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. 2008 – Dec. 2009

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Foreword

Welcome to the 2008-2009 issue of the CERFACS Scientific Activity Report.

To start with it is worth recalling three main events which took place during the period :

- firstly, on October 1^{st}, 2008, TOTAL, the international, France-based, energy group, became the seventh CERFACS shareholder. This brought new support to CERFACS' research activities, especially in the field of applied mathematics and parallel algorithms ;
- secondly, on November 9^{th}, 2009, INRIA[1] and CERFACS signed the agreement establishing a new joint laboratory. The first research action to be implemented within this laboratory is called "HiePACS", for "High-end parallel algorithms for challenging numerical simulations". Jean ROMAN is the director of the joint laboratory, while Iain DUFF is involved as its senior scientific advisor. We expect that this joint laboratory will provide increased manpower and efficiency for addressing the crucial issues linked to solvers and algorithms for new massively parallel many-core computer architectures ;
- thirdly, on December 1^{st} and 2^{nd}, 2009, AERES[2] , the French evaluation agency, reviewed the past activity and the proposed future programme of SUC[3] , the associated research group with CNRS[4] . The evaluation committee worked under the chairmanship of Philippe COURTIER, member of CERFACS Scientific Council. We later heard that SUC received the highest possible grade, i.e. A+.

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. As for previous years, our activity report is written in such a way that the reader interested in a particular scientific issue should be able to find both a detailed description of the work that has been achieved, as well as a complete list of references, including papers in the reviewed literature and internal reports (which can be made available upon request). CERFACS scientific production is still high :

- the number of high-standard publications, i.e. in internationally-refereed journals, is over 120 for the two-year period, showing a continued increase as compared to past years when the mean rate of publications was closer to 30 to 45 per year ; CERFACS' researchers have also produced over the period more than 210 technical reports, book chapters, and papers in conference proceedings ;
- training of new researchers is still very intense, with 23 Ph. D. theses being awarded over the period ;
- finally CERFACS researchers and engineers are also very active in applied research, with more than 50 grants per year being held over the period, awarded either by national funding agencies or industrial partners.

During 2008 and 2009, the mean total number of (full-time equivalent) people working at CERFACS has been 110 (see Tables ii to viii), with a global annual budget rising from 7.9 to 8.8 M€.

[1] Institut National de Recherche en Informatique et en Automatique
[2] Agence d'Evaluation de la Recherche et de l'Enseignement Supérieur
[3] Sciences de l'Univers au CERFACS
[4] Centre National de la Recherche Scientifique

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

CERFACS Structure

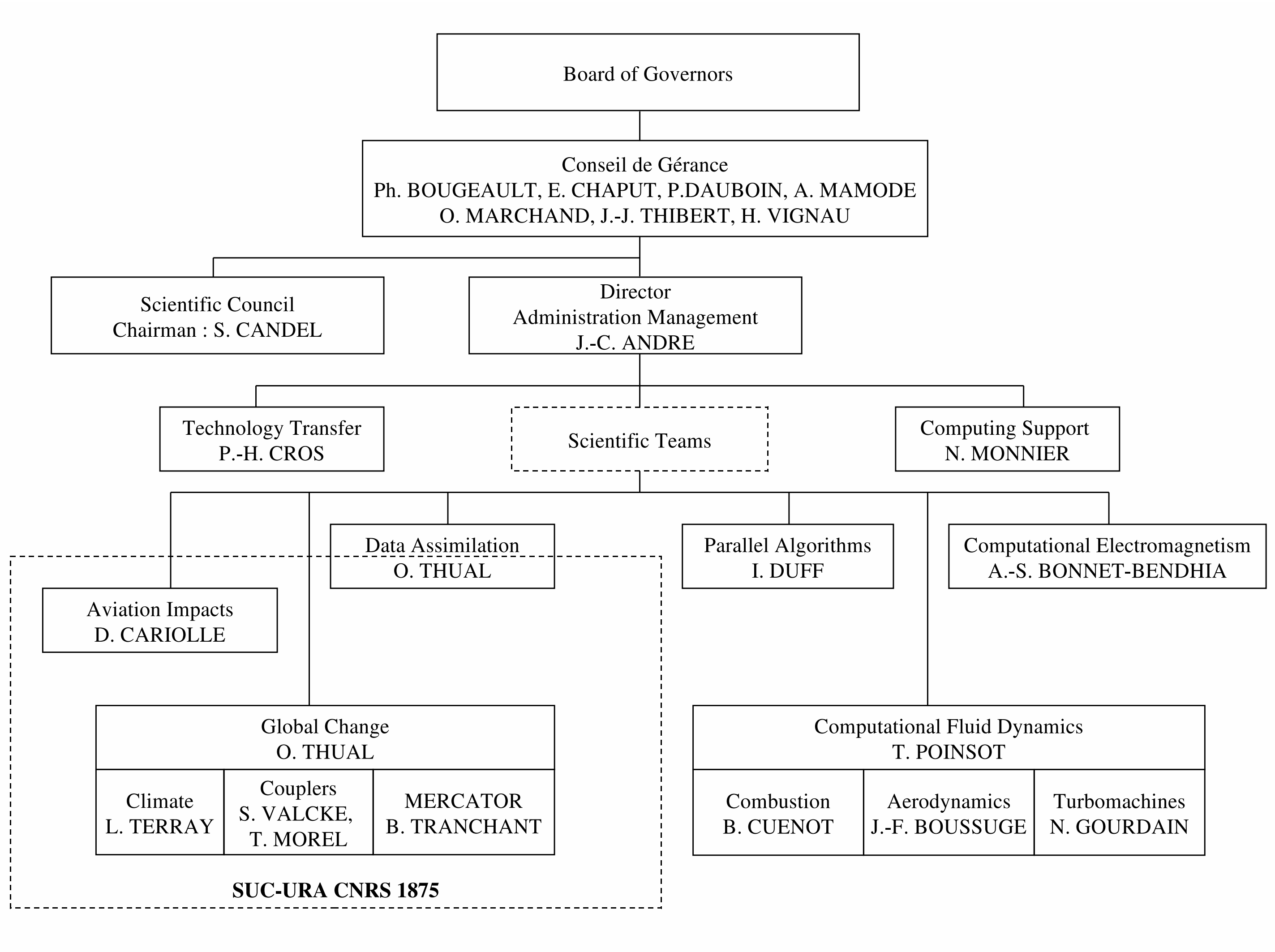
As a ”Société Civile” CERFACS is governed by two bodies.
Firstly, the ”Conseil de Gérance”, composed of only 7 managers (in French, ”Gérants”) nominated by the 7 shareholders (see table i, where the 7th shareholder, TOTAL, joined on Oct. 1st, 2008), follows quite closely the CERFACS activities and the financial aspects. It met 8 times during the period (9 April 2008, 12 June 2008, 5 September 2008, 18 December 2008, 20 April 2009, 8 July 2009, 11 September 2009 and 18 December 2009).
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 5 times during the period (16 January 2008, 10 September 2008, 7 October 2008, 21 January 2009 and 25 September 2009).

CERFACS Scientific Council met for the eleventh time, on 11 January 2008, under the chairmanship of Prof. Jean-François MINSTER, and for the twelfth time on 23 January 2009, under the chairmanship of Prof. Sébastien CANDEL.

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

CENTRE NATIONAL D’ÉTUDES SPATIALES (CNES)	21.3%
ÉLECTRICITÉ DE FRANCE (EDF)	21.3%
MÉTÉO-FRANCE	21.3%
EUROPEAN AERONAUTIC DEFENCE AND SPACE COMPANY (EADS)	9 %
SAFRAN	9%
OFFICE NATIONAL D’ÉTUDES ET DE RECHERCHES AÉROSPATIALES (ONERA)	9%
TOTAL	9%

Table i : Société Civile Shareholders



CERFACS chart as of Dec. 31, 2009

CERFACS Staff

NAME	POSITION	PERIOD
DUFF	Project Leader	1988/11
CHATELIN	Group leader	1988/09
VASSEUR	Senior	2007/05
AVERY	Senior	2008/11-2009/10
BABOULIN	Post Doc	2006/04-2008/03
FUCHS	Post Doc	2009/06
GARCIA ARAUJO	Post Doc	2006/04-2008/03
JIRANEK	Post Doc	2008/11
KAYA	Post Doc	2009/09
TSHIMANGA	Post Doc	2007/11-2009/10
UCAR	Post Doc	2007/01-2008/12
HAIDAR	Ph.D student	2005/03-2008/08
MOUFFE	Ph.D student	2005/10-2009/03
PINEL	Ph.D student	2006/10
SLAVOVA	Ph.D student	2005/03-2009/05
TROELTZCH	Ph.D student	2007/05
AHMADNASAB	Engineer Ph.D student	2008/05-2008/07 2003/08-2008/02
BONNEMENT	Student	2008/02-2008/08
THAM	Student	2008/06-2008/09
VILAR	Student	2008/06-2008/09
LANGOU	Trainer	2009/07-2009/08
GIRAUD	INRIA	2009/11
GRATTON	Visitor	2007/07

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

NAME	POSITION	PERIOD
POINSOT	Project Leader	1992/09
CUENOT	Senior	1996/10
DENIAU	Senior	2006/11
DUFOUR	Senior Post Doc	2009/06 2007/06-2009/05
GICQUEL	Senior	2004/02
GOURDAIN	Senior Post Doc	2008/02 2006/02
JOUHAUD	Senior	2001/10
MONTAGNAC	Senior	2000/11
PUIGT	Senior	2005/12
STAFFELBACH	Senior Post Doc	2008/11 2006/06-2008/01
VERMOREL	Senior	2007/11
BOUSSUGE	Research Engineer	2002/02
ALBOUZE	Post Doc Ph.D student	2009/02 -2009/04 2005/10-2009/01
BOUDIER	Post Doc	2007/10-2008/06
BRACONNIER	Post Doc	2007/01-2008/12
CABRIT	Post Doc Ph.D student	2009/10 2006/10-2009/09
CHENY	Post Doc	2009/09
DAUPTAIN	Post Doc	2008/04
DECHAUME	Post Doc	2009/04
DUCHAINE	Post Doc	2007/11-2009/10
GARCIA	Post Doc Ph.D student	2009/02 2005/10-2008/12
GOUGEON	Post Doc	2008/07
HALLEZ	Post Doc	2009/09
LAMARQUE	Post Doc Ph.D student	2009/07 2007/11-2008/06
LANDMANN	Post Doc	2006/08-2008/08
LAURENCEAU	Post Doc	2008/07
MENDEZ	Post Doc	2007/11-2008/10
MOUFFE	Post Doc	2009/05
POITOU	Post Doc	2009/12
PORTA	Post Doc	2007/04-2008/06
RIBER	Post Doc	2008/05
AMAYA	Ph.D student	2006/10
BLANC	Ph.D student	2006/09-2009/08
BODOC	Ph.D student	2007/07
COLIN	Ph.D student	2004/12-2008/01
COLLADO	Ph.D student	2009/09
ENAUX	Ph.D student	2006/10
EYSSARTIER	Ph.D student	2008/10
FOSSO	Ph.D student	2007/10

TAB. iii: List of members of the COMPUTATIONAL FLUID DYNAMICS project (1/3).

FRANZELLI	Ph.D student	2008/01
GRANET	Ph.D student	2008/10
GULLAUD	Ph.D student	2007/11
GUEDENEY	Ph.D student Student	2008/11 2008/02-2008/08
GUTIERREZ	Ph.D student	2006/12-2009/11
HANNEBIQUE	Ph.D student Student	2009/10 2009/03-2009/08
HERMETH	Ph.D student	2009/03
HERNANDEZ VERA	Ph.D student	2008/11
JAEGLE	Ph.D student	2006/09-2009/12
JAURE	Ph.D student Engineer Student	2009/04 2008/10-2009/03 2008/04-2008/09
KRAUSHAAR	Ph.D student	2008/10
LACAZE	Ph.D student	2005/11-2009/04
LAVEDRINE	Ph.D student	2004/10-2008/05
LEGRAS	Ph.D student	2007/11
LEYKO	Ph.D student	2006/09
MAGLIO	Ph.D student	2007/07
NYBELEN	Ph.D student	2004/11-2008/03
OZEL	Ph.D student	2007/09
PEDOT	Ph.D student	2008/10
RICHARD	Ph.D student	2009/10
ROCCHI	Ph.D student Engineer	2009/11 2009/02-2009/10
ROUX A	Ph.D student	2005/10-2009/05
RUIZ	Ph.D student Student	2008/10 2008/03-2008/09
SAN JOSE	Ph.D student	2006/10-2009/12
SCHMITT	Ph.D student	2005/10-2009/05
SENONER	Ph.D student	2007/01
SENSIAU	Ph.D student	2005/03-2008/10
SICOT	Ph.D student	2006/09-2009/09
SIERRA SANCHEZ	Ph.D student	2008/10
SILVA GARZON	Ph.D student	2007/08
WAGNER	Ph.D student	2006/10-2009/09
WIECZOREK	Ph.D student	2007/06
WLASSOW	Ph.D student Student	2009/03 2008/07-2008/12
WOLF	Ph.D student	2007/10
WUNSCH	Ph.D student	2006/12-2009/11
ZEREN	Ph.D student	2006/12-2009/11
ZUZIO	Ph.D student	2007/08
BARRE	Engineer	2009/11
BARTH	Engineer	2008/06-2008/09
BOILEAU	Engineer	2007/05-2008/10
BOCQUET	Engineer	2009/07-2009/12

List of members of the COMPUTATIONAL FLUID DYNAMICS project (2/3).

DUBUC	Engineer	2009/12
ESTIVAL	Engineer	2009/04
FERRIER	Engineer	2008/06-2009/11
HARRY	Engineer Student	2009/02-2009/07 2008/09-2009/01
JOUBERT	Engineer	2007/06-2008/11
MILLOT	Engineer	2008/02-2008/08
ROUMEAS	Engineer	2007/06-2008/10
SAILLOFEST	Engineer	2008/11
AUBERT	Student	2009/03-2009/08
BOGER	Student	2008/04-2008/09
BRUYAT	Student	2008/06-2008/08
BURNAZZI	Student	2009/10
CARDENAS	Student	2008/10-2009/01
CHEN	Student	2009/07-2009/08
COMBE	Student	2007/09-2008/06
DEVILLERS	Student	2008/03-2008/08
FRANCOIS	Student	2009/05-2009/11
GIRET	Student	2009/07-2009/09
GU	Student	2009/03-2009/08
LEGAC	Student	2008/01-2008/03
LINKES	Student	2009/03-2009/09
LEONARD	Student Student	2009/10-2009/12 2009/03-2009/09
MAHMOUDI	Student	2009/03-2009/08
OTERO	Student	2009/03-2009/09
QUILLATRE	Student	2009/06-2009/08
QUINT	Student	2009/06-2009/11
RAUSCHENBER	Student	2008/04-2008/09
SALAS	Student	2009/03-2009/08
SIMSONT	Student	2008/04-2008/09
VAN HAUWERT	Student	2008/03-2008/10
VU	Student	2009/04-2009/09
ZHU	Student	2009/07-2009/09
BIBRZYCKI	Visitor-PhD	2009/09
KAESS	Visitor-PhD	2008/02-2008/03
KANEVA	Visitor-PhD	2009/07-2009/12
KOZOLUB	Visitor-PhD	2009/09
LANG	Visitor-PhD	2009/04-2009/06
NAJAFIYAZDI	Visitor-PhD	2009/11
MOREAU	Trainer	2009/04
TROUVE	Trainer	2009/06-2009/07
COMTE	Trainer	2009/09
MULLER	Visitor	1997/11
NICOUD	Visitor	2001/10
RIZZI	Visitor	1987/10
SAGAUT	Visitor	2003/12-2009/07
SCHONFELD	Visitor	2001/01

List of members of the COMPUTATIONAL FLUID DYNAMICS project (3/3).

NAME	POSITION	PERIOD
THUAL	Project Leader	1991/09
ROGEL	Senior	1998/10
TERRAY	Senior	1992/10
WEAVER	Senior	1999/11
MASSART	Senior	2004/12
BOURIQUET	Research Engineer	2006/08
MAISONNAVE	Research Engineer	2000/12
MOREL	Research Engineer	2000/03
PAGE	Research Engineer Engineer	2009/07 2008/01-2009/06
VALCKE	Research Engineer	1997/02
THEVENIN	Research Engineer Engineer	2008/09 2007/12-2008/08
DAMASIO DA COSTA	Post Doc	2006/10-2008/09
MOINE	Post Doc	2008/12
MUNOZ	Post Doc	2007/10-2008/10
PANGAUD	Post Doc	2009/12
RICCI	Senior Post Doc	2008/11 2007/11-2008/10
SWINGEDOUW	Post Doc	2008/03-2009/12
CORRE	Ph.D Student Student	2008/10 2008/02-2008/06
DAGET	Ph.D Student	2005/05-2008/04
MIROUZE	Ph.D Student	2007/10
BOE	Engineer	2007/12-2008/02
BOUSQUET	Engineer	2009/01-2009/12
DARDEL	Engineer	2008/03-2008/07
LATOUR	Engineer	2009/05
NAJAC	Engineer Ph.D Student	2008/10-2008/12 2005/10-2008/09
MINVIELLE	Engineer Ph.D Student	2008/10-2009/04 2005/09-2008/09
SANCHEZ	Engineer	2009/05
VALDIVIESO	Engineer	2009/01-2009/01
CHABOT	Student	2008/01-2008/06
ELYAKIME	Student	2009/03-2009/07
IVANOFF	Student	2009/03-2009/09
PAJOT	Student	2008/06-2008/09
TABURET	Student	2009/06-2009/09
WATIOTIENNE	Student	2009/06-2009/08
ARGAUD	EDF	2006/07
BURILLON	IPSL	2008/12
DEANDRIS	IPSL	2009/10
CASSOU	CNRS	2002/11
COQUART	CNRS	2006/12
PIACENTINI	Visitor	2007/06

TAB. iv: List of members of the CLIMATE MODELLING & GLOBAL CHANGE project.

NAME	POSITION	PERIOD
DREVILLON	Senior	2006/06-2009/02
TRANCHANT	Senior	2001/07-2009/12
LELLOUCHE	Senior	2002/10-2009/03
REMY	Senior	2003/12
BOURDALLE-BADIE	Research Engineer	2001/01
DERVAL	Research Engineer	2003/07
DRILLET	Research Engineer	1999/03-2008/02

TAB. v: List of members of the MERCATOR group.

NAME	POSITION	PERIOD
BONNET	Project Leader	2006/05
BENDALI	Project Leader	1996/01
FARES	Senior	1992/06
MILLOT	Senior	1995/11
PERNET	Senior	2007/03
COSSONNIERE	Ph.D student	2008/10
PEYNAUD	Ph.D student Student	2009/10 2008/06-2008/09
PICOT	Student	2009/02-2009/08
STEIF	Ph.D student	2008/10
PEYRUSSE	Student	2008/05-2008/07
PIGERON	Student	2009/03-2009/05
VAN OLMEN	Student	2008/06-2008/09
COLLINO	Visitor	1994/04

TAB. vi: List of members of the COMPUTATIONAL ELECTROMAGNETISM project.

NAME	POSITION	PERIOD
CARIOLLE	Project Leader	2003/08
PAOLI	Senior	2004/07
CHOSSON	Post Doc	2006/05-2008/04
CRESPIN	Post Doc	2009/01
NYBELEN	Post Doc	2008/04-2009/12
SARRAT	Post Doc	2008/11-2009/12
PAJOT	Ph.D Student	2008/11
PAUGAM	Ph.D Student	2005/01
PICOT	Ph.D Student	2009/10
LE BERRE	Engineer	2007/01-2008/02
CAHUZAC	Student	2008/04-2008/09
SAUNIER	Student	2008/07-2008/11
PIACENTINI	Visitor	2007/10

TAB. vii: List of members of the ENVIRONMENTAL IMPACT OF AVIATION project.

NAME	POSITION	PERIOD
CROS	Project leader	1997/04
JONVILLE	Engineer	2000/10
MILHAC	Engineer	2004/01
OLIVEIRA	Technician	2007/06
SCOTTO	Student	2009/06-2009/07

TAB. viii: List of members of the TECHNOLOGY TRANSFER group.

NAME	POSITION	PERIOD
MONNIER	Project Leader	1996/12
D'AST	Engineer	1996/10
LAPORTE	Engineer	1988/04
DEJEAN	Technician	1990/11
DUPRAT	Technician	2008/09-2008/11
FLEURY	Technician	1999/10
LABARBE	Student	2009/04-2009/06

TAB. ix: List of members of the COMPUTER SUPPORT group.

CERFACS Wide-Interest Seminars

Angelique Poncot (EDF R&D) : *Assimilation de données pour la dynamique du xénon dans les coeurs de centrale nucléaire.* (September 22th, 2008)

Julien Boe (CERFACS) : *Changement global et cycle hydrologique : Une étude de régionalisation sur la France (Thesis defense).* (November 23th, 2008)

David Pardo (Basque Center for Applied Mathematics) : *Incorporating minimum Frobenius Norm Models in Direct Search.* (January 9th, 2009)

Philip Avery (CERFACS) : *Domain decomposition and FETI-DP : an introduction with applications.* (May 28th, 2009)

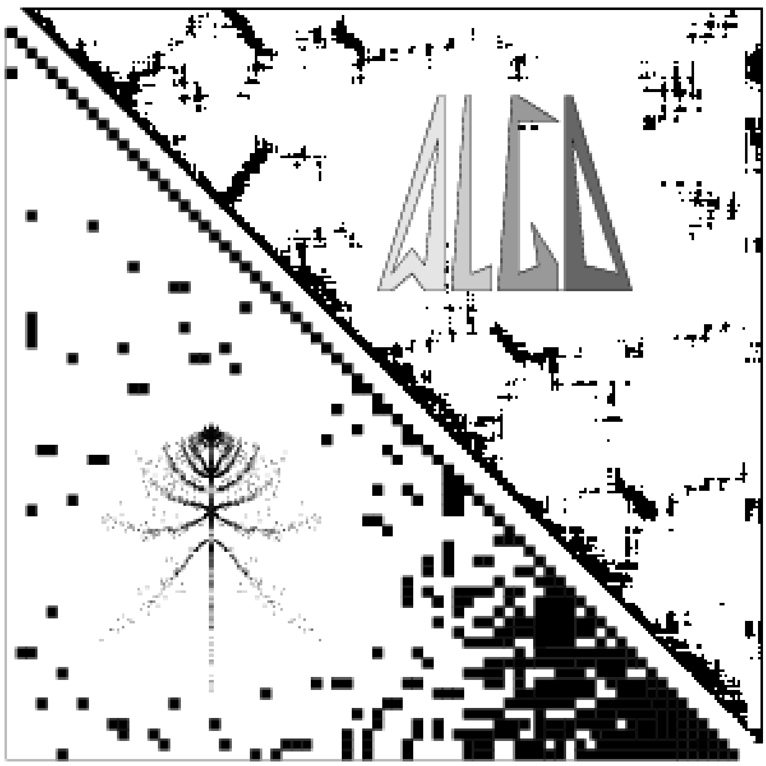
Philippe Gaspar (CERFACS) : *Coupling 3-D models of ocean physics and biogeochemistry to a marine animal population dynamics model to study the combined impacts of fisheries and climate change.* (June 4th, 2009)

Peter Oke (CSIRO, Hobart, Tasmania) : *Ensemble data assimilation : theory and practice.* (June 24th, 2009)

Arnaud Trouvé (Department of Fire Protection Engineering, University of Maryland) : *Fire Modeling : a Flaming Cocktail Made of CFD, Combustion Modeling, Data Assimilation and Forecasting.* (July 1st, 2009)

1

Parallel Algorithms Project



1 Introduction

1.1 Introduction

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 the Parallel Algorithms Project can be found from the statistics of accesses to the CERFACS Web pages where a major part of all the hits for CERFACS projects are on the Algo web pages.

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, INRIA-Lyon, and INRIA-Bordeaux. The release currently being distributed is Version 4.9.2. Some research work that will most likely have an impact on future releases is discussed in the following sections, in particular in Sections 3.2,3.4,3.6,3.9. There are around 1,000 downloads of the code each year. The complex version has been accessed extensively and used in many applications, particularly in electromagnetics. We have been collaborating with our colleagues from ENSEEIHT, Lyon, and Bordeaux, through a large ANR grant, called SOLSTICE. The main tasks in this grant supplement and overlap our research work for sparse linear solvers including development of techniques that might be implemented in future releases of MUMPS and the combined use of direct and iterative methods for solving very large problems from numerical simulation. Some of the work described in Sections 3 and 4 is supported by this ANR programme. We continued our collaborations with our colleagues in France and California on sparse direct methods through a Franco-Berkeley Fund grant with several visits between Toulouse and Berkeley in 2008 and 2009.
Most of the work discussed in Section 3 is concerned with the direct factorization of symmetric indefinite and general sparse matrices. Considerable work has been done to understand and develop robust approaches to the case of symmetric indefinite matrices. Research on examining the out-of-core parallel solution for

one or many right-hand sides is progressing well and will hopefully also result in future improvements to `MUMPS`. The current *A*chilles Heel of parallel direct methods is in the preliminary analysis stages involving mainly symbolic and combinatorial aspects. This is being addressed by some tasks from SOLSTICE and we discuss some of this work in Section 3 (e.g. Sections 3.5, 3.6, 3.10).

The development of robust and general purpose preconditioners and an analysis of their properties is discussed in many of the contributions to Section 4. Although iterative methods can usually avoid the memory restrictions of direct methods, 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. We have continued this work, including two-level and spectral schemes that effectively and explicitly remove error components in a subspace spanned by eigenvectors corresponding to small eigenvalues of the already preconditioned system. Much of the work has been to extend these techniques so that they can be applied to a wide range of problems in different application areas. Many of the contributions include a detailed analysis of these methods and their application to large two and three dimensional problems in geophysics and aeronautics and their extension to handle additional right-hand sides efficiently. Some of this work involves novel ways of combining direct methods and iterative methods to obtain powerful hybrid methods for tackling problems of the order of many millions of variables. Other work examines partitioning techniques that can greatly enhance some of the kernel operations of iterative methods on parallel architectures, in particular of matrix-vector multiplication. Some of our software, in particular the GMRES and FGMRES routines that are available on our web pages are high on the “google” list, are very widely used, and have been downloaded over 5000 times.

The main area of interest in Qualitative Computing concerns a deep understanding of the influence of finite-precision computation on complex scientific numerical applications. Of particular concern are a deeper understanding of the role of nonlinearities and singularities in the context of floating-point arithmetic. A major tool in this work continues to be the use of homotopic deviations, a technique pioneered at CERFACS. Over the last two years, Françoise Chatelin has distilled much of the research conducted by herself, students, and colleagues into a book that will be published shortly (see Section 5).

A major focus of our work on nonlinear systems and optimization has been in joint work with the PALM Project and the Climate Modelling Group on data assimilation. This area is becoming one of the main interdisciplinary focus points at CERFACS. We were awarded a large grant from RTRA to look into this area in conjunction with colleagues in CNES, ENSEEIHT-IRIT and Météo-France. This project, named ADTAO, started in the spring of 2009 and will continue until 2012. We are involved in a study of solution techniques for linear least-squares computations that lie at the heart of data assimilation algorithms, and we have investigated several aspects of this including further studies on Gauss-Newton methods and model reduction techniques. Some of this work has been done in collaboration with scientists from the UK through a grant from the Alliance programme. We are also continuing the development of software for solving large dense linear least-squares in a parallel environment and have studied component conditioning and parallel tools for cases when the least-squares problem has constraints added in an incremental manner. Much of our optimization work involves trust region methods including the innovative combination of multilevel schemes with trust region methods for optimization problems including those arising in the solution of partial differential equations. We are greatly aided in our optimization work by Philippe Toint who is now a consultant to CERFACS in this area.

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 open to the shareholders of CERFACS. In collaboration with Olivier Boiteau and Jean-Philippe Argaud from

EDF/SINETICS, we organized a two-day seminar on High-Performance Computing and Numerical Linear Algebra held at EDF in Clamart in April 2009. The lectures strongly emphasized the use of backward errors in numerical linear algebra, advanced domain decomposition algorithms, and open source libraries for scientific computing. We are 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. In this reporting period, we had three stagiaires (Audrey Bonnement, Léon Tham and François Vilar) from MATMECA in Bordeaux. Members of the Team have assisted in many lecture courses at other centres, including Ecole Nationale de la Météorologie, ENSEEIHT, ENSICA-ISAE, INSA and the University of Toulouse 1. Azzam Haidar completed his PhD thesis “On the parallel scalability of hybrid linear solvers for large 3D problems” in June, 2008. Two PhD theses were successfully defended in 2009. Melodie Mouffe defended her thesis entitled “Multilevel optimization in infinity norm and associated stopping criteria” in February and I am delighted to record that the thesis was of such a high standard that Melodie was awarded a Prix Léopold Escande by INPT. This maintains our impressive record and is the fourth Algo thesis to receive this accolade. Mila Slavova successfully defended her thesis on “Parallel triangular solution in the out-of-core multifrontal approach for solving large sparse linear systems ” in April 2009. In addition, Caroline Boess, who worked for a year on her thesis at CERFACS, was awarded a PhD by the University of Bremen in Germany in August 2008. Her thesis title was “Using model reduction techniques within the incremental 4D-Var method”.

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. In addition to inviting our visitors to give seminars, some of which are of general interest to other teams, we also run a 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.

A worldwide celebration commemorating the memory of Gene Golub was held on February 29th 2008, a day that would have been his nineteenth birthday. On this day, thirty events in twenty three countries were organized. The Gene Golub Day organized at CERFACS was attended by about twenty five people. Eleven talks covering both theory and applications in high performance computing, optimization and data mining were presented by young researchers (most of them being PhD students) coming from several centres in France. The main idea behind this was to remember that Gene Golub had an amazing ability to communicate and inspire young people, often greatly influencing their future career. This was the only event in France in the February 29th commemoration of the memory of Gene Golub.

We continue to have a “Sparse Days at CERFACS” meeting each year. On 23-24 June 2008, we combined forces with the VECPAR 2008 meeting that was being held in Toulouse from 24-27 June. Thus the theme of our Sparse Days on that occasion was on vector and parallel computing, including also work on modern architectures like multicores, graphics processing units etc., although, as always, we encouraged any contributions relevant to our research programme. The joint workshop attracted 48 people from 10 countries. In 2009, the theme for our Sparse Days held from 18-19 June was hybrid solvers and we again attracted a good attendance from many countries in Europe and beyond. We are now planning the 2010 Sparse Days that will be combined with the wrap up meeting for the ANR Solstice project. Also planned for 2010 is a workshop on Optimization and Control that is being sponsored by the RTRA programme. More on this in our next Activity report !

I am very pleased to record that, over the reporting period, we have continued our involvement in joint research projects with shareholders and with other teams at CERFACS.

Perhaps the most significant event in this period involved a collaboration with INRIA with whom we have had a long-standing and close relationship although they are not a partner. This was the formation late in 2009 of a project on high performance numerical computation, called HiePACS, under the umbrella of a joint CERFACS-INRIA agreement on the foundation of a common laboratory. The HiePACS Project is led by Jean Roman from Bordeaux but Luc Giraud (who is now a research director at INRIA) is the main resident INRIA person on this project. It is great to welcome back Luc to CERFACS in this new capacity.

We have continued the collaboration with Airbus on shape optimization for drag minimization under lift constraints (this is the topic of the PhD thesis of Anke Tröltzsch). This is a challenging area since both the cost function and the gradient are noisy, and because heavy CFD computations with the elsA code are involved. Meta-model based optimization with noisy data and derivative free optimization algorithms have been studied in this context. Related research on algorithms for aerodynamic shape optimization have also been investigated in the framework of a DTP optimization project. This has been done in strong collaboration with the CFD team (Aerodynamics group) at CERFACS and both EADS and ONERA.

We have continued to support CNES in the GOCE mission on orbitography. Indeed we have developed a strong collaboration on the parallel distributed generation of normal equations and their subsequent Cholesky factorization for applications in geodesy. We have also developed a fruitful collaboration related to integer ambiguity resolution with André Lannes and colleagues at CNES/GRGS.

We have continued detailed discussions with EDF/SINETICS on parallel sparse direct methods for the solution of industrial problems in structural mechanics in the framework of the ANR Solstice project to be finished in June 2010. We have also participated in the study of algorithms for data assimilation in neutronics in collaboration with the Climate Modelling and Global Change Group (PhD thesis of A. Ponçot).

Our work on the optimization and linear algebraic aspects of data assimilation has been of great interest to and has been the subject of some discussions with the Climate Modelling and Global Change Group and Météo France. In the context of this collaboration, we have also hosted visits from Kristian Mogensen (ECMWF, UK), and from Patrick Laloyaux and Annick Sartenaer of the University of Namur, Belgium. This collaboration on data assimilation will continue in the coming years in the framework of the RTRA funded ADTAO project where efficient techniques for solving nonlinear least-squares problems will be developed.

We have been working closely with TOTAL on the development of solvers on massively parallel computers for Helmholtz problems arising in their geophysical applications (PhD of Xavier Pinel). In this context, we have solved huge indefinite linear systems efficiently with preconditioned Krylov subspace methods. During the PRACE Petascale Summer School held in Stockholm on August 26th-29th 2008, we successfully ported a three-dimensional Helmholtz solver to the IBM Blue Gene P at Juelich, Germany. We achieved almost perfect scalability on up to 65,536 cores both in the weak sense (when the computation per processor is kept constant) and in the strong sense (when the same problem is run on an increasing number of processors) on academic model problems. This opens the route to new projects related to inverse problems that are of crucial interest in seismics at TOTAL.

We assist the other Projects at CERFACS at all levels from the “over-a-coffee” consultancy to more major collaborations. These include advice on the elsA and the AVBP codes of CFD, in particular advice on the accuracy of their computations in a parallel environment, and many aspects of numerical algorithms with CFD and Global Change. We have also interacted with the CSG group on issues concerning new computer chips and technologies.

In a sense I have only now one senior in the team, Xavier Vasseur, to whom I am deeply indebted to the smooth day-to-day functioning of the Team. However, he has been ably abetted by Serge Gratton who became a Professor at ENSEEIHT in 2009 and more recently by Luc through the HiePACS project with INRIA. I am very pleased to say that Xavier is also well supported in his efforts by our enthusiastic and talented postdocs and our students who all contribute hugely to the ambience and atmosphere that many visitors remark on with great appreciation and fondness.

I should also pay tribute to the support we receive from our ex-team members who are now working at ENSEEIHT. Patrick Amestoy jointly supervised one student and collaborates strongly in our programmes on direct and hybrid solvers. As mentioned earlier, Serge is involved in many research projects in particular in optimization and least squares. Daniel Ruiz is collaborating with us on aspects of the SOLSTICE project and Michel Daydé interacts closely with us on networking, computing, and GRID topics. It is our local diaspora in action !

Iain S. Duff.

Visitors to Parallel Algorithm Project in 2008-2009

In alphabetical order, our visitors in the years 2008-2009 included :
MORAD AHMADNASAB (University Toulouse I, France),
PATRICK AMESTOY (ENSEEIHT-IRIT, France),
NECULAI ANDREI (Institute for Informatics, Romania),
MARIO ARIOLI (RAL, U.K.),
MICHELE BENZI (Emory University, U.S.A),
PAOLO BIENTINESI (Duke University, U.S.A),
PAOLA BOITO (University Paul Sabatier, Toulouse, France),
VINCENT BOYER (LAAS, Toulouse, France),
LUIZ MARIANO CARVALHO (Universidade do Estado do Rio de Janeiro, Brazil),
ANTHONY CHRONOPOULOS (University of Texas at San Antonio, U.S.A),
MICHEL DAYDÉ (ENSEEIHT-IRIT, France),
CÉDRIC DOUCET (University Grenoble I, France),
TONY DRUMMOND (Lawrence Berkeley National Laboratory, Berkeley, U.S.A.),
LUC GIRAUD (ENSEEIHT-IRIT, France),
FRANÇOIS GLINEUR (University of Leuwen, Belgium),
ABDOU GUERMOUCHE (INRIA-Bordeaux Sud-Ouest, France),
AZZAM HAIDAR (ENSEEIHT-IRIT, France),
ISAAC HAILPERIN (DESY and FU Berlin, Germany),
MICHAL KOCVARA (University of Birmingham, U.K.),
PATRICK LALOYAUX (The University of Namur, Belgium) ,
JULIEN LANGOU (The University of Colorado at Denver, U.S.A.),
JEAN-YVES L'EXCELLENT (INRIA-ENS, Lyon, France),
ANDREW LYONS (Argonne National Laboratory, U.S.A.),
GÉRARD MEURANT (CEA, Bruyères-le-Châtel, France),
DUBRAVKA MIJUCA (University UNION, Belgrade, Serbia),
KRISTIAN MOGENSEN (ECMWF, U.K.),
FRÉDÉRIC NATAF (University Paris VI, France),
ESMOND NG (Lawrence Berkeley National Laboratory, Berkeley, U.S.A.),
VITALIY OGARKO (Student, Russia),
SAULIUS PAKENAS (Student, Lithuania),
JASON RIEDY (Lawrence Berkeley National Laboratory, U.S.A.),
JEAN ROMAN (INRIA Futurs, LaBRI, Talence, France),
DANIEL RUIZ (ENSEEIHT-IRIT, France),
ANNICK SARTENAER (The University of Namur, Belgium),
JENNIFER SCOTT (Rutherford Appleton Laboratory, U.K.),
PETE (G.W.) Stewart (University of Maryland, USA),
ZDENEK STRAKOS (Academy of Sciences of the Czech Republic, Czech Republic),
CLAUDE TADONKI (University of Orsay, France),
PHILIPPE TOINT (The University of Namur, Belgium),
DENIS TRYSTRAM (IMAG, Grenoble, France),
BORA UCAR (INRIA-ENS, Lyon, France),
LUIS NUNES VICENTE (University of Coimbra, Portugal),
ICHITARO YAMAZAKI (Lawrence Berkeley National Laboratory, Berkeley, U.S.A.),

2 List of Members of the Algo Team

IAIN DUFF - Project Leader
FRANÇOISE CHAITIN-CHATELIN - Qualitative Computing Group Scientific Advisor
PHILIP AVERY - Senior Researcher, from October 2008 until October 2009
SERGE GRATTON - Senior Researcher and ENSEEIHT-IRIT, France
XAVIER VASSEUR - Senior Researcher
MARC BABOULIN - Post. Doc., until March 2008
MARTIN FUCHS - Post. Doc., from June 2009
MILAGROS GARCIA - Post. Doc., until August 2008
PAVEL JIRANEK - Post. Doc., from October 2008
KAMER KAYA - Post. Doc., from September 2009
JEAN TSHIMANGA - Post. Doc., until October 2009
BORA UÇAR - Post. Doc., until December 2008
AZZAM HAIDAR - Ph.D. Student, until June 2008
MÉLODIE MOUFFE - Ph.D. Student, until March 2009
XAVIER PINEL - Ph.D. Student
TZVETOMILA SLAVOVA - Ph.D. Student, until May 2009
ANKE TRÖLTZSCH - Ph.D. Student
MORAD AHMADNASAB - Visitor, University Toulouse I, France, until September 2008
PATRICK AMESTOY - Senior Visitor, ENSEEIHT-IRIT, France
LUC GIRAUD - Senior Visitor, ENSEEIHT-IRIT, France
XUEPING GUO - Senior Visitor, East China Normal University, Shanghai, China (June 2008-May 2009)

VINCENT MALMEDY - Junior PhD Visitor, University of Namur, Belgium (June-August 2008)
AUDREY BONNEMENT - Trainee (February-August 2008)
LÉON THAM - Trainee (June-August 2008)
FRANÇOIS VILAR - Trainee (June-August 2008)
NICOLE BOUTET - Administration, until March 2009
BRIGITTE YZEL - Administration

3 Dense and Sparse Matrix Computations

3.1 Using FGMRES to obtain backward stability in mixed precision

M. Arioli : RUTHERFORD APPLETON LABORATORY, *England* ; **I. S. Duff** : CERFACS, *France and* RUTHERFORD APPLETON LABORATORY, *England*

In [ALG2] we consider the triangular factorization of matrices in single precision arithmetic and show how these factors can be used to obtain a backward stable solution. Our aim is to obtain double precision accuracy even when the system is ill-conditioned. We examine the use of iterative refinement and show by example that it may not converge. We then show both theoretically and practically that the use of FGMRES will give us the result that we desire with fairly mild conditions on the matrix and the direct factorization. We perform extensive experiments on dense matrices using MATLAB and indicate how our work extends to sparse matrix factorization and solution.

3.2 Parallel matrix scaling algorithms

P. R. Amestoy : ENSEEIHT-IRIT, *France* ; **I. S. Duff** : CERFACS, *France and* RUTHERFORD APPLETON LABORATORY, *England* ; **D. Ruiz** : ENSEEIHT-IRIT, *France* ; **B. Uçar** : CERFACS, *France*

Based on [2], we worked on an iterative procedure which asymptotically scales the infinity norm of both rows and columns of a given matrix to 1. In [ALG59], we propose a parallelization of the scaling procedure. We argue that the parallelization requires a careful partitioning of two diagonal matrices in addition to a standard sparse matrix partitioning for parallel matrix-vector multiply operations. We propose a method based on an all-reduce operation to partition the diagonal matrices. We present performance results on a PC cluster where good speedups are obtained for matrices having a reasonable number of nonzeros and the results are presented at the VECPAR'08 conference. The parallel algorithms are implemented in Fortran, and the resulting codes are integrated into MUMPS [1].

