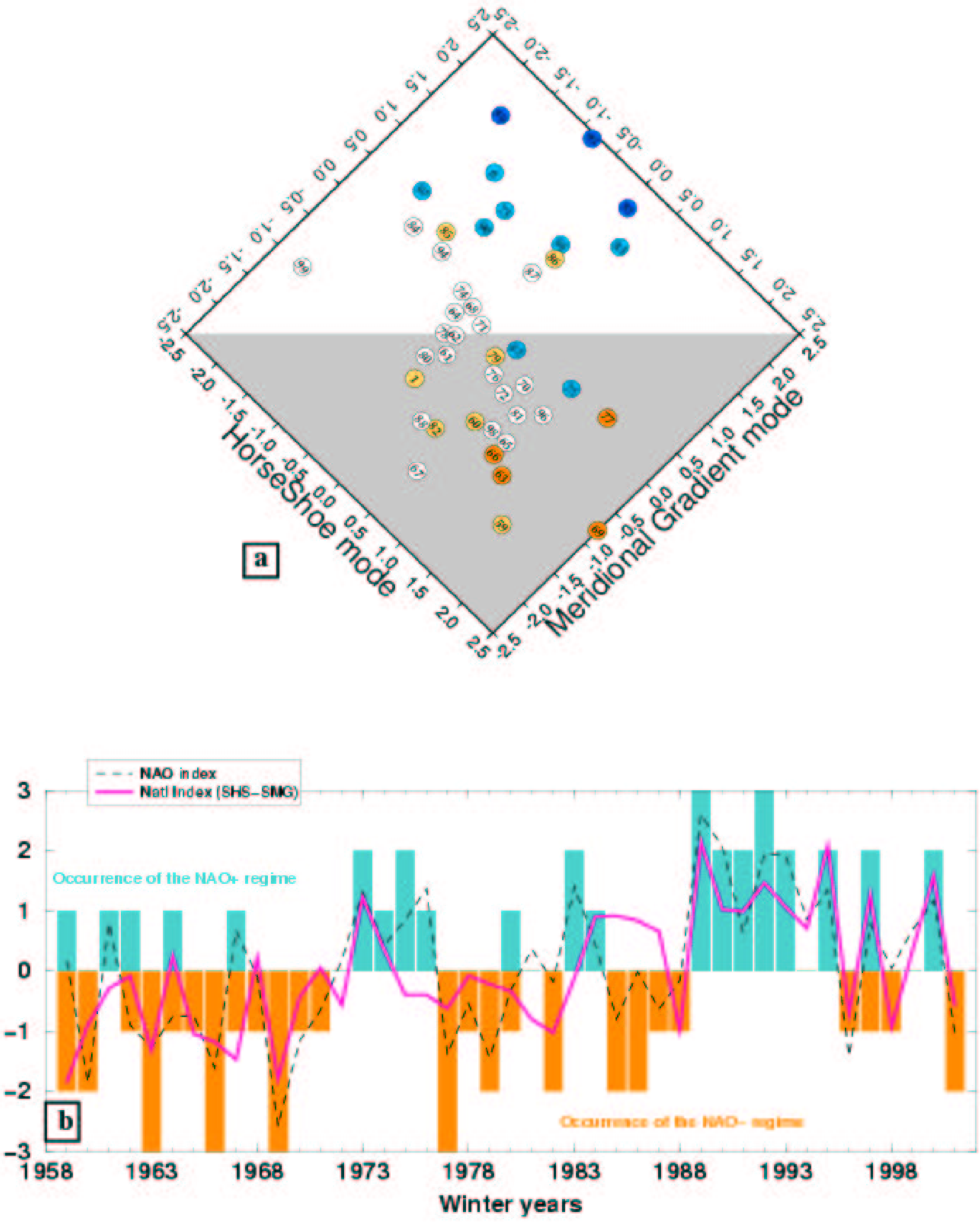


Figure 3

Figure viii: a) Normalized projection coefficient of the August SST anomali es between 1958 to 2000 in the phase-space spanned by the two summer SST modes. Each dot represents a given year and the color indicates the predominance of the winter NAO regimes. White dots refer to winters where NAO regimes are not dominant. Blue (yellow) dots stands for winters primarily dominated (2 months out of 3) by the positive (negative) NAO regime whereas deep-blue (orange) dots represent winters where the positive (negative) NAO regime is exclusively present (3 months out of 3). The included number refers to the year of the considered winter. b) Time series of the observed winter NAO index and the