[1] P. R. Amestoy, I. S. Duff, J.-Y. L'Excellent, and J. Koster, (2001), A fully asynchronous multifrontal solver using distributed dynamic scheduling, *SIMAX*, **23**, 15–41.

[2] D. Ruiz, (2001), A scaling algorithm to equilibrate both rows and columns norms in matrices, Tech. Rep. RAL-TR-2001-034 and RT/APO/01/4, Rutherford Appleton Laboratory, Oxon, UK and ENSEEIHT-IRIT, Toulouse, France.

3.3 Solving incremental dense least squares problems in parallel

M. Baboulin : CERFACS, *France* ; **L. Giraud** : ENSEEIHT, *France* ; **S. Gratton** : ENSEEIHT-IRIT, *France* ; **J. Langou** : THE UNIVERSITY OF COLORADO AT DENVER AND HEALTH SCIENCES CENTER, *USA*

We present a parallel distributed solver that enables us to solve incremental dense least squares arising in some parameter estimation problems. This solver is based on ScaLAPACK and PBLAS kernel routines. In the incremental process, the observations are collected periodically and the solver updates the solution with new observations using a QR factorization algorithm. It uses a recently defined distributed packed format (see [3]) that handles symmetric or triangular matrices in ScaLAPACK-based implementations. We provide performance analysis on an IBM pSeries 690. We also present an example of application in the area of space geodesy for gravity field computations with some experimental results. More details can be found in [ALG8].

[3] M. Baboulin, L. Giraud, S. Gratton, and J. Langou, (2005), A distributed packed storage for large parallel calculations., Technical Report TR/PA/05/30, CERFACS.

3.4 Towards parallel bipartite matching algorithms

I. S. Duff : CERFACS, *France and* RUTHERFORD APPLETON LABORATORY, *England* ; **D. Ruiz** : ENSEEIHT-IRIT, *France* ; **B. Uçar** : CERFACS, *France*

One of the most powerful preprocessing methods for direct solvers is known as the maximum product matching ordering. Given an $n \times n$ matrix A, the objective is to find a permutation M such that the diagonal product of the permuted matrix, $\prod \mathrm{diag}(AM)$, is maximum (in magnitude) among all permutations. It is well known that the standard algorithms (see [6]) for this problem are not amenable to parallelization. We follow a different path. We start from the property that an optimal diagonal is invariant under suitable matrix scaling. Based on this, we have designed the following algorithm : (1) Scale the matrix in parallel such that each row and column contains one entry of magnitude 1.0 ; (2) find a maximum cardinality matching using only the entries of magnitude 1.0 ; (3) if the matching is perfect, we are done. (4) If not, select a particular entry and update the scaling factors as well as the matching. This process is repeated until a perfect matching is found. We have observed that on many matrices, applying the first three steps above is sufficient to obtain the optimal matching where the algorithm happens to reduce to selecting a maximum entry in each row or column. For the others we have envisaged an approximate approach, where the resulting matching is not guaranteed to be of maximum product, but is empirically observed to have an almost equal impact on the factorization as a maximum product one. The results obtained so far have been discussed in a SIAM conference in March 2008 [4]. Further investigations were performed and additional results have been presented later [5] where it is concluded that our efforts, more or less, amount to reinventing a known algorithm.

[4] P. R. Amestoy, I. S. Duff, D. Ruiz, and B. Uçar, (2008), Computing a class of bipartite matchings in parallel. Presented at *SIAM Conference on Parallel Processing for Scientific Computing (*PP08), Atlanta, USA. 12–14 March, 2008.

[5] P. R. Amestoy, I. S. Duff, D. Ruiz, and B. Uçar, (2009), Towards parallel bipartite matching algorithms. Presented at *Scheduling for large-scale systems*, , Knoxville, Tennessee, USA, May 13–15, 2009.

[6] I. S. Duff and J. Koster, (2001), On algorithms for permuting large entries to the diagonal of a sparse matrix, *SIAM J. Matrix Analysis and Applications*, **22**, 973–996.

3.5 The block triangular form of symmetric matrices

I. S. Duff : CERFACS, *France and* RUTHERFORD APPLETON LABORATORY, *England* ; **B. Uçar** : CERFACS, *France*

We report observations on the block triangular form of symmetric, structurally rank deficient, square, sparse matrices. As the matrix is square and structurally rank deficient, it has at least one underdetermined and one overdetermined block. We prove that these blocks are transposes of each other. Furthermore, we show that the fine decomposition of the square block consists of matrices whose row is set equal to its column set or whose row set and column sets are disjoint. The properties shown help us recover symmetry around the anti-diagonal in the block triangular matrix. The main results are carried over to full rank symmetric matrices as well. The paper [ALG45] has been accepted to be published in SIAM Review.

3.6 Combinatorial problems in solving linear systems

I. S. Duff : CERFACS, *France and* RUTHERFORD APPLETON LABORATORY, *England* ; **B. Uçar** : CNRS *and* ENS LYON, *France*

We have done a survey on the symbiotic interaction between numerical linear algebra and combinatorial optimization. The survey has been presented at a Dagstuhl workshop by Duff.
Numerical linear algebra and combinatorial optimization are vast subjects ; as is their interaction. In virtually all cases there should be a notion of sparsity for a combinatorial problem to arise. Sparse matrices therefore form the basis of the interaction of these two seemingly disparate subjects. As the core of many of today's numerical linear algebra computations consists of the solution of a sparse linear system by direct or iterative methods, we surveyed some combinatorial problems, ideas, and algorithms relating to these computations.
On the direct methods side, we discussed issues such as matrix ordering ; bipartite matching and matrix scaling for better pivoting ; and task assignment and scheduling for parallel multifrontal solvers. On the iterative method side, we discussed preconditioning techniques including incomplete factorization preconditioners, support graph preconditioners, and algebraic multigrid. In a separate part, we discussed the block triangular form of sparse matrices.
This survey has been invited to be included in an edited book on combinatorial scientific computing.

3.7 On accurate and time efficient solution of primal-mixed finite-element equations in multiscale solid mechanics

I. S. Duff : CERFACS, *France and* RUTHERFORD APPLETON LABORATORY, *England* ; **D. Mijuca** : UNIVERSITY UNION, *Belgrade, Serbia*

In [ALG10] in order to identify the best technique to solve a class of geometrically multiscale model problems in thermoelasticity, we examine a combination of a primal–mixed finite element approach and direct sparse solvers and matrix scaling routines. The criteria for optimality are robustness, accuracy and execution time. It will be shown that the present finite element approach, where displacement and stress variables are simultaneously solved from large scale indefinite poorly scaled systems of equations using the sparse HSL solver `MA57` with the aid of the matrix scaling routines `MC64` or `MC30` during the factorization process, enables a reliable solution even if hexahedral finite elements in a mesh differ in size up to six orders of magnitude. A number of tests in multiscale elasticity and thermoelasticity are examined to test the accuracy and execution time efficiency of the proposed solution approach on a standard PC computing platform.

3.8 Performance analysis of maximum cardinality matching algorithms for sparse matrices

I. S. Duff : CERFACS, FRANCE AND RUTHERFORD APPLETON LABORATORY, *England* ; **K. Kaya** : CERFACS, *France* ; **B. Uçar** : ENS LYON, *France*

We review the algorithms in the literature for solving the problem of finding a maximum cardinality matching in bipartite graphs. We also discuss two heuristic algorithms for the same problem which can precede the exact algorithms for the same problem. We have implemented all these heuristics and algorithms and performed extensive tests. Our aim is to present these algorithms and discuss implementation details which are often necessary to have fast codes for sparse matrices. We have realized a simple improvement to one of the existing algorithms which improves the performance of the original algorithm in most of the cases. To the best of our knowledge, the existing implementations of the exact algorithms use only one of the heuristics as a preprocessing step. By means of experiments, we show that the second is much more efficient. At the time of writing, a technical report [7] was under preparation.

[7] K. Kaya, I. S. Duff, and B. .Uçar, (2009), Performance analysis of maximum cardinality matching algorithms for sparse matrices. Manuscript, in preparation.

3.9 Parallel triangular solution in the out-of-core multifrontal approach for solving large sparse linear systems

Tz. Slavova : CERFACS, *France*

We consider the solution of very large systems of linear equations with direct multifrontal methods. In this context the size of the factors is an important limitation for the use of sparse direct solvers. We will thus assume that the factors have been written on the local disks of our target multiprocessor machine during parallel factorization. Our main focus is the study and the design of efficient approaches for the forward and backward substitution phases after a sparse multifrontal factorization. These phases involve sparse triangular solution and have often been neglected in previous works on sparse direct factorization. In many applications, however, the time for the solution can be the main bottleneck for the performance. This thesis consists of two parts. The focus of the first part is on optimizing the out-ofcore performance of the solution phase. The focus of the second part is to further improve the performance by exploiting the sparsity of the right-hand side vectors. More details can be found [ALG31].

3.10 On the matrix symmetrization problem

B. Uçar : CERFACS, *France*

We consider the following variant of the matrix symmetrization problem. Given a square, unsymmetric sparse matrix, find a permutation of the columns of the matrix to yield a zero-free diagonal and to maximize the structural symmetry. The problem is known to be NP-hard. We had proposed a fairly fast heuristic and performed extensive tests empirically demonstrating results around 75% of the optimum [ALG64]. A solution to the matrix symmetrization problem can be used in different contexts. First, the method can be used as a preprocessing tool for some algorithms which are originally designed for structurally symmetric matrices. We have obtained promising results with the algorithms that are used for reducing bandwidth, and also with those that are used for obtaining doubly bordered block diagonal forms. Second, direct solvers for unsymmetric systems can take advantage of structural symmetry. We tried modifications of the proposed approach in the context of direct methods. Although these modifications did not lead to significant changes in the performance of the direct solver, we have identified new research problems to pursue later. One of them is to develop effective scaling algorithms for a given set of diagonal entries so that all diagonal entries become one in magnitude and the maximum magnitude of an off-diagonal entry that is larger than one is minimized. We plan to investigate such scaling methods in the forthcoming periods with new recruits.

4 Iterative Methods and Preconditioning

4.1 The FETI family of domain decomposition methods for inequality-constrained quadratic programming : Application to contact problems with conforming and nonconforming interfaces

P. Avery : CERFACS, *France* ; **C. Farhat** : INSTITUTE FOR COMPUTATIONAL AND MATHEMATICAL ENGINEERING, STANFORD, *USA*

Two domain decomposition methods with Lagrange multipliers for solving iteratively quadratic programming problems with inequality constraints are presented. These methods are based on the FETI and FETI-DP substructuring algorithms. In the case of linear constraints, they do not perform any Newton-like iteration. Instead, they solve a constrained problem by an active set strategy and a generalized conjugate gradient based descent method equipped with controls to guarantee convergence monotonicity. Both methods possess the desirable feature of minimizing numerical oscillations during the iterative solution process. Performance results and comparisons are reported for several numerical simulations that suggest that both methods are numerically scalable with respect to both the problem size and the number of subdomains. Their parallel scalability is also illustrated on a Linux cluster for a complex 1.4 million degree of freedom multibody problem with frictionless contact and nonconforming discrete interfaces. More details can be found in [ALG3].

4.2 A Padé-based factorization-free algorithm for identifying the eigenvalues missed by a generalized symmetric eigensolver

P. Avery : CERFACS, *France* ; **C. Farhat** : STANFORD UNIVERSITY, *USA* ; **U. Hetmaniuk** : UNIVERSITY OF WASHINGTON, *USA*

When computing the solution of a generalized symmetric eigenvalue problem of the form $Ku = \lambda Mu$, the Sturm sequence check, also known as the inertia check, is the most popular method for reporting the number of missed eigenvalues within a range $[\sigma_L, \sigma_R]$. This method requires the factorization of the matrices $K - \sigma_L M$ and $K - \sigma_R M$. When the size of the problem is reasonable and the matrices K and M are assembled, these factorizations are possible. When the eigensolver is equipped with an iterative solver, which is nowadays the preferred choice for large-scale problems, the factorization of $K - \sigma M$ is not desired or feasible and therefore the inertia check cannot be performed. To this effect, the purpose of this paper is to present a factorization-free algorithm for detecting and identifying the eigenvalues that were missed by an eigensolver equipped with an iterative linear equation solver within an interval of interest $[\sigma_L, \sigma_R]$. This algorithm constructs a scalar, rational, transfer function whose poles are exactly the eigenvalues of the symmetric pencil (K, M), approximates it by a Padé expansion, and computes the poles of this approximation to detect and identify the missed eigenvalues. The proposed algorithm is illustrated with an academic numerical example. Its potential for real engineering applications is also demonstrated with a large-scale structural vibrations problem. More details can be found in [ALG4].

4.3 Multi-level direct K-way hypergraph partitioning with multiple constraints and fixed vertices

C. Aykanat : Bilkent University, *Turkey*; **B. B. Cambazoglu** : Ohio State University, *USA*; **B. Uçar** : CERFACS, *France*

K-way hypergraph partitioning has an ever-growing use in parallelization of scientific computing applications. In [ALG5], we claim that hypergraph partitioning with multiple constraints and fixed vertices should be implemented using direct K-way refinement, instead of the widely adopted recursive bisection paradigm. Our arguments are based on the fact that recursive-bisection-based partitioning algorithms perform considerably worse when used in the multiple constraint and fixed vertex formulations. We discuss possible reasons for this performance degradation. We describe a careful implementation of a multi-level direct K-way hypergraph partitioning algorithm, which performs better than a well-known recursive-bisection-based partitioning algorithm in hypergraph partitioning with multiple constraints and fixed vertices. We also experimentally show that the proposed algorithm is effective in standard hypergraph partitioning.

4.4 Numerical study on incomplete orthogonal factorization preconditioners

Z.-Z. Bai : Chinese Academy of Sciences, *Beijing, China*; **I. S. Duff** : CERFACS, *France and* Rutherford Appleton Laboratory, *England*; **J.-F. Yin** : Chinese Academy of Sciences, *Beijing, China*

We design, analyse and test a class of incomplete orthogonal factorization preconditioners constructed from Givens rotations, incorporating some dropping strategies and updating tricks, for the solution of large sparse systems of linear equations. Comprehensive accounts about how the preconditioners are coded, what storage is required and how the computation is executed for a given accuracy are presented. A number of numerical experiments show that these preconditioners are competitive with standard incomplete triangular factorization preconditioners when they are applied to accelerate Krylov subspace iteration methods such as GMRES and BiCGSTAB. More details can be found in [ALG9].

4.5 A dimensional split preconditioner for Stokes and linearized Navier-Stokes equations

M. Benzi : Department of Mathematics and Computer Science, Emory University, Atlanta, *USA*; **X.-P. Guo** : Department of Mathematics, East China Normal University, Shanghai, *China and* CERFACS, *France*

In this paper we introduce a new preconditioner for linear systems of saddle point type arising from the numerical solution of the Navier Stokes equations. Our approach is based on a dimensional splitting of the problem along the components of the velocity field, resulting in a convergent fixed-point iteration. The basic iteration is accelerated by a Krylov subspace method like restarted GMRES. The corresponding preconditioner requires at each iteration the solution of a set of discrete scalar elliptic equations, one for each component of the velocity field. Numerical experiments showing mesh-independent convergence on a standard finite element discretization of the Stokes and Oseen problems are included.

4.6 Iterative methods applied to large rank-deficient sparse matrices

A. Bonnement : CERFACS, *France* ; **S. Gratton** : ENSEEIHT-IRIT AND CERFACS, *France* ; **X. Vasseur** : CERFACS, *France*

The analysis of the rank deficiency of large matrices is an open problem occurring in various algorithms. Whereas various rank-revealing procedures have been proposed for dense matrices, this question is rarely addressed for large sparse matrices. During her Master thesis, A. Bonnement has studied an algorithm based on the use of the GMRES Krylov subspace method to compute a null space basis of sparse rank-deficient matrices. Special attention has been paid to the stopping criteria used in the linear solver. This algorithm has been evaluated when computing null space informations of large sparse matrices coming from academic problems and structural mechanics (collaboration with O. Boiteau EDF R&D within the ANR Solstice project) and electromagnetism. On this set of semidefinite symmetric positive matrices, it has been found that the proposed algorithm did obtain reliably both the deficiency and an accurate null space basis.

4.7 Block GCR for the solution of three-dimensional wave propagation problems

H. Calandra : TOTAL, *France* ; **S. Gratton** : ENSEEIHT-IRIT, *France* ; **J. Langou** : UNIVERSITY OF COLORADO DENVER, *US* ; **X. Pinel** : CERFACS, *France* ; **X. Vasseur** : CERFACS, *France*

The goal of our research was to speed up the CERFACS home-grown code developed during Xavier Pinel's PhD thesis project. This application code solves the Helmholtz equation in the frequency domain and in three dimensions. Gratton, Pinel and Vasseur had already shown that the iterative method FGMRES combined with a two grid-inner solver for a preconditioner leads to a robust and scalable solver which was unheard of for this type of problem. Based on this, we wanted to further exploit the fact that the linear system of equations needed to be solved for multiple right-hand sides (say a thousand). We applied an iterative method developed by Langou in 2004, namely BlockGCR with deflation, in the context of this application code. For a standard test case (Segsalt, 5Hz, 24 RHS on 512 processors of egee.cerfacs.fr), the BlockGCR with deflation solver compares favourably with existing methods. The best time with existing methods was achieved using 8 synchronized FGMRES (each using 64 processors) three times (to handle the 24 right-hand sides) and was 248 seconds (for 240 matrix-vector products). Note that all existing block solvers were noticeably slower than this. BlockGCR needed 169 seconds (for 97 matrix-vector products). This represents a 31% time decrease. We have similar positive results on other test cases. A question is left open. While it is clear that mono-right-hand-side iterative methods have a time to solution that increases linearly with the number of right-hand sides, we do not know what the trend is for iterative methods with multiple right-hand sides for this application. Do we have a sublinear behaviour ?

4.8 Algorithm 881 : A Set of Flexible GMRES Routines for Real and Complex Arithmetics on High-Performance Computers

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In this article we describe our implementations of the FGMRES algorithm for both real and complex, single and double precision arithmetics suitable for serial, shared-memory, and distributed-memory computers. For the sake of portability, simplicity, flexibility, and efficiency, the FGMRES solvers have been implemented in Fortran 77 using a reverse communication mechanism for the matrix-vector product, the preconditioning, and the dot-product computations. For distributed-memory computation, several orthogonalization procedures have been implemented to reduce the cost of the dot-product calculation, which is a well-known bottleneck of efficiency for Krylov methods. Furthermore, either implicit or explicit calculation of the residual at a restart is possible depending on the actual cost of the matrix-vector product. Finally, the implemented stopping criterion is based on a normwise backward error. Further details can be found in [ALG13].

4.9 Newton's method for the common eigenvector problem

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In [8], we have proved the sensitivity of computing the common eigenvector of two matrices A and B, and we have designed a new approach to solve this problem based on the notion of the backward error. If one of the two matrices (say A) has n eigenvectors then to find the common eigenvector we have just to write the matrix B in the basis formed by the eigenvectors of A. But if there are eigenvectors with multiplicity > 1, the common vector belongs to a vector space of dimension > 1 and such a strategy would not help to compute it. In this paper, we use Newton's method to compute a common eigenvector for two matrices, taking the backward error as a stopping criteria. We mention that no assumptions are made on the matrices A and B. More details can be found in [ALG14].

[8] A. E. Ghazi, S. E. Hajji, L. Giraud, and S. Gratton, (2006), A short note on backward errors for the common eigenvector problem, Technical Report TR/PA/06/13, CERFACS.

4.10 Flexible GMRES with deflated restarting

L. Giraud : INRIA BORDEAUX SUD-OUEST, *France* ; **S. Gratton** : ENSEEIHT-IRIT, *France* ; **X. Pinel** : CERFACS, *France* ; **X. Vasseur** : CERFACS, *France*

There are many situations in scientific computing where variable preconditioners have to be considered for the iterative solution of a linear system. In that framework we have proposed a novel algorithm that attempts to combine the numerical features of GMRES-DR and the flexibility of FGMRES. The new algorithm, referred to as FGMRES-DR, inherits attractive numerical properties from its two parents. We have shown, on a set of small test examples as well as on two real life applications in wave propagation, that, after the first restart of the method, FGMRES-DR may outperform FGMRES ; the benefit obtained is problem dependent. More details can be found in [ALG52].

4.11 Sparse approximations of the Schur complement for parallel algebraic hybrid solvers in 3D

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In this work [9], we study the computational performance of variants of an algebraic additive Schwarz preconditioner for the Schur complement for the solution of large sparse linear systems. In earlier works, the local Schur complements were computed exactly using a sparse direct solver. The robustness of the preconditioner comes at the price of this memory and time intensive computation that is the main bottleneck of the approach for tackling huge problems. In this work, we investigate the use of sparse approximations of the dense local Schur complements. These approximations are computed using a partial incomplete LU factorization [11]. Such a numerical calculation is the core of the multi-level incomplete factorization such as the one implemented in pARMS [10]. The numerical and computing performance of the new numerical scheme is illustrated on a set of large 3D convection-diffusion problems ; preliminary experiments on linear systems arising from structural mechanics are also reported.

[9] L. Giraud, A. Haidar, and Y. Saad, (2010), Sparse approximations of the Schur complement for parallel algebraic hybrid linear solvers in 3D, *Numerical Mathematics : Theory, Methods and Applications*, **in press**.

[10] Z. Li, Y. Saad, and M. Sosonkina, (2003), pARMS : a Parallel Version of the Algebraic Recursive Multilevel Solver, *Numerical Linear Algebra with Applications*, **10**, 485–509.

[11] Y. Saad, (1994), ILUT : A dual threshold incomplete ILU factorization, *Numerical Linear Algebra with Applications*, **1**, 387–402.

4.12 Using multiple levels of parallelism to enhance the performance of domain decomposition solvers

L. Giraud : INRIA BORDEAUX - SUD-OUEST, *France* ; **A. Haidar** : UNIVERSITY OF TENNESSEE, DEPARTMENT OF COMPUTER SCIENCE, *USA* ; **S. Pralet** : BULL SAS, *France*

Large-scale scientific simulations are nowadays fully integrated in many scientific and industrial applications. Many of these simulations rely on models based on PDEs that lead to the solution of huge linear or nonlinear systems of equations involving millions of unknowns. In that context, the use of large high performance computers in conjunction with advanced fully parallel and scalable numerical techniques is mandatory to efficiently tackle these problems.
In this work [12], we consider a parallel linear solver based on a domain decomposition approach. Its implementation naturally exploits two levels of parallelism, that offers the flexibility to combine the numerical and the parallel implementation scalabilities. The combination of the two levels of parallelism enables optimal usage of the computing resource while preserving attractive numerical performance. Consequently, such a numerical technique appears as a promising candidate for intensive simulations on massively parallel platforms.
The robustness and parallel numerical performance of the solver is investigated on large challenging linear systems arising from finite-element discretizations in structural mechanics applications.

[12] L. Giraud, A. Haidar, and S. Pralet, (2009), Using multiple levels of parallelism to enhance the performance of domain decomposition solvers, *Parallel Computing*, **(in press)**.

4.13 Parallel algebraic hybrid solvers for large 3D convection-diffusion problems

L. Giraud : INRIA BORDEAUX - SUD-OUEST, *France* ; **A. Haidar** : UNIVERSITY OF TENNESSEE, DEPARTMENT OF COMPUTER SCIENCE, *USA*

In this work [ALG15] we study the parallel scalability of variants of an algebraic additive Schwarz preconditioner for the solution of large three-dimensional convection diffusion problems in a non-overlapping domain decomposition framework. To alleviate the computational cost, both in terms of memory and floating-point complexity, we investigate variants based on a sparse approximation or on mixed 32- and 64-bit calculations. The robustness and the scalability of the preconditioners are investigated through extensive parallel experiments on up to two thousand processors. Their efficiency from a numerical and parallel performance view point are reported.

4.14 Toward robust hybrid parallel sparse solvers for large scale applications

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As supercomputer platforms continue to gain ground in the High Performance Computing world, new advances in simulation require the continuing development of new algorithms and numerical methods. The solution of this challenging research area requires a multidisciplinary approach involving advanced numerical schemes, massively parallel computing and the design of highly scalable algorithms and codes to be executed on future Petaflop machines. In this direction, we have developed the hybrid hierarchical solver (MaPHyS) in order to take advantage of the architectural features of these new platforms. MAPHYS, maintained and supported by the HiePACS project (INRIA-CERFACS joint Lab), is a hybrid approach that combines iterative and direct methods. The focus of this solver is to develop effective parallel algebraic preconditioners that are suitable and scalable for high performance computation. It is based on substructuring domain decomposition techniques. Furthermore, we investigate work on multi-level parallel approaches to be able to exploit large numbers of processors with reasonable efficiency.

4.15 On the parallel scalability of hybrid linear solvers for large $3D$ problems

A. Haidar : UNIVERSITY OF TENNESSEE, DEPARTMENT OF COMPUTER SCIENCE, *USA*

Large-scale scientific applications and industrial simulations are nowadays fully integrated in many engineering areas. They involve the solution of large sparse linear systems. The use of large high performance computers is mandatory to solve these problems. The main topic of this research work of my thesis at CERFACS was the study of a numerical technique that had attractive features for an efficient solution of large scale linear systems on large massively parallel platforms. The goal is to develop a high performance hybrid direct/iterative approach for solving large 3D problems. We focus specifically on associated domain decomposition techniques for the parallel solution of large linear systems. We have investigated several algebraic preconditioning techniques, discussed their numerical behaviour, their parallel implementation and scalability. We have compared their performance on a set of 3D grand challenge problems. Details about this research area can be found in the thesis [ALG29] and in the papers [ALG15, ALG16].

4.16 Stopping criteria for LSQR based on the backward error

P. Jiránek : CERFACS, *France* ; **D. Titley-Peloquin** : MCGILL UNIVERSITY, *Canada*

In [ALG57] we propose practical and efficiently computable stopping criteria for the iterative solution of large sparse linear least squares problems based on the estimation of the backward error. We focus mainly on the LSQR algorithm but many ideas are to some extent applicable to other equivalent methods like the CGLS method. We recall the importance of the 2-norm of the projection of the residual vector onto the range of the system matrix, how it is useful for measuring the convergence, and we provide formulae that can be used to efficiently estimate this quantity at every iteration of LSQR. In addition we concentrate on the efficient estimation of the backward error. The backward error in least-squares problems is given by the smallest singular value of a certain matrix, which we approximate using the quantities computed during the Golub-Kahan bidiagonalization in LSQR. It appears that the resulting estimate of the backward error has similar properties to the estimate of the 2-norm of the projected residual vector. We also use a similar approach for computing a certain asymptotically equivalent estimate of the backward error.

4.17 Numerical stability of Simpler GMRES and GCR

P. Jiránek : CERFACS, *France* ; **M. Rozložník** : ACADEMY OF SCIENCES OF THE CZECH REPUBLIC, *Czech Republic* ; **M. H. Gutknecht** : ETH ZURICH, *Switzerland*

In [ALG21] we analyse the numerical behaviour of several minimum residual methods which are mathematically equivalent to the GMRES method. We compare two main approaches : one that computes the approximate solution in terms of a Krylov subspace basis from an upper triangular linear system for the coordinates, and one where the approximate solutions are updated with a simple recursion formula. We show that a different choice of the basis has a significant influence on the numerical behaviour of the resulting implementation. While the Simpler GMRES and ORTHODIR are less stable due to the ill-conditioning of the basis, the residual basis is well-conditioned as long as we have a reasonable residual norm decrease. These results lead to a new implementation, which is conditionally backward stable, and they explain the experimentally observed fact that the GCR method delivers very accurate approximate solutions when it converges fast enough without stagnation.
In [ALG62] we observe that the Simpler GMRES basis is well-conditioned if and only if the residual norms (nearly) stagnate, while the (normalized) residuals remain well-conditioned if and only if the convergence is fast. This results in a new implementation [ALG20] of the Simpler GMRES method which adaptively combines both bases using a criterion based on the intermediate residual decrease and was proved to be backward stable. A similar improvement can be made for the GCR method as well.

5 Qualitative Computing

Group members : Françoise Chaitin-Chatelin, Morad Ahmadnasab, CERFACS and Université Toulouse 1.

The main activity of the Qualitative Computing group in 2008-2009 has been the writing of "Qualitative Computing : A computational journey into nonlinearity" to be published by World Scientific, Singapore. This book, written in mathematical language, is about the domain of *mathematical computation* which extends *beyond modern calculus* and *classical analysis* when numbers are not restricted to belong to a commutative field. It describes the dynamics of complexification, resulting in an endless remorphing of the computational landscape. Computation weaves a colourful tapestry always in a state of becoming. In the process, some meta-principles emerge which guide the autonomous evolution of mathematical computation. These organic principles are essential keys to analyse very large numerical simulations of unstable phenomena.
High tech industries are in desperate need for adequate tools to assess the validity of simulations produced by ever faster computers for ever more unstable problems. In order to meet these industrial expectations, the applied mathematicians are facing a formidable challenge summarized by the two words 1) nonlinearity and 2) coupling. This book is unique of its kind in proposing to explore truly new paths in the unchartered jungle of nonlinear computation.

- 1) Use hypercomputation in *quadratic* algebras, rather than the computation in *linear* vector spaces that is traditional since the early 20th century.
- 2) Complement the classical linear logic (based on the sequence of natural integers) with a complex logic which expresses the potential of the complex plane for organic intelligence.

The book illustrates how Qualitative Computing has been the driving force behind the evolution of mathematical logic from the beginnings, when Pythagoras presented the first known incompleteness result, the proof of the irrationality of $\sqrt{2}$. It is a fact of experience that the classical logic of Aristotle is too limited to capture the dynamics of nonlinear computation. Mathematics provides us with the missing tool, an organic logic (based on $\{\mathbb{R}, \mathbb{C}, \infty\}$) which is tailored to the dynamics of nonlinearity. This organic logic can tame the computing paradoxes stemming from measurements in the absence of associativity ; it represents the internal clockwork of computation. It makes full use of the computing potential of rings of numbers with 1,2,4 and 8 dimensions. The necessity to limit the frame of interpretation to 3 dimensions at most brings to light some mechanisms by which computation turns the complex into the simple without reduction.

The book is primarily intended for graduate students, researchers and engineers seriously involved in the challenges of intensive scientific computing at the edge of turbulence and chaos. At the same time, the philosophically oriented reader will enjoy the historical and epistemological perspectives on Computation which accompany the mathematical text all along.
The presentation of the technical content is almost everywhere kept at an undergraduate level. The prerequisites are classical calculus, analysis and numerical linear algebra.
The subject of Qualitative Computing covers theoretical and practical aspects of nonlinear computation. Multiplication is the lead actor : multiplication of numbers, vectors and matrices. The theoretical aspects which have been chosen for presentation in the book describe hypercomputation over vectors in Dickson algebras (Chapters 2 to 6, 9 and 11), the theory of Homotopic Deviation for matrices (Chapter 7), and Fourier analysis for complex signals (Chapter 10). As for Chapter 8, it addresses more practical

aspects. Inter alia, it clarifies why the scientific computer not only is a most efficient tool to speed-up intractable computations in every corner of our technological society, but also has an epistemological potential which begs to be put to good use in our attempt to decipher the organic evolution of life. Then, the final Chapter 12 concludes with organic intelligence for dicksonian numbers and wraps up some of the lessons in computation that were taught in the book. A few of them follow. Numbers need not be confined to commutative fields. They can be vectors or matrices in algebras equipped with a *noncommutative* multiplication that is the source of evolution. And Nature's computation based on electromagnetic information coming from physical light can be paradoxical ! Moreover, the informations processed by computation in A_k, $k \geq 5$, cannot have a purely electromagnetic origin. The Sharkovski order (derived from the fixed points of $x = f^{(n)}(x)$) reveals an *algorithmic* connection between the actual ∞ and the four qualities (discrete, continuous, real, complex) that numbers can possess when they are the building blocks of classical calculation (arithmetic, calculus, analysis). The logistic computation realises an approximate *numerical synthesis* between Uniqueness and Multiplicity by the magic of successive iterations over $\mathbb{R}$ in finite precision. And this magic is revealed by the evolution of a real parameter.
Only a few snapshots of the infinite computational landscape lying beyond modern calculus and analysis can be shown in one single book. The door is open for further investigation. If scientists want it to happen, the multimillennary evolutive art of computing will come back to life, awakened from a sleep which is now lasting for more than a century.
Further information can also be found in [ALG60].

5.1 A study of round-off propagation in massively parallel codes for Large Eddy Simulation (LES)

M. Ahmadnasab : CERFACS, *France*

During three months Morad Ahmadnasab has studied the growth of rounding errors on parallel computers occurring when considering Large-Eddy Simulation (LES) problems handled in the CFD Group at CERFACS. The main concern is the sensitivity of the physical model to the spatial discretization combined with explicit time-stepping approaches such as Runge-Kutta, and the sensitivity to parameters such as the number of processors used for parallel simulation, changes in initial conditions, and machine precision. It has been notably recommended to pay special attention to accurate summation and dot product algorithms for floating-point numbers to minimize the propagation of rounding errors in such an environment. An implementation of an existing algorithm due to Rump, Ogita and Oishi (2008) has been realised that could be used later in AVBP. More details can be found in [ALG32].

6 Nonlinear Systems and Optimization

6.1 Analysis of the Conditioning of the Components of a Linear Least Squares Solution

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In this paper, we address the accuracy of the results for the overdetermined full rank linear least squares problem. We recall theoretical results obtained in [13], on conditioning of the least squares solution and the components of the solution when the matrix perturbations are measured in Frobenius or spectral norms. Then we define computable estimates for these condition numbers and we interpret them in terms of statistical quantities. In particular, we show that, in the classical linear statistical model, the ratio of the variance of one component of the solution by the variance of the right-hand side is exactly the condition number of this solution component when perturbations on the right-hand side are considered. We also provide fragment codes using LAPACK routines to compute the variance-covariance matrix and the least squares conditioning and we give the corresponding computational cost. Finally we present a small historical numerical example that was used by Laplace in Théorie Analytique des Probabilités, 1820, for computing the mass of Jupiter and experiments from the space industry with real physical data. More information can be found in [ALG7]

[13] M. Arioli, M. Baboulin, and S. Gratton, (2007), A Partial Condition Number for Linear Least Squares Problems, *SIAM Journal on Matrix Analysis and Applications*, **29**, 413–433.

6.2 Using dual techniques to derive componentwise and mixed condition numbers for a linear function of a linear least squares solution

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We prove duality results for adjoint operators and product norms in the framework of Euclidean spaces. We show how these results can be used to derive condition numbers especially when perturbations on data are measured componentwise relatively to the original data. We apply this technique to obtain formulas for componentwise and mixed condition numbers for a linear function of a linear least squares solution. These expressions are closed when perturbations of the solution are measured using a componentwise norm or the infinity norm and we get an upper bound for the Euclidean norm. More details can be found in [ALG6].

6.3 The Optimization Test Environment

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The TEST ENVIRONMENT is an interface to efficiently test different optimization solvers. It is designed as a tool for both developers of solver software and practitioners who just look for the best solver for their specific problem class. It enables users to :
– Choose and compare diverse solver routines ;
– Organize and solve large test problem sets ;
– Select interactively subsets of test problem sets ;
– Perform a statistical analysis of the results, automatically produced as LaTeX and PDF output.
The TEST ENVIRONMENT is free to use for research purposes. It will be published in 2010, cf. [14].

[14] F. Domes, M. Fuchs, and H. Schichl, (2010), The Optimization Test Environment. Submitted.

6.4 SVD-tail : a new linear-sampling reconstruction method for inverse scattering problems

M. Fares : CERFACS, *France* ; **S. Gratton** : ENSEEIHT-IRIT, *France* ; **Ph.L. Toint** : FUNDP-UNIVERSITY OF NAMUR, *Belgium*

A new efficient numerical procedure (SVD-tail) is proposed for the reconstruction of the shape and volume of unknown objects from measurements of their radiation in the far field. At variance with previously published linear-sampling methods where the solution is constructed as a regularized solution of the far-field equations using a variant of the TikhonovMorozov type, the new algorithm uses a new eigenspace recovery technique which exploits the combined presence of error in the operator and of eigenvalue clusters. Its performance on a battery of examples and its comparison with existing methods are shown to be promising. More details can be found in [ALG12]

6.5 A splitting technique for discrete search based on convex relaxation

M. Fuchs : CERFACS, *France* ; **A. Neumaier** : UNIVERSITY OF VIENNA, FACULTY OF MATHEMATICS, *Austria*

In mixed integer programming, branching methods are a powerful and frequently employed tool. This paper presents a branching strategy for the case when the integer constraints are associated with a finite set of points in a possibly multidimensional space. We use the knowledge about this discrete set represented by its minimum spanning tree and find a splitting based on convex relaxation. Typical applications include design optimization problems where design points specifying several discrete choices can be considered as such discrete sets.
This work was presented at the 20th International Symposium of Mathematical Programming (ISMP) 2009 and is accepted for publication in 2010, cf. [15]. Latest developments will be presented at the 81st Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM) 2010 and at Complex Systems Design & Management (CSDM) 2010, cf. [16].

[15] M. Fuchs and A. Neumaier, (2009), A splitting technique for discrete search based on convex relaxation, *Journal of Uncertain Systems, Special Issue on Global Optimization and Intelligent Algorithm*. Accepted.

[16] M. Fuchs and A. Neumaier, (2010), Discrete search in design optimization. Submitted.

6.6 Cloud based design optimization

M. Fuchs : CERFACS, *France*

Cloud based design optimization (CBDO) is an approach to significantly improve robustness and optimality of solutions sought in engineering design. One of the main features is the possibility to capture and model high-dimensional uncertainty information, even in the case that the information available is incomplete or unformalized.

Continuing our past studies we present the graphical user interface for CBDO in this paper. Also we mention the latest improvements of our methods, we give an illustrative example demonstrating how unformalized knowledge can be captured, and we highlight relations to different uncertainty models, such as p-boxes, Dempster-Shafer structures, and α-level optimization for fuzzy sets.

This work has been presented at the International Fuzzy Systems Association World Congress (IFSA) 2009, cf. [ALG61].

6.7 Numerical experience with a recursive trust-region method for multilevel nonlinear optimization

S. Gratton : ENSEEIHT-IRIT, *France* ; **M. Mouffe** : CERFACS, *France* ; **A. Sartenaer** : FUNDP UNIVERSITY OF NAMUR, *Belgium* ; **Ph. Toint** : FUNDP UNIVERSITY OF NAMUR, *Belgium* ; **D. Tomanos** : FUNDP UNIVERSITY OF NAMUR, *Belgium*

We consider an implementation of the recursive multilevel trust-region algorithm proposed by Gratton, Mouffe, Toint, Weber in [ALG18] for bound-constrained nonlinear problems, and provide numerical experience on multilevel test problems. A suitable choice of the algorithm's parameters is identified on these problems, yielding a satisfactory compromise between reliability and efficiency. The resulting default algorithm is then compared to alternative optimization techniques such as mesh refinement and direct solution of the fine-level problem. More details can be found in [ALG58].

6.8 Stopping rules and backward error analysis for bound-constrained optimization

S. Gratton : ENSEEIHT-IRIT, *France* ; **M. Mouffe** : CERFACS, *France* ; **Ph.L. Toint** : FUNDP UNIVERSITY OF NAMUR, *Belgium*

Termination criteria for the iterative solution of bound-constrained optimization problems are examined in the light of backward error analysis. It is shown that the problem of determining a suitable perturbation on the problem's data corresponding to the definition of the backward error is analytically solvable under mild assumptions. Moreover, a link between existing termination criteria and this solution is clarified, indicating that some standard measures of criticality may be interpreted in the sense of backward error analysis. The backward error problem is finally considered from the multicriteria optimization point of view and some numerical illustration is provided. Find more information in [ALG54].

6.9 Multilevel Trust-Region Methods in Nonlinear Optimization

S. Gratton : ENSEEIHT-IRIT, *France* ; **A. Sartenaer** : FUNDP, *Belgium* ; **Ph.L. Toint** : FUNDP, *Belgium*

A class of trust-region methods is presented for solving unconstrained nonlinear and possibly nonconvex discretized optimization problems, like those arising in systems governed by partial differential equations. The algorithms in this class make use of the discretization level as a means of speeding up the computation of the step. This use is recursive, leading to true multilevel/multiscale optimization methods reminiscent of multigrid methods in linear algebra and the solution of partial differential equations. A simple algorithm of the class is then described and its numerical performance is shown to be numerically promising. This observation then motivates a proof of global convergence to first-order stationary points on the fine grid that is valid for all algorithms in the class. More details can be found in [ALG19].

6.10 An observation-space formulation of variational assimilation using a restricted preconditioned conjugate gradient algorithm

S. Gratton : ENSEEIHT-IRIT, *France* ; **J. Tshimanga** : CERFACS, *France*

We consider parameter estimation problems involving a set of m physical observations, where an unknown vector of n parameters is defined as the solution of a nonlinear least-squares problem. We assume that the problem is regularized by a quadratic penalty term. When solution techniques based on successive linearization are considered, as in the incremental four-dimensional variational (4D-Var) techniques for data assimilation, a sequence of linear systems with particular structure has to be solved. We exhibit a subspace of dimension m that contains the solution of these linear systems, and derive a variant of the conjugate gradient algorithm that is more efficient in terms of memory and computational costs than its standard form, when m is smaller than n. The new algorithm, which we call Restricted Preconditioned Conjugate Gradient (RPCG), can be viewed as an alternative to the so-called Physical-space Statistical Analysis System (PSAS) algorithm, which is another approach to solve the linear problem. In addition, we show that the non-monotone and somehow chaotic behaviour of the PSAS algorithm when viewed in the model space, experimentally reported by some authors, can be fully suppressed in RPCG. Moreover, since preconditioning and re-orthogonalization of residuals vectors are often used in practice to accelerate convergence in high-dimensional data assimilation, we show how to reformulate these techniques within subspaces of dimension m in RPCG. Numerical experiments are reported, on an idealized data assimilation system based on the heat equation, that clearly show the effectiveness of our algorithm for large-scale problems. More details can be found in [ALG17].

6.11 Semilocal and global convergence of the Newton-HSS method for systems of nonlinear equations

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Newton-HSS methods, that are variants of inexact Newton methods different from Newton-Krylov methods, have been shown to be competitive methods for solving large sparse systems of nonlinear equations with positive definite Jacobian matrices [17]. In that paper, only local convergence was proved. In this paper, we prove a Kantorovich-type semilocal convergence. Then we introduce Newton-HSS methods with a backtracking strategy and analyse their global convergence. Finally, these globally convergent Newton-

HSS methods are shown to work well on several typical examples using different forcing terms to stop the inner iterations. This work will be described in the forthcoming technical report [18] that has been accepted for publication in Numerical Linear Algebra and its Applications.

[17] Z. Bai and X. Guo, (2010), The Newton-HSS methods for systems of nonlinear equations with positive-definite Jacobian matrices., *Journal of Computational Mathematics*, **28**, 235–260.

[18] X.-P. Guo and I. S. Duff, (2010), Semilocal and global convergence of the Newton-HSS method for systems of nonlinear equations, Tech. Rep. TR/PA/10/14, CERFACS.

6.12 GNSS Networks in Algebraic Graph Theory

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A new approach to the GNSS network is presented. Here, this approach is restricted to the case where the user handles the network data for his or her own objectives : the satellite-clock biases are not estimated. To deal with the general case where some data are missing, the corresponding theoretical framework appeals to some elementary notions of algebraic graph theory. As clarified in the paper, the notion of closure delay (CD) then generalizes that of double difference (DD). The body of the paper is devoted to the implications of this approach in GNSS data processing. One is then led to define local variables, which depend on the successive epochs of the time series, and a global variable which remains the same all over these epochs with, however, possible state transitions from time to time. In the period defined by two successive transitions, the problem to be solved in the least-square sense is governed by a linear equation in which the key matrix has an angular block structure. This structure is well suited to recursive QR factorization. The state transitions included by the variations of the GNSS graph are then handled in an optimal manner. Solving the integer-ambiguity problem via LLL decorrelation techniques is also made easier. At last but not the least, is centralized mode ; this approach particularly well suited to quality control. More information can be found in [ALG22].

6.13 QR Implementation of GNSS Centralized Approaches

A. Lannes : CNRS/LSS, *France* ; **S. Gratton** : ENSEEIHT-IRIT, *France*

When processing times series of global positioning data, one is led to introduce ”local variables,’ which depend on the successive epochs of the time series, and a ’global variable’ which remains the same all over these epochs with however possible state transitions from time to time. For example, the latter occur when some satellites appear or disappear. In the period defined by two successive transitions, the problem to be solved in the least-square sense is governed by a linear equation in which the key matrix has an angular block structure. The structure is well suited to recursive QR factorization. The corresponding techniques prove to be very efficient for GNSS data processing and quality control in real-time kinematics. The main objective of this paper is to show how the QR implementation of GNSS centralized approaches combines the advantages of all the methods developed hitherto in this field. The study is conducted by considering the simple case of continuous observations with a local-scale single baseline. The extension to networks is simply outlined. More information can be found in [ALG23].

6.14 Approximate Gauss-Newton methods for optimal state estimation using reduced-order models

A. S. Lawless : DEPARTMENT OF MATHEMATICS, UNIVERSITY OF READING, *UK*; **N. K. Nichols** : DEPARTMENT OF MATHEMATICS, UNIVERSITY OF READING, *UK*; **C. Boess** : CERFACS, FRANCE AND ZENTRUM FUER TECHNOMATHEMATIK, UNIVERSITAET BREMEN, *Germany*; **A. Bunse-Gerstner** : ZENTRUM FUER TECHNOMATHEMATIK, UNIVERSITAET BREMEN, *Germany*

The Gauss-Newton (GN) method is a well-known iterative technique for solving nonlinear least-squares problems subject to dynamical system constraints. Such problems arise commonly in optimal state estimation where the systems may be stochastic. Variational data assimilation techniques for state estimation in weather, ocean and climate systems currently use approximate GN methods. The GN method solves a sequence of linear least-squares problems subject to linearized system constraints. For very large systems, low-resolution linear approximations to the model dynamics are used to improve the efficiency of the algorithm. We propose a new method for deriving low-order system approximations based on model reduction techniques from control theory. We show how this technique can be combined with the GN method to retain the response of the dynamical system more accurately and improve the performance of the approximate GN method. More details can be found in [ALG24].

6.15 Using Model Reduction Methods within Incremental Four-Dimensional Variational Data Assimilation

A. S. Lawless : DEPARTMENT OF MATHEMATICS, UNIVERSITY OF READING, *UK*; **N. K. Nichols** : DEPARTMENT OF MATHEMATICS, UNIVERSITY OF READING, *UK*; **C. Boess** : CERFACS, FRANCE AND ZENTRUM FUER TECHNOMATHEMATIK, UNIVERSITAET BREMEN, *Germany*; **A. Bunse-Gerstner** : ZENTRUM FUER TECHNOMATHEMATIK, UNIVERSITAET BREMEN, *Germany*

Incremental four-dimensional variational data assimilation is the method of choice in many operational atmosphere and ocean data assimilation systems. It allows the four-dimensional variational data assimilation (4DVAR) to be implemented in a computationally efficient way by replacing the minimization of the full nonlinear 4DVAR cost function with the minimization of a series of simplified cost functions. In practice, these simplified functions are usually derived from a spatial or spectral truncation of the full system being approximated. In this paper, a new method is proposed for deriving the simplified problems in incremental 4DVAR, based on model reduction techniques developed in the field of control theory. It is shown how these techniques can be combined with incremental 4DVAR to give an assimilation method that retains more of the dynamical information of the full system. Numerical experiments using a shallow-water model illustrate the superior performance of model reduction to standard truncation techniques. More details can be found in [ALG25].

6.16 Multilevel optimization in infinity norm and associated stopping criteria

M. Mouffe : CERFACS, *France*

This thesis concerns the study of a multilevel trust-region algorithm in infinity norm, designed for the solution of nonlinear optimization problems of high size, possibly subject to bound-constraints. The multilevel algorithm that we study has been developed on the basis of the algorithm of Gratton, Sartenaer and Toint in [ALG19]. In this work, we look at both theoretical and numerical properties of the new algorithm. In a first part, the main features of the new algorithm are exposed. We then look at several stopping criteria for nonlinear bound-constrained optimization algorithms. In particular we define stopping criteria that are meaningful in terms of backward error analysis. We finally compare numerically our method to competing algorithms in the same field in order to show its remarkable efficiency. More information can be found in [ALG30].

6.17 Limited-memory preconditioners, with application to incremental four-dimensional variational data assimilation

J. Tshimanga : FUNDP, NAMUR, BELGIUM AND CERFACS/SUC URA 1875, *France*; **S. Gratton** : ENSEEIHT-IRIT, *France*; **A. T. Weaver** : CERFACS/SUC URA 1875, *France*; **A. Sartenaer** : FUNDP, NAMUR, *Belgium*

Incremental four-dimensional variational assimilation (4D-Var) is an algorithm that approximately solves a nonlinear minimization problem by solving a sequence of linearized (quadratic) minimization problems of the form $\min_x F[x] = \frac{1}{2}x^T Ax - b^T x + c$, where x is the control vector, A is a symmetric positive-definite matrix, b is a vector containing data and prior information, and c is a constant. This paper proposes a family of limited-memory preconditioners (LMPs) for accelerating the convergence of conjugate-gradient (CG) methods used to solve quadratic minimization problems such as those encountered in incremental 4D-Var. The family is constructed from a set of vectors $\{s_i : i = 1, ..., l\}$, where each s_i is assumed to be conjugate with respect to the (Hessian) matrix A. In incremental 4D-Var, approximate LMPs from this family can be built using conjugate vectors generated during the CG minimization on previous outer iterations. The spectral and quasi-Newton LMPs employed in many operational 4D-Var systems are shown to be special cases of the family of LMPs proposed here. In addition, a new LMP based on Ritz vectors (approximate eigenvectors) is derived. The Ritz LMP can be interpreted as a stabilized version of the spectral LMP. Numerical experiments performed with a realistic global ocean 4D-Var system are presented, to test the impact of the three different preconditioners. The Ritz LMP is shown to be more effective than, or at least as effective as, the spectral and quasi-Newton LMPs in our 4D-Var experiments. Our experiments also demonstrate the importance of limiting the number of CG (inner) iterations on certain outer iterations to avoid possible divergence of the cost function on the outer loop. The optimal number of CG iterations will depend on the specific preconditioner used, and can be computed a priori, albeit at the expense of several evaluations of the cost function on the outer loop. In a cycled 4D-Var system, it may be necessary to perform this computation periodically to account for changes in the Hessian matrix arising from changes in the observing system and background-flow field. More details can be found in [ALG27].

7 Conferences and Seminars

7.1 Conferences, seminars, and meetings attended by members of the Parallel Algorithms Project

February

Gene Around the World. Meeting at University of Oxford, UK. 29 February 2008. I.S. DUFF, After dinner speaker.

March

13th SIAM Conference on Parallel Processing for Scientific Computing, Atlanta, USA. 12–14 March 2008. MARC BABOULIN *Computing the conditioning of dense linear least squares with (Sca)LAPACK*.

13th SIAM Conference on Parallel Processing for Scientific Computing, Atlanta, USA. 12–14 March 2008. BORA UÇAR *Computing a class of bipartite matchings in parallel*, joint work with P. R. Amestoy, I. S. Duff, and D. Ruiz, Contributed talk.

April

Copper Mountain Conference on Iterative Methods, Copper, Colorado, USA. 6-11 April 2008. M.ARIOLI AND I.S. DUFF†, *Using FGMRES to obtain backward stability in mixed precision*, Talk, Workshop Chair, Organizing Committee.

Meeting of ICIAM Board, Vancouver, Canada. 12 April 2008. I.S. DUFF, Member of Board.

May

SIAM Conference on Optimization, Boston, Massachusetts, USA. 10-13 May 2008. M. MOUFFE, *Numerical results with a multilevel trust-region method in infinity norm*, joint work with S. Gratton, A. Sartenaer, Ph.L. Toint and D. Tomanos, Seminar.

SIAM Conference on Optimization, Boston, Massachusetts, USA. 10-13 May 2008. S. GRATTON, *Multi-Secant Equations, Approximate Invariant Subspaces and Multigrid Optimization*, joint work with Ph.L. Toint, Minisymposium Talk.

Meeting at CEA/DEN Grenoble on uncertainties. 27 May 2008. X. VASSEUR, *Partial condition numbers for the linear least squares problems*, joint work with S. Gratton.

June

Householder Symposium XVII, Zeuthen, Germany. 1-6 June 2008. I.S. DUFF, *Practical rank determination for square and rectangular sparse matrices,* Talk.

Householder Symposium XVII, Zeuthen, Germany. 1-6 June 2008. S. GRATTON, *Quasi-Newton formula, matrix nearness problems and preconditioning* , joint work with A. Sartenaer, Ph.L. Toint and J. Tshimanga, Talk.

EAGE Rome 2008 : 70th EAGE Conference & Exhibition incorporating SPE EUROPEC, Rome, Italy. 9-12 June 2008. X. PINEL *Massively parallel computation for the solution of the 3D Helmholtz equation in the frequency domain*, joint work with H. Calandra, I. Duff, S. Gratton and X. Vasseur, Talk.

Numerical Analysis and Its Applications : 4th International Conference, NAA 2008 Lozenetz, Bulgaria. 16-20 June 2008. M. AHMADNASAB *Some Contributions of Homotopic Deviation to the Theory of Matrix Pencils*, joint work with F. Chaitin-Chatelin, Talk.

PMAA'08 - 5th Parallel Matrix Algorithms and Applications, Neuchâtel, Switzerland. 20-22 June 2008. X. PINEL *Solution of three-dimensional Helmholtz equation in the frequency domain, using Krylov methods preconditioned by multigrid*, joint work with H. Calandra, I. Duff, S. Gratton and X. Vasseur, Talk.

PMAA'08 - 5th Parallel Matrix Algorithms and Applications, Neuchatel, Switzerland. 20-22 June 2008. BORA UÇAR *A matrix partitioning interface to PaToH in MATLAB*, joint work with Ü. V. Çatalyürek and C. Aykanat, Contributed talk.

PMAA'08 - 5th Parallel Matrix Algorithms and Applications, Neuchâtel, Switzerland. 20-22 June 2008. A. HAIDAR, *Algebraic preconditioners for parallel hybrid solvers on large 3D problems*, joint work with L. Giraud, S. Pralet, Contributed talk.

VECPAR'08 - 8th International Meeting High Performance Computing for Computational Science, Toulouse, France. 24-27 June 2008. BORA UÇAR *A parallel matrix scaling algorithm*, joint work with P. R. Amestoy, I. S. Duff, and D. Ruiz, Contributed talk.

July

SIAM Annual Meeting, San Diego, USA. 8-16 July 2008. I.S. DUFF, Chairman of the SIAM Board of Trustees.

LMS Durham Symposium on Computational Linear Algebra for Partial Differential Equations, Durham University. 14-24 July 2008. I. DUFF, Invited attendee.

August

PRACE Petascale Summer School, Stockholm, Sweden. 26-29 August 2008. X. PINEL AND X. VASSEUR, participants.

September

CCGSC'08 - Clusters and Computational Grids for Scientific Computing, Flat Rock, NC, USA. 14-17 September 2008. BORA UÇAR *Exact algorithms for a task assignment problem*, joint work with Kamer Kaya, Invited Talk.

Bath-RAL Numerical Analysis Day, University of Bath, England. 23 September 2008. I. DUFF, Attendee.

October

International Workshop on Numerical Analysis and Scientific Computing (NASCom08), Rostov-on-Don, Russia. 13-17 October 2008. I. DUFF, *Exploiting the backward stability of FGMRES,* Keynote talk.

Ninth European Multigrid Conference, Bad Herrenalb, Germany. 20-23 October 2008. X. VASSEUR, *Algebraic and geometric multigrid preconditioners for the solution of Helmholtz problems,* joint work with S. Gratton and X. Pinel, Talk.

8th Mathias Seminar, Workshop organized by TOTAL, Cannes, France. 23-24 October 2008. S. GRATTON *Massively parallel computations for the solution of optimisation problem using multigrid techniques*, joint work with H. Calandra, X. Pinel and X. Vasseur, Invited Talk.

November

Second International Conference on Numerical Algebra and Scientific Computing (NASC08), Beijing, China. 1-5 November 2008. I. DUFF, *Using FGMRES to obtain backward stability in mixed precision*, Keynote talk and co-chair of the meeting. Also on Advisory Board for ANA Prize.

EPSRC Workshop on NA/HPC. Interface between applications and algorithms, Oxford. 5-7 November 2008. I.S. DUFF, co-organizer.

SIAM Board of Trustees, Philadelphia, Pennsylvania, USA. 12-13 December 2008. I.S. DUFF, Chairman of Board.

EPSRC Workshop on NA/HPC. Interface between applications and algorithms, Manchester. 8-9 November 2008. I.S. DUFF, co-organizer.

January

Complex Networks across the Natural and Technological Sciences, University of Strathclyde, Glasgow. 27-30 January 2009. I.S. DUFF[†] AND B. UÇAR, *Combinatorial problems in numerical linear algebra,* Invited speaker.

February

Dagstuhl Seminar on Combinatorial Scientific Computing, Dagstuhl Castle, Germany. 1-6 February 2009. I.S. DUFF[†] AND B. UÇAR, *Combinatorial problems in numerical linear algebra,* Invited plenary talk.

Seminar on Numerical Analysis and Winter School SNA'09, Ostrava, Czech Republic. 2-6 February 2009. P. JIRÁNEK, *On a stable variant of Simpler GMRES and GCR*, joint work with M. Rozložník, contributed talk.

Winter school "New trends in scientific computing", CIRM, Marseille, France. 9-13 February 2009. P. JIRÁNEK, *A posteriori error estimates and stopping criteria for iterative solvers,* joint work with Z. Strakoš and M. Vohralík, poster.

March

SIAM Conference on Computational Science and Engineering (CSE09) Miami, Florida, USA. 2-6 March 2009 P. AVERY, *The FETI Family of Domain Decomposition Methods for Inequality Constrained Quadratic Programming : Application to Contact Problems,* Minisymposium talk.

Fourth International Conference on High Performance Scientific Computing. Modeling, Simulation and Optimization of Complex Processes, Hanoi, Vietnam. 2-6 March 2009. I.S. DUFF, *The solution of really large sparse linear equations from three-dimensional modelling,* Keynote talk.

SIAM Conference on Computational Science & Engineering (CSE09), Miami, Florida, USA. 2-6 March 2009. I.S. DUFF, *Preconditioning Techniques,* Minisymposium co-organizer with Sherry Li.

Center of Computational Mathematics colloquium (UCD), Denver, USA. 19 March 2009. X. PINEL *Theoretical and experimental analysis of a perturbed two-grid preconditioner for indefinite Helmholtz problems*, joint work with H. Calandra, S. Gratton and X. Vasseur, Invited Talk.

Copper09 : Fourteenth Copper Mountain conference on multigrid methods, Copper Mountain, USA. 22-27 March 2009. X. PINEL *Theoretical and experimental analysis of a perturbed two-grid preconditioner for indefinite Helmholtz problems*, joint work with H. Calandra, S. Gratton and X. Vasseur, Talk.

CEA-EDF-INRIA school : Methods and algorithms for solving large algebraic systems on modern high performance computing systems, Centre de recherche INRIA Sophia-Antipolis-Méditerranée, 30 March - 3 April 2009. I.S. DUFF, Invited lecturer.

April

Numerical Analysis Seminar, CWI Amsterdam, The Netherlands. 6 April 2009. X. VASSEUR, *A two-grid method used as a preconditioner for the solution of Helmholtz problems,* joint work with S. Gratton and X. Pinel, Invited Seminar.

Department of Mathematics, TU Delft, The Netherlands. 8 April 2009. X. VASSEUR, *Massively parallel computations for the solution of Helmholtz problems in geophysics,* joint work with H. Calandra, S. Gratton and X. Pinel, Invited Seminar.

EDF/CERFACS Seminar on HPC and Numerical Linear Algebra, EDF Clamart, Paris. 19-30 April 2009. P. AVERY, S. GRATTON AND X. VASSEUR, two days of lecture, seminar jointly organized with O. Boiteau and J.P. Argaud (EDF).

May

Optimization Days, Montreal, Canada. 4-6 May 2009. M. MOUFFE, *Multilevel trust-region method in infinity-norm for bound-constrained optimization*, joint work with S. Gratton and Ph. Toint, Seminar.

Meeting on sparse solvers, TOTAL, Paris. 18 May 2009. X. VASSEUR, *Overview on MUMPS.*, invited talk.

Meeting of ICIAM Board, Oslo, Norway. 21 May 2009. I.S. DUFF, Member of Board.

June

The 2nd International Conference on Mathematical Modelling and Computation and The 5th East Asia SIAM Conference, Universiti Brunei Darussalam, Brunei. 8-13 June 2009. I. DUFF, *Solving very large sparse linear equations from three-dimensional modelling*, Keynote talk.

23rd Biennial Conference on Numerical Analysis, University of Strathclyde, Glasgow. 23-26 June 2009. I. DUFF, *Exploiting sparsity in the solution phase for large sparse systems*, Talk.

The 4th IMACS Conference on Mathematical Modelling and Computational Methods in Applied Sciences and Engineering Modelling 2009, Rožnov pod Radhoštěm, Czech Republic. 22-26 June 2009. P. JIRÁNEK, *A posteriori error estimates and stopping criteria for iterative solvers*, joint work with Z. Strakoš and M. Vohralík, contributed talk.

ENUMATH 2009, Uppsala, Sweden. 29 June - 3 July 2009. P. JIRÁNEK, *A posteriori error estimates and stopping criteria for iterative solvers*, joint work with Z. Strakoš and M. Vohralík, contributed talk.

July

SIAM Annual Meeting, Denver, USA. 8-16 July 2009. I.S. DUFF, Chairman of the SIAM Board of Trustees.

Sparse Matrices for Scientific Computation : In Honour of John Reid's 70th Birthday, The Cosener's House, Abingdon. 15-16 July 2009. I. DUFF, *Multifrontal methods*, Invited talk

International Fuzzy Systems Association World Congress (IFSA), Lisbon, Portugal. 20-24 July 2009. M. FUCHS,*Cloud based design optimization*, Contributed Talk.

Joint Assembly on meteorologic, oceanic and cryospheric sciences (MOCA), Montreal, Canada. 19-29 July 2009. J. TSHIMANGA ILUNGA *A Reduced Dimension Conjugate Gradient-like Method for Data Assimilation Problems*, Contributed Talk.

August

20th International Symposium of Mathematical Programming (ISMP), Chicago, Illinois, USA. 23-28 August 2009. S. GRATTON, *Stopping Criteria for Bound-constrained Optimization Problems*, Contributed talk.

20th International Symposium of Mathematical Programming (ISMP), Chicago, Illinois, USA. 23-28 August 2009. M. FUCHS, *Design Optimization Under Uncertainty Using Clouds*, Contributed Talk.

20th International Symposium of Mathematical Programming (ISMP), Chicago, Illinois, USA. 23-28 August 2009. A. TROELTZSCH, Attendant.

September

The 8th International Conference on Parallel Processing and Applied Mathematics (PPAM 2009), Wroclaw, Poland. 13-16 September 2009. I. DUFF, *Solving large sparse linear equations from discretizations of three-dimensional PDEs*, Keynote talk.

BFG09 14th Belgian-French-German Conference on Optimization, Special Topic : Optimization in Engineering, Leuven, Belgium. 14-18 September 2009. J. TSHIMANGA ILUNGA *An observation-space formulation of variational assimilation using a restricted preconditioned conjugate gradient algorithm*, Invited minisymposium talk.

BFG09 14th Belgian-French-German Conference on Optimization, Special Topic : Optimization in Engineering, Leuven, Belgium. 14-18 September 2009. A. TROELTZSCH *Experiments on a self-correcting geometry technique for derivative free unconstrained optimization*, joint work with S. Gratton and Ph.L. Toint, Invited minisymposium talk.

Eighth Bath-RAL Numerical Analysis Day, Rutherford Appleton Laboratory, Oxfordshire. 29 September 2009. P. AMESTOY, I. DUFF†, M. SLAVOVA, AND B. UÇAR, *Exploiting sparsity in the solution phase for large sparse equations,* Invited speaker.

October

9th Mathias Seminar, Workshop organized by TOTAL, Cannes, France. 15-16 October 2009. X. PINEL *Perturbed two-level preconditioner for the solution of three-dimensional Helmholtz problems in the frequency domain*, joint work with H. Calandra, S. Gratton and X. Vasseur, Invited Talk.

SIAM Conference on Applied Linear Algebra, Monterey, California, USA. 26-29 October 2009. I. DUFF, *Hybrid techniques in the solution of large scale problems,* Invited minisymposium talk.

SIAM Conference on Applied Linear Algebra, Monterey, California, USA. 26-29 October 2009. I. DUFF, *Development and history of sparse direct methods,* Invited minisymposium talk.

SIAM Conference on Applied Linear Algebra, Monterey, California, USA. 26-29 October 2009. I. DUFF, *Role of linear algebra in industrial applications,* Invited panel member.

SIAM Conference on Applied Linear Algebra, Monterey, California, USA. 26-29 October 2009. P. JIRÁNEK, *On a stable variant of Simpler GMRES and GCR*, joint work with M. Rozložník, contributed talk.

November

Sparse Day at Lawrence Berkeley National Lab, Berkeley, California, USA. 2 November 2009. P. AMESTOY, I. DUFF†, M. SLAVOVA, B. UÇAR, AND F.-H. ROUET, *Exploiting sparsity in the solution phase for large sparse equations,* Invited speaker.

December

SIAM Board of Trustees, Philadelphia, Pennsylvania, USA. 12-13 December, 2009. I.S. DUFF, Chairman of Board.

† Indicates the speaker in multiply authored presentations.

7.2 Conferences and seminars organized by the Parallel Algorithms Project

January

ANR SOLSTICE project meeting, 29-30 January 2008 at CERFACS, Toulouse, France.

February

Gene around the world at CERFACS 2009 February 2008 at CERFACS, Toulouse, France.

June

Sparse Days Meeting at CERFACS 23-24 June 2008 at CERFACS, Toulouse, France.

June

Sparse Days Meeting at CERFACS 18-19 June 2009 at CERFACS, Toulouse, France.

7.3 Internal seminars organized within the Parallel Algorithms Project

February

Parallel Computing for General Purpose Optimisation and New Generation HPC Architectures., February 20, 2008. C. TADONKI.

April

On the multiscale simulations by mixed finite element method in thermoelasticity., April 18, 2008. D. MIJUCA.

May

Eigenvalue spectrum of twisted mass lattice QCD., May 15, 2008. I. HAILPERIN.
Block S-Step Krylov Iterative Methods., May 22, 2008. A. CHRONOPOULOS.

June

On the parallel scalability of hybrid linear solvers for large 3D problems., June 23, 2008. Ph.D. thesis defence. A. HAIDAR.

July

On the numerical behaviour of Simpler GMRES and GCR., July 31, 2008. P. JIRANEK.

August

Multi-Secant Equations, Approximate Invariant Subspaces and Multigrid Optimization., August 3, 2008. V. MALMEDY.

December

Robust design optimization via potential clouds., December 16, 2008. M. FUCHS.
Auctions for Distributed (and Possibly Parallel) Matchings., December 17, 2008. J. RIEDY.
Hybrid method for solving highly-indefinite linear systems of equations., December 17, 2008. I. YAMAZAKI.

January

Incorporating Minimum Frobenius Norm Models in Direct Search.., January 9, 2009. L. VICENTE.
Optimal antireflective preconditioners for signal and image deblurring., January 20, 2009. P. BOITO.
A posteriori error estimates and stopping criteria for iterative solvers., January 20, 2009. P. JIRANEK.

February

Multilevel optimization in infinity norm and associated stopping criteria., February 10, 2009. Ph.D. thesis defence. M. MOUFFE.

April

Parallel multifrontal solution of large sparse linear systems in an out-of-core environment., April 28, 2009. Ph.D. thesis defence. T. SLAVOVA.

May

Core problem theory in linear approximation problems., May 28, 2009. Z. STRAKOS.
Domain decomposition and FETI-DP : an introduction with applications., May 28, 2009. P. AVERY.

July

Translation and modern Interpretation of thirteen pages of Laplace's 1820 treatise., July 30, 2009. J. LANGOU.

November

Solution of sparse linear systems of equations for electrical engineering : the case study of FLUX software., November 18, 2009. C. DOUCET.

December

Solving Knapsack problems on GPU., December 17, 2009. V. BOYER.

8 Publications

8.1 Journal Publications

[ALG1] P. Amestoy, I. Duff, A. Guermouche, and T. Slavova, (2009), Analysis of the solution phase of a parallel multifrontal approach, *Parallel Computing*. DOI : 10.1016/j.parco.2009.06.001.

[ALG2] M. Arioli and I. S. Duff, (2008), Using FGMRES to obtain backward stability in mixed precision, *Electronic Transactions on Numerical Analysis*, **33**. Special issue commemorating 60th anniversary of Gérard Meurant.

[ALG3] P. Avery and C. Farhat, (2009), The FETI Family of Domain Decomposition Methods for Inequality-Constrained Quadratic Programming : Application to Contact Problems with Conforming and Nonconforming Interfaces, *Computer Methods in Applied Mechanics and Engineering*, **198**, 1673–1683.

[ALG4] P. Avery, C. Farhat, and U. Hetmaniuk, (2009), A Padé-based factorization-free algorithm for identifying the eigenvalues missed by a generalized symmetric eigensolver, *Int. J. Numer. Methods. Eng.*, **79**, 239–252.

[ALG5] C. Aykanat, B. B. Cambazoglu, and B. Ucar, (2008), Multi-level direct K-way hypergraph partitioning with multiple constraints and fixed vertices, *Journal of Parallel and Distributed Computing*, **68**, 609–625.

[ALG6] M. Baboulin and S. Gratton, (2009), Using dual techniques to derive componentwise and mixed condition numbers for a linear functional of a linear least squares solution., *BIT*, **49**, 3–19.

[ALG7] M. Baboulin, J. Dongarra, S. Gratton, and J. Langou, (2009), Computing the Conditioning of the Components of a Linear Least Squares Solution, *Numerical Linear Algebra with Applications*, **16**, 517–533.

[ALG8] M. Baboulin, L. Giraud, S. Gratton, and J. Langou, (2009), Parallel tools for solving incremental dense least squares problems : application to space geodesy, *Journal of Algorithms and Computational Technology*, **3**, 117–133.

[ALG9] Z.-Z. Bai, I. S. Duff, and J.-F. Yin, (2009), Numerical study on incomplete orthogonal factorization preconditioners, *J. Computational and Applied Mathematics*, **226**, 22–41.

[ALG10] I. S. Duff and D. Mijuca, (2009), On accurate and time efficient solution of primal-mixed finite-element equations in multiscale solid mechanics, *Communications in Numerical Methods in Engineering*. DOI : 10.1002/cnm.1296.

[ALG11] I. S. Duff, (2009), The design and use of a sparse direct solver for skew symmetric matrices, *J. Computational and Applied Mathematics*, **226**, 50–54.

[ALG12] M. B. Fares, S. Gratton, and P. L. Toint, (2009), SVD-tail : a new linear-sampling reconstruction method for inverse scattering problems,, *Inverse Problems*, **25**, 095013.

[ALG13] V. Frayssé, L. Giraud, and S. Gratton, (2008), Algorithm 881 : A Set of Flexible GMRES Routines for Real and Complex Arithmetics on High-Performance Computers, *ACM Trans. Math. Softw.*, **35**, 1–12.

[ALG14] A. E. Ghazi, S. Hajji, L. Giraud, and S. Gratton, (2008), Newton's method for the common eigenvector problem, *Journal of Computational and Applied Mathematics*, **219-2**, 398–407.

[ALG15] L. Giraud and A. Haidar, (2009), Parallel algebraic hybrid solvers for large 3D convection-diffusion problems, *Numerical Algorithms*, **51**, 151–177.

[ALG16] L. Giraud, A. Haidar, and L. T. Watson, (2008), Parallel scalability study of hybrid preconditioners in three dimensions, *Parallel Computing*, **34**, 363–379.

[ALG17] S. Gratton and J. Tshimanga, (2009), An observation-space formulation of variational assimilation using a restricted preconditioned conjugate gradient algorithm, *Quarterly Journal of the Royal Meteorological Society*, **135**, 1573–1585.

[ALG18] S. Gratton, M. Mouffe, P. Toint, and M. Weber-Mendonca, (2008), A recursive l_∞ trust-region method for bound-constrained nonlinear optimization, *IMA J Numer Anal*, **28**, 827–861.

[ALG19] S. Gratton, A. Sartenaer, and P. L. Toint, (2008), Recursive Trust-Region Methods for Multiscale Nonlinear Optimization, *SIAM Journal on Optimization*, **19**, 414–444.

[ALG20] P. Jiranek and M. Rozloznik, (2009), Adaptive version of Simpler GMRES, *Numerical Algorithms*, **53**, 93–112.

[ALG21] P. Jiránek, M. Rozložník, and M. H. Gutknecht, (2008), How to make Simpler GMRES and GCR more stable, *SIAM J. Matrix Analysis and Applications*, **30**, 1483–1499.

[ALG22] A. Lannes and S. Gratton, (2009), GNSS Networks in Algebraic Graph Theory, *Journal of Global Positioning Systems*, **8**, 1–23.

[ALG23] A. Lannes and S. Gratton, (2009), QR Implementation of GNSS Centralized Approaches, *Journal of Global Positioning Systems*, **7**, 133–147.

[ALG24] A. S. Lawless, N. K. Nichols, C. Boess, and A. Bunse-Gerstner, (2008), Approximate Gauss-Newton methods for optimal state estimation using reduced order models, *Int. J. Numer. Methods in Fluids*, **56**, 1367–1373.

[ALG25] A. S. Lawless, N. K. Nichols, C. Boess, and A. Bunse-Gerstner, (2008), Using model reduction methods within incremental four-dimensional variational data assimilation, *Monthly Weather Review*, **136**, 1511–1522.

[ALG26] A. Trefethen, N. Higham, I. Duff, and P. V. Coveney, (2009), Developing a high- performance computing/numerical analysis roadmap, *Int. J. of High Performance Computing Applications*, **23**, 423–426.

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8.2 Theses

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2

Data Assimilation

1 Introduction

As for most of CERFACS activities, the data assimilation activities are balanced between software development and scientific research, and involve close collaboration with external groups. This is the case for the ocean data assimilation activities which are centred on the development of NEMOVAR. Initiated ten years ago to accompany the first steps of MERCATOR-Océan, this activity has been strongly reinforced, during the last five years, through collaboration with ECMWF, the Met Office, and INRIA/LJK.

In the case of the atmospheric chemical data assimilation activities, the PALM software, originally built for the MERCATOR Ocean data assimilation system, has been used as a collaborative tool between several laboratories involved in the field. The collaboration with CNRM and ECMWF, among others, has led to significant progress with the development of the MOCAGE-PALM system that now assimilates data from numerous different satellites. Beyond the development of these assimilation suites, CERFACS is now a recognized scientific actor of the field .

The expertise of CERFACS in more than one field of data assimilation, its skills in the development of generic tools and the interest of its partners, has motivated data assimilation activities in other domains for which numerical modelling plays an important role. This is the case of nuclear core modelling which combines neutronics and thermo-hydraulics and for which a tight collaboration with EDF/R&D exists. Noticeable activities in hydrology through collaboration with CNRM or SCHAPI are to be mentioned. The scientific maturation of these more recent activities has not yet reached the level of the two previous ones.

2 Data assimilation for oceanography

The ocean data assimilation activities have been aimed at furthering the scientific and technical development of a variational assimilation system for the OPA model. For the past two years, the activities have covered developments to physical and numerical aspects of the assimilation system, applications of the assimilation system to global ocean reanalysis, and the development of a new variational data assimilation system for OPA to fit within the framework of NEMO. A summary of the main results obtained during the period 2008–2009 is given below.

2.1 Correlation modelling using an implicit diffusion equation diffusion (I. Mirouze, A. Weaver)

An important aspect of background-error covariance modelling is the design of a spatial correlation model. Application of the correlation model must be computationally efficient for problems of large dimension. In addition, the correlation model should be sufficiently general to allow for the representation of inhomogeneous and anisotropic correlation functions. Several papers discuss the theoretical basis for employing a diffusion equation to represent the action of an inhomogeneous and anisotropic correlation operator. Extending these early works, an alternative 3D correlation operator has been developed as part of the PhD thesis of I. Mirouze. The new operator is formulated as a symmetric product of 1D implicit diffusion operators. The implicit formulation has several advantages over a previous formulation based on an explicit diffusion algorithm, the most important being the ability to reduce significantly the number of diffusion iterations particularly at high resolution and with inhomogeneous and anisotropic versions of the diffusion algorithm. A novel technique has also been developed to estimate economically the normalization coefficients required to compute unit-amplitude (correlation) functions from the diffusion algorithm. These new developments are described in a recently submitted article by [DA29].

2.2 Ensemble estimation of background-error covariances (N. Daget, A. Weaver)

The background-error covariance model requires the specification of several parameters such as location-dependent variances and length scales. A procedure for estimating the covariance parameters using ensembles of ocean analyses and forecasts was developed as part of the PhD thesis of N. Daget ([DA12]). The method is based on the assumption that the covariance matrix estimated from a sample of ensemble analysis/forecast states is a good approximation to the true error covariance matrix of the analysis/forecast. In our approach, ensembles of 3D-Var ocean analyses and model forecasts were generated by randomly perturbing surface forcing fields (windstress, precipitation) and the observations used for assimilation (sea surface temperature, temperature and salinity profiles). The ensemble-generation procedure is similar to the Monte Carlo step of the Ensemble Kalman Filter. [DA3] studied the impact of two flow-dependent background-error variance formulations on the quality of global ocean analyses. One formulation was based on a simple, parameterized scheme, while the other formulation employed variances estimated from the ensemble. The ensemble estimates were shown to lead to better balanced analyses and to improvements in fields not directly constrained by the assimilated data, such as zonal velocities in the equatorial Pacific. Deficiencies in the ensemble method were also identified, such as an underestimation in the ensemble spread, and thus points to the need to improve aspects of the ensemble-generation procedure.

2.3 Global ocean reanalysis (A. Weaver, N. Daget, P. Rogel)

As described above, the ensemble system was used for improving the estimates of the background-error covariances. In the ENSEMBLES project, the ensemble system was used for providing samples of initial conditions for probabilistic seasonal and decadal forecasts with coupled models at CERFACS and Météo-France ([DA11]). The ocean reanalyses generated by CERFACS for ENSEMBLES have also been used by different groups for climate diagnostics and intercomparison studies (e.g., [DA5]). Figure 2.1 shows a multi-decadal time-series of global heat anomalies computed from the CERFACS ensemble 3D-Var reanalysis. The increase in decadal variability compared to a reanalysis without data assimilation is a striking feature in this figure. Various results from diagnostic studies which include the CERFACS reanalyses were presented in a series of white papers at the international OceanObs'09 conference ([DA21, DA15, DA16]). The CERFACS ocean reanalysis data-set produced for ENSEMBLES is publicly available through an OPeNDAP Server at ECMWF. (http ://www.ecmwf.int/research/EU_projects/ENSEMBLES/data/data_dissemination.html).

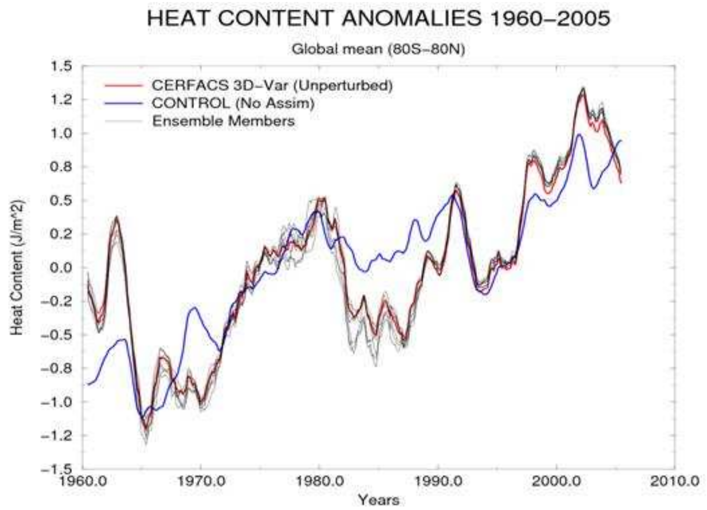

FIG. 2.1: Multi-decadal time-series of global ocean heat content anomalies averaged over the upper 300 meters. Shown are the control (no assimilation) experiment (blue curve), and the 3D-Var reanalyses from the unperturbed (red curve) and eight perturbed experiments (black curves).

2.4 Development of NEMOVAR (A. Weaver, I. Mirouze, A. Piacentini)

A collaborative project was initiated between CERFACS and ECMWF to develop a variational assimilation system for NEMO. The new system is called NEMOVAR ([DA19]). Since the project's initiation, the Met Office and researchers from INRIA/JLK have joined the project. The consolidation of a large part of European ocean modelling activities around NEMO was a key factor in deciding to develop NEMOVAR. NEMOVAR has inherited the basic algorithmic structure of the OPAVAR system developed at CERFACS for NEMOVAR's predecessor OPA8.2. The current version of NEMOVAR employs a close variant of the multivariate 3D-Var (FGAT) method of [1]. Initial experimentation has focused on the use of delayed-mode temperature and salinity profiles from the ENACT/ENSEMBLES data-set and a 1° global configuration. Other data-types have been incorporated (altimeter, SST, TAO currents, sea-ice concentration) but have not been tested yet in assimilation mode. Multi-decadal 3D-Var experiments with NEMOVAR show significant improvements over experiments produced without assimilating data. NEMOVAR is not yet as mature as OPAVAR in terms of algorithmic options and scientific assessment, but is already a significant improvement over OPAVAR in terms of computer performance, code structure, and its capacity to run with different global resolutions and to use real-time data-sets. In France, NEMOVAR research and development has been supported by ANR-COSINUS (VODA project), LEFE-ASSIM, CNES-TOSCA and the GMMC.