normalized difference between the projections of the August SST field onto the SMG and SHS modes. The NAO index is defined by the principal component time series of the leading EOF of the seasonal (December to February) SLP anomalies over the NAE sector. Blue (orange) bars represent the number of months occupied by the NAO+ (NAO-) regimes.

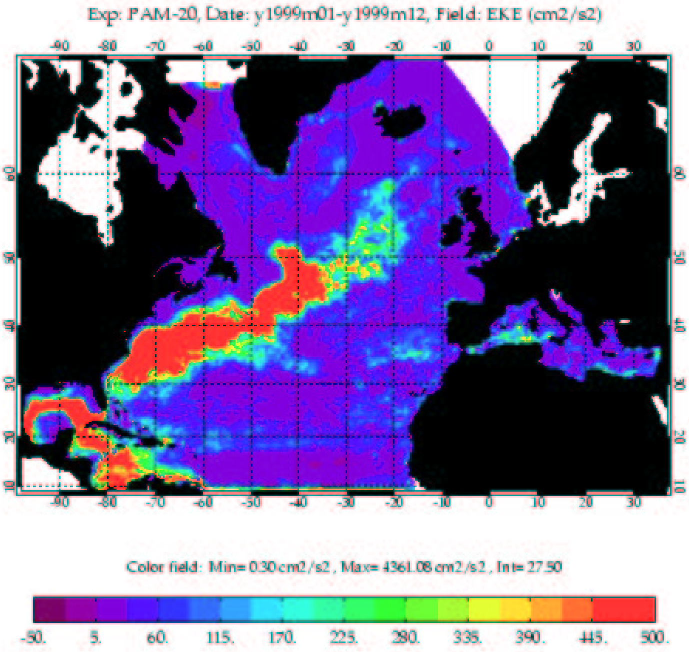


Figure ix: Annually averaged eddy kinetic energy (cm^2/s^2) as calculated by the in terannual simulation over the 3rd year.

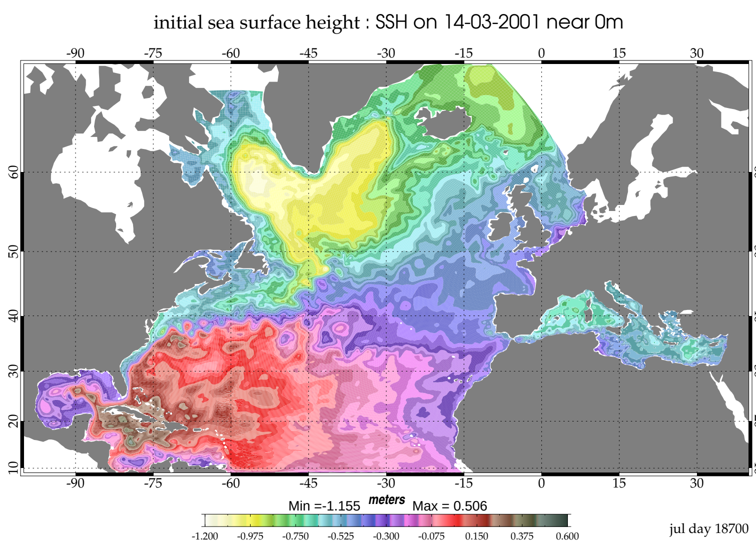


Figure x: Example of Initial sea surface height (SSH) calculated by the SAM-1/PAM syst em on 14 March 2001. In an operational mode, SLA tracks from TOPEX and ERS-2 are assimilated every week