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3 Data assimilation for atmospheric chemistry

The assimilation of minor atmospheric trace species is a very promising technique to obtain global and regional datasets for the monitoring and the forecasting of the atmospheric composition. The challenge lies in the optimal combination of measurements having very different resolutions in space and time, with for examples in-situ data from ground-based stations, aircrafts, low Earth orbiting and geosynchronous satellite measurements. Obtaining datasets that combine in an optimal manner all those types of data is a necessity for the validation of 3D predictive chemical models and the GMES program of the European Union and ESA. All the measurement types must be combined within the models in an optimal manner using data assimilation techniques. For several years, we used at CERFACS the MOCAGE-PALM data assimilation suite. MOCAGE-PALM is developed at CERFACS, in close collaboration with the Météo-France/CNRM, since the beginning of the EC-FP5 ASSET European project in January 2003. In 2005, the system was proposed as a common collaborative tool for the whole community involves in the ADOMOCA project of the PNCA (latter replaced by the LEFE program). We had therefore added a lot of flexibility to MOCAGE-PALM, so it could satisfies the different applications of the ADOMOCA project.
In parallel of the development work, we have improved the MOCAGE-PALM system in order to increase its quality. The most noticeable improvement came from the work on the characterization of the forecast error. This work was conducted in synergy with CERFACS assimilation studies in the area of oceanography. To improve the analyses, several other ways were explored : four dimensional assimilation method, a re-linearization iterative process and a control in the spectral space. Moreover, we have developed linear chemical scheme for other species than ozone that prove to be very computationally efficient for data assimilation.
Recently, the assimilation system was made independent to the MOCAGE model in order to apply the assimilation suite to any other chemistry-transport model. The assimilation part, still developed under the PALM framework, was renamed Valentina. Nowadays, the Valentina system could work with various geometries of the CTM (regular or Gaussian global grid, various vertical grids and resolution), at different resolutions. Moreover, Valentina can now work with regional CTMs.

3.1 Improvement of the assimilation system

3.1.1 Horizontal correlation of the forecast errors (S. Massart, A. Piacentini)

From the beginning of the assimilation system development, the horizontal correlations of the forecast errors were modelled using a diffusion equation on the sphere. But the original finite difference-time explicit implementation of the diffusion equation solver could not treat the polar regions on a rectangular longitude-latitude grid. As a consequence, the observations beyond $80°$ latitude were not assimilated. As this was a major restriction because it prevented the detailed study of the ozone evolution within the polar latitudes, a formulation was developed by projecting the horizontal fields for each pressure level onto the spherical harmonic basis. The diffusion equation was then solved in this basis, and projected back to the physical space. This fast numerical approach for modelling the horizontal correlations of the forecast errors allowed to assimilate all the available observations. But this approach implies a homogeneous length scale for the correlations. Studies based on an ensemble of assimilations showed us that in the stratosphere, the length

scales for the ozone forecast errors are strongly heterogeneous [DA7, DA17]. To be able to represent such heterogeneities in the correlations, we modelled them still using a diffusion equation but solved by a finite difference-time implicit scheme. Such a scheme allows to treat not only the whole sphere domain but also limited area regional domains (cf. 3.1.6). As a drawback, it requires to invert a huge size matrix. The inversion was thus realized with the MUMPS parallel solver. As this solver was not efficient on the Météo-France NEC vector supercomputers, a preconditioned GMRES iterative solver was also implement.
At the present time, the Valentina assimilation software disposes of two options for specifying the length scales of the horizontal correlations of the forecast errors. For homogeneous length scales, the solver is based on the spherical harmonic basis. For heterogeneous length scales, the solver is based on a finite difference-time implicit scheme and the user has to provide the estimated length scales in a NetCDF file.

3.1.2 Vertical correlation of the forecast errors (S. Massart, A. Piacentini)

In a similar way to the modelling of the horizontal correlations of the forecast errors, the vertical correlation were modelled using a diffusion equation. In fact, the previous formulation of the vertical correlations did not produced the desired shape for heterogeneous length scales. Contrary to the horizontal correlations, the vertical ones presents boundaries both on the ground and at the top of the model. In this particular case, the difficulty is to well specify the boundary conditions of the diffusion equation to ensure correlation functions. As proposed by the PhD work of Isabelle Mirouze [DA18], we solved this matter by combining Neumann and Dirichlet boundary conditions. The advantage of such an approach is to build correlation functions with an heterogeneous length scale. But this requires the computation of the square root of a number of small matrices equal to the number of grid points for each assimilation window. As for the horizontal modelling, the computation of the vertical correlation, based on the calculation of the square root of matrices, is more efficient on scalar computers than on vector processors.

3.1.3 Resurrection of the 4D-Var for the advection part (S. Massart, A. Piacentini)

Since the first release and till recently, the only assimilation method implemented in the Valentina assimilation system was 3D-FGAT. This hybrid assimilation method was selected because it is more precise than a classical 3D-Var and does not require the adjoint of the model as 4D-Var. Few tests were performed several years ago to diagnose the benefit of using a 4D-Var scheme. The diagnosis revealed that the benefit was low compared to the required computational time. The project of implementing a full 4D-Var to Valentina was thus postponed.
Recently, in a situation driven by dynamical effects, the 3D-FGAT has shown its limits. In order to overcome these limitations, we have reconsidered the choice of using a 4D-Var scheme. The adjoint of the transport layer of MOCAGE was thus developed under the constrain of saving computational time. Running on scalar computers, the 4D-Var computational cost is similar to the 3D-FGAT one using two 12h–assimilation windows for the 4D-Var instead of eight 3h–windows for the 3D-FGAT. But on the Météo-France NEC computer, the 4D-Var computational cost is extremely expensive and it optimization is still in progress.
As the 4D-Var analysis provided better results than 3D-FGAT on specific tests, the 4D-Var was experimented on a real situation. The Microwave Limb Sounder (MLS) ozone profiles were analyzed during the whole 2008 year with the 4D-Var, providing good quality ozone fields compared to independent data (cf. 3.3.2). Due to this pretty good behaviour of the 4D-Var, it will be part of the future releases of Valentina provided that it can be optimized on vector machines.

3.1.4 Spectral control to increase the horizontal resolution (B. Pajot, S. Massart, A. Piacentini)

Most of the new datasets from the last generation of spacecraft instruments have higher spatial resolutions than the standard horizontal resolution (about 250 km) of the MOCAGE model in its global configuration.

In particular, the IASI data have a pixel size of 12 km. To assimilate these new datasets, the observations have to be averaged toward the model grid, which results in a significant loss of information. The model resolution can of course be increased to avoid this, but this will significantly increase the numerical cost (in terms of memory and computational time) of the assimilation process. Rather, we are developing a multi-scale assimilation strategy in the spectral space. The assimilation process will be first performed at the T42 truncation (64 points of discretization for the latitude), thus capturing the largest structures of the fields, followed by two successive optimizations at the T85 truncation (128 points) and T170 truncation (256 points).
First of all, we adapted MOCAGE and Valentina to be able to take into account the three target truncations. Preliminary assimilation results obtained at each truncation are encouraging and are promising for the multi-scale strategy to come ([4]).

3.1.5 Development of linear chemistry schemes (D. Cariolle, *et al.*)

During those past years a linerized ozone photochemical scheme has been developed for use within GCMs and CTMs [2]. This scheme is widely used for climate simulations and data assimilation studies. The computational cost of this scheme is very low since it only requires an additional continuity equation to be solved in the large scale models. We have therefore extended the methodology to treat other chemical species, in particular a linerized scheme has been derived for CO and used within the MOCAGE model to assimilate the CO data from the MLS and MOPIT satellite instruments. The results show the ability of the scheme to capture the essential features of the CO distribution. An article summarizing those results has been published in Atmospheric Chemistry and Physic Discussion [3].

3.1.6 Limited area analysis (A. Piacentini)

Up to now, the Valentina assimilation system has been involved in programs dealing with the global atmospheric chemical composition, from the upper troposphere to the lower mesosphere. The system has been recently extended to produce chemical analyses on a limited area when it is coupled with a regional version of MOCAGE. Those developments occurred in the framework of the FP7 collaborative MACC project, and the POGEQA (RTRA/STAE) national project. Both project address the monitoring of air quality.
The MOCAGE model has the advantage of offering the possibility to work on four nested domains, from the global scale to the regional scale. Working with the regional domain is essential for the modelling of air quality in order to have a sufficient horizontal resolution. For computational reasons it is not possible to increase the resolution of the global domain up to scales useful for air quality studies. On the other hand, simulations within regional domains require boundary conditions that must be provided from the simulations on the global domain. As a consequence, the data assimilation techniques have to be used on the two domains. The Valentina system can now provide separate assimilations for the global and regional domains. The global assimilation has already been evaluated in numerous studies. The regional assimilation is currently evaluated on two types of data : in-situ surface measurements and measurements from geostationary satellites.

3.2 Improvement of the methodology

3.2.1 Using ensemble forecasts to diagnose forecast errors (S. Massart)

As the covariance matrix of the forecast errors is a key point for the quality of the Valentina analysis, a special effort has been devoted to better specify it. Among the different possible techniques, the one based on an ensemble of perturbed forecasts was selected. The key idea of this technique is to run in parallel an ensemble of assimilations of the same set of observations (same time, same location) but having values randomly perturbed with a Gaussian distribution. Statistics on the ensemble forecasts from the ensemble analyses allows to diagnose both variances and correlations of the forecast errors.

This methodology was applied to the July 2003 Michelson Interferometric Passive Atmosphere Sounder (MIPAS) ozone data [DA7]. The aim was to diagnose length-scales associated with the horizontal correlations of the forecast errors. It was then applied to the MLS ozone profiles during the winter 2007 [DA6, DA28]. The aim was there to diagnose the standard deviation (square root of the variance) of the forecast errors and the length-scale associated with the vertical correlation (Fig. 3.1). At least, we explored how important is to use diagnosed background errors covariance for the atmospheric ozone analysis [DA17, DA28].

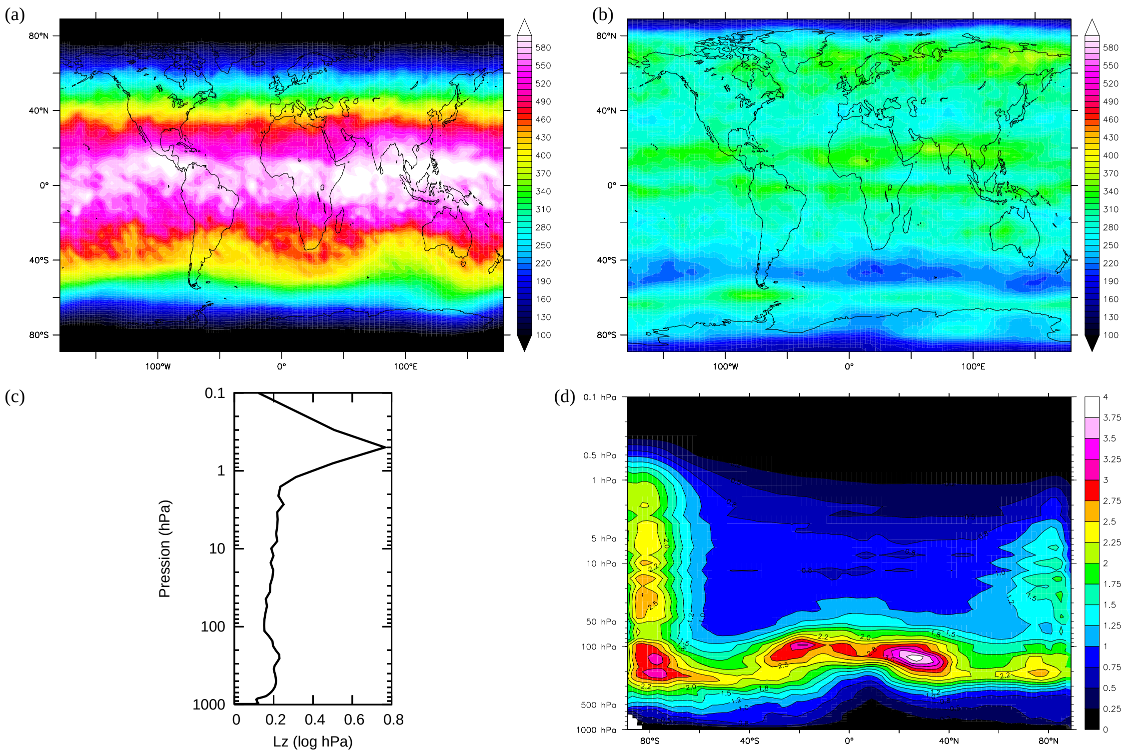

FIG. 3.1: Example of diagnosed covariance of the ozone forecast errors for the winter 2007. (a) Stratospheric zonal length scales (in km) of the horizontal correlations. (b) Stratospheric meridional length scales (in km). (c) Length scales (in log(hPa)) of the vertical correlations. (d) Zonal average of the standard deviation (in %.) of the ozone forecast errors.

3.2.2 The outer loop (B. Pajot, A. Piacentini, S. Massart)

When planning to carry on a re-analysis of the chemical composition of the atmosphere, it is of uttermost importance to find a trade off between accuracy and overall computing time. As 3D-FGAT appears to be an attractive compromise, it was choosen from the very beginning to be implemented in our Valentina assimilation system. To reduce the deficiencies of this approach with respect to the full featured 4D-Var, the iterative process known as the outer loop can be used in conjunction with 3D-FGAT. As the use of an outer loop within a 3D-FGAT has been rarely reported, we planned to include this feature in Valentina to test it. While analysing the MLS ozone profiles during the winter 2007, we found that the 3D-FGAT with the outer loop produced sometimes an overestimation of the ozone increment. To explore this phenomenon, some experiments were performed with a one-dimensional advection model of a passive tracer. By several representative situations, experiments showed the benefits of the outer loop, except for practical situations driven by very rapid dynamics [DA27]. This results explained the overestimation encounter while assimilating the MLS data within Valentina as the overestimation appeared in regions where the wind speed was high compared to the time length of the assimilation window.

3.3 Studies based on the Valentina assimilation system

3.3.1 The assimilation of IASI ozone data (S. Massart, A. Piacentini, D. Cariolle, *et al.*)

With the use of data assimilation, we studied the quality of the Infrared Atmospheric Sounding Interferometer (IASI) total ozone column measurements. The IASI data were provided by the inversion of IASI radiances performed at the Laboratoire ATmosphères, Milieux, Observations Spatiales (LATMOS). This data set was initially compared on a five-month period to a three-dimensional time varying ozone field that we take as a reference. This reference field resulted from the combined assimilation of ozone profiles from the MLS instrument and of total ozone columns from the Scanning Imaging Absorption Spectrometer for Atmospheric CHartographY (SCIAMACHY) instrument. It had low systematic and random errors when compared to ozonesondes and Ozone Monitoring Instrument (OMI) data. The comparison showed that on average, the LATMOS-IASI data tended to overestimate the total ozone columns by 2% to 8%. The random observation error of the LATMOS-IASI data was estimated to about 7%. Using this information, the LATMOS-IASI data are then assimilated, combined with the MLS data. This first LATMOS-IASI data assimilation experiment shows that the resulting analysis is quite similar to the one obtained from the combined MLS and SCIAMACHY data assimilation. The differences are mainly due to the lack of SCIAMACHY measurements during polar night, and to the higher LATMOS-IASI random errors especially over the southern polar region.

3.3.2 Efficient analysis of the 2008 ozone content (S. Massart)

In order to validate the IASI ozone data provided by several teams as we proceeded with the LATMOS-IASI data, we decided to build an efficient ozone analysis for the year 2008. As a difference with the previous study, only ozone profiles from the MLS instrument were assimilated. But to increase the quality of the analysis, the assimilation was conduced with the 4D-Var. Moreover it used the monthly averaged diagnosed covariance matrices of the forecast errors obtained by an ensemble of assimilations. The analysed ozone fields have very low systematic and random errors when compared to ozonesondes and OMI data. They are currently used by the Laboratoire d'Aérologie as a stratospheric background since it is a requirement to produce ozone profiles from IASI radiance measurements with a 1D-Var algorithm. They will also soon be used as a reference to compare with the LATMOS-IASI data produced by a new algorithm.

3.3.3 Studies based on the Valentina assimilation system (S. Massart, A. Piacentini, D. Cariolle, *et al.*)

One major constraint imposed to the Valentina assimilation system is to keep its flexibility. This allows Valentina to participate to a large range of studies, even if it was for instance always coupled with MOCAGE for scientific studies. As an example, the assimilation of spaceborne carbon monoxide (CO) observations

has allowed to explore the transport pathways of CO in the African upper troposphere during the monsoon season [DA1]. The assimilation of ozone measurements helped to deduce the ozone loss in the 2002-2003 Arctic vortex [DA4]. The ozone analysis from Valentina were also helpful to extract wind information in Météo-France 4D-Var operational Numerical Weather Prediction suite [DA8].
Moreover, we had recently implemented in MOCAGE a simplified scheme for the potential temperature. The key idea was to produce temperature analyses that differ from the temperatures provided by the ECMWF analyses as forcings for the MOCAGE thermodynamic. Actually, it is known that there is a bias of few degrees in the ECMWF stratospheric temperatures. As species concentrations are also driven by temperatures, especially for ozone, we expected to reduce the MOCAGE bias using the Valentina analysed temperatures instead of ECMWF ones. But preliminary results showed that the modification of the temperature does not affect a lot the ozone concentration.

3.4 References

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4 Other Data assimilation applications

CERFACS has acquired a good expertise in data assimilation and its application in oceanography and atmospheric chemistry. Other applicative fields are now considering the use of data assimilation techniques. It is CERFACS's and its shareholders' will to widen the scope of application of data assimilation and to build new collaborations around data assimilation. For that purpose, the assimilation group has been involved in different innovative projects.

4.1 Use of data assimilation schemes with EDF neutronics model (B. Bouriquet, S. Massart, S. Ricci)

The collaboration between CERFACS and the department SINETICS of EDF/R&D on data assimilation started in 2003. As of today, the collaborative project ARTEMIS (2008-2010) aims at using data assimilation schemes to improve the modelisation of the neutronic state of power plants nuclear cores as well as the estimation of model parameters. Making the most of this collaborative work, data assimilation is becoming a constitutive part of neutronics studies and several prototypes were already build on top of the current neutronics model COCAGNE.

These experiments proved that the assimilation of the observed neutronic state with the BLUE algorithm allows the correction of the neutronic state itself, namely the thermal flux of neutrons ([DA14]). It was also shown that the BLUE algorithm allows the correction of some model parameters such as the reflector parameters, the irradiation of the in core assemblies or the power to activity parameters (P/A). These results were presented in [DA22] and corroborate the previous studies carried out on the neutronic model COCCINELLE during the CERFACS/EDF R&D ADONIS project (2003-2008). We now expect that data assimilation could provide a global procedure to tune several model parameters at once.

Specific work was done regarding the use of heterogeneous observations coming from different instruments ([DA23]). In the assimilation framework, data coming from heterogeneous sources are used in a transparent way with no major adjustment of the method. Using various instrumental configurations, it was shown that the influence of the instruments on the analysis is related to :
– the granularity of the instruments, *i.e* the density and the in core repartition,
– the accuracy of the instrument,
– the global in core instrumentation configuration.

Further works focused on the impact of the loss or removal of instruments in core. The quality of the reconstruction of the neutronic field with data assimilation was represented as a decreasing function of the number of removed or lost instruments. It was shown that the quality of the reconstruction is mainly governed by the spatial repartition of the instruments. Depending on this repartition, the decrease consists in two or three distinct phases. The ultimate stagnation phase can be explained by statistical effects and by the heterogeneity of the influence of the instruments. This study required numerous data assimilation analysis.

In order to reduce the associated computational cost of the former study , the formulation of the gain matrix in the BLUE algorithm was optimized. An hybrid method using either a fast matrix inversion based on the Schur complement or the direct inversion was developed. This approach made it possible for numerous analysis to be achieved at reasonable computational cost : a global gain of 64% of time computing was obtained with respect to the standard inversion method. Moreover in the most studied cases of very few instrument removals, the gain can reach 97% of computational time.

The study of the impact of instrument removal raised the issue of the individual effect of the instruments ([DA23]). A method to identify the most or the least usefull instruments for the analysis was developed. It was shown that :
– the location of an instrument has more impact than it's accuracy,
– the optimal position of a new instrument mainly depends on the existing instrumental configuration,
– the positioning of the instruments in a network must be done at once and not through an iterative process.

The application of data assimilation in neutronics also aims at providing relevant information for the validation of the neutronics model. This question is of great interest since EDF's neutronics model is currently being enhanced. Assimilation studies on COCAGNE supports the validation of the numerical model and it's input data such as the assemblies irradiation or cross section libraries. So far, all experiments were done in the framework of twin experiments. The neutronics model still being developed, the use of real observations was not possible so far. A main objective for 2010 is to carry out the previously described experiments with real data and to improve the knowledge of COCAGNE.

A PhD was initiated in 2005 in the framework of CERFACS and EDF R&D collaboration in data assimilation to study the optimization of the PWR control and operation. This PhD investigated the enhancement of the xenon dynamics forecast for PWR guiding systems using variational data assimilation. A 4D-Var scheme was implemented on top of a coupled model simulating the xenon dynamics and the neutronic state. This PhD work was successfully defended by Angé lique Ponçot in October 2008 ([DA13]). The time evolving coupled model and it's adjoint developed for this PhD offer a great framework for the application of advanced data assimilation algorithms in neutronic. This work leads also to an international conference presentation ([DA20])

4.2 Data assimilation applications in hydrology (S. Ricci)

A fruitful collaboration with CNRM has been conducted since 2005 on data assimilation in their hydrological modeling system (ISBA-MODCOU) leading to joint publications in the context of G. Thirel's PhD. Even though METEO-FRANCE owns a leading position in the field of data assimilation, the scientific and technological skill of CERFACS (such as the use of PALM) is appreciated in this collaboration. On the one hand, PALM experts at CERFACS provided support for the implementation of the SIM-assimilation prototype. On the other hand, the choice of the assimilation method was guided by both assimilation experts at CNRM and CERFACS. This studies shows that the assimilation of observed flows at about 200 to 900 stations in SIM improves the flow simulations through the correction of soil humidity. The improvement of the simulated flows enables the improvement of the initial condition for the flows ensemble forecasts with SIM. These results are of great interest as the SIM ensemble forecasts are used by SCHAPI for real time flooding forecast.

In 2007 CERFACS and SCHAPI started a collaboration on the assessment of the use of data assimilation techniques with hydrology and hydraulics. A first prototype, built on top of the hydrological model ATHYS, has proved that the assimilation of observed discharges allows to fruitfully tune the most sensible model parameters, leading to an improvement in the water level forecast scores. The second prototype assimilates water level observations in the hydraulics model MASCARET and enables the estimation of the water level and discharge. These results initiated a collaboration between CERFACS and the department LNHE of EDF R&D on the use of data assimilation for hydraulic 1D and hydraulic 3D.

In addition, CERFACS has reinforced its competences in data assimilation for hydrology with its participation to the “Lez project” in collaboration with Hydro-Science Montpellier lab. This project gathers experts in hydrology, hydraulics, biology and geology to improve the knowledge of the Lez hydrosystem.

4.3 Generic use of data assimilation (B. Bouriquet, S. Massart, S. Ricci)

The results from both ADONIS and ARTEMIS projects on data assimilation for neutronics offer proof that the use of data assimilation techniques for other fields than meteorology or oceanography is a promising approach. Inter-disciplinary exchanges on data assimilation methods and applications has been promoted both by CERFACS and EDF R&D. Various EDF R&D departments showed their interest to data assimilation and applications to mechanics, hydraulics and hydrology are being considered. In order to facilitate the access to data assimilation for these new applicative fields, the collaborative work between CERFACS and SINETICS was thought with a generic point of view.

The basic operators for data assimilation were implemented in an experimental data assimilation platform. This platform was used in the framework of neutronics and mechanics. Additional tools focused on the validation of the algorithms, the enhancement and the use of the methods were also included. For instance, major work is still being done on the modeling of covariance matrices ([DA24]). The CERFACS-EDF R&D collaboration also aims at implementing general assimilation tools in the framework of the EDF integrated study and physics coupling platform SALOME.

In order to diffuse CERFACS competences in data assimilation and also to initiate new collaborations, great efforts are made to provide some informative material about data assimilation such as presentations, seminars, technical notes, tutorials or training courses.

This question is partly addressed in the PALM/Assimilation training course ([DA25]). This 3-day training presents the main features of the coupling software PALM that are of interest for data assimilation. Simple to advanced variational methods are first explained and then applied to a simple ocean model. Examples of data assimilation prototypes are presented along with the use of algebra or optimization packages in PALM. This training is particularly fitted to scientists with a basic previous knowledge of data assimilation willing to apply this technique to their own studies. Two sessions of this program were organised at CERFACS over 2008-2009.

Additionally, a PALM independent training course on data assimilation was established. This 2-days training aims at presenting data assimilation concepts and objectives. Classical applications of data assimilation are described and the impact of data assimilation is highlighted. An inventory of the simple assimilation methods is proposed along with a description of their advantages and disadvantages. A synthesis of the major questions to address when setting up an assimilation system is made. This program was presented at EDF-Clamart in 2009.

5 Publications

5.1 Journal Publications

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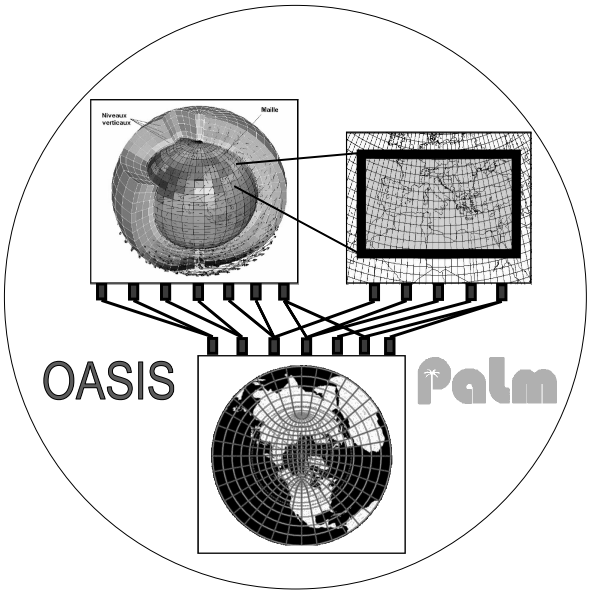
3

Coupling tools and HPC Climate Modeling



1 Introduction

Research activities of the Global Change team are characterized by a balanced mix of scientific studies and development of tools and methods supporting these studies. The scientific studies define the tools and methods to develop which in return increase the efficiency of the purely scientific work. Sharing tools and methods with other research laboratories is also good way to establish long-lasting scientific links.

During the 2005-2009 period, the Global Change team has continued to ensure the maintenance, support and development of the PALM and OASIS coupling software. These tools, produced and distributed by our team for many years capitalize the Global Change team expertise in code coupling. They share some basics characteristics but have different specific features and target different communities. PALM is a dynamic coupler which is now used in many industrial applications and few data assimilation suites for which it was originally conceived. OASIS specializes in climate modelling coupling and offers a highly parallel interpolation library. Finally, the behaviour of our coupled climate models on the always-evolving computing platforms has gain considerable interest in our team during the last few years, especially with the massively parallel platforms starting to impose themselves as one of the main future computing solution for the next decades of climate modelling.

2 The OASIS coupler

The OASIS coupler is open source software developed at CERFACS since 1991, used to couple numerical codes modelling the different components of the Earth System (oceanic and atmospheric general circulation, sea-ice, land, atmospheric chemistry, etc.) developed independently by different research groups. In a numerical coupled model, OASIS acts as a separate executable, which main function is to interpolate the coupling fields exchanged between the component codes, and as a library linked to the component models, the OASIS PRISM Model Interface Library (OASIS PSMILe), which performs the exchange of data. Since the PRISM project funded by the European Commission over the 2002-2004 period [CC6] which objective was to share the development, maintenance and support of software and metadata environments for Earth System Modelling, OASIS has been developed through an active collaboration between CERFACS, CNRS and NLE-IT from Sankt-Augustin in Germany.

OASIS is used by about 30 climate modelling groups in France and in other European countries, but also in many other countries world-wide. For example, OASIS is used by : ECMWF for their operational seasonal prediction suite, the EC-Earth consortium gathering 11 ECMWF member states in which ECMWF seasonal forecast system is developed into an Earth System Model, MPI-M in Germany in the framework of the COSMOS project, NCAS and UKMO in the UK, SMHI in Sweden, KNMI in the Netherlands, INGV and ENEA in Italy, but also in the USA (IRI, NASA JPL, etc.), in Canada (MSC), in Japan on the Earth Simulator super computer (JAMSTEC), in China (ICCES) and in Australia (BMRC and the University of Tasmania), etc. The central position of OASIS in the climate modelling community was confirmed by the success of the 2009 OASIS User meeting that gathered about 40 researchers and engineers from around the world i.e. from Australia, Denmark, Finland, France, Germany, Italy, Ireland, Japan, The Netherlands, United-Kingdom, Sweden [CC24].

Since 2005, OASIS has been used in particular at CERFACS and at CNRM to couple different versions of the Météo-France atmospheric model ARPEGE-climat including the land model ISBA, the ocean model OPA9/NEMO developed at LOCEAN including CNRM sea-ice model GELATO, and TRIP, a runoff model from University of Tokyo. This coupled model was run to realize seasonal prediction experiments and global change simulation over the XXIth century in the framework of the European project ENSEMBLES and to participate in the IPCC Fourth Assessment Report in 2007. It has also been used by the Global Change team in the ANR funded project ESCARSEL for climate simulation over the last millennium. The EU funded CIRCE project is another example of a CNRM coupled modelling project using OASIS, here to assemble a 3-component coupled model : a Mediterranean regional configuration of the ocean model NEMO-V2, a global configuration of NEMO-V2, and ARPEGE-climat V3 with variable resolution (50 km over the Mediterranean).

Furthermore, OASIS is the coupling software used by the main climate modelling CNRS group, the Institut Pierre Simon Laplace (IPSL). At IPSL, OASIS has been used for the IPCC AR4 and in the framework of the ANR funded CICLE project ([CC23], [CC21], [CC22]) to assemble the IPSL-CM4 Earth System Model based on the atmosphere/surface model LMDZ-ORCHIDEE and the ocean and sea-ice model OPA/NEMO-LIM. OASIS is currently used for the IPSL-CM5 ESM which also includes the atmospheric chemistry model INCA ; this ESM will be used by IPSL for the next IPCC AR-5 due in 2013. In the past 4 years, the Global Change team has also provided active support to its community of users.

Today, two different versions of OASIS are available, OASIS3 and OASIS4 . Besides few bug fixes and minor improvements, the main achievement done during the 2005-2009 period regarding OASIS3 ([CC9], [CC12], [CC8], [2]), which includes standard 2d interpolations (bilinear, bicubic, nearest neighbour) and 2D conservative remapping, is its parallelisation on a field-per-field basis. Thanks to this improvement, done in collaboration with IPSL, it is now possible within a coupled model to use more than one OASIS interpolation executable, each one treating a different subset of the coupling fields. This parallelisation represent a great improvement for the coupled models into which the one-executable OASIS was becoming a bottle-neck of the simulation but it is of course limited by the number of coupling fields.

This limitation explains why most of the effort since 2005 was devoted to the development of the new fully parallel version of the coupler, OASIS4, in collaboration with CNRS and NLE-IT ([CC4], [1]). OASIS4 is developed since 2002 to address higher resolution climate simulations run on massively parallel platforms with coupling exchanges involving a higher number of (possibly 3D) coupling fields at a higher coupling frequency. The configuration of the coupling parameters (coupling fields, interpolation, frequency, etc.) is done externally by the user through XML files. OASIS4 coupling includes the commonly known point based 2d and 3d interpolations (bilinear, trilinear, bicubic, tricubic, 2D and 3D nearest neighbour), and 2D conservative remapping. The interpolation of the coupling fields needed to express on the grid of the target component the coupling fields provided by the source component on its grid imply : (1) identifying the neighbours of each target point, i.e. the source grid points that will contribute to the calculation of the target grid point value, (2) calculating the weights of the different neighbours and (3) performing the calculation of the grid point values. With OASIS3, the source coupling field is entirely gathered in the OASIS3 executable which performs these 3 steps and then redistributes the resulting coupling field to the target model. To minimize the transfer of source data, it was decided with OASIS4 to perform the neighbour search (1) by the PSMILe of each source model process for the intersection of the source process local domain with each target process local domain and to transfer only the useful source grid points to the parallel interpolation executable which then performs the interpolation or remapping per se i.e. (2) and (3) above. Furthermore, the neighbourhood search is done with a multi-grid schemes ensuring low CPU cost of the search, at the same time showing a good scalability and identical results when applied to grid partitioned domains. OASIS4 has been used in the framework of the GEMS project (lead by ECMWF) by Mto-France, KNMI (Netherlands), and MPI-M (Germany) for 3D coupling between atmospheric dynamic and atmospheric chemistry models, and is currently by SMHI (Sweden) for 2D ocean-atmosphere coupling.

Through its expertise in coupled climate modelling, the Global Change team has also played a key role in the set-up of the METAFOR and IS-ENES projects, which have both been funded by European Community (EC) under the 7th Framework Plan. METAFOR, which started in March 2008 with a funding of 2.2 MEuros over 3 years, aims at defining metadata to describe in a standard way climate data and the coupled models that produced the data ([CC10], [CC5]). Standard metadata are essential to ensure that key data and models can be described, identified, understood and shared between modellers and users. Based on its experience with OASIS4 metadata, the Global Change team is particularly active in the definition of metadata describing the coupled composition and exchanges. IS-ENES started exactly one year later and is funded for 7.6 MEuros over the 2009-2012 period. IS-ENES proposes to develop a virtual Earth System Modelling Resource Centre integrating the European ESM) and their hardware, software, and data environment. METAFOR and IS-ENES will be the main source of external funding for development of the OASIS coupler in the year to come.

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3 The PALM coupler

3.1 Introduction

PALM is a software tool allowing the concurrent execution and the intercommunication of programs developed independently one from the other and not having been especially designed for that. In addition to the data exchange, this coupler offers a number of services, such as intermediate computations on the exchanged data, grid to grid interpolations, and parallel data redistribution. The couplings therefore span from simple sequential code assembling (chaining) to complex applications involving tens of components run in parallel and/or sequentially. Sometimes the components must run in parallel, especially if the coupling exchanges take place in the inner iterative processes of the computational entities. Furthermore, an important aspect of PALM is that it allows the components to be launched at any point during the run ; in this sense, PALM is a dynamic coupler. The main characteristics of PALM are its easy set-up, its flexibility, its performances, the simple updates and evolutions of the coupled application (one can add a model to the coupled application without changing the structure of the algorithm) and the many side services it offers.

More generally, the component coupling approach followed by PALM allows splitting a system into elementary computational entities that can then be more easily handled and maintained. This approach has proven to be very effective for the design, the management and the monitoring of large complex systems as, for instance, data assimilation suites.

The ongoing development of the final MPMD version of PALM, denoted by PALM_MP, started in 2002. A first running version was released in April 2003. The current available version, PALM_MP 3.0.4, implements most of the originally committed functions. Some tools such as the algebra toolbox (toolbox that interfaces the most common linear algebra operations) or the opportunity to read/write in NetCDF files have been developed. In add, some useful functionalities like the dynamic objects or the possibility to run the units in the driver process have been implemented. One of the major enhancements of the coupler was to adapt it on new high massively parallel calculators. Because on this kind of calculators the MPI-2 standard is often imperfectly implemented or even not implemented at all (IBM Blue Gene L), an MPI-1 version of PALM has been developed. Still in this scope, a brand new communication scheme is being implemented. More and more users (ONERA, SNECMA) would like to couple commercial codes like Fluent or Abaqus with PALM. The standard use of PALM imposes to the users to have access to the code sources they want to couple, which is usually not possible with commercial codes. In general, with these computation codes a breach is nevertheless possible by calling routines developed in the form of dynamic library (*.so). New functions allowing these codes to be dynamically connected to the coupler have been developed using MPI functionalities. More portable methods are under evaluation like the socket mechanism.

In parallel the PALM team has granted the maintenance of the previous versions and has provided extensive user support, including training sessions both on the use of the coupler itself and on its application to parallel coupling and data assimilation suites ([CC13]).

Today, the PALM coupler has proven to be a flexible and powerful parallel dynamic coupler with application domains extending far beyond data assimilation. The user community is constantly increasing and the software is ceaselessly evolving to deal with new functional requirements and new hardware technologies.
For more information, one can consult the PALM website : http ://www.cerfacs.fr/globc/PALM_WEB/index.html

3.2 Usage of PALM

3.2.1 Data assimilation with PALM

As a data assimilation framework, the PALM coupler is used in the operational suite of the MERCATOR ocean forecasting system and for research purposes by the ”Research and development” teams (selected by the GMMC) and by DRM. CNES and LA use PALM in the French project ADOMOCA for atmospheric chemistry data assimilation. EDF utilized PALM in the ADONIS project for data assimilation methods in neutronics simulation. CNRM takes advantage of PALM to build a hydro-meteorological data assimilation suite based on the Safran-Isba-Modcou chain.

3.2.2 Code coupling with PALM

As a code coupler, PALM has started to be used at CERFACS by the CFD TEAM in RANS (N3S-Natur) and LES (AVBP) coupled applications ([CC1]). Having proven its efficiency, it is now spreading in the scientific and engineering community. Among its users, we list SNECMA (DMA and SPS) and ONERA which both use PALM in CFD coupled applications. CESBIO and INRIA (Avignon) are involved in the SEVE working group and use PALM to couple a large number of models in order to evaluate the impact of human activities and the expected climatic change on environmental resources. In the NitroEurope research project, INRIA (Rennes, Grignon), AARHUS UNIVERSITET, FZK, RWTH and the Technical University of Madrid use PALM to couple models in order to study the flows and transformations of nitrogen at the landscape scale. TOTAL tested PALM to build a parallel data loader. IFREMER is coupling a coast model with a waves’ one with PALM. Other users are MINES Paris, IFP (Institut Francais du ptrole), MINES Albi, ECP, CORIA, IMT (Institut mathmatique de Toulouse), SCHAPI, BRGM, LMTG, LEGOS, UMR CNRS 5805 EPOC, DRM (Environnement Canada), LMMC (Algrie) and FUNDP (Facult Univesitaire Notre-Dame de La Paix, belgium).

4 HPC Climate Modeling

(E. Maisonnave)

Climate modellers, who conceived, developed, optimized their codes for vector machines have to face the rapid supercomputer market evolution and start porting their codes onto MPP architectures : the top 500 most powerful machines all belong to this category. Like several european, american and japanese laboratories, we have tested our coupled configuration ARPEGE-NEMO on those new platforms, developing high resolution configuration to exhaustively examine weak and strong scaling issues.

As a first step, a Grid compliant version of the low resolution ARPEGE-NEMO coupled model has been developed and evaluated in the framework of the ANR funded project LEGO. Its performance has been measured in a realistic multi-parametric study. The main result is that enhancements realized on simulation tasks scheduling are efficient and should be transposed to other architectures ([CC3], [CC2])

Furthermore, several steps have been taken since 2005 to port the ARPEGE/NEMO climate model on the new massively parallel platforms and test its performance. Like most of European models, the ARPEGE-NEMO climate model consists of different components, developed separately by different scientific communities and technically assembled through the MPI-based coupler OASIS. Adapting a climate model to MPP platforms not only requires a deep modification of each component architecture, but also the verification that the coupler can efficiently drive a coupled experiment on these platforms.

Due to the complexity of their structure, climate model codes are often missing from computer vendor benchmarks. To have a clear idea of the behaviour of current coupled systems on MPP machines, porting of the ARPEGE-NEMO climate model has been done on massive cluster assembling of weak clock speed CPUs (IBM Blue Gene L and P) and on faster CPU machines using less processors (SGI Altix ICE, IBM JS21, [CC18], [CC16]).

Some existing model features have been selected to reach the highest degree of internal parallelism currently possible, in particular latitude-longitude partitioning for ARPEGE physics, partitioning on the spectral modes and on the altitude for its dynamics, and latitude-longitude partitioning for NEMO. In spite of this, scalability of the T159 resolution version rapidly decreases and only can be enhanced by increasing the problem size, as can be seen on Fig 4.1. The alternative, which is not yet planned on the short or midterm time scale, would be to completely rewrite the architecture of the atmospheric code.

This is why a high resolution version of the coupled model was developed. Started on the Japanese Earth Simulator in collaboration with IPSL developers, the current prototype (ARPEGE t359-NEMO 1/12 degrees) reached 400 Gflops during the NEC SX9 Mto France Operational Health Check in spring 2009 [CC24]. This higher resolution version helped us to reveal good scalability performances up to about 1000 processes and necessity to go to even higher resolution to fully benefit from MPP platforms computing power.

Beside evaluating the scalability of each model component, it appeared necessary to test if the original mono-process OASIS3 coupling field interpolations and exchanges were not becoming a bottleneck for

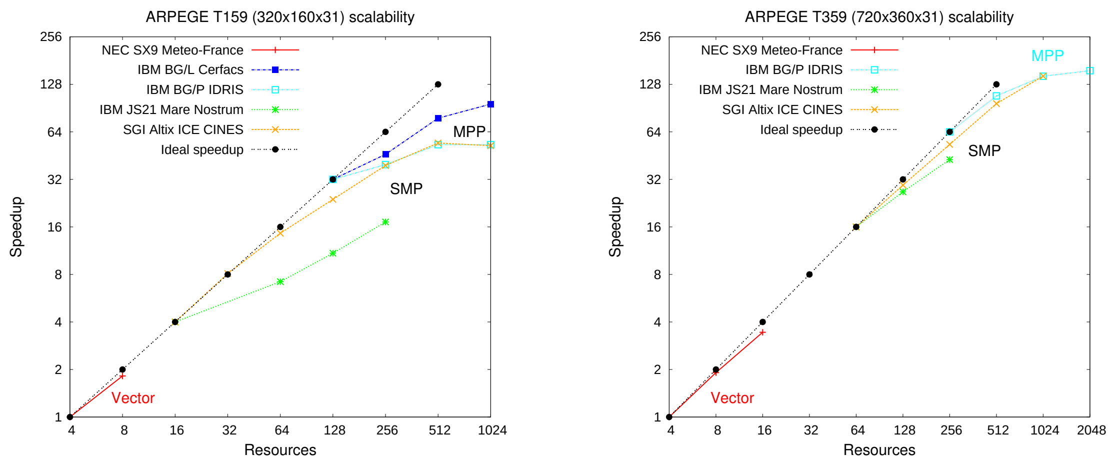

FIG. 4.1: Speed-up of low (t159) and high (t359) resolution configuration of climate model atmospheric component (ARPEGE) on several MPP platforms.

the coupled system and to quantify the benefits brought by the field-per-field parallelisation of OASIS3 (see section II). Evaluating the high resolution model behaviour on vector machine, we concluded that even after some optimisation, the extra cost of coupling can reach, in wall-clock time, 25 % of the slowest components when the component are well balanced. This seems to indicate that OASIS3 limits are reached. At highest resolutions, OASIS3 communications and calculations are slowing the coupled model (probably even more on MPP platforms) : an OASIS4 configuration will be soon set up to try to reduce this coupling extra cost.

5 Publications

5.1 Journal Publications

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5.3 Technical Reports

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4

Climate Variability and Global Change

1 Introduction

The Climate group conducts basic and applied research in the field of climate variability and global change. Our main scientific and technical objectives are the following :

- To improve the understanding of climate processes underlying the natural variability of the main climate natural modes, such as the North Atlantic Oscillation (NAO), the Atlantic Meridional Overturning Circulation (AMOC) and the El Nino Southern Oscillation (ENSO) and of the response of the NAO, AMOC and ENSO to climate change.
- To detect, attribute and describe anthropogenic climate change on global to regional scales using high resolution atmospheric models and long-term high quality observations.
- To assess the impacts of anthropogenic climate change at regional scale with specific interest in the changes of the hydrological cycle and to provide uncertainty bounds in future climate projections.
- To study the potential of decadal predictability due to both external forcing and oceanic initial conditions.
- To explore and develop the appropriate tools to make the most efficient use of the new supercomputer architectures for high-resolution climate modelling exercises.

The methodology relies upon a dual approach combining observations and simulations performed with state-of-the-art general circulation models of the atmosphere, ocean, land surface, sea-ice and the coupled climate system. Most of our objectives are endorsed by national and/or international programs through coordinated projects and collaborations with other partners mainly at the french and European levels (European Framework Program 6, FP6 : ENSEMBLES, DYNAMITE ; Agence Nationale de la Recherche ANR : CLIMATOR, ESCARSEL, VALIDATE ; Ministère de l'écologie, de l'énergie, du Développement Durable et de l'Aménagement du Territoire MEDAD : REXHYSS, ACCIES ; Ministère de la Recherche, Action Concertée Incitative : CYPRIM).

2 Climate variability and predictability

Interest in weather/climate fluctuations has been rapidly growing over the last two decades or so, following the recent recurrence of meteorological extremes and the more pressing evidence for anthropogenic influences on climate. In such a context, demand for predictability of climate variability logically emerged from the decision-makers sphere. The estimation of the predictability relies on deeper understanding on the physical processes that controls both intrinsic and externally forced climate variability. To address those issues, a dual approach based on observational and modelling studies has been adopted by the climate group with the aim of improving climate forecasts as well as impact studies from intra-seasonal to decadal time scales.

2.1 Tropical-extratropical connections (C. Cassou, E. Sanchez, S. Bielli, L. Terray)

A special attention has been devoted to tropical-extratropical connections leading to potential predictability over a broad NAE region. At intraseasonal timescale, observational evidence has been provided for a lagged relationship between some specific phases of the MJO in the tropics and the occurrence of the North Atlantic weather regimes in winter (ENSEMBLES project, Figure 2.1), The NAO regimes are the most affected in response to low-frequency Rossby waves that are initiated in the North Pacific by the MJO-related bursts/suppression of convection, and that propagate eastward towards the NAE domain along the circumpolar jet waveguide. Wave breaking in the NAE domain is concurrently altered and appears to act as a relay prior to the full development of the NAO regimes. These findings have a direct application in terms of monthly prediction and have been compiled in a Nature paper [CM8]. Collaboration with Météo-France (Direction de la production) has been initiated on this issue using operational monthly forecasts from ECMWF.
A dedicated study of the 2003 climate dynamics also suggests that tropical-extratropical connections are important in summertime for NAE variability. Combining observational results and model experiments (ANR/CHAMPION project) we had previously demonstrated that anomalous convective activity over a broad tropical Atlantic basin alters the occurrence statistics of the NAE weather regimes and consequently modify the associated probability of heat waves to occur. Targeted simulations for 2003 (ANR/IRCAAM project) further highlight that the ocean-atmosphere extratropical coupling is important to reinforce the primary tropical-extratropical atmospheric signal. Seasonal forecasts get a direct benefit from these results through a sustained collaboration with Météo-France (Direction de la Climatologie) and Mercator-Océan within the framework of the Seasonal Forecast. For instance, relevant diagnostics based on regime occurrences and anomalous tropical circulation (assessed through predicted divergent and rotational flow) have been implemented on EUROSIP operational forecasts.

Tropical-extratropical connections are also found to be a relevant actor at decadal timescales. We showed through coordinated model experiments carried out within the EU-DYNAMITE project that the observed warming of the Indo-Pacific warmpool favours the occurrence for positive NAO regimes and could explain in part the NAO positive trend observed at the end of the last century [CM16]. Two mechanisms have been proposed for the remote tropical-NAE relationship : the direct route through the North Pacific following the

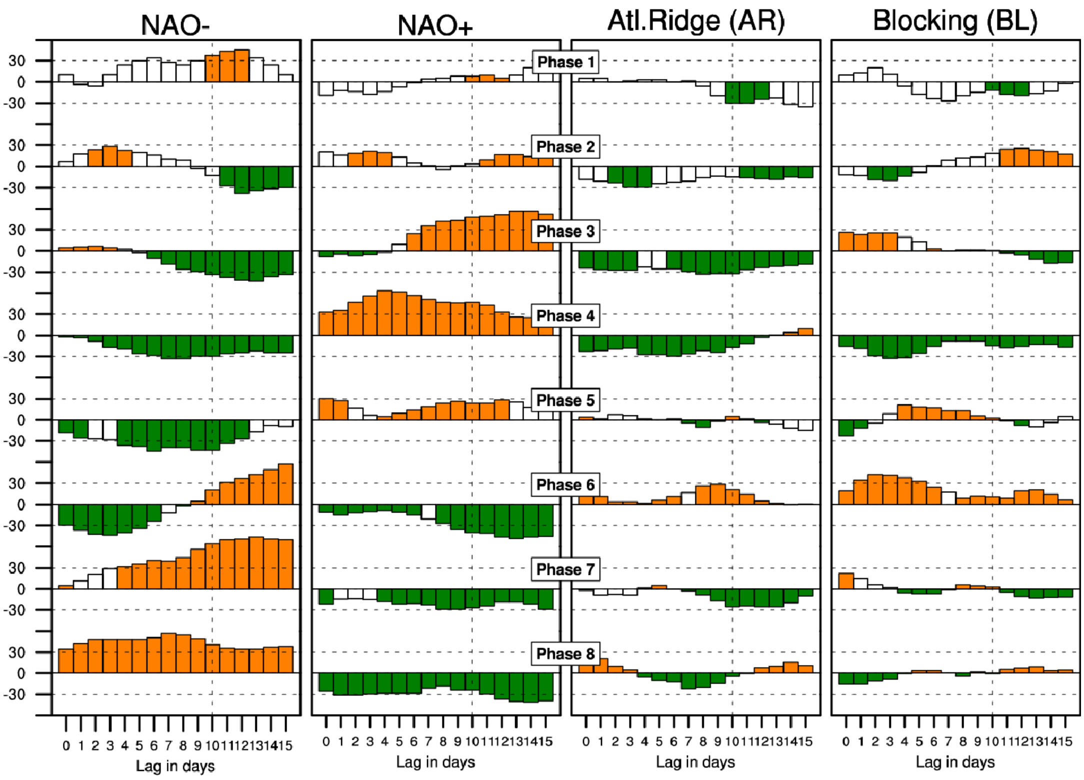

FIG. 2.1: Table of contingency between the MJO phases (rows) and the NAE weather regimes (columns). For each MJO phase, the anomalous percentage occurrence of a given regime is given as a function of lag in days, with regimes lagging MJO phases.

jet waveguide, and the indirect route through the modification of the Walker cells between tropical Atlantic and Indo-Pacific basins leading to the excitation of Rossby waves that propagate towards Europe from the western part of the tropical Atlantic.

2.2 North Atlantic-European dynamics (E. Sanchez, C. Cassou, L. Terray)

Previous studies realized at CERFACS have shown that weather regimes can be considered as elementary bricks for NAE atmospheric dynamics whose seasonal-to-decadal variability can be interpreted to the first order as the time integration of their anomalous occurrence (Figure 2.2). In addition to occurrence, transitions between regimes also appear a relevant criterion especially to link large-scale variability and extreme events. In the Mediterranean region, we show for instance that intense precipitations episodes mostly occur during transition days between two NAE regimes where strong southerlies develop in the western basin. (ACI/CYPRIM project, [CM16])

Those conclusions hold for present-day climate variability (20^{th} century) but are expected to be more and more contested in the future due to global warming. Additional factors such as land-atmosphere interaction (FP6/ENSEMBLES project, [CM3] or local sea surface temperature coupling around Europe (ANR/IRCAAM project) also act as positive feedbacks for dynamically-induced signals for temperature and precipitation especially in summer. We show from IPCC-AR4 experiments that the weight of these two mechanisms with respect to the NAE anomalous atmospheric dynamics itself varies with models for the mid-to-late 21^{st} century [CM3], [CM2]. This weight is largely responsible for the huge uncertainties of surface continental variables over Europe, together with the parameterization of the evapotranspiration processes.

2.3 Decadal to centennial variability and predictability (P. Rogel, D. Swingedouw, M. Minvielle, C. Cassou, L. Terray)

Low frequency predictability (from interannual to multidecadal timescale) mostly relies on the ocean influence on the overlying atmosphere. Analyses have been carried out to estimate the predictability of the climate system over the NAE domain at decadal timescale. A basic decadal hindcast exercise has been completed using initial conditions obtained from assimilation from 1960 to 2005 and provided by the climate group (ENSEMBLES project). Preliminary results confirm that some predictability, although weak, can be found over the NAE domain associated with the use of observed ocean initial conditions. Diagnostics highlight however some difficulties in extracting predictable signals because traditional diagnostics used for seasonal-to-interannual forecasts cannot be applied to decadal predictions due to strong interactions between model mean biases/drift and variability beyond one year of integration of the coupled system. Further investigations are clearly needed in the future to better understand the interactions between the model biases and the decadal variability and predictability.

Coupled IPCC-like models are known to be very poor in the reproduction of the North Atlantic ocean dynamics mostly because of the representation of several physical processes that would require a higher horizontal and vertical resolution, and because of the estimation of the ocean-atmosphere fluxes by the models. To address those issues, we have implemented a novel statistical forcing method based on weather regimes (DESAGO project, [CM19]) to reconstruct the surface ocean variables derived from the CNRM-CM3 IPCC-AR4 model and used to force two high resolution configurations of the ORCA ocean model (ORCA05 and NATL4). Those simulations allowed us to investigate by which mechanisms the ocean integrates high frequency atmospheric changes from 1960-to-present. Those analyses appear to be a prerequisite to better quantify and understand the low-frequency modifications of the ocean due to anthropogenic forcings. Additional model experiments based on reconstructed variables from CNRM-CM3 scenarios suggest that changes in the NAE atmospheric dynamics estimated through occurrence statistics of the NAE regimes is not responsible for the significant slowdown (30%) of the thermohaline circulation at the end of the 21^{st} century ; the latter is mostly controlled by the direct thermodynamical warming trend at the surface ocean leading to stabilization of the oceanic column. This projected change and associated processes are in agreement with the last millennium climate evolution estimated from model simulations (ANR/ESCARSEL project) in response to solar forcings, even if signals are much weaker for the latter case. Decreased solar activity is associated with an increase of the modelled thermohaline circulation due to radiative/thermal effects that dominate the counteracting wind-driven slackening of the oceanic Atlantic gyres due to predominant negative NAO induced by the solar forcing through a Pacific-Atlantic teleconnection.

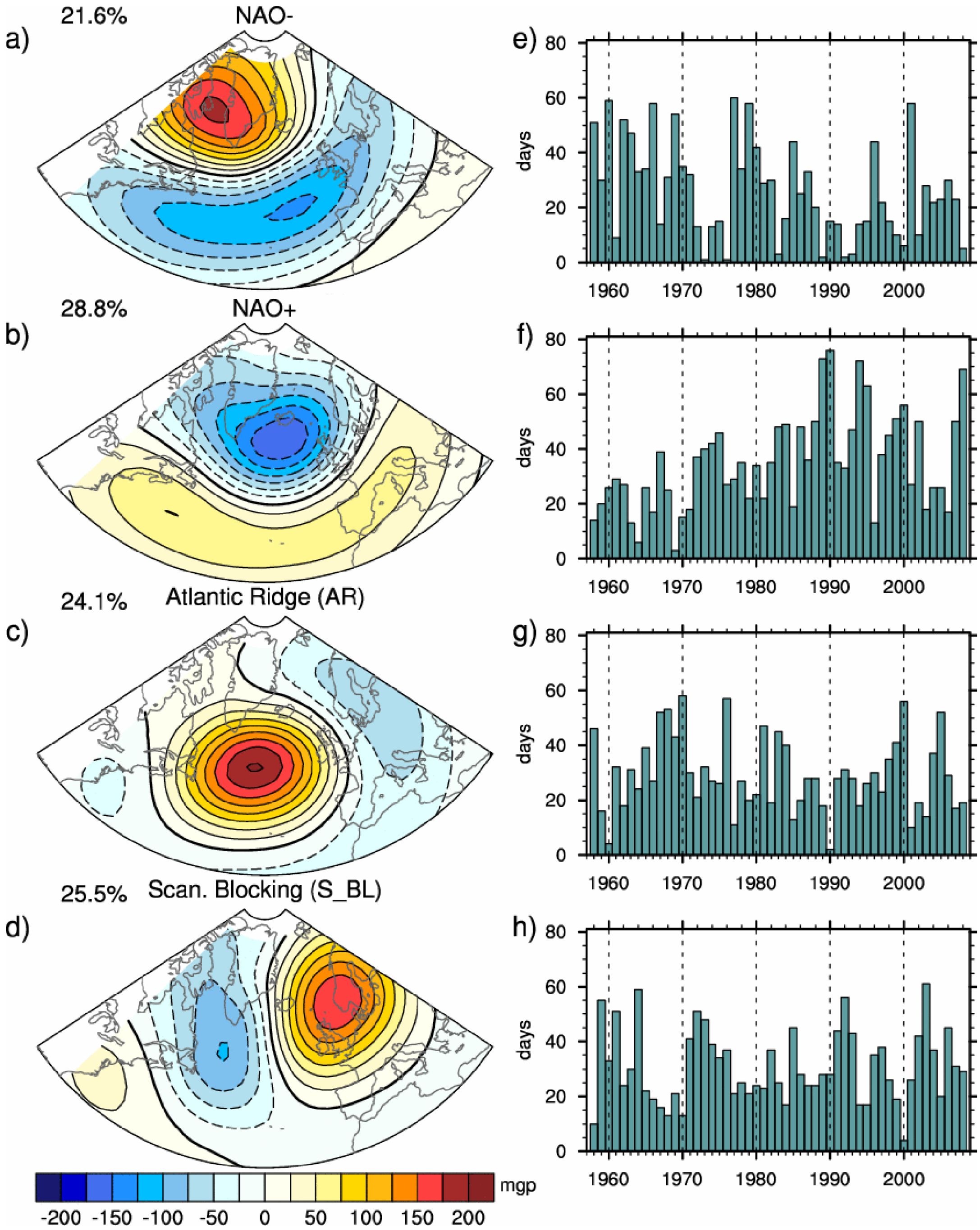

FIG. 2.2: (a-d) Centroids of the four wintertime NAE Z500 weather regimes (m). (e-h) Number of days of occurrence of each regime per winter from 1958 to 2009

3 Climate change and impact studies

3.1 Statistical and mixed statistical-dynamical downscaling

The downscaling activities have been aimed at developing new statistical or mixed dynamical-statistical downscaling methodologies and using them in climate change impact studies at regional to local scale. Since 2005, the activities have covered developments to the physical basis and technical aspects of the (dynamical-)statistical downscaling algorithms and their application to the impacts of climate change upon the hydrological cycle in the main French river basins and France wind energy potential. A summary of the main results obtained during the period 2008-2009 is given below.

3.1.1 Statistical downscaling scheme : algorithm development for hydrology (J. Boé, C. Pagé, L. Terray)

Our main objective was to develop a relevant methodology to study the impacts of climate change on the hydrological cycle in the main French river basins, with a special focus on the different uncertainties involved. First, when it comes to studying the impacts of climate change, the relevant spatial scales for the physical processes involved are much smaller than the ones that CGCMs are currently able to treat. An intermediary step, called downscaling, is thus necessary to derive from the global climate models regional climate scenarios at the relevant spatial scales. Second, studying the impacts of climate change involves a large number of uncertainties. The main steps necessary to evaluate the impacts of climate change can be summarized as follows : (1) construction of emission and/or concentration scenario ; (2) global climate modeling ; (3) downscaling ; (4) impact modeling. For instance, the uncertainties associated with step 2 includes here both epistemic (linked to biases in the model representation of the climate system) and natural variability uncertainty. To address these uncertainties, a large ensemble of climate models is needed. This implies that it is necessary to downscale many climate projections, which has some practical implications concerning the choice of the downscaling method. The main advantage of statistical downscaling over dynamical downscaling is that it is computationally inexpensive and as such, it fitted our objectives.

Statistical downscaling schemes (SDS) consist of building an empirical relationship based on observations or pseudo-observations between large-scale atmospheric predictors and the local variables necessary as input to the impact model. Then the large-scale predictors from the climate models are used to derive the high-resolution climate scenarios on the basis of this empirical relationship. Two atmospheric predictors are used in the new SDS scheme : sea level pressure (SLP) and surface temperature averaged over Western Europe. The 1981-2005 SAFRAN analysis data set developed at Météo-France provides the pseudo-observed local variables in the learning period. The atmospheric predictors for the learning period are extracted from the NCEP reanalysis.

The SDS method is based on weather typing and conditional resampling of the days of the learning period. There are three main steps involved in the development of the SDS method over the learning period. First, weather types based on SLP and discriminating for French precipitation are extracted [CM4], using an automatic partitioning algorithm and taking into account precipitation properties during the classification process. The four seasons are treated separately, and between 9 and 10 weather types are obtained depending on the season. The second step is intended to represent the within-type variability of precipitation and account for the dynamical variability within the weather types [CM4]. There is generally a strong link between the distance of the SLP pattern of a given day to the weather types and the intensity of precipitation. In order to take this effect into account, several multivariate regressions are used with predictors being the daily Euclidean distances between the SLP pattern of a given day and the weather types of the corresponding season. For each regression, the predictand (defined as a precipitation index) is the root mean square of daily precipitation averaged over a given area. The performance of the algorithm is not very sensitive to the precise choice of the number and exact repartition of the precipitation indices. Surface temperature is also used as a secondary predictor in the downscaling algorithm in order to account for processes not related to dynamical changes (for instance radiative ones). The final step of the downscaling algorithm consists of conditional resampling of the days of the learning period, by searching for the day of the learning period in the same weather type with the closest precipitation and temperature indices ([CM6], [CM21]).

3.1.2 Full recoding of the algorithm : the DSCLIM software (C. Pagé)

The previous downscaling methodology has been recoded completely in C language in a highly-configurable manner, under the CeCILL open-source license. This made possible the strong optimization of the code, the writing of modular libraries of basic functions, the automatisation of the processes, and the standardization of the file format used (NetCDF CF-1.0 convention). It also rendered the code unix platform-independent and easy to port (building of the code through GNU standard autotools). Some inconsistencies in the initial implementation of the methodology were corrected : seasonal cycle of shortwave radiation, horizontal domains, temperature variable index (land-sea mask). Scientific, technical and source-code documentations were written. Finally, some basic plotting and post-processing scripts were also developed, e.g. calculation of potential evapotranspiration, relative humidity, minimum and maximum daily temperature and relative humidity ; monthly, seasonal, annual and climatological means [CM21].

3.1.3 Statistical and mixed downscaling schemes : algorithm development for wind resources(J. Najac, J. Boé, L. Terray)

Similar ideas were also used and adapted within Julien Najac PhD to extend the statistical downscaling algorithm for the estimation of the climate change impacts upon the surface winds over France. The previous statistical downscaling method has been adapted to estimate daily mean 10 m wind speeds and directions at specific sites (a set of 78 meteorological stations over France) using large-scale atmospheric circulation predictors. Daily 850 hPa wind field has been selected as the optimal large scale circulation predictor. As for the original one, the method is based on a classification of the daily wind fields into a few synoptic weather types and multiple linear regressions. Years are divided into an extended winter season from October to March and an extended summer season from April to September, and the procedure is conducted separately for each season. ERA40 reanalysis and observed station data have been used to build and validate the downscaling algorithm over France for the period 1974-2002 [CM12].

To overcome the sparse nature of the existing wind observations, another statistical-dynamical downscaling method has also been developed to estimate projections of the mean 10m wind speed and direction distributions at high spatial resolutions using the weather-type based approach combined with a mesoscale model [CM20]. Daily 850hPa wind fields (predictors) from ERA40 reanalysis and daily 10m wind speeds and directions (predictands) measured at 78 meteorological stations over France were used to build and validate the downscaling algorithm over the period 1974-2002. First, the daily 850hPa wind fields are classified into a large (O(100)) number of wind classes and one day is randomly chosen inside each wind class. Simulations with a non-hydrostatic mesoscale atmospheric model (MESO-NH developed at CNRM and Laboratoire d'Aérologie) were then performed for the selected days over three interactively nested domains over France, with finest horizontal mesh size of 3km over the Mediterranean area. The initial and coupling fields (lateral boundaries) are derived from the ERA40 reanalysis. Finally, the 10m wind distributions are reconstructed by weighting each simulation by the corresponding wind class frequency (the observed ones from ERA40 in the validation step and the ones derived from climate model scenario simulation for the impact case study) [CM13].

3.2 Impact studies

3.2.1 Impact of climate change on the hydrological cycle in the main French river basins(J. Boé, C. Pagé, L. Terray)

Using the SDS scheme described above and the predictors from the CMIP3 model database, an ensemble of climate scenarios have been statistically downscaled in order to force a hydrometeorological model (the SAFRAN-ISBA-MODCOU suite, developed at CNRM) over France. Then, the main changes in different variables of the hydrological cycle have been investigated. Despite large uncertainties linked to climate models (the so-called structural uncertainty), some robust signals already appear in the middle of the 21^{st} century. In particular, a decrease in mean discharges in summer and fall, a decrease in soil moisture, and a decrease in snow cover, especially pronounced at the low and intermediate altitudes, are simulated. The low flows become more frequent but generally weak, and uncertain changes in the intensity of high flows are simulated. Another objective was to study the different uncertainties at stake, in particular, the relative importance of modelling uncertainty versus that of downscaling uncertainty. To evaluate downscaling uncertainties and assess the robustness of the results obtained with the statistical downscaling method, two other downscaling approaches have been used. The first one is a dynamical downscaling methodology based on a variable resolution atmospheric model, with a quantile-quantile bias correction of the model variables. The second approach is based on the so-called anomaly method that simply consists of perturbing present climate observations by the climatological change simulated by global climate models. After hydrological modelling, some discrepancies exist among the results from the different downscaling methods. However, they remain limited and to a large extent smaller than climate model uncertainties (Figure 3.1). This was confirmed recently in the framework of the REXHYSS project where both downscaling and hydrological modelling uncertainties have been shown to be smaller (but significant) than climate model uncertainty. These results are fully described in [CM6].

3.2.2 Impact of climate change on surface winds in France (J. Najac, L. Terray)

The purely statistical and mixed statistical-dynamical downscaling schemes described above have been used to perform a multimodel (using the CMIP3 model database) study of the impact of climate change on the wind resources over France. The analysis was carried out for both 2046-2065 and 2081-2100 periods with the 1971-2000 period as a reference. For the cold season (ONDJFM), we have found significant changes in the Southeast (decrease of the mean wind speed and the number of high wind days, and an increase in the number of low wind days) and in the North (increase in the mean wind speed and the number of high wind days, and decrease of the number of low wind days). For the warm season (AMJJAS), we found significant changes all over France with a decrease of the mean wind speed and the number of high wind days, and an increase of the number of low wind days in all stations. For both seasons, changes are larger for 2081-2100 than for 2046-2065. We have also found good agreement between the models with regard to the sign of the changes in most stations for the warm season, and in a few stations for the cold season. Moreover, the magnitude of the changes remains uncertain in most cases as the intermodel dispersion is of the same order of magnitude as the amplitude of the changes. Finally, we showed that those changes are due to both intratype and intertype modifications. The results from the two methods are in good agreement and consistent with direct simulation results from dynamical models.

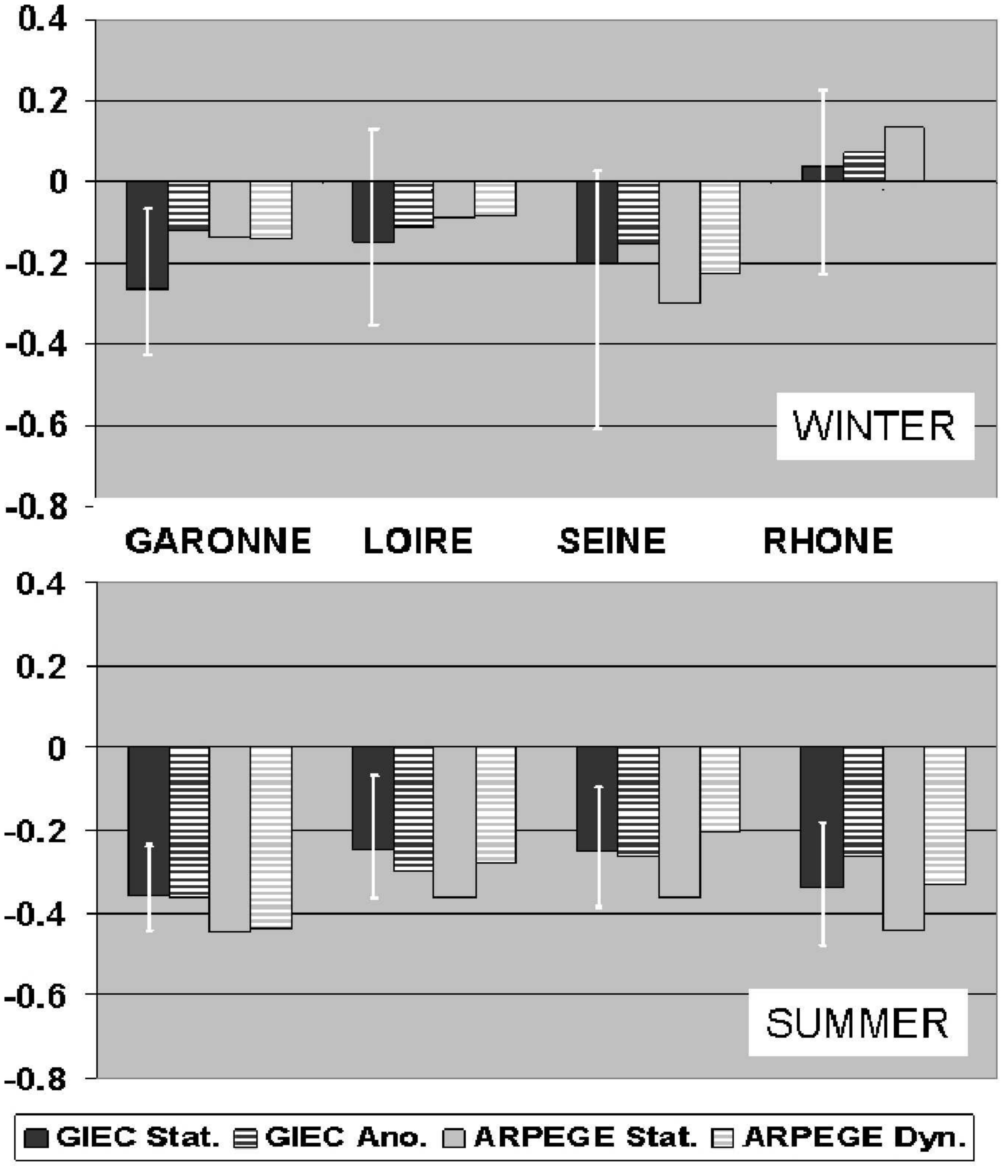

FIG. 3.1: Relative changes in the discharges of the Garonne, Loire, Seine, and Rhône (without units) in winter and summer given by the anomaly method (GIEC ano.), the statistical downscaling method of the CMIP3 models (GIEC Stat.), dynamical downscaling with ARPEGE-Var.Res. after bias correction (ARP Dyn.), and the statistical downscaling of ARP-VR (ARP Stat.). The white error bar gives the intermodel spread (given by the minimum and maximum) of CMIP3 Stat.

We have also analyzed the various sources of errors from the methods. The main drawbacks of the statistical-dynamical downscaling method are the addition of two sources of errors (errors that originate from the day sampling and errors that originate from the mesoscale simulations) and the assumption that the climate change signal may be entirely captured by changes in the wind class frequency of occurrence. Furthermore, while a sample of 200 days appeared to be satisfactory to represent the 10m wind speed and direction distributions, the current version of the method is not adapted for extreme wind studies. The main advantage of this method is that it can provide crucial information at the scale of interest for policymakers. Moreover, given the mesoscale simulations, it can be easily applied to a wide range of GCMs for different time periods, which is essential to carry out relevant impact studies. Results of this work are detailed in [CM20] as well as in [CM13].

3.2.3 Distribution of high-resolution scenario for impact studies (C. Pagé, L. Terray)

We have used the DSCLIM software to produce a set of multimodel high resolution climate scenarios for France (at a horizontal resolution of 8 km). We have performed the downscaling all CMIP3 models for the scenario SRES A1B as well as several simulations forced by a wider range of SRES scenarios made with the ARPEGE model at CNRM and SUC [CM22]. This set of regional scenarios, named SCRATCH08, has been primarily used for a number of applications linked to climate change impact assessment through our participation to funded projects. The latter cover a large spectra ranging from hydrology (REXHYSS) , agronomy (ANR/CLIMATOR and ANR/VALIDATE), biodiversity (ANR/QDIV) to health questions (GICC/ACCIES). Furthermore we have also provided SCRATCH08 data to other public and private institutions and entities in relation with their own climate impact and adaptation projects. Indeed we have always provided simultaneously the expertise on the correct use of these scenarios in order to account for the various sources of uncertainty. The SCRATCH08 have also been transferred to Mété-France/DCLIM and are to be included in Météo-France high-resolution scenarios catalog for both internal and external use.

4 Publications

4.1 Journal Publications

[CM1] J. André, J. Royer, and F. Chauvin, (2008), Les cyclones tropicaux et le changement climatique, *Comptes Rendus Geosciences*, **340**, 575–583.

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[CM3] J. Boé and L. Terray, (2008), Uncertainties in summer evapotranspiration changes over Europe and implications for regional climate change, *Geophys. Res. Letters*, **35**, L05702, doi :10.1029/2007GL032417.

[CM4] J. Boé and L. Terray, (2008), A weather type approach to analysing France winter precipitation : twentieth century trends and influence of anthropogenic forcing, *J. Climate*, **21**, 3118–3133.

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4.2 PhD Thesis

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[CM20] J. Najac, (2008), Impacts du changement climatique sur le potentiel éolien en France : une étude de régionalisation, thèse de doctorat de l'université paul sabatier.

4.3 Technical Reports

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[CM22] C. Pagé, L. Terray, and J. Boé, (2008), Projections climatiques à échelle fine sur la France pour le 21ème siècle : les scńarii SCRATCH08, Technical Report TR/CMGC/08/64, CERFACS.

5

MERCATOR project

1 CERFACS contribution to MERCATOR-OCEAN

This report summarizes the CERFACS contribution to the Mercator-Ocean project. The GIP Mercator-Ocean is a French centre of operational oceanography. The CERFACS team is mainly working in research and development tasks for the next generation of ocean forecasting systems. Yann Drillet, Marie Drevillon and Jean-Michel Lellouche were hired by the GIP between 2008 and 2009.
Mercator-Ocean is involved in the MyOcean project, the implementation project of the GMES Marine Core Service, aiming at deploying the first integrated European capacity for Ocean Monitoring and Forecasting. MyOcean Service should provide information on the Ocean from global to regional scales.
During the GODAE experiment, Mercator-Ocean achieved a real time operation of a 1/4^o global ocean system (PSY3) and a 1/12^o Atlantic ocean system (PSY2) based upon primitive equations with data assimilation of *in situ* and satellite observations.
Mercator-Ocean is now aiming at consolidate the operational exploitation of the systems, routinely monitor them and assess the products quality in order to fulfil the user needs. One of the current challenges is the development of a high resolution global ocean forecasting system. The CERFACS team brings to Mercator-Ocean an expertise on development of model configuration and assimilation, as well as a scientific expertise on analysing the ocean circulation.

1.1 High resolution ocean forecasting system at 1/12^o (R. Bourdallé-Badie, C. Derval, B. Tranchant)

Weekly analysis and a 14-days forecast are produced for the North Atlantic ocean with a 1/12^o model assimilating altimetry, in situ and climatology data sets. The new target is a 1/12^o global ocean analysis and forecasting system, called PSY4. Its development requires strong technical efforts due to an important computational cost and storage requirements. The setup of the configuration begun in 2007 and the integration with the assimilation begun in 2008.
It is based on the new version of the LOCEAN primitive equation ocean model, NEMO, coupled with the LIM ice model. The CERFACS's team has worked on the switch of all Mercator's systems to this new version.

1.1.1 Ocean model improvements for the 1/12^o global configuration

The first task was to compute a new bathymetry file from the latest available bathymetry data bases, ETOPO1 (1') and GEBCO08 (30"). An important difference between the old bathymetry file and the new one is that no smoothing was applied as it usually does. New numerical schemes should be able to work well even in region of high bathymetric variability. Various tests performed by different research teams with regional models of the Kerguelen area and the Labrador Sea show better results with an unsmoothed bathymetry.
The other tasks to improve this configuration are in one hand on the model himself, with the add of new parameterizations and numerical schemes, and in other hand a specific work on the ocean-atmosphere interaction and the forcing fluxes.

1.1.1.1 New parameterizations for ORCA12

New parameterizations were available in the new NEMO code and in the NEMO community.

To improve the representation of observed small scale features and their impact on water masses evolution, different advection schemes for tracers (Zalezak, QUICKEST and PPM) were tested, first on a Mediterranean configuration at 1/12^o and after in the global 1/12^o itself. The general patterns of the Mediterranean circulation are correctly reproduced with all of them. The variability is more realistic with the QUICKEST and PPM schemes which are of a higher order than the Zalezak one and does not require an explicit diffusion. In the global configuration, we have found the same conclusions in term of variability than in the Mediterranean model but the representation of the North Atlantic Current is less realistic. The reason is the absence of an isopycnal diffusion. So we finally recommended the use of the Zalezak scheme for the global 1/12^o configuration. The figure 1.1 shows a snapshot of the ocean current at 50 meters depth in the 1/12^o system.

An important weakness of the first ORCA12 reference simulation was the representation of the ice. This was the first attempt to run the LIM ice model with a high spatial resolution and some parameters were not well tuned. Short sensitivity experiments over few months were performed to tune a set of parameters for this configuration. We have worked too on the new elastic-viscous-plastic model for the sea ice which allows a more realistic representation of the sea ice dynamic. Those new parameterization, parameter sets and new forcing fields have led to a much more realistic ice representation.

A new routine, to take into account the light penetration in the ocean depending on climatology of chlorophyll, was available in the latest NEMO version. This routine induces a modification of the penetration of the solar heat flux depending on the turbidity of the ocean. The DRAKKAR project have successfully tested it in a lower resolution configuration. We adapted this routine to be able to run it with the global 1/12^o configuration. We obtain the same results : warmer temperature in the first levels of the model in the turbid areas and where the mixed layer depth was shallow.

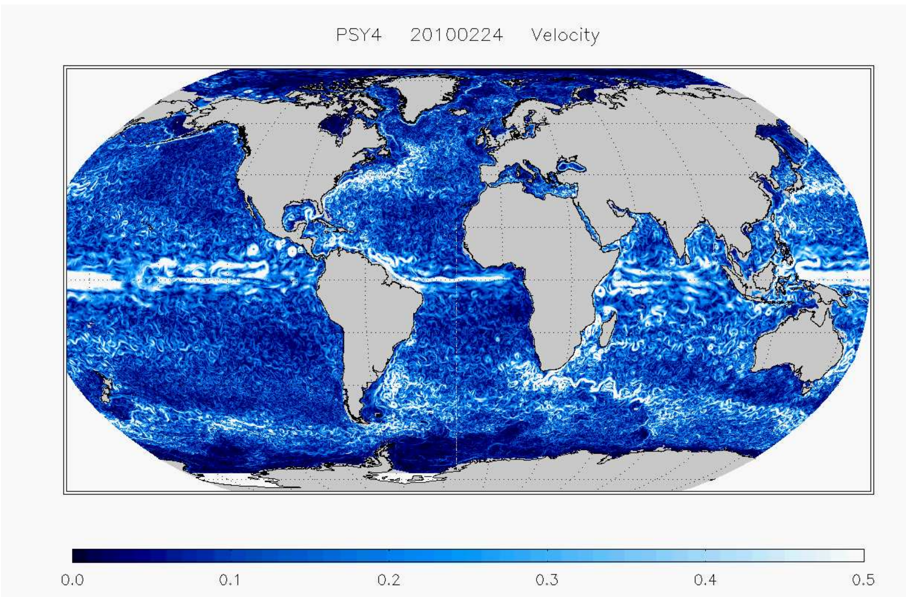

FIG. 1.1: Current intensity forecast at 50 meters depth with the PSY4 system.

1.1.1.2 High frequency atmospheric forcing

Up to now, the ocean models were forced by atmospheric forcing fields at a daily frequency. To be more realistic and better represent the ocean-atmosphere interaction, we assessed the impact of a high frequency forcing (3h) on the ocean and of new parameterizations linked to this topic : solar penetration with a diurnal cycle and mixing due to the wind stress. Due to the numerical cost of the high resolution model, most of the sensitivity experiments have been performed with the global 1/4^{o} model.
The impact of high frequency wind stress, 3h versus 24h, has been tested with 3-year simulations. The high frequency wind stress induces a little more variability of the surface circulation in some regions : south-east pacific, north-west tropical pacific and Gulf Stream area. There is a significant impact on the mixed layer depth (MLD) representation. At the mid-latitude, where the variability of the wind stress is stronger, the MLD simulated with the 3h wind forcing are deeper. This compares better with the observations in all regions except in the convective area in the Labrador Sea where the MLD is deeper with daily mean wind stress. The high frequency variation of the wind stress induces high frequency variation in the MLD and more homogeneous water in the first meters. The ice representation is also changed. A large improvement is induced in the southern hemisphere but the solution, in summer, in the northern hemisphere is less satisfying. A new set of parameters for the ice model has been proposed to solve this problem. The drag coefficient between the atmosphere and the ice, the rigidity of the ice, etc were tuned.
The effect of applying an analytical diurnal cycle of the solar heat flux on the ocean was also studied. The diurnal cycle is estimated with an analytical formulation applied to the daily flux. The impact on the subsurface temperature is larger than on the sea surface temperature. Even if the daily mean energy input is the same over one day, the diurnal cycle induces a destratification and restratification which allow to capture warm water in the subsurface where the mixed layer depth is weak. The difference and the RMS computed with the observed temperature observations show a significant improvement between 50 and 200 meters depth in the simulation with the diurnal cycle.
Those experiments suggest a beneficial impact of a higher frequency wind forcing and a representation of the diurnal cycle for the solar heat flux. The simulated ocean has then a more realistic mixed layer depth and level of energy in the surface layers.
Atmospheric forcing fields are applied to the ocean using “bulk formulae” introducing dependencies of the applied fluxes to the ocean state. Different so called bulk formulations are proposed in the literature. Here the CLIO, CORE and ECUME formulations are compared. When the ECUME bulk formulation is applied, eddy kinetic energy and current intensity are weak. The surface temperature tends to unrealistically rise due to stronger heat fluxes compared to the observed data. The sea surface temperature is also too cold with the CLIO formulation. The currents with the CORE formulation are weak too, but this could be corrected by taking into account the ocean current intensity to compute the fluxes. The sea surface temperature is realistic. The CORE bulk formulation is the most appropriate for ORCA12.

1.1.2 Integration and qualification of the high resolution global ocean forecasting system PSY4

A new operational global ocean forecasting system at 1/12 ^{o} has been developed and is routinely operated since December 2009. It has been designed to meet the next requirements of the future operational oceanography.
It consists on :

- A global eddy resolving ocean model at 1/12^{o} named ORCA12 built from the OGCM NEMO 1.09 coupled to the sea ice model LIM2 [1].
- A data assimilation scheme named SAM2v1 based on the SEEK filter equations, see [2] that uses an ensemble of anomalies to represent the background error covariances, a localization technique, and an adaptative scheme. This method assimilates jointly satellite SLA and SST, and in situ profiles of temperature and salinity.

- The FGAT (First Guess at Appropriate Time) method is used and allows to compare the observations with their model equivalent at the observation time. However, instead of propagating the innovation, FGAT assumes the innovation vector to be constant both in time and space within the assimilation window.

- Corrections are applied with the Incremental Analysis Update (IAU) method.

Before being operated routinely, the system is running during about a year in order that the model trajectory is adjusted by the assimilation scheme. It also allows to control that the system behaviour is in agreement with the required quality. This period starting from April 2009, covers about 8 months of 2009 before the weekly operational procedure. The validation procedure includes assimilation and physical diagnostics, comparison to climatology, and independent observations, especially drifters and ice coverage. The existing operational systems, global 1/4^o and regional 1/12^o, are also a basis for comparison performances. First conclusions show that this new ocean forecasting system improves analysis and forecasts compared to the other systems excepted for the temperature field in the sub-surface. The figure 1.2 shows the anomalies of temperature at the equator in the three main basins (Indian, Pacific and Atlantic) coming from the SST RTG, a combination of in-situ and satellite data, and those coming from our system. It shows that this system is able to reproduce the seasonal cycle with a very good precision even along the coasts. Note that warm anomalies found in the tropical Pacific ocean from october to february are also found in the data of the TAO/TRITON mooring array. At 2^{o}S, when the seasonal signal is removed with a digital filter, tropical instability waves appear, see figure 1.3. We note that there is a good agreement with data in term of intensity and propagation velocities.

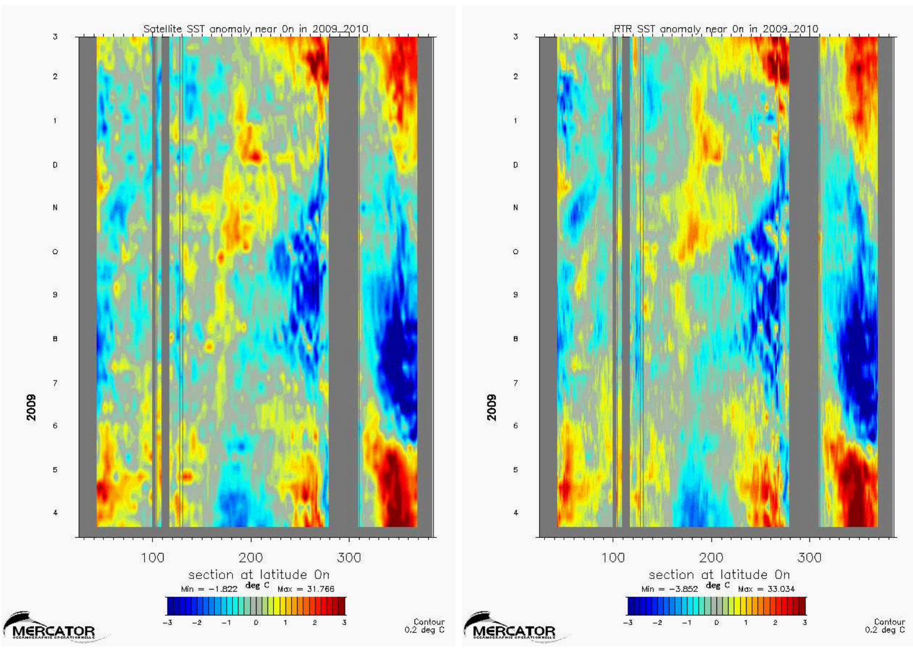

FIG. 1.2: Hovmuller diagram of SST anomalies at the equator calculated from SST RTG (left) and from PSY4 (right). Period : April 2009 - March 2010

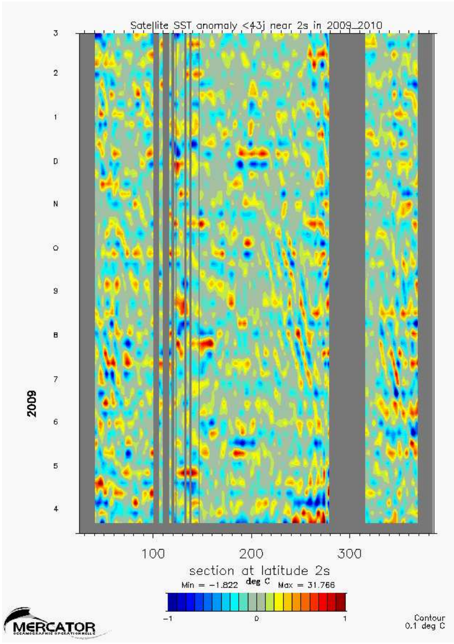

FIG. 1.3: Hovmuller diagram of SST anomalies (sesonal signal removed) at 2°S calculated from SST RTG (left) and from PSY4 (right). Period : April 2009 - March 2010

1.2 Scientific qualification of the systems forcasting and reanalysis (M. Drevillon, J.M. Lellouche)

A thorough scientific assessment of the upgrade of the operational systems, for instance PSY2 and PSY3, is necessary to ensure a sufficient quality of the analysis and forecasts.

Scientific calibration and validation of the analysis and forecasts are the two major phases of the scientific qualification process. A new system has to go through the whole process before it becomes fully operational and its “outputs” are made available for users.

Some operational oceanography metrics have been defined in the context of the MERSEA European project, ended in 2008, and the international GODAE and GODAE-Oceanview initiatives for operational oceanography.

A calibration procedure is necessary to document the range of values for the various metrics as well as the ability of an analysis and forecasting system to capture the major ocean processes it was built to describe. The calibration process is thus conducted on a reference numerical experiment of a given system and is derived from the scientific assessment of ocean reanalyses. The key physical processes are also studied in relation with the configuration representativity whether it is a global or regional system, coarse or high resolution etc...

The spin-up of the system from a restart with climatological conditions to catch up with real time is generally used as the reference simulation. This simulation usually covers several months up to a year in order to cover one seasonal cycle at least. In the case of PSY3, the GLORYS reanalysis is also available as a very valuable reference experiment, even if there are some important differences between the two systems, for instance the Incremental Analysis Update scheme is implemented in GLORYS.

The scientific calibration process requires several men/month per system to be efficient. At the end of the process, the strength and weaknesses of the system, as well as remaining questions and recommendations

for future developments are drawn. It has to be homogeneous over the different systems to make intercomparisons possible.
The first attempt of applying a homogeneous calibration procedure was made on the last major scientific upgrade of PSY2 and PSY3. Later on the assessment of GLORYS also followed the same scheme.
The quality of the statistics in the observation space is first assessed using data assimilation statistics on SLA, SST, T and S profiles, as well as comparisons with independent data, velocity measurements at 15 meters depth from drifters, Sea Ice coverage and drift. The consistency of the analysis characteristics with the input hypothesis is checked : the prescribed observation and model error before and after analysis should not be biased, have a gaussian distribution and be consistent with the prescribed errors in the assimilation scheme.
The physics in the model space was checked, especially seasonal signals, high frequencies fluctuations with respect to mooring observations. The realism of equatorial waves was also assessed, showing an improvement with respect to the previous systems. The consistency of integrated quantities such as volume transports was also verified by comparing to values given by the literature. The systematic biases, the modes and tendencies were also quantified.
Weaknesses of the system such as a systematic underestimation of surface currents (10 to 20%) and weak temperature and salinity corrections at depth were identified. It was found that the behaviour of PSY2 and PSY3 is often comparable, despite the different spatial resolutions. This result is very important as this shows that the system NEMO/SAM2 system is robust and performs well as most metrics reach state of the art values.
One of the major recommendations issued from the calibration was that further versions of PSY2 should tune the data assimilation system and the input data resolution to take better advantage of this high resolution configuration.

1.3 Ocean reanalysis (E. Rémy)

Ocean reanalysis became an important activity at Mercator-Ocean. They do not only provide historical times series for ocean climate monitoring but also allow to study the behaviour of the forecasting systems over long time period. System failures, slow model drifts can only be identified in such simulation. Advanced assimilation techniques are explored in the context of reanalysis.

1.3.1 Low resolution 3DVar ocean reanalysis

A low resolution global ocean reanalysis was produced based on the ORCA 2° model configuration and the OPAVAR assimilation code in its 3DVar version [3]. It covers the period 1960-2005. In situ temperature and salinity observations are assimilated with along track Sea Level Anomalies. The ability of the assimilation to reproduce the observed interannual variability of the subsurface heat content and sea level variability was demonstrated. Experiments were also conducted showing the sensitivity of the estimated large scale ocean circulation to the type of observations assimilated and the mean dynamical topography chosen as a reference for the Sea Level Anomaly data. The salinity, especially at depth appears to be the more sensitive variable. Less salinity observations exist to constrain the model trajectory than temperature observations.
We participate to a multi analysis intercomparison in the framework of the GSOP project (Global Synthesis and Observations Panel). Different estimations of the interannual variability of the ocean and related indices were computed over the last 50 years from ocean model reanalysis and observations based estimation. The goals were to evaluate the quality of the estimations, identify their strength and weaknesses and also compute ocean climate indicators with their error bars. Those indicators were build to monitor well known ocean climate phenomena as the ocean component of El Nino, the indian ocean dipole... The dispersion of the ensemble members provides an error estimate on the different quantities computed. Some estimates

were surprisingly close for given variables, as heat content, on certain period and regions. The different estimates tend to diverge in the late 2000.

1.3.2 Interannual variability in the Glorys Reanalysis

A first reanalysis simulation, called Glorys1v1 covering the period 2002-2008, was produced with the 1/4^o forecasting system. The calibration procedure described before was applied. More specific physical diagnostics were studied.
The Meridional Overturning Circulation (MOC) of the Atlantic basin was computed. This quantity represents as a stream function the zonal mean transport depending on latitude and depth. It shows the intensity and paths of the water masses. The evaluation of the MOC is extremely difficult from in situ observations or current meters. Ocean models constrained with observations are a way to explore the variability of the thermohaline circulation in the North Atlantic, and its variability. In the Glorys simulation, we did not found significant interannual variability of the integrated transport. The decomposition in an Ekman induced transport, and a barotropic and baroclinic component did not show more time variability. The estimated values at 26^{o}N are in agreement with the estimates from observations. In the equatorial region, an unrealistic recirculation pattern appears. Experiments with ORCA2 shown that the MOC is very sensitive to the chosen MDT. Unrealistic patterns, like seen in GLorys, also appear. They are not seen in the simulations without assimilation.
One of the major convection region of the world ocean is situated in the Labrador sea. It is a key region for water mass formation. Deep convection is still difficult to represent in numerical models. The events occur very rapidly and locally after a preconditioning phase by the surface forcing and currents. In the simulation without assimilation, the convection events do not show enough interannual variability and the convection depth is too high. The characteristics of the convection events represented in Glorys in terms of depth and duration are in agreement with the Yashayev analysis from temperature and salinity profile observations. The figure 1.4 shows the mean temperature profile evolution in the convection area of the Labrador estimated from in situ profile observations and from the reanalysis.

1.4 Publications

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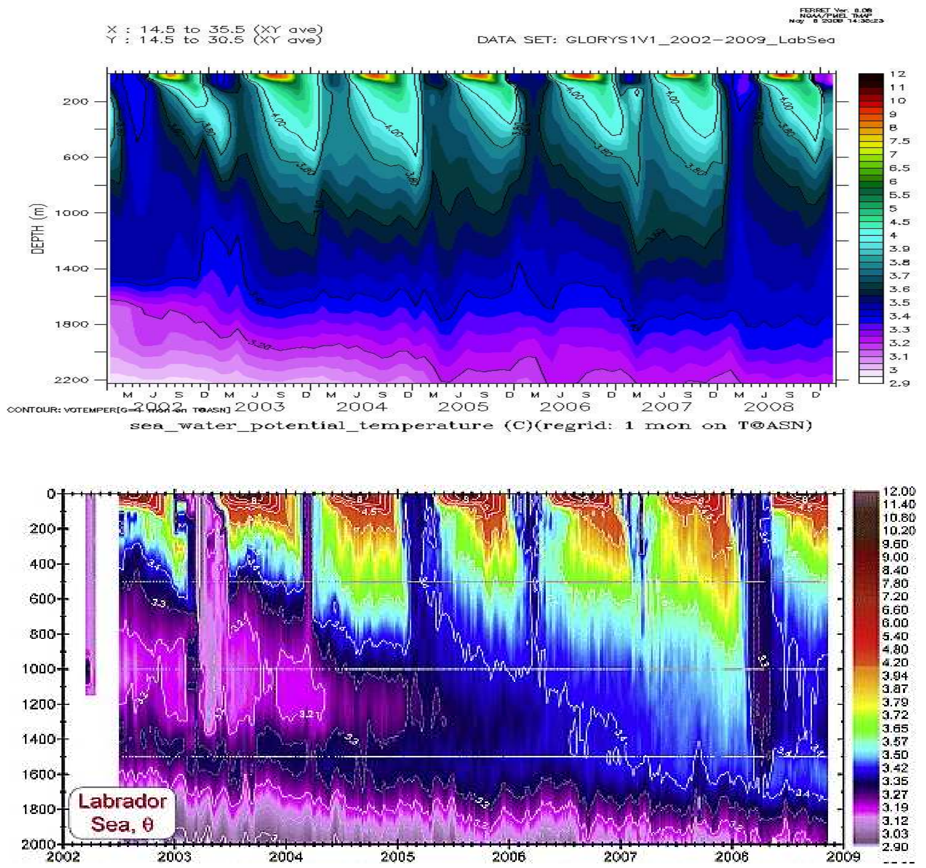
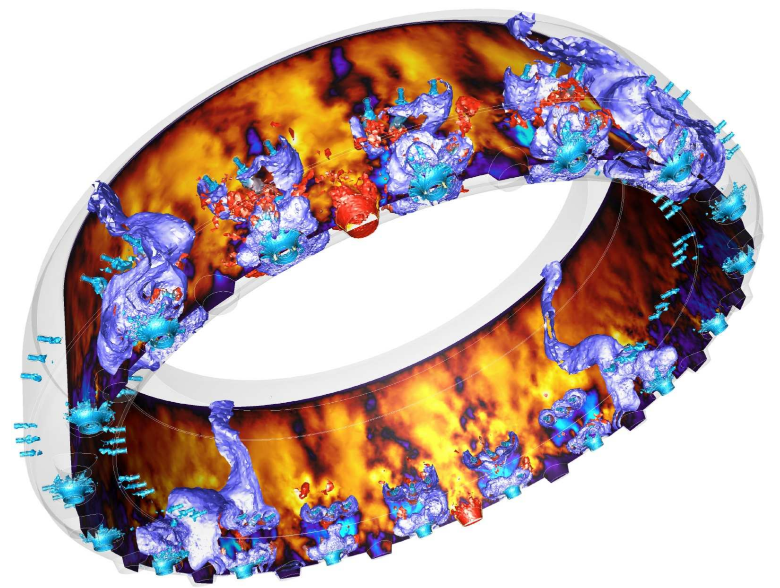


FIG. 1.4: Mean temperature profile evolution in the convection area of the Labrador sea in Glorys (top) and from observations (bottom)

6

Combustion



1 Combustion

The combustion team at CERFACS continues the development of efficicent numerical tools for combustion applications. Besides the CFD code AVBP and the acoustic code AVSP, these tools now also include a code for thermal transfer in solids (AVTP) and a radiation code (PRISSMA). Still dedicating important efforts to modelling and fundamentals, necessary to guarantee accurate descriptions of the involved physics, the CFD team is more and more involved in multiphysics coupling and extension of the solvers to a wide range of applications. This of course implies constant renewal of numerical methods and computational techniques, to obtain the best results in the most efficient way.
Current applications include aeronautical burners, piston engines, rocket engines, large size gas turbines and industrial furnaces.

1.1 Combustion basics

1.1.1 Chemistry (B. Franzellli, G. Albouze, E. Riber, M. Sanjosé, T. Poinsot)

Chemical kinetics are one of the controlling factors in all combustion applications. Although detailed schemes are available for most fuels, their use in LES of complex configurations is still impossible because of their huge computational cost. Alternative techniques such as tabulation methods are promising in academic configurations [COMB56, COMB1] but their extension to industrial configurations remains a problem because of the large number of parameters to be accounted for (heat losses, fresh gas temperature and pressure, dilution by recirculating gases (EGR), number of streams feeding combustion,...) [7]. CERFACS collaborates with IFP, CORIA and EM2C to develop tabulation methods in AVBP. In parallel the team has also proposed a strategy to build two-step reduced schemes accounting for fuel oxidation reaction and $CO - CO_2$ equilibrium, which are valid for a wide range of equivalence ratio, fresh gas temperature and pressure, and EGR dilution. Two schemes for methane-air (2S_CH4_BFER) and kerosene-air (2S_KERO_BFER) schemes are now available. They are fast and use little memory, and their coupling with compressible codes and turbulent combustion models is straightforward. The evolution of ame quantities such as laminar ame speed, adiabatic ame temperature or ignition delay is accurately predicted over a wide range of operating conditions. For example, Fig. 1.1 displays the dependence of laminar flame speed versus equivalence ratio for fresh gas pressure varying from 1 to 12 atm [4] .

1.1.2 Euler modelling of particle dispersion (P. Sierra, E. Riber, B. Cuenot, L. Gicquel, T. Poinsot, E. Masi, O. Simonin)

To model dispersion and preferential concentration of liquid fuel droplets before they evaporate, the mesoscopic Euler-Euler approach proposed by [3] has been developed in collaboration with IMFT since 2003 : the particle velocity is decomposed into a correlated velocity shared by all the particles and an uncorrelated velocity defined for each particle, this latter becoming non negligible for very inertial particles. The Eulerian equations for the dispersed phase are obtained by ensemble averaging of a Boltzman-like equation for several moments of a particle probability density function. When neglecting the Random Uncorrelated Motion (RUM), comparisons between Euler-Lagrange and Euler-Euler LES in a particle-laden

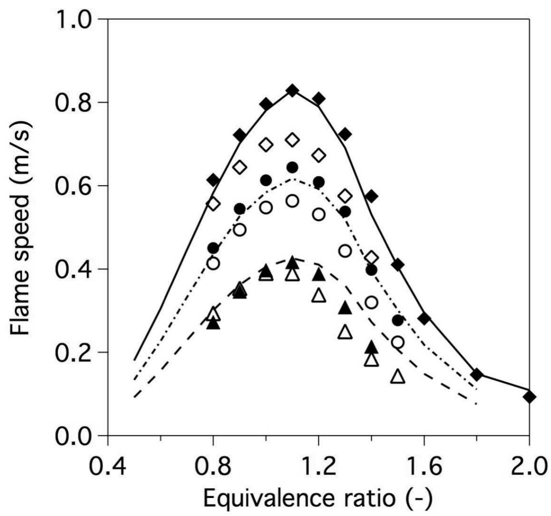


FIG. 1.1: Laminar flame speed versus equivalence ratio at fresh gas temperature $T_f = 473K$. Comparison between 2S_KERO_BFER scheme (lines), LUCHE skeletal mechanism (plain sybols) and DAGAUT detailed mechanism (empty symbols) for pressure P = 1, 3, 12 atm.

turbulent bluffbody flow have shown promising results [COMB33]. However, the particle fluctuations are largely underestimated by the Eulerian simulations, showing than the RUM must be accounted for. One possibility is to solve an additional transport equation for particle Random Uncorrelated Energy (RUE) which contains several terms to be closed. The closures proposed by [14] showed good results in particle-laden Homogeneous Isotropic Turbulence [COMB22] but failed in mean-sheared turbulent particle-laden ows [10].
In her PhD, P. Sierra works with E. Masi, PhD student at IMFT directed by Pr. O. Simonin to develop new closures for partie RUE. The models are tested *a priori* and *a posteriori* in a particle-laden turbulent planar jet.

1.1.3 Radiation (D. Poitou, J. Amaya, B. Cuenot, M. El Hafi)

Radiation plays an important role in combustion : it contributes to thermal fluxes to the walls, but also plays a role in the chemical structure of the flame and its emissions. In the case of sooty flames, radiation is essential as soot particles are very absorbing. However coupling radiation to LES is a difficult task as the equations to solve are very different, with different time and length scales. Moreover, due to the spectral nature of radiation, the CPU cost associated to radiation of gases is extremely high. In collaboration with Ecole des Mines d'Albi, a DOM solver for radiation (PRISSMA) [COMB20], including various models for the spectral properties of gases, has been developed and coupled to AVBP through the PALM interface. The interaction of radiation, turbulence and combustion has been studied in detail and concluded that no sub-model was required for the sub-grid scale radiation processes. Application to a laboratory configuration illustrated the impact of radiation on the flame structure.

1.1.4 Numerical methods for CFD (A. Roux, M. Kraushaar, S. Jauré, V. Granet, O. Vermorel, L. Gicquel, T. Poinsot, V. Moureau)

The quality of Large Eddy Simulation of turbulent flows is strongly conditioned on the accuracy and robustness of numerical schemes. This is even more critical for compressible and reacting flows, where sharp velocity or density gradients may appear. Note also that the performance of the numerical schemes is altered near boundaries where the mathematical problem may not be well posed. Therefore a compromise must be found between accuracy and stability, that depends on the numerical scheme, the geometry and the flow. Such difficulties are further emphasized in the context of multi-phase flows where the liquid phase transport equations exhibit major difficulties. In the Euler-Euler framework, the governing set of equations generates local accumulation of the liquid phase with very large discontinuities. Likewise, in the context of the Euler-Lagrange framework, regions of low particle concentrations generate large numerical oscillations due to coupling of a discrete singularity with the gaseous phase. Both methods are very difficult to handle numerically in LES and preliminary studies obtained in the PhD thesis of N. Lamarque and M. Porta (both defended in 2007) have been further investigated by A. Roux and M. Kraushaar. To increase stability while preserving accuracy, one possible alternative to the centered schemes used today in AVBP is the distributed residuals method, that leads to partially upwinded schemes. The difficulty is to determine the best distribution of nodes weight to reach the accuracy and stability target.

In parallel to the development of fully compressible implicit schemes, an incompressible LES solver may be of use since the associated stability criterion scales with the local flow velocity. This change of governing equations induces a clear gain when compared to the speed of sound scaling stability law of fully compressible solvers. Recent developments for Poisson equation solvers show good behavior and massively parallel scaling of such algorithms is now possible contrarily to older solutions. Ongoing developments are being pursued by M. Kraushaar in collaboration with V. Moureau from CORIA to offer massively parallel LES incompressible flow capabilities in AVBP.

Finally, work is conducted on boundary conditions, being a weak point of compressible solvers especially for LES or DNS in the subsonic regime. For these unsteady solvers, the capacity to let vortices and acoustic waves leave the domain without generating reected waves is mandatory but difficult to ensure in multiple applications. Methods based on the classical NSCBC technique [9] usually assume one dimensional and inviscid non reacting flows on the boundary, which is incorrect in industrial applications. Recent methods originally developed for structured grids [15] allow to take into account transverse terms as well as viscous and source terms. A major issue for these methods is to determine the Mach number to be used in the specification of the transverse terms. This approach has been extended in the PhD thesis of V. Granet to unstructured grids in AVBP [5] and tested on different complex applications, like turbine blades or piston engines.

1.1.5 Wall phenomena (O. Cabrit, S. Mendez, F. Nicoud, T. Poinsot)

One crucial but complex physical issue is linked to wall phenomena. Turbulent gaseous flows along walls become very complex in the presence of a flame or hot gases. This is particularly the case in aerospace applications such as the flow through the nozzle of solid propellant motors. In this case, multicomponent, high temperature combustion products chemically interact with the carbon-carbon nozzle which undergoes thermal pyrolysis. Computing such large scale systems requires relevant wall models in order to assess mass or heat transfers at the solid-gas interface. Developing such a model was the objective of the PhD work of O. Cabrit (defended in fall 2009) for SPS Bordeaux, who realized Direct Numerical Simulations (DNS) of representative periodic channel flows and built appropriate wall models [COMB7, COMB58].

1.2 LES of two-phase reacting flows

Most combustors studied in the team burn liquid fuel. To take into account the dispersed liquid phase, two solvers are now available in AVBP : an Eulerian solver based on the approach of Février *et al.* [3]

([COMB3, COMB33]) and a classical Lagrangian solver. Both solvers are fully parallel and use the same physical models for momentum, heat and mass transfer to the gas.

1.2.1 LES of non-reacting two-phase flows (M. Garcia, F. Jaegle, J.M. Senoner, M. Sanjosé, B. Cuenot, T. Poinsot)

To validate LES of two-phase flows, an experimental configuration has been measured at ONERA (MERCATO test bench, R. Lecourt) and compared to a series of simulations using Euler-Euler, Euler-Lagrange (monodisperse) and Euler-Lagrange (polydisperse) formulations [COMB39]. To perform such simulations, a specific model (FIMUR) has been developed to represent the liquid injection without simulating primary atomisation.
Comparison with experimental data showed that both solvers are able to reproduce both the gaseous and liquid flows with good accuracy ([COMB77]). The effect of polydispersion appeared to stay moderate in this configuration. The injection model also proved to correctly represent the flow at injection.

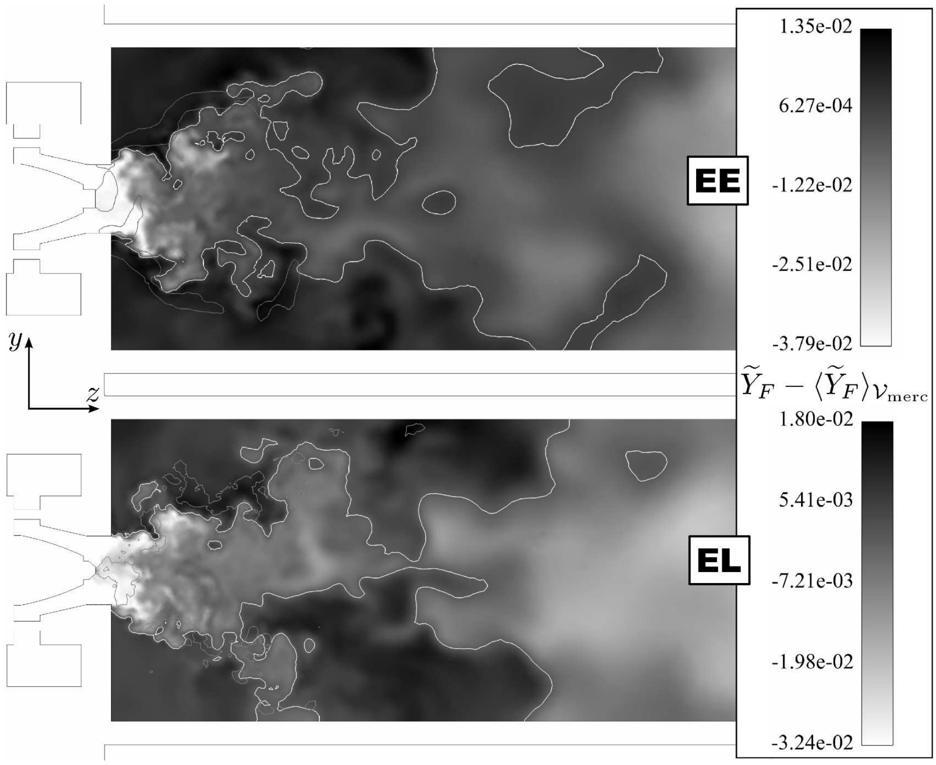


FIG. 1.2: Field of fuel vapor in the MERCATO configuration : comparison between the Euler-Euler and the Euler-Lagrange formulations.

1.2.2 LES of two-phase flames based on Euler-Euler formulation (M. Sanjosé, F. Jaegle, A. Eyssartier, G. Hannebique, J. Laédrine B. Cuenot, T. Poinsot)

The Euler-Euler formulation of two-phase flows has been used to simulate reacting flows in various configurations, including the MERCATO configuration and an industrial configuration, the multi-point injector of SNECMA [COMB68] tested experimentally at ONERA (C. Guin). It appeared that the numerical methodology developed for non-reacting flow was also efficient on reacting flows and good qualitative agreement has been obtained between experimental and numerical results [COMB49].

1.3 Unsteady combustion

1.3.1 LES of combustion instabilities (P. Wolf, G. Staffelbach, A. Roux, B. Enaux, V. Granet, S. Hermeth, I. Hernandez, L. Gicquel, O. Vermorel,T. Poinsot)

The development of LES tools in the last ten years at CERFACS has been driven first by the study of combustion instabilities. Initiated first for Siemens and Alstom, these studies are now performed for SNECMA, TURBOMECA and ANSALDO. In 2008 and 2009, multiple studies have been devoted to LES of combustion instabilities with specific demands oriented towards the prediction of azimuthal instabilities that can only be captured if the full annular burner is treated numerically.

The role of azimutal modes in annular chambers has become a theme of major importance. These modes have been out of reach of LES for a long time because most LES codes were able to compute only one sector of the real turbine instead of the 15 to 24 which compose the turbine. A major breakthrough achieved at CERFACS in 2007 is the first LES of a complete gas turbine chamber. Since then successive computations with increasing degrees of geometrical complexities have been obtained [COMB6, COMB42, COMB45, COMB89]. These studies complemented by LES of non-reacting flow injection system, have reached maturity and are now used by CERFACS partners to build understanding and apprehend azimuthal thermoacoustic instabilities.

Contrarily to azimuthal modes, longitudinal acoustic modes are mainly governed by the inflow and outflow acoustic boundary conditions. Two possible strategies have been investigated to go beyond this limitation :

- The first simplest option consists in computing the entire flow domain including regions where the inflow and outflow conditions are known (i.e. shocked nozzles) as illustrated in the case of the ONERA experimental ramjet burner [COMB36]. For this specific case, fully predictive LES predictions could be obtained provided that the proper chemistry model si employed [11].
- The second solution is most often needed since full computations are rarely possible (computation in rotating parts, undetermined conditions...) and relies on the identification of the inflow and outflow acoustic impedances based on 1D flow approximations [COMB26, COMB27, COMB34].

The baseline solver for unsteady combustion studies at CERFACS is AVBP. It is used with various submodels for combustion (one and two-step reduced schemes, FPI methods for more complex kinetics), subgrid scale tensor (WALE [2], dynamic model, one-equation model), gray gas models for radiation, law-of-the-walls for heat transfer.

Analyzing LES results can be difficult and additional tools are useful to understand the unsteady flow activity. This includes tools to construct maps of spectral activity, POD (proper orthogonal decomposition) [COMB36] which have been coupled to AVBP but also acoustic solvers such as AVSP described in Section 1.3.2.

LES results remain very sensitive to numerical parameters (scheme order), acoustic parameters (impedances) and models (chemical schemes). For example, taking into account radiation and heat losses at walls modifies the frequency and the amplitude of modes [13, 12]. Real configurations also operate with liquid fuel lines with specific responses to the acoustic forcing. Multiple transfer function and models are needed to properly take into account these effects [COMB3, COMB33].

As an example, Fig. 1.3 displays the temperature field (right picture) in a complete TURBOMECA combustion chamber in which an azimutal mode appears under certain extreme conditions [COMB42]. This LES was performed on 700 processors of a Cray XT 3 machine. The left figure shows the geometry used to predict the longitudinal thermoacoustic behavior of the ONERA ramjet burner [COMB35, COMB36].

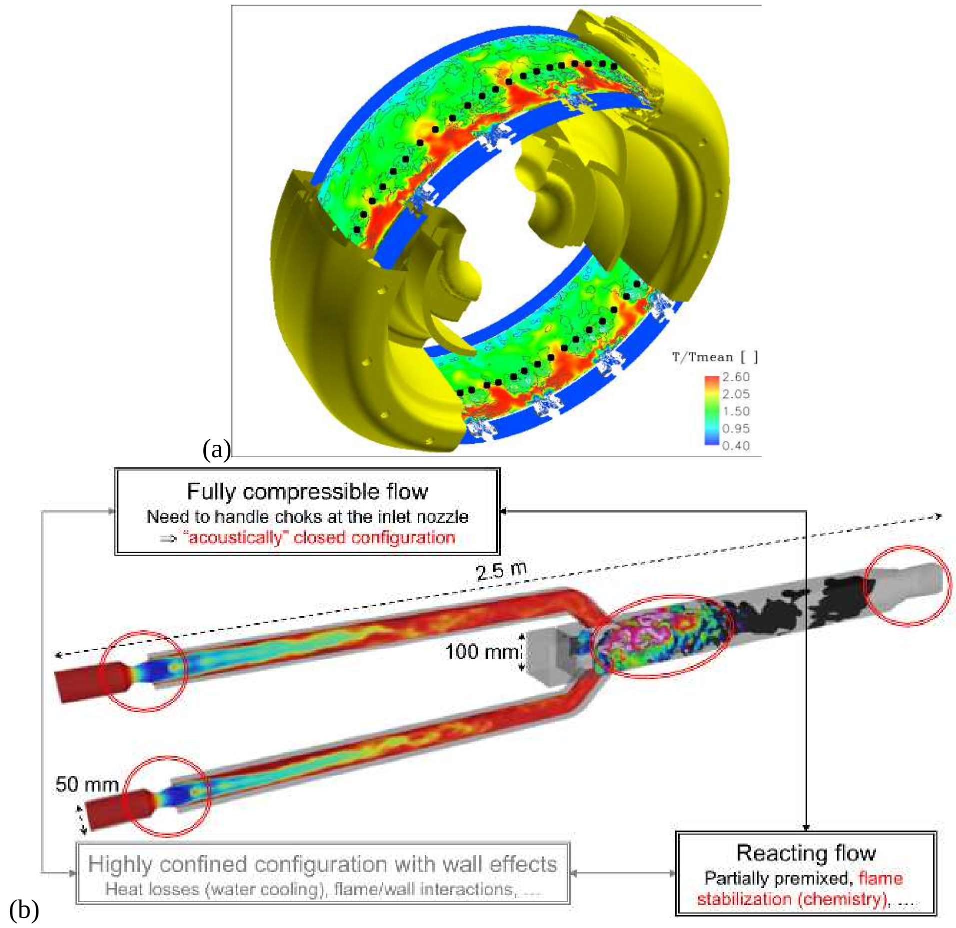
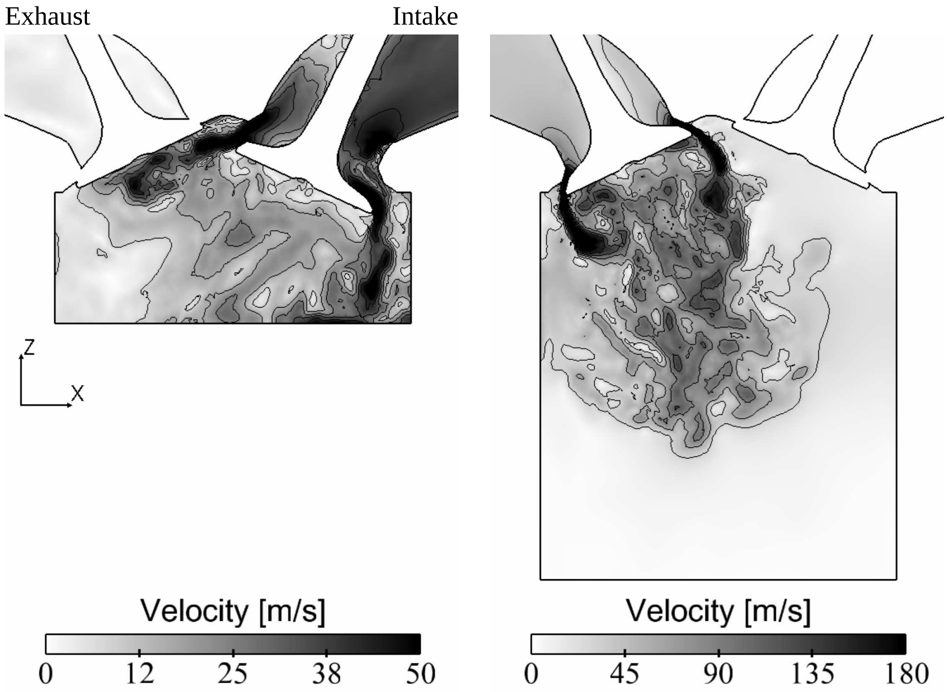


FIG. 1.3: Visualization of (a) flame and hot gases in a LES of a helicopter gas turbine combustion chamber and (b) the computational domain needed to compute the longitudinal stability of the ONERA ramjet burner.

In piston engines, cycle-to-cycle variations (CCV) are detrimental in terms of combustion efficiency, and are thus essential to understand and control in an attempt to further optimize overall engine efficiency. The difficulty is that many different mechanisms can lead to CCV, and that their importance and interactions can hardly be studied using only standard engine experiments based on cylinder pressure analysis. The multi-cycle LES performed during the PhD thesis of B. Enaux and V. Granet have confirmed the high potential of LES to accurately capture cyclic combustion variations in piston engines ([COMB44]). The computational domain considered in these simulations covers almost the whole experimental setup (intake and exhaust plenums, intake and exhaust ducts, flame-arrestors, cylinder) to account for acoustic phenomena. It was shown that LES can now be performed over 25 to 30 consecutive cycles and is able to distinguish between stable operating points (i.e. operating points with low CCV levels) and unstable operating points (high CCV levels) and can bring a new insight into the causes and mechanisms of cyclic variability. This collaborative work with IFP clearly illustrates why and how LES can be used to study and understand unsteady phenomena in piston engine applications.



[300 CAD before TDC] [145 CAD before TDC]

FIG. 1.4: Instantaneous velocity fields (LES) in a vertical cross-section of the 10th cycle.

1.3.2 Acoustic tools for combustion instabilities and noise (E. Gullaud, K. Wieczorek, C. Silva, M. Leyko, C. Sensiau, J. Richard, F. Nicoud, T. Poinsot)

Acoustics play a key role in combustion and must be accounted for both experimentally and numerically. To understand confined flames, the LES codes presented in Section 1.3.1 are powerful tools but they are also extremely expensive. An alternative and complementary path is to develop acoustic codes solving the wave equation in complex geometries for reacting flows. CERFACS is developing a full three-dimensional Helmholtz solver (called AVSP) solving the Helmholtz equation in the frequency domain. It is coupled to the LES code AVBP : they use the same data structure ; the fields of mean temperature, mass fraction and local flame transfer function required by AVSP are obtained by post-processing AVBP simulations. As an example, Fig. 1.5 shows how the geometry description influences the structure and frequency of the second annular mode in a full annular chamber with 15 burners. These modes are often crucial for the stability of the combustor and for its noise emission. The AVSP code has now been used to study a variety of academic [8] and industrial [COMB40] configurations. The major recent development is the implementation of a model for the acoustic damping of multi-perforated walls [COMB19, COMB28]. Besides, a preliminary version of a generalized acoustic tool which accounts for the mean flow effects has been developed [COMB31]. AVSP has also been adapted to handle issues related to the combustion noise thematic. This AVSP-forced version of the code (as opposed to the AVSP-modal tool used for thermo-acoustic modes analysis) uses acoustic sources from AVPB to compute the acoustic spectrum in the near field region. This methodology was used to represent the direct noise from an academic combustor studied experimentally at Ecole Centrale Paris. The indirect noise generation (noise generated from entropy spots interacting with regions of strong mean velocity gradient) has also been addressed from a theoretical

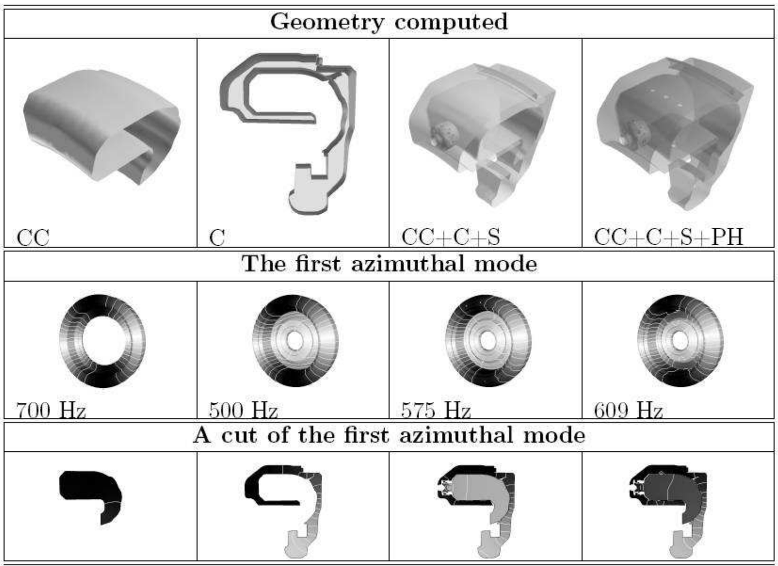


FIG. 1.5: Acoustic analysis of a gas turbine annular chamber. Influence of the geometry on the first azimuthal eigenmode calculated by AVSP (light grey denotes a pressure anti-node and black gray a pressure node).

point of view and a simple analytical model has been developed to assess the direct-to-indirect noise ratio [COMB26]. Besides, the theory of propagation in compact nozzles [6] was extended in order to propose an appropriate representation of the Entropy Wave Generator [1] experiment developed at DLR [COMB27].

1.3.3 LES of ignition (G. Lacaze , B. Enaux, J.-P. Rocchi, B. Cuenot, T. Poinsot)

Ignition, and high-altitude relight, are critical phases for aeronautical burners, which directly affect their design. They are also complex processes, which require good premixing of the gaseous reactants and favourable flow dynamics. In rocket engines, ignition must be performed with a minimum pressure peak, to avoid damage to the engine. In piston engines, ignition is also crucial and CERFACS leads research on ignition for both turbines and piston engines.

Ignition is a transient process for which LES is the best adapted CFD tool. However the very first moments of ignition (either by a spark plug, a hot jet or a laser) correspond to very small scale, out-of-equilibrium thermodynamical processes, that are out of reach of standard CFD solvers : a model is required to represent this first phase of ignition, still guaranteeing a correct evolution of the igniting gases afterwards.

This model implemented in AVBP allowed to successfully compute various industrial configurations : rockets, aeronautical burners or piston engines. Interesting results were obtained in terms of optimized location of igniters and allowed a better understanding of the flame developments, propagation and stabilisation [COMB4, COMB23, COMB24].

1.4 LES of transcritical flow and combustion (T. Schmitt, A. Ruiz, B. Cuenot), L. Selle

Liquid propulsion for rocket engines involves fluids in a transcritical or supercritical thermodynamic state. This means that, to compute flows and flames in such systems with the correct mass flow rate and thermodynamic conditions, one has to use real gas thermodynamics.
This has been done in AVBP (in collaboration with EM2C and IMFT), where the perfect gas thermodynamics have been replaced by thermodynamics issued from a cubic equation of state. This implied not only to change the computation of thermodynamic variables, but also to modify the numerics and boundary conditions according to the modified behavior of the governing equations.
The resulting code was applied first to non reacting turbulent jets [COMB78, COMB37], then to the MASCOTTE (ONERA Palaiseau) configuration where the flame could be reproduced with the correct characteristics (in particular the correct length). AVBP-real-gas is now part of the official AVBP suite, and the simulation of a new injector for the VINCI engine is underway to help for its final design.

1.5 Coupled simulations (F. Duchaine, J. Amaya, T. Pedot, Y. Hallez, B. Cuenot, T. Poinsot)

Multiphysics has become a major topic in the team, as it is an essential step for industrial problems : being able to include for example thermal transfer in combustion simulations makes the result much closer to reality and allows to better understand the behaviour of the complete system.
Multiphysics implies not only to master different physics ans their associated solvers, but also the way they should be coupled. This raises the question of when, where and which variables should be exchanged between the solvers.
For computation efficiency, multiphysics simulations must be distributed on the processors of a parallel machine in an optimal way. This is done through a dedicated CERFACS software (PALM, which is written by the Global Change Team) that controls the different solvers and their exchanges.
The coupling of thermal transfer in solids with CFD showed very interesting results on the efficiency of cooling systems [COMB12, COMB11]. The coupling of combustion with radiation also showed interesting results on the flame structure and thermal transfer to the walls [COMB57, COMB2]. In his PhD, J. Amaya coupled all three solvers (Combustion-AVBP, therma transfer-AVTP and radiation-PRISSMA), which opens the door to a wide range of new problems and applications.

1.6 Software engineering (G. Staffelbach, O. Vermorel, P. Estival, E. Riber, A. Dauptain)

CERFACS has a very significant experience in having multiple users (engineers, PhD students, post-doc.) run large LES codes on massively parallel machines. This experience shows that CPU time, disk usage and first of all, human time are easily wasted when research codes are simply distributed to users. The CFD team has developed two main actions to improve the efficiency of LES : the first one is the training of users with a one-week hands-on course organized at CERFACS two or three times a year and which has allowed more than 80 attendants to learn LES in a high-level practical formation. The second action is the encapsulation of AVBP in an interface software called C3S which controls pre-, run and post-processing phases of AVBP and hides from the users most of the delicate options of an LES research code.
C3S is a large scale (9 person-years since 2007) project to make LES useful for industry engineers but also to minimize users time and errors in organizing the running, pre- and post-processing of LES.

C3S started on April, 23rd, 2007. The version 3.1 of the C3S software has been delivered to the partners on February, 20th 2010. The engineers of Turbomeca and Safran Villaroche have a daily use of C3S now. The engineers Vacheslav Anisimov and Carmine Russo are using C3S in the frame of the Ansaldo contract. C3S is also distributed in CNRS laboratories (EM2C, IMFT), and will be available at IFP and PSA soon.

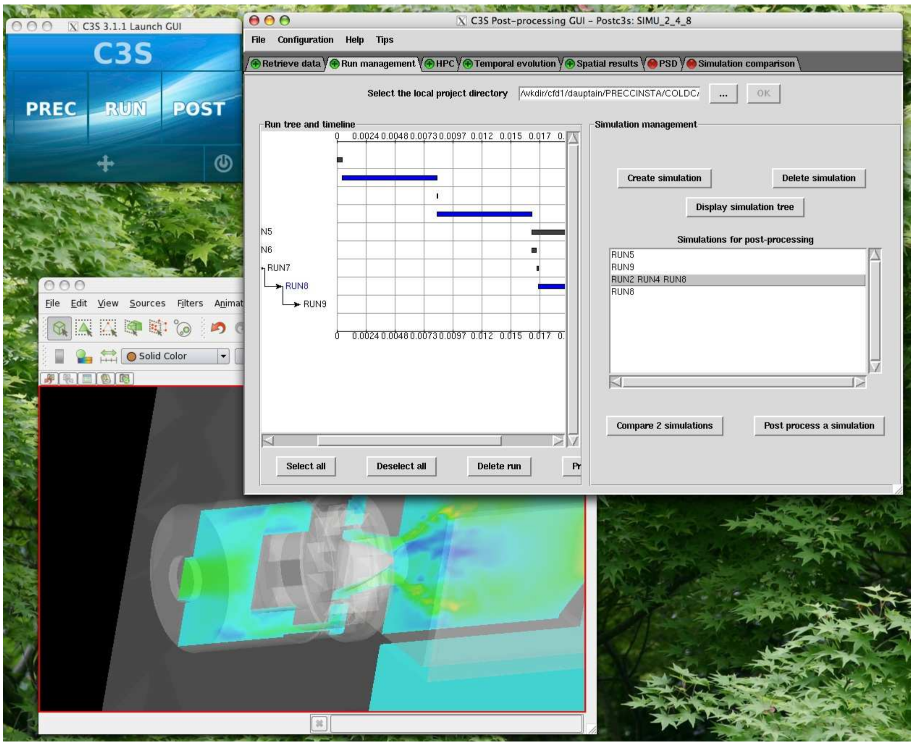


FIG. 1.6: A C3S session, upper left the control panel, upper right a run management graph, bottom, a Paraview session launched fron C3S.

More than just giving access to LES simulations, C3S introduces a new standard in performing LES : the runs are stored with a high level of tracability, high performance computing statistics and memory usage statistics are constantly presented, and a wide range of post-processing tools are included in the C3S distribution. This explains why the C3S users community is increasing, in particular when LES simulations have to be exchanged between CERFACS and its partners.

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7

Aviation and Environment

1 Introduction

Jean-François Boussuge

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Our mission is to be a bridge between academic research and industrial applications in such a way that industry can benefit as soon as possible from recent developments associated to CFD. To fulfil this, we develop and improve methods and tools that are or will be daily used in industry. The core activity is dedicated to the structured CFD solver *elsA* which belongs to ONERA and for which Cerfacs has an official agreement to participate to its development.

During the past two years, the capability of *elsA* has been enhanced in various directions connected to modelisation, meshing flexibility and multi-physics applications. Major points are high-order methods for acoustics simulations, the development of the next generation of flow solver based on structured/unstructured meshes and last the growth of multiphysics simulations.

Besides *elsA*, we have access to in-house solvers : AVBP for unstructured Large Eddy Simulation (LES) and NTMIX for Direct Numerical Simulation (DNS) applications. NTMIX has been rewritten in order to make it more efficient on massively parallel machines and also to increase its scope (ability to handle semi-complex configurations with a multiblock approach).

The next sections are structured into three parts : the first one covers the activities related to numerical methods (Time Spectral Method approach, high order schemes, surrogate model based on proper orthogonal decomposition, adjoint method...) ; the second part deals with the applications (aircraft and turbomachine simulations) ; the last one concerns software engineering.

This work is done in collaboration with national and European research actors through various projects : ONERA, LMFA, LEA, DLR, UPMC, University of Sherbrooke and University of Montpellier for the research part ; on the industrial side, Airbus, Snecma and Turbomeca. A new collaboration is currently beginning with DynFluid (ex SINUMEF).

2 Simulations of aircraft wakes and rocket launch emissions

2.1 Wake chemistry and microphysics in the vortex regime (L. Nybelen, R. Paoli, J. Picot, D. Cariolle)

A chemical/microphyscal module fully integrarted with the dynamics (on line coupling) was developed for wake simulations inside NTMIX solver. This objective of this research was to develop a chemical and microphysical model for the simulation of gaseous and particulate emissions in the near-field of an aircraft wake. The approach consists in solving the three-dimensional Navier-Stokes equations together with the conservation equations for each chemical species. The numerical code used for the simulations is NTMIX developed at CERFACS. This gives directly access to all dynamics/chemistry interactions that are important during the jet expansion and its interaction with the wake vortices. The kinetic scheme consisted of 14 species including $\mathrm{NO_x}, \mathrm{HO_x}$ and $\mathrm{HNO_3}$, 34 gaseous reactions and 2 heterogeneous reactions that take place on ice particles surface. The latter are treated as Lagrangian clusters that are followed throughout the flow. The simulation were carried out in consists in two steps : first solve the near-field wake, i.e. $0 < t < 10\,s$ on a small domain and a very fine mesh. These simulations include the exhaust jet and its interaction with the trailing vortex. These at $t = 10\,s$ where then averaged averaged in the axial direction and interpolated on a coarser mesh and a larger domain commensurate with the vortex Crow instability wavelength (about $400\,m$). The advantage of this methodology is that the data can be smoothly recovered from one domain to another, and the same model and numerical solver is used. Figure 2.1 shows the distribution of particles around vortices in the two-engines and four-engines aircraft case, respectively. In the four-engine case, the wake is much larger because of the double entrainment of the external inboard jet which is initially far from the trailing vortex. This impact the initiliazation in the following far-field and in particular a significant part of the particles are not entrained by the system of the two-corating vortices as shown in Fig. 2.2.

2.2 Wake microphysics in the diffusion regime (R. Paugam, R. Paoli, C. Sarrat, A. Crespin, D. Cariolle)

2.2.1 Three-dimensional simulations (R. Paugam, R. Paoli, C. Sarrat, D. Cariolle)

Three-dimensional numerical simulations of the evolution of a contrail in diffusion regime were carried using the MesoNH code. The initial conditions were taken from the data at $t = 40\,min$ obtained by R. Paugam in his thesis. Four hours of the transition contrail to cirrus are simulated. The results show the horizontal contrail spreading over 3200 m width, while the vertical extent remains limited (see Fig. 2.3). At this stage of the dissipation regime, the primary and secondary wakes are not separated any more. The model is able to maintain a high optical depth as a result of an ice density decrease coupled with an increase of the mean radius of the particles in the growing contrail by condensation of ambient water vapor (see Fig. 2.4).

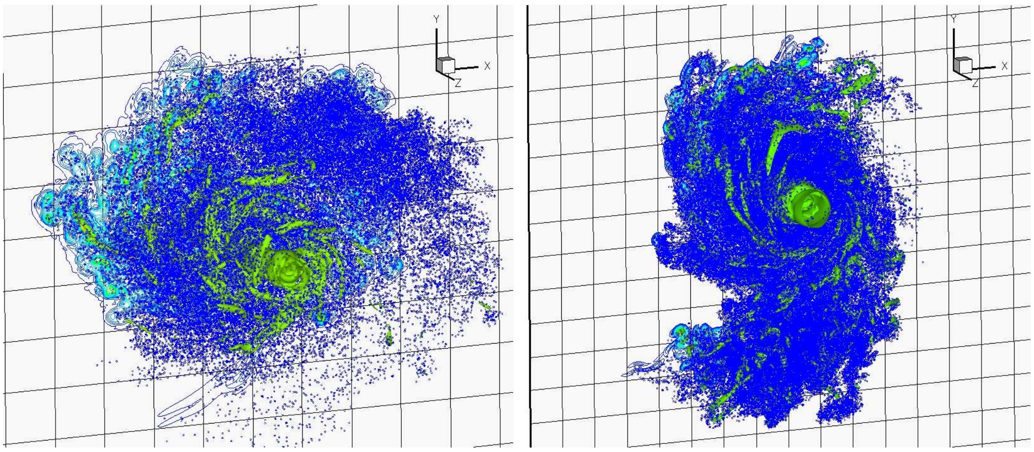

FIG. 2.1: Vorticity isosurface (green) and particle distribution in two-engine (left panel) and four-engine (right panel) aircraft at $t = 8\,s$.

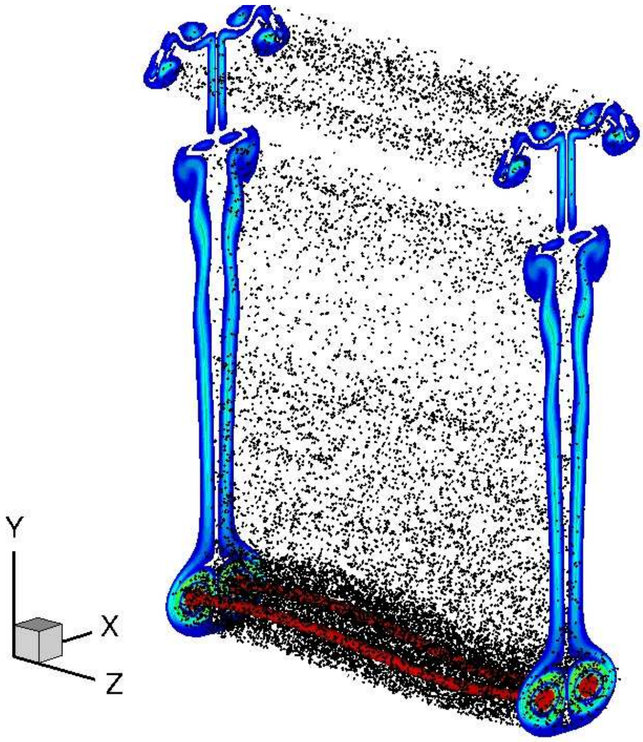

FIG. 2.2: Vorticity contour and particle distribution at $t = 100\,s$ showing the first and secondary wake and the exhaust non-entrained by the trailing vortex.

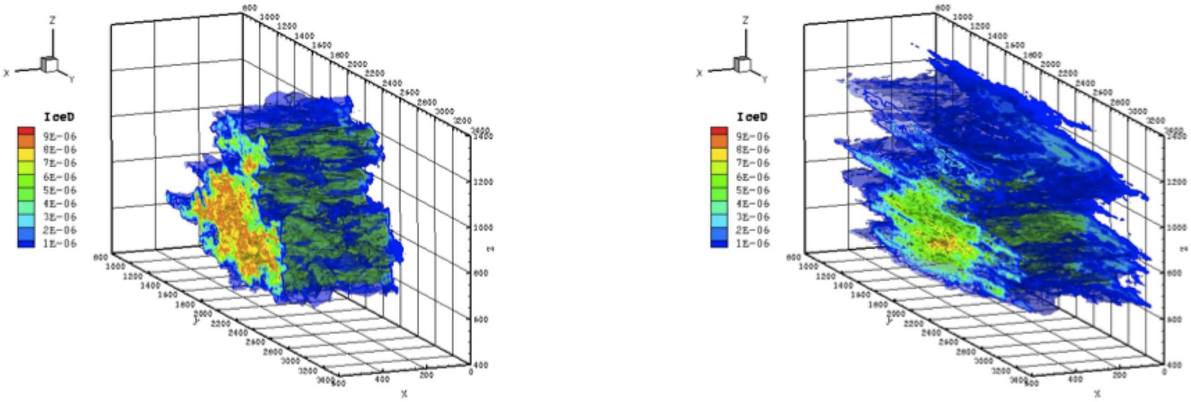

FIG. 2.3: Three-dimensional view of the contrail, over a 500m portion. The aircraft flight is along the x-axis. The colored iso-surfaces represent the ice density : (a) at $t = 2320\,s$ and (b) at $t = 10120\,s$.

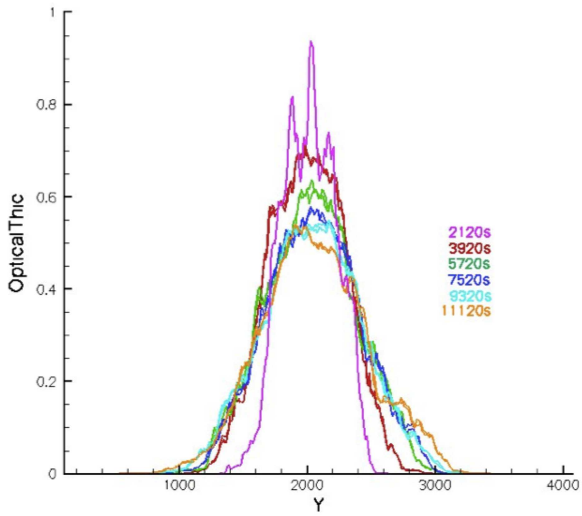

FIG. 2.4: Contrail optical thickness as a function of the horizontal axis, perpendicular to the flight direction. The optical thickness is integrated over the vertical, each colored line represents a time of the evolution.

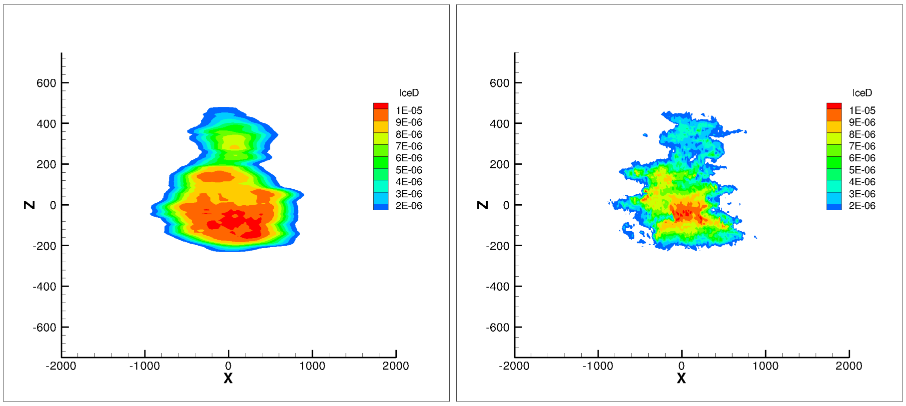

FIG. 2.5: Two-dimensional maps (cross section perpendicular to the flight direction) of ice density (in kg m^{-3}) one hour after the exhausts emissions by the airplane, with the diffusion-condensation model (left panel, with $Dx = 10m^2s^{-1}$ and $Dz = 0.001m^2s^{-1}$), and with Meso-NH (right panel).

2.2.2 Simulations with a diffusion-condensation model (A. Crespin, R. Paoli)

A two-dimensional diffusion-condensation model (in a plan perpendicular to the flight direction) at high resolution (10m et 1s) have been developed to simulate the spreading of a contrail ("condensation trail") in a sursaturated environment, from a few hours to several days after the passage of an airplane. The model has the same microphysics than the NTMIX and Meso-NH models.

The model is initialized with Meso-NH fields at the beginning of the diffusion phase (at 30min).The model outputs have been compared with Meso-NH meso-scale model. The contrail evolution with the diffusion-condensation model shows good consistency with Meso-NH (see Fig. 2.5). The size of the ice particules increases by condensation of available humidity. Ice density is greater in the center of the contrail where more nucleation particules are available. On the edges of the contrail, ice particules are larger because more water vapor is available for condensation. The good agreement between particule density in the diffusion model and in Meso-NH shows that, to a first order, the contrail evolution can be represented by diffusion processes coupled to microphysics. However the condensation appears too large in the diffusion model, in particular on contrail edges where particule radius are larger than Meso-NH outputs. Further simulations are under way to assess the impact of the level of sursaturation on the ice crystal size and on the optical thickness. The ultimate goal is to obtain a relationship between optical depth, turbulence level and sursaturation.

2.3 Impact of Ariane V launches on atmospheric O_3 (C. Sarrat, D. Cariolle)

Rockets with solid propellant like Ariane V or Titan IV emit in the atmosphere a large number of chemical species and particles. In the stratosphere, from about 10 km to 70 km, the boosters are used and the largest part of the exhausts are emitted. Although the environmental impact of such rockets in the troposphere have been performed, there are few studies on the stratospheric impact despite that most of the ozone layer is encountered at those altitudes.

The rockets use propergol that emits a large amount of chlorine species with a significant proportion in form of radicals that can destroy the ozone layer. Measurement campaigns have been performed in May and December 1996 during two Titan IV launches. Aircraft measurements made inside or outside the rocket

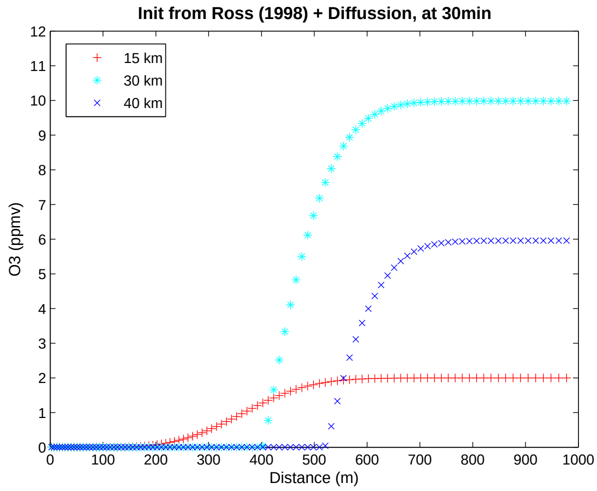

FIG. 2.6: Impact of a Titan IV rocket on the ozone content at 15 km, 30 km et 40 km altitude, 30 mn after the launch.

plumes show that few minutes after the launch the ozone content inside a 8 km wide plume is severely depleted.

Using a chemical-diffusion model we have calculated the ozone evolution expected after a Titan IV launch and found that the chlorine radical are very efficient to deplete ozone from about 15 to 40 km. Those results (see Fig. 2.6) are consistent with measurements and with previous calculation previously published.

We have repeated the same calculations for the Ariane V case but, due to the uncertainties in the chlorine emission indices of that rocket the resultas are very preleminary. To reduce uncertainties a cooperation have been developed with the SNPE at Bordeaux that will calculate more precise values for the emission indices, in particular with the account of species transformation during the post-combustion phase. Given the importance of those studies, CNES has decided to further support our studies and more results are expected in the years to come.

3 Large scale ozone distribution and emissions from aircraft and ships

3.1 Introduction of plume chemistry into large-scale atmospheric models : application to aircraft NO_x emissions (D. Cariolle, B. Cuenot, R. Paoli, R. Paugam)

We have developed a new method to account for the non-linear chemical effects during plume dispersion (Cariolle et al. 2009). The method is suitable for isolated NOx emissions from local sources and leads to a parameterization that is implemented in a global model and use to evaluate the impact of aircraft emissions. Compared to previous approaches that introduce corrected emissions or corrective factors to account for the non-linear chemical effects, our parameterization is based on the description of the plume effects via a fuel tracer and a lifetime during which the non-linear interactions between species are important and operate with effective reaction rates (ERR). The implementation of the parameterization insures mass conservation and allows the transport of non-diluted emissions in plume-form by the model dynamics. With inclusion of the plume effects, the simulations with the LSCE model of the impact of aircraft emissions are in rather good agreement with previous work. We found that the ozone production is decreased by 10 to 15 $\%$ in the northern hemisphere with the largest effects in the north Atlantic corridor when we account for plume effects on the chemistry (see Fig. 3.1). These figures are consistent at the global scale with evaluations made with corrected emissions, but regional differences are noticeable due to the possibility offered by our parameterization to transport emitted species in plume-form before operating at large scale.

3.2 Introduction of plume chemistry into large-scale atmospheric models : application to ship emissions (D. Cariolle, B. Cuenot, R. Paoli)

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The ERR method described above (Cariolle et al. 2009), has been adapted by Huszar et al. 2009 to treat the NO_x emission by ship within the near Atlantic european corridor. In this study the chemistry transport model CAMx has been used. CAMx is an Eulerian photochemical dispersion model developed by ENVIRON Int. Corp. (http ://www.camx.com). Model results show that the ship traffic emissions strongly modify NO_x levels not only over remote ocean but also at coastal areas and to some extent over land at greater distances from the sea. High NO_x levels occur along major shipping routes enfolding Western Europe from south of the Iberian Peninsula heading north around the British Islands to Northern and Baltic Seas. Highest levels of 4-6 ppbv are found over the English Channel during both seasons with peaks up to 8 ppbv in summer.NO_x is enhanced by more than 1 ppbv almost everywhere along the vessel corridors. Over the distant ocean, shipping traffic enhances NO_x surface levels by hundreds of pptv. Due to transport over the land, ship emissions affect also inland concentrations.

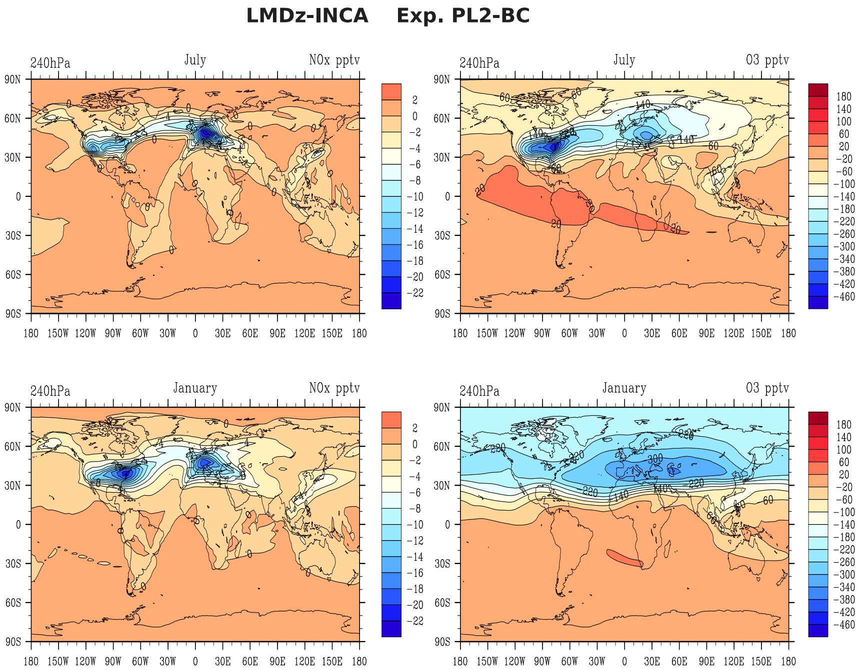

FIG. 3.1: LMDz-INCA model distributions of the NO_x (left) and O_3 (right) variations at 240 hPa in January (bottom panels) and July (upper panels) due to plume effects using the ERR method.

With the inclusion of the ERR plume parameterization (with $\tau = 1$ hour), the average surface large-scale NO_x concentration decreases by up to 0.1 ppbv over remote sea during both seasons. The reduction in the main corridors is much more intensive and exceeds 1 ppbv at peak levels in both summer and winter. This can be also interpreted as the modification of the NO_x perturbation caused by ship emissions. In relative numbers, model simulations show that ship NOx perturbation is reduced by more than 10 % along shipping routes. Areas of intensive ship traffic (coastal regions and the most important shipping corridors) indicate larger reduction up to 20-25 %. As a consequence, ozone production due to the ship emission is lessened. The ship plume effects lead to decrease of ozone in both summer and winter seasons. The reduction occurs on the whole area of the European domain with the largest effects in the shipping corridors where the ozone reduction reaches values of about 0.4-0.7 ppbv in winter and 1-2 ppbv for summer conditions.

4 Publications

4.1 Journal Publications

[PAE1] Barret, B., P. Ricaud, C. Mari, J.-L. Attié, N. Bousserez, B. Josse, E. Le Flochmoen, N. L. Livesey, S. Massart, V.-H. Peuch, A. Piacentini, B. Sauvage, V. Thouret, and J.-P. Cammas. Transport pathways of CO in the African upper troposphere during the monsoon season : a study based upon the assimilation of spaceborne observations. *Atmos. Chem. Phys.*, 8, pp. 3231-3246, 2008

[PAE2] Cariolle, D., M. J. Evans, M.P. Chipperfield, N. Butkovskaya, A. Kukui and G. Le Bras. Impact of the new HNO_3 forming channel of the $HO_2 + NO$ reaction on the tropospheric budgets of HNO_3, NO_x, HO_x and ozone. *Atmos. Chem. Phys.*, 8, 4061-4068, 2008.

[PAE3] Cariolle, D., D. Caro,R. Paoli, D. Hauglustaine, B. Cuenot, A. Cozic, and R. Paugam. Parameterization of plume chemistry into large-scale atmospheric models : application to aircraft NO_x emissions. *J. Geophys. Res.*, 114, D19302, 2009.

[PAE4] Chosson, F., R. Paoli, and B. Cuenot (2008) Ship plume dispersion rates in convective boundary layer for chemistry models, *Atmos. Chem. Phys.*, 8,4841-4853.

[PAE5] El Amraoui, L., V.-H. Peuch, P. Ricaud, S. Massart, N. Semane, H. Teyssedre, D. Cariolle, and F. Karcher. Ozone loss in the 2002-2003 Arctic vortex deduced from the assimilation of Odin/SMR O_3 and N_2O measurements : N_2O as a dynamical tracer *Q. J. R. Met. Soc.*,134, 217-228, 2008.

[PAE6] Filippi, J.-B., F. Bosseur, C. Mari, C. Lac, P. Le Moigne, B. Cuenot, D. Veynante, D. Cariolle, and J.-H. Balbi. Coupled atmosphere-wildland fire modeling *Journal of Advances in Modeling Earth Systems*, Vol. 1, art. 11, 2009.

[PAE7] Huszar, P., D. Cariolle, R. Paoli, T. Halenka, M. Belda, H. Schlager, J. Miksovsky, and P. Pisoft. Modeling the regional impact of ship emissions on NO_x and ozone levels over the Eastern Atlantic and Western Europe *Atmos. Chem. Phys. Disc.*, Vol. 9, pp. 26735-26776, 2009.

[PAE8] Massart, S., C. Clerbaux, D. Cariolle, A. Piacentini, S. Turquety, and J. Hadji-Lazaro. First steps towards the assimilation of IASI ozone data into the MOCAGE-PALM system *Atmos. Chem. Phys.*, 9, pp. 5073-5091, 2009.

[PAE9] Nybelen, L. and R. Paoli. Direct and large-eddy simulations of merging in corotating vortex system. *AIAA Journal*, 47, 157-167, 2009.

[PAE10] Pannekoucke, O., and S. Massart. Estimation of the local diffusion tensor and normalization for heterogeneous correlation modelling using a diffusion equation *Q. J. R. Met. Soc.*, 134, 1425-1438, 2008.

[PAE11] Paoli, R., X. Vancassel, F. Garnier, and P. Mirabel (2008), Large-eddy simulation of a turbulent exhaust jets and a vortex sheet interaction : particle formation and evolution in the near field of an aircraft wake. *Meteorologische Zeitschrift*, 17, 131-144.

[PAE12] Paoli, R. and K. Shariff. Turbulent Condensation of Droplets : Direct Simulation and a Stochastic Model. *J. Atmos. Sci.*, 66, 723-740, 2009.

[PAE13] Paugam, R., R. Paoli, and D. Cariolle (2009) Three-dimensional numerical simulations of the evolution of a contrail and its transition into a contrail-cirrus , *Atmos. Chem. Phys. Disc.*, 9,20429-20469.

[PAE14] Semane, N., V.-H. Peuch, S. Pradier, G. Desroziers, L. El Amraoui, P. Brousseau, S. Massart, B. Chapnik, and A. Peuch. On the extraction of wind information from the assimilation of ozone profiles in Météo-France 4D-Var operational NWP suite *Atmos. Chem. Phys.*, 9, pp. 4855-4867, 2009

4.2 Technical reports

[PAE15] Massart, S., B. Pajot, A. Piacentini and O. Pannekoucke On the deficiencies of the 3D-Fgat assimilation method. *CERFACS Technical Report*,TR/AE/09/87, 2009.

[PAE16] Massart, S., C.Clerbaux, D.Cariolle, A.Piacentini, S.Turquety and J.Hadji-Lazaro First steps towards the assimilation of IASI ozone data into the MOCAGE-PALM system. *CERFACS Technical Report*,TR/AE/09/04, 2009.

[PAE17] Pannekoucke, O., and S. Massart Estimation of the local diffusion tensor and normalization for heterogeneous correlation modeling using a diffusion equation. *CERFACS Technical Report*,TR/AE/08/13, 2008

8

Aerodynamics and Multiphysics

1 Introduction

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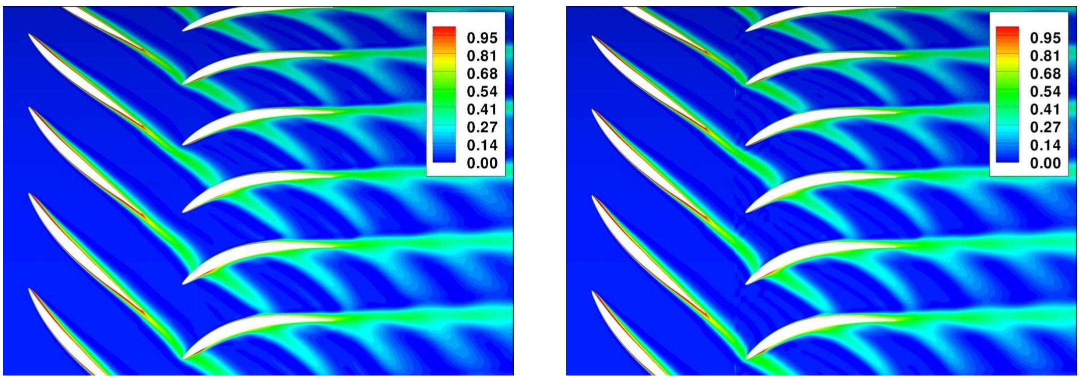
2 Numerical aerodynamics

2.1 Numerical methods

2.1.1 Development of phase-lagged boundary conditions for the Time Spectral Method (F. Sicot, G. Dufour)

The Time Spectral Method (TSM) is a numerical method dedicated to the simulation of time-periodic flows. It aims at providing a physical precision close to classical unsteady RANS techniques but at a much lower computational cost. After being successfully applied at Cerfacs to external aerodynamic flows, a new phase of development was needed to target turbomachine configurations. The so-called phase-lag periodic condition has been implemented in *elsA*, as it allows to solve for only one blade per row regardless of each row blade count. It has been adapted to the TSM, and the proposed method is an intermediate between the direct-store and shape correction methods. The row interface is based on a sliding non-abutting block boundary condition and requires sophisticated space-time interpolations, together with anti-aliasing filtering. Developments have been validated for a rotor/stator configuration. Figure 2.1 compares entropy contours in a blade to blade plane for a compressor stage, showing good agreement between the TSM solution and a classical unsteady time integration scheme. For this case, the CPU gain is four.



(a) Classical unsteady scheme (b) TSM computation with five harmonics

FIG. 2.1: Computation of rotor/stator interactions in a compressor stage : comparison of the TSM solution with a reference solution for entropy contours.

2.1.2 Harmonic Balance Technique for multistage compressors (T. Guedeney, G. Dufour)

The Time Spectral Method (and its associated phase-lagged boundary conditions) is based on the assumption that only one frequency and its harmonics are needed to model the flow field (for example the blade passing frequency of the rotor in the domain of the stator). Therefore, the TSM allows to simulate only one stage of a turbomachine. To extend this method to multistage turbomachines, we need to take into account several frequencies which are not necessarily multiples of a base frequency. To implement this method called Harmonic Balance Technique (HBT), we adapted all the features developed for the TSM to a multi-frequency formulation. TSM and HBT give the same results on a compressor stage. However, conditioning problems may appear in HBT and will need more work. Figure 2.2 presents the flow field in a compressor, coloured with entropy. It shows the interaction process between the incoming wakes (generated by the upstream rotor) and the stator.

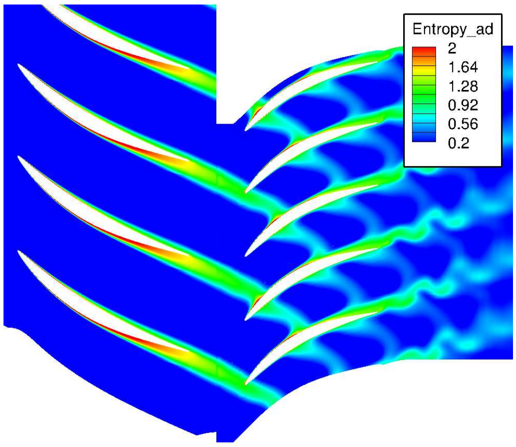


FIG. 2.2: HBT simulation in a multistage compressor. Flow field coloured with entropy on a blade to blade plane.

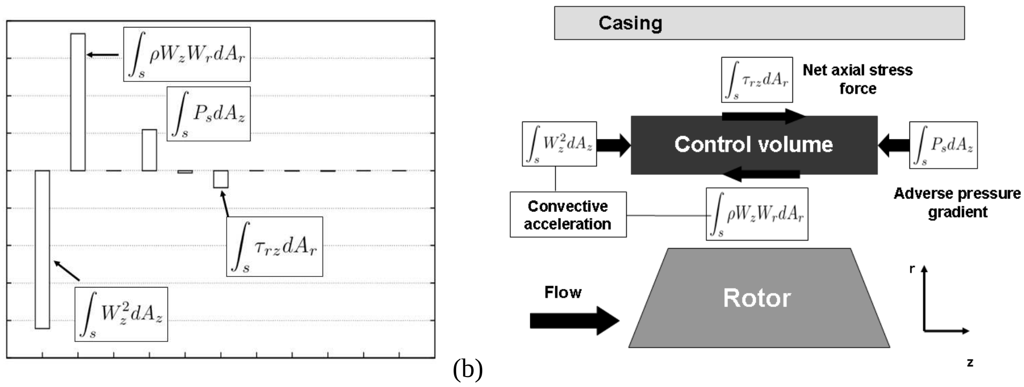
2.1.3 Advanced methods for post-processing in turbomachines (G. Legras, F. Wlassow, N. Gourdain)

Design of turbomachines leads to complex geometries that make the analysis of results often very difficult. Sophisticated post-processing methods are required, for example to analyse rotor-stator interactions or the development of instabilities. The modal analysis of unsteady signals (in time and space) taken in a multi-stage components is complex due to row interactions. A first method has been developed at CERFACS, based on the application of :

1. a spatial Discrete Fourier Transform (DFT),
2. a temporal DFT on the spatial modes,
3. the Tyler & Sofrin model [1] to determine the origin of spatial modes and their rotating speed.

The results give a mapping of spatial vs. temporal modes. This tool is well adapted to the analysis of rotor-stator interactions at all operating points but also when rotating stall phenomena occur.

A second tool has been developed, based on the model of Shabbir & Adamczyk [2] who proposed a new approach for the analysis of near wall flows (originally for the analysis of casing treatment performance near the rotor casing). Their idea was to perform a budget of the axial momentum equation on a control volume located in the region of interest. This approach has been developed at CERFACS and expanded to all RANS equations (steady or unsteady flows, Cartesian or cylindrical formulation, etc.). The tool has been validated for the flow analysis in the transonic test case NASA ROTOR37 with axisymmetric casing treatment and is now used to study casing treatment mechanisms in an industrial multistage compressor.



(a) (b)

FIG. 2.3: Application of the Shabbir & Adamczyk model to the flow analysis in the NASA ROTOR37 test case. (a) Balance of the axial momentum equation and (b) sketch illustrating the axial forces acting on the casing control volume.

Figure 2.3 illustrates the application of the Shabbir & Adamczyk method on a control volume located near the casing of a single transonic rotor. Preliminary results highlight the tool capabilities to analyse the flow physics in turbomachines and design casing treatments in compressors.

[1] Tyler, J.M. and Sofrin, T.G., *Axial flow compressor noise studies*, SAE Transactions, Vol. 70, pp. 309-332, 1962
[2] Shabbir, A. and Adamczyk, J.J., *Flow mechanism for stall margin improvement due to circumferential grooves casing on axial compressors* J. Turbomach., Vol. 127, Issue 4, pp. 708 -718, 2005

2.1.4 *elsA* upgrade for aeroacoustics (H. Deniau, A. Fosso-Pouangué)

2.1.4.1 Numerical scheme

During the last years, the need of high fidelity simulations on complex geometries for aeroacoustics predictions has grown. Most high fidelity numerical schemes, in terms of low dissipative and low dispersive effects, are based on Finite-Difference (FD) approaches. But for industrial applications, FD schemes are less robust than Finite-Volume (FV) ones. Thus the present study focuses on the development of a new compact high-fidelity scheme for two- and three- dimensional applications.
This scheme is formulated in physical space and not in computational space so that they are more appropriate for general grids. They are based on compact interpolation to approximate interface-averaged field values using known cell-averaged values. For each interface, the interpolation coefficients are determined by matching Taylor series expansions around the interface centre. The scheme is formally sixth-order accurate in a preferred direction almost orthogonal to the interface and at most fourth-order accurate in transverse directions. Concerning the multiblock treatment, good spectral resolution, conservativeness and low computational costs are guaranteed.

Numerous test cases as the linear convection of a Gaussian wave, the convection of a Lamb-Oseen vortex and the diffraction of an acoustic wave on a plane have been used to validate the schemes. The most efficient schemes are shown to be at least fifth-order accurate on linear and non-linear convection problems. They are also less dissipative and less dispersive on non-uniform curvilinear grids than schemes using implicit interpolation with constant coefficients of the same order on uniform Cartesian grids [1].

2.1.4.2 Boundary conditions

For aero-acoustic computations, non reflecting boundary conditions are needed and two kinds of these conditions have been implemented in *elsA* : the non radiative Tam's boundary conditions and the NSCBC ones following the Poinsot-Lele method. For the later approach, many formulations have been implemented corresponding to subsonic inflow or outflow conditions. A sponge layer treatment has been associated with these conditions to dump the wave arriving at the boundary or to impose inflow conditions with Tam's conditions.

2.1.4.3 High-order chimera interpolation

Handling complex geometries with structured grids is not always possible by using only matching multiblocks boundaries. It is sometimes necessary to use overset grids also called Chimera technique. These overset grids are exchanging information using interpolation methods. Although this method is not conservative, it makes meshing easier and facilitates the treatment of mobile parts. Moreover it allows scaling by giving the possibility to use refined grids around small geometry details.

To keep high precision, low dispersion and low dissipation properties when Chimera technique is used, a high order interpolation method has been implemented. It can use either a Lagrangian interpolation technique or an improved Lagrangian method which is optimised in Fourier space.

Validation has been done by convecting a vortex through a periodic domain composed of three overset grids. All grids have 65$\times$65 nodes (see Fig. 2.4).

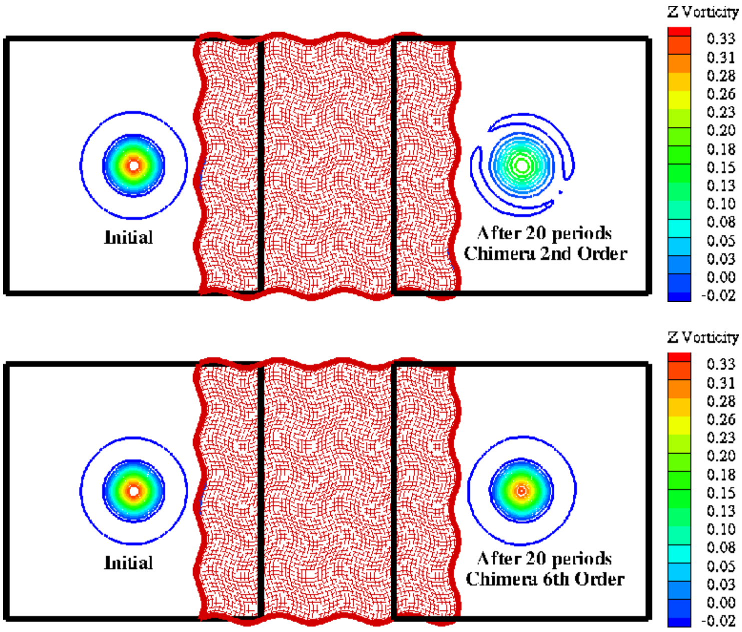


FIG. 2.4: Vortex convection test case : three overset grids are considered.

[1] Pouangué, A.F., Deniau, H., Sicot, F. and Sagaut, P., *Curvilinear Finite-Volume Schemes using High-Order Compact Interpolation*, JCP, In press 2010

2.1.5 Optimisation (M. Montagnac, J. Laurenceau, M. Mouffe)

Numerical optimisation is a central discipline for aircraft design. Cerfacs is involved in optimisation since 2005 and works mainly in preliminary and detailed design phases of an aircraft [1], [AAM13, AAM22, AAM8]. Typical industrial shape optimisations encountered at these levels usually consider several hundreds of design variables and a few constraints. All shapes must be assessed through a high-fidelity analysis with an aerodynamic solver. In this field, the choice of the optimisation algorithm is heavily constrained by the computational cost implied by one function evaluation. Thus, gradient-based optimisation algorithms are particularly valued for their speed of convergence although they only give a local optimum. In a tight collaboration with the Cerfacs Parallel Algorithms team, many different algorithms solving nonlinear optimisation problems were tested and are now used on a daily basis in the industrial context. In addition, the gradient-based choice is enhanced by the use of the discrete adjoint method that can give the gradient of the objective function with respect to the shape variables by solving only a single linear system. As a comparison, the finite difference method requires as many non-linear system resolutions as the number of shape variables. As a consequence, many numerical features have been linearized and integrated in the *elsA* software to enable optimisations on complex aircraft configurations.
Numerical optimisations are performed within the OPTaliA framework of Airbus France which includes the *elsA* software that handles both aerodynamic simulations and discrete adjoint state computations.
During the last two years, the aerodynamics team has initiated, jointly with Airbus, a project on the Multidisciplinary Design Optimisation of an aeroelastic wing. The OSYCAF project funded by the STAE foundation and starting in 2010 will involve four major players from Toulouse (Cerfacs, Onera, ISAE, UPS) that share many disciplinary scientific objectives such as computational fluid dynamics, mathematical algorithms, optimisation and structural mechanics. The unified or integrated approach for coupling the two disciplines in a fully industrial automatic process applied to a full aircraft is a long term objective.

[1] Laurenceau, J., Meaux, M., Montagnac, M. and Sagaut, P., *Comparison of Gradient Based and Gradient Enhanced Response Surface Based Optimizers*, AIAA Journal, In press 2010

2.1.6 Gas-kinetic schemes for industrial flows (H. Deniau, G. Puigt, M. Boger)

The standard discretization of the Navier-Stokes equations is based on separated schemes for convection and for diffusion. In particular, diffusion schemes generally need accurate gradient reconstruction at mesh interfaces and this task can be very challenging on multi-element unstructured grids. Gas-kinetic schemes derived from the Boltzmann equation can be seen as an alternative to classical diffusion operators. Within this approach, diffusion operator are obtained through algebraic relations as moments of a particle distribution function.
Solutions obtained with several versions of the Bhatnagar-Gross-Krook (BGK) scheme and with second-order MUSCL Roe's scheme coupled with centred schemes for diffusion are comparable (Fig. 2.5).
Our current efforts concern the validation of the scheme for complex flows, the extension of the BGK schemes to multi-dimension distribution functions and the analysis of the schemes for hybrid grids composed of structured and unstructured zones.

2.2 Flexible CFD

2.2.1 Hybrid grid approach for CFD (G. Puigt, M. Montagnac)

In CFD, structured grids are suitable for obtaining flows with anisotropy : the user has to align mesh lines with the anisotropy direction. Most numerical schemes use this property of structured grids to accelerate convergence and finally, for a complex geometry, most of the time is spent on the mesh generation process.

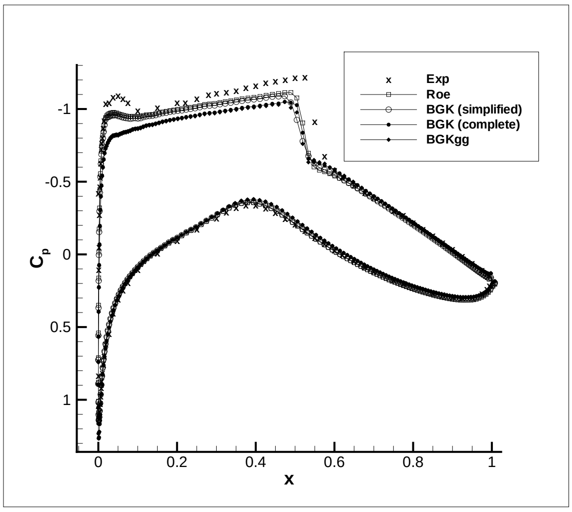


FIG. 2.5: RAE2822, comparison of pressure distribution with experimental data. Classical Roe scheme and three different versions of the gas-kinetic scheme based on BGK.

Even with the help of advanced meshing techniques like chimera or non-abutting mesh interfaces, some configurations can not be meshed nor computed with structured grids at reasonable cost.

On the other hand, unstructured meshes have become widespread as complex geometries can be meshed with little effort. Most unstructured mesh generators can account for skewed prisms and / or hexahedra for the boundary layer but on complex geometries, the unstructured hexahedral generation algorithms often produce meshes with irregular cells in the boundary layer leading to significant precision losses.

One solution is to be able to treat inside the same CFD code structured blocks and unstructured ones composed of hexahedra, prisms, pyramids and tetrahedra : structured meshes in boundary layers (except in regions of very complex geometry) and unstructured grids elsewhere. At the beginning of 2008, ONERA developed with our help a demonstrator of unstructured / hybrid CFD code based on the *elsA* code. The success lead to the implementation of unstructured capabilities in *elsA*. The *elsA* code architecture and most new lines have been implemented at CERFACS. In December 2009, Euler schemes were validated for unstructured grids (Fig. 2.6) and the work will continue.

2.2.2 Chimera technique (F. Blanc, B. Landmann, M. Montagnac)

Two techniques related to the overset grid mechanism have been improved since 2008 : the Implicit Hole Cutting approach and the patch assembly algorithm.

The main issue is to perform the ”grid assembly”, which means that each cell of the computational domain must know whether it is calculated, blanked or interpolated. Because most existing setup techniques require a tedious iterative process and a high degree of user input, two automated assembly algorithms have been developed. The implicit hole cutting algorithm is based on a grid quality criterion whereas the patch assembly algorithm gives priority of user-defined blocks over the other blocks. Both algorithms have proven to be efficient and robust on industrial configurations [AAM11, AAM16], [1-2].

[1] Landmann, B. and Montagnac, M., *A highly automated parallel chimera method for overset grids based on the implicit hole cutting technique*, International Journal for Numerical Methods in Fluids, In press 2010

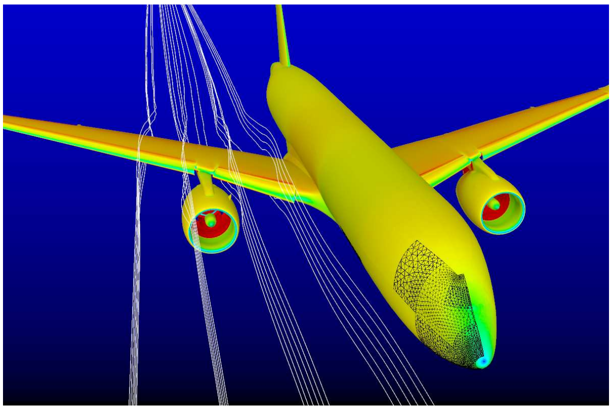
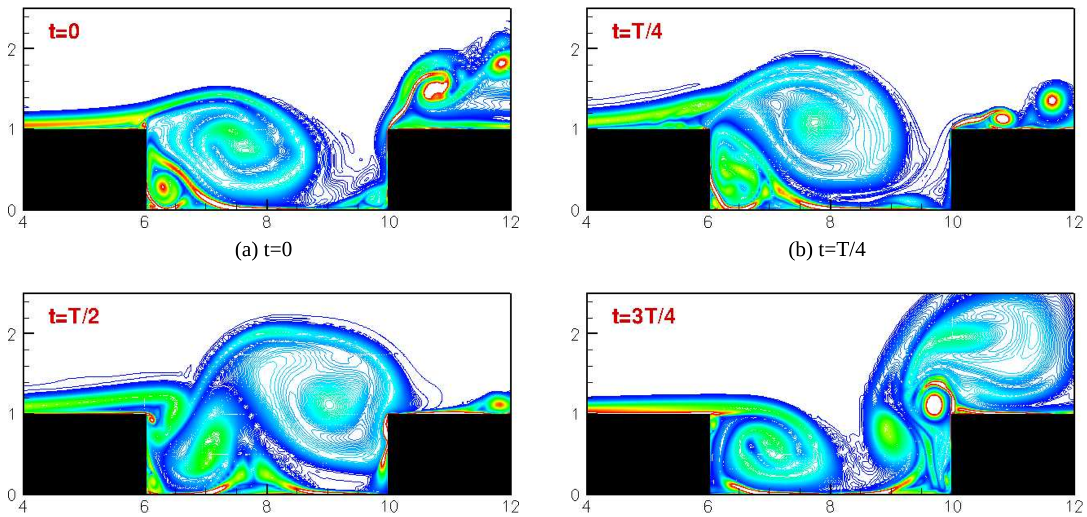


FIG. 2.6: Industrial high-lift configuration computed with the *elsA* code. Fully unstructured mesh composed of 41 million cells, splitted for computation on 64 CPUs.

[2] Blanc, F., *Patch Assembly : An Automated Overlapping Grid Assembly Strategy*, Journal of Aircraft, Vol. 47, No 1, 2010

2.2.3 NTMIX (L. Gougeon, H. Deniau)

DNS is an effective tool to achieve fundamental studies and validate models but remains expensive and often limited to simple geometries. Because of the increased complexity of simulations (physics, complex geometry), high performance computing for DNS has become a scientific challenge. In the framework of the project SND-Super (funded by the EADS foundation), a rewriting of the DNS/LES solver NTMIX has been undertaken in order to suit it to modern super-computers architectures and to increase the applications fields. The code was rewritten using current programming methods (modularity, genericity, simplified workflow based on CGNS format) and multiblock capability was added.
New implementations have been done on boundary conditions. An extension to three-dimensional cases of characteristic boundary conditions of Poinsot-Lele has been taken into account with the method of Lodato. Moreover, boundary conditions suitable for acoustic simulations are now available in the code. These are the far field boundary conditions initially developed by Tam and Dong and generalised in three-dimension by Bogey and Bailly. After successful validation and non-regression tests of the new NTMIX's release, applications of unsteady flow over a two-dimensional cavity have been performed (Fig. 2.7).



(a) t=0 (b) t=T/4

(c) t=T/2 (d) t=3T/4

FIG. 2.7: Instantaneous vorticity contours at four different times (over a period T).

3 Applications

3.1 Aircraft

3.1.1 Aircraft aeroelastic stability computations with the Time Spectral Method (G. Dufour, F. Sicot, G. Puigt)

Forced motion computations can be used to predict the aeroelastic stability of flexible structures. The Time Spectral Method (TSM) has been applied to a complete aircraft model, including turbofan intakes and mobile surfaces. The aircraft is put in forced pitching oscillation. The results are analysed by a Fourier decomposition of the unsteady pressure signal on the aircraft skin, and compared to a classical unsteady time integration scheme, the Dual Time Stepping (DTS) approach. Figure 3.1 compares the TSM results with the DTS reference. It shows a good agreement between the two methods. For this case, the TSM method is about two times faster than the DTS approach.

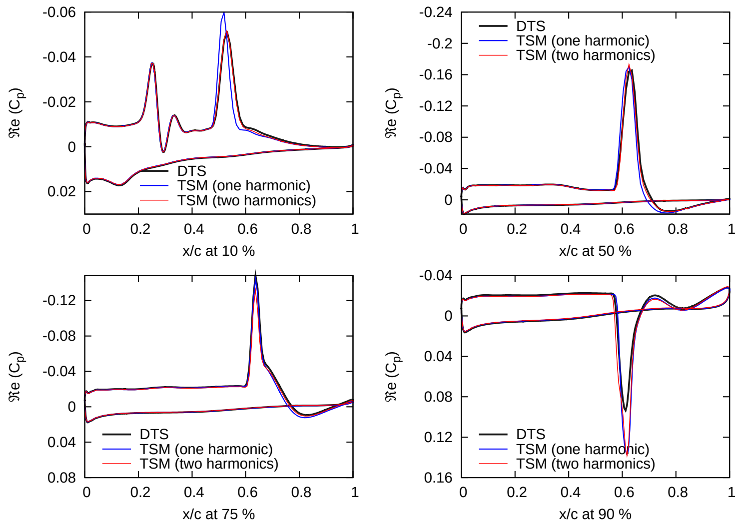


FIG. 3.1: TSM computation of a full aircraft in forced pitching motion, real part of the first harmonic of pressure.

3.1.2 Time Spectral Method for aeroelasticity simulations (F. Blanc)

Classical solutions for aeroelasticity are based on a time marching algorithm that couples a CFD solver and a structural model and require high computation times because long transient regimes must be computed before getting a stabilised periodic state, especially when the damping of the aeroelastic system is low. The Time Spectral Method allows to speed-up simulations of unsteady flows by reducing the computational time of transients. Following this idea, an extension of the TSM for aeroelastic solvers based on a coupling between a CFD solver and a structural model has been developed [AAM11, AAM16].

TSM applied to CFD computes an unsteady flow using a set of steady flow solvers coupled by a source term. In the same manner, TSM applied to aeroelasticity solves a dynamic aeroelasticity problem using a set of coupled *static* aeroelasticity problems. This technique has been applied to industrial configurations such as the computation of the periodic deformations of an aircraft due to the periodic forced motion of its control surfaces. Results are identical to those obtained with classical time marching algorithms with a computational time reduced by one order of magnitude.

3.1.3 Stability and control : dynamic derivatives (J.-C. Jouhaud, G. Joubert)

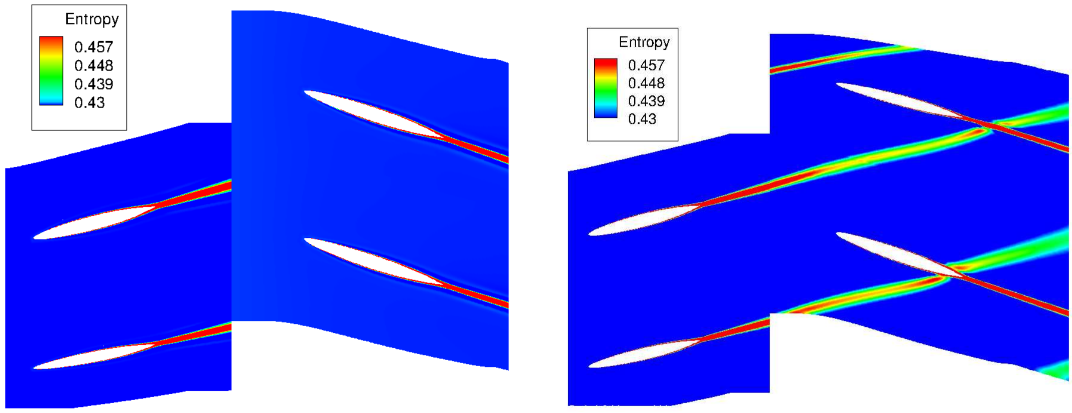
The first stages of the design process of a new aircraft focus on the sizes of the main components. The designer refers to some stability and control characteristics as a guidance of the design process. Up to now, the aerodynamic data considered in these early design steps were mostly based on tabulated data, issued from previous experience and/or semi-empirical approaches. Although satisfactory when determining some high level parameters (e.g. areas and planforms of lifting surfaces), such simplified approaches can lead to errors, especially when used in final conceptual design steps (e.g. sizing or allocation of control surfaces).
Generally, these errors can only be detected when a significant increase in the fidelity of the aerodynamic data base is made available, typically with wind tunnel data or even flight test data leading to high correction costs. Thus, the interest for an increase in the fidelity level of the aerodynamic data base is obvious, at all steps of the design process : this is one of the main objectives of the SimSAC project. This FP7 European project gathers a total of 17 partners including CERFACS and is coordinated by Professor Arthur Rizzi from KTH.
More precisely, one part of the work was the assessment and improvement of CFD tools for predicting the stability and control dynamic derivatives. Then, a numerical benchmark has been conducted in order to establish the ability as well as the productivity of different tools to predict stability and control derivatives. Different levels of fidelity have been included, from quasi-steady linear aerodynamics (VLM) to fully unsteady RANS solvers. The numerical data have been successfully compared with experimental ones.

3.1.4 Simulation of counter rotating open rotors (G. Dufour, M. Burnazzi)

Efficiency and cost of aeroengines have become a major issue for airframers as well as engine manufacturers. One way to achieve such improvements is the open rotor (OR) architecture (also referred to as prop-fan or counter rotating open rotor).
In the first step of this project, a steady simulation, based on the mixing plane approach, has been made. This simulation is fast, but neglects the interaction between the two rotors (Fig. 3.2-(a)) : the wake of the front rotor does not reach the rear rotor.
However, rotor/rotor interaction is the source of many challenges raised by this architecture (namely, vortex interactions, noise generation and whirl flutter for instance). Therefore, an unsteady approach based on the phase-lagged boundary condition has been set up. Figure 3.2-(b) shows the interaction of the wake of the first rotor in the second one, obtained by a chorochronic time reconstruction of the unsteady field.

3.1.5 Jet (A. Fosso-Pouangué, N. Lamarque, H. Deniau)

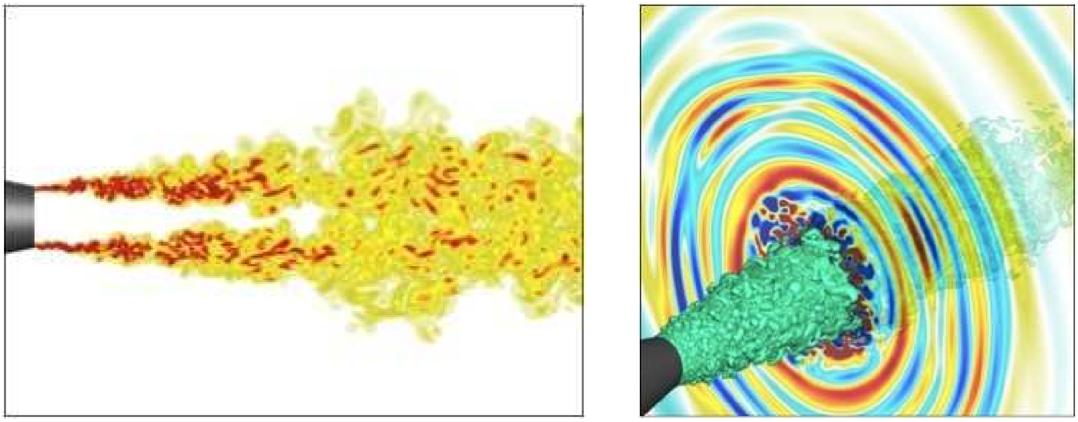
elsA can be used to perform numerical simulations for the prediction of jet-noise reduction produced by fluidic control. The validation will be done by comparison with the experimental data of the Laboratoire d'Etudes Aérodynamique (LEA). The main jet is at Mach number 0.3 and a Reynolds of 300.000. The control device consists in eight pairs of two convergent micro-jets.
At the moment, ongoing computations focus on a single jet. The new implemented sixth-order accurate compact scheme (section 2.1.4) is used together with Tam's boundary conditions. The instantaneous snapshots seems promising (see Fig. 3.3), the first exploited statistics are well in line with experimental data.



(a) Mixing plane computation

(b) Chorochronic computation

FIG. 3.2: Counter rotating open rotor simulations : color contours of entropy on a cut located close to the spinner.



(a) Vorticity magnitude field

(b) Iso-surface of vorticity and dilatation field in one plane

FIG. 3.3: Instantaneous fields obtained with *elsA*. *Free jet at Re = 300 000*

3.2 Turbomachinery

3.2.1 Flow control in compressors (G. Legras, N. Gourdain)

A challenge for compressor designers is to avoid the development of aerodynamic instabilities, such as rotating stall or surge. The difficulty to predict these phenomena lead to an over-sizing of the compressor that is detrimental for the performance (and thus for pollutant emissions). Casing treatments, which consist of slots, grooves or cavities within the rotor casing, are known to have the potential of bringing substantial stability and surge margin improvement. Unfortunately, although many studies have been published about these methods, the mechanisms related to casing treatment are not well understood. In this context, CERFACS is working in collaboration with SAFRAN and Ecole Centrale de Lyon (LMFA) to :

1. assess the capacity of *elsA* to predict the effect of casing treatments (boundary conditions, flow solvers, etc.),

2. test a wide range of configurations for casing treatments, from conventional (axisymmetric/non-axisymmetric) to more innovative (honeycomb) designs [AAM3],
3. develop a diagnostic tool to improve/optimise the casing treatment design,
4. understand the physical mechanisms that can improve stall margin and compressor performance.

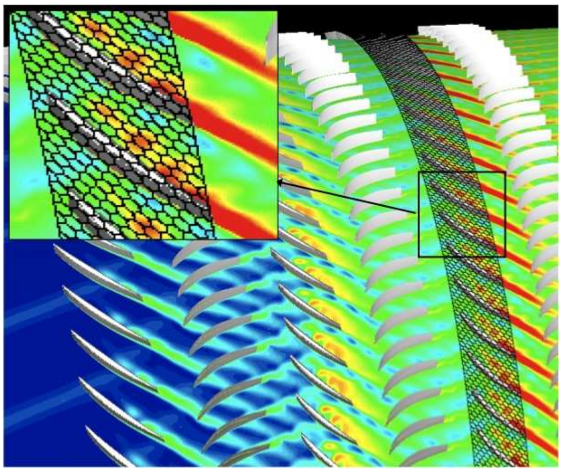


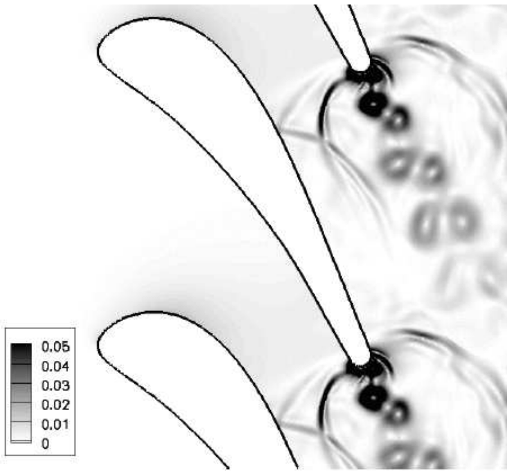
FIG. 3.4: Unsteady flow simulation in a 3-stage high-pressure compressor with a control solution, based on a honeycomb design. The stability is increased by 40% in this compressor.

This work already indicated that physical mechanisms to control are completely different in transonic and subsonic compressors. Interesting results have been obtained in a multistage compressor, showing that rotating stall can be suppressed and stability (in terms of operating range) increased by 40% (Fig. 3.4).

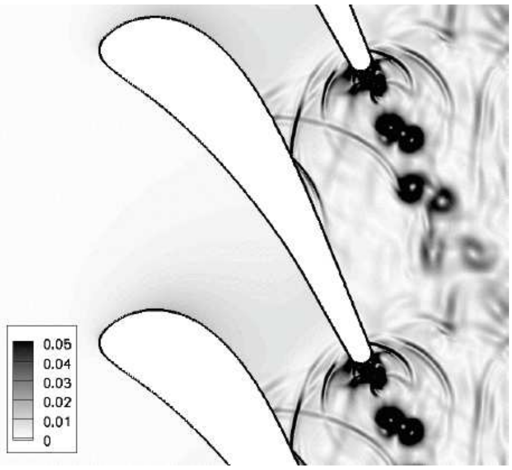
3.2.2 High fidelity methods for aerodynamics (L. Gicquel, T. Leonard, N. Gourdain)

Large Eddy Simulation (LES) has clearly demonstrated its potential in predicting and improving CFD predictions of turbulent reacting flows, not only in laboratory scale burners but also in real combustors [AAM17]. Its application to wall bounded flows, as encountered in compressors and turbines, remains however to be investigated. Indeed, the numerical modelling involved by the wall treatment of such complex systems in LES still remains under investigation and the relevancy of the LES potential is still to be demonstrated or even confronted to more conventional methods based on a RANS approach. In a first attempt to address these issues, LES simulations have been conducted for a fixed transonic blade exhibiting large unsteady flow motions and for which a detailed experiment database is available [1-2]. For this test case, both LES codes available at CERFACS (*i.e. elsA* and AVBP) have been tested and compared to RANS and unsteady RANS as illustrated on Fig. 3.5. While increasing the cost with respect to the URANS approach by a factor 100, LES shows very satisfying results with both flow solvers and better predicts the frequency of vortex shedding behind the blade trailing edge than other methods.

[1] Sieverding, C., Richard, H. and Desse, J.-M., 2003. *Turbine blade trailing edge ow characteristics at high subsonic outlet mach number*, Transaction of the ASME, Vol. 125, pp. 298-309, 2003
[2] Sieverding, C., Ottalia, D., Bagnera, C., Comadoro, A., Brouckaert, J.-F. and Desse, J.-M., *Unsteady turbine blade wake characteristics*, J. of Turbomach., Vol. 126, pp. 551-559, 2004



(a) URANS



(b) LES

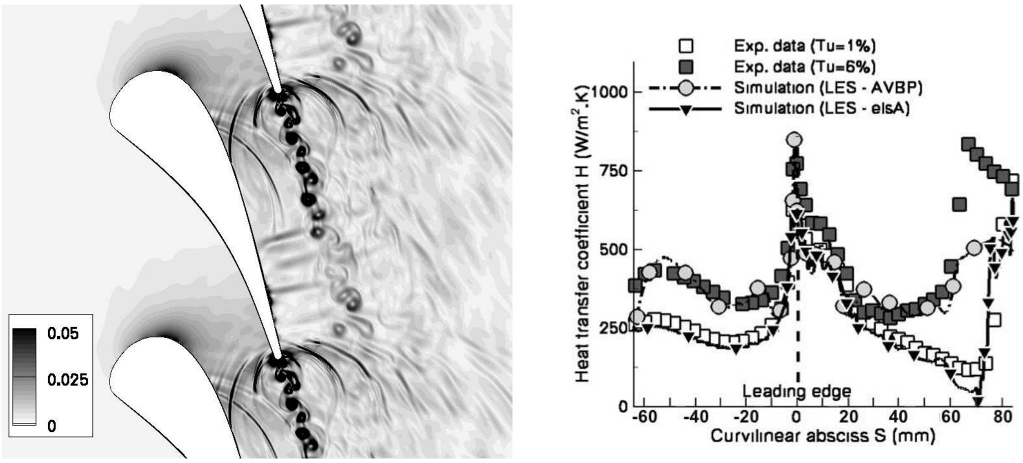
FIG. 3.5: Unsteady flow simulation (*elsA*) in an inlet guide vane. Density gradient.

3.2.3 High fidelity methods for aerothermal effects (E. Collado, F. Wlassow, F. Duchaine, L. Gicquel, N. Gourdain)

A critical problem in high pressure turbines of modern engines is the vane and blade reliability as it is subjected to high thermal constraints. Considering that a small variation of the blade temperature leads to a strong reduction of its life duration, accurate numerical tools are required to estimate the blade temperature. To develop innovative methods, CFD flow solvers (both *elsA* and AVBP) are used first to investigate flows in well documented test cases. The methods are then applied to industrial test cases. Different problems must be solved such as (1) the description of unsteady flows and laminar to turbulent transition, (2) coupling between thermal and dynamic boundary layers, and (3) technological devices for cooling.

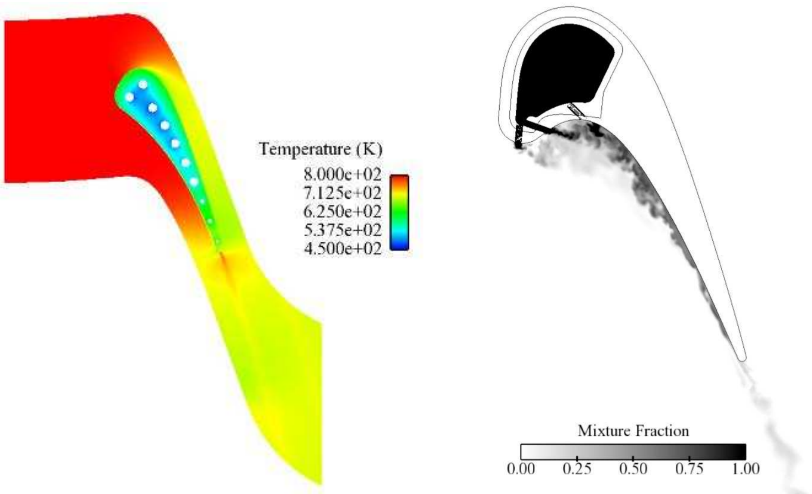
For the prediction of transition, LES is used to predict the flow in the LS89 configuration [1]. Results indicate that LES predicts the effects of transition (Fig. 3.6) but depends strongly on the inlet turbulence intensity.
In complex geometries, the blade wall temperature heterogeneities require to use a fluid/solid coupling strategy. To solve such Conjugate Heat Transfer (CHT) problems, a multi-physics approach has been developed. It consists in solving each set of equations separately with dedicated solvers and to exchange information at the interface thanks to boundary conditions (this technique allows thus to use existing state-of-the-art codes). A Navier-Stokes flow solver (that can be based on either RANS or LES approach) is coupled with a conduction solver (AVTP). This strategy was first applied to the well documented configuration NASA C3X [2] to study the influence of the fluid/solid interface boundary condition (fig. 3.7(a)). Results show that the predicted wall temperature is in good agreement with experimental results.
The effect of cooling devices was also investigated in the T120D blade [3]. A method based on a coupling between a LES flow solver and solid heat conduction solver successfully demonstrated its capacity to improve the prediction of cooling hole effectiveness (Fig. 3.7(b)) [AAM2]. In the frame of a cooperative work with the university of Stanford (at the summer program of the Center for Turbulence Research Lab.), this method has been applied to study the effect of hot spots coming from the combustion chamber.

[1] Arts, T., Lambert de Rouvroit, M., and Rutherford, A. W., *Aero-thermal investigation of a highly loaded transonic linear turbine guide vane cascade*, Technical Note, no 174, Von Karman Institute, 1990



(a) LES (*elsA*) (b) Prediction of heat transfer with *elsA* and AVBP.

FIG. 3.6: Aerothermal investigations in the LS89 test case.



(a) NASA C3X vane (RANS, *elsA*) (b) T120D configuration (LES, AVBP)

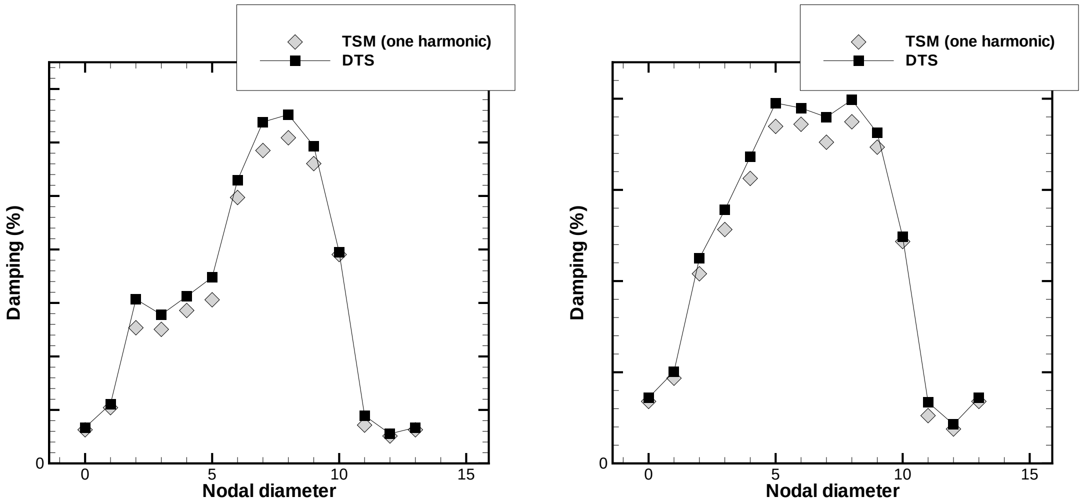
FIG. 3.7: Temperature prediction in the fluid and solid.

[2] Hylton, L., Mihelc, M., Turner, E., Nealy, D., and York, R., *Analytical and experimental evaluation of the heat transfer distribution over the surfaces of turbine vanes*, Tech. Rep., CR 168015, NASA, 1983
[3] Gomes, R. A. and Niehuis, R., *Film cooling effectiveness measurements with periodic unsteady flow on highly loaded blades with main flow separation*. Proceedings of ASME Turbo Expo : Power for Sea, Land and Air, Orlando, Florida, USA, 2009

3.2.4 Time Spectral Method computations for compressor aeroelasticity (G. Dufour, F. Sicot)

Unsteady aerodynamics is a major issue for aircraft manufacturers and designers, for flutter assessment, flight dynamics data generation, or turbomachine multistage predictions. In this context, the Time Spectral

Method (TSM), previously applied to external aerodynamics flows, has been extended to blade flutter using a weak coupling approach. Since the blades do not necessarily vibrate in phase, a specific phase-lagged boundary condition has been implemented in *elsA*. The originality of the present development is that it is done purely in the time domain, as opposed to the mixed treatment in the Fourier space often used in the literature.
The proposed method has been validated for an axial compressor blade undergoing forced motion along its first bending mode. In Fig. 3.8 the results are verified against computations performed with a classical time integration scheme (dual time stepping). The agreement between the two methods is quite good. In particular, the critical diameter is correctly predicted. The TSM method is found to be about 5 times faster than the DTS approach for this case. The method is currently being applied to a centrifugal compressor, and other test cases will be tackled within the European project FUTURE.



(a) Low rotation speed (b) High rotation speed

FIG. 3.8: Time Spectral Method prediction of aerodynamic damping for a compressor blade in forced motion.

3.2.5 High fidelity methods for aeroacoustics (F. Sicot, S. Moreau, N. Gourdain)

An analytical model has been developed at University of Sherbrooke (Canada) for the predictions of the fan tonal and broadband noises. CERFACS cooperates with the Sherbrooke's team to validate such an acoustic model by comparing the model predictions with unsteady blade loading provided by numerical unsteady simulations. Different configurations are investigated, from a simple flat plane cascade to a whole stage of a subsonic compressor test case [1]. Unsteady RANS and spectral methods (TSM) are used for each configuration to compare with the model. In the simple case of a blade slice (Fig. 3.9), both numerical methods compare very well up to the sixth harmonics. Unfortunately, comparisons with the model do not match very well, mainly because flow simulations exhibit large velocity fluctuations close to the leading edge (due to a local flow separation) that cannot be predicted by the analytical model. In the full 3D case, this flow separation is removed and a better agreement is observed between the URANS and the analytical model.

[1] Michon, G. J., Miton, H. and Ouayahya, N., 2005. *Experimental study of the unsteady flows and turbulence structure in an axial compressor from design to rotating stall conditions*, 6th European Conference on Turbomachinery, paper 015-03/39, Lille, France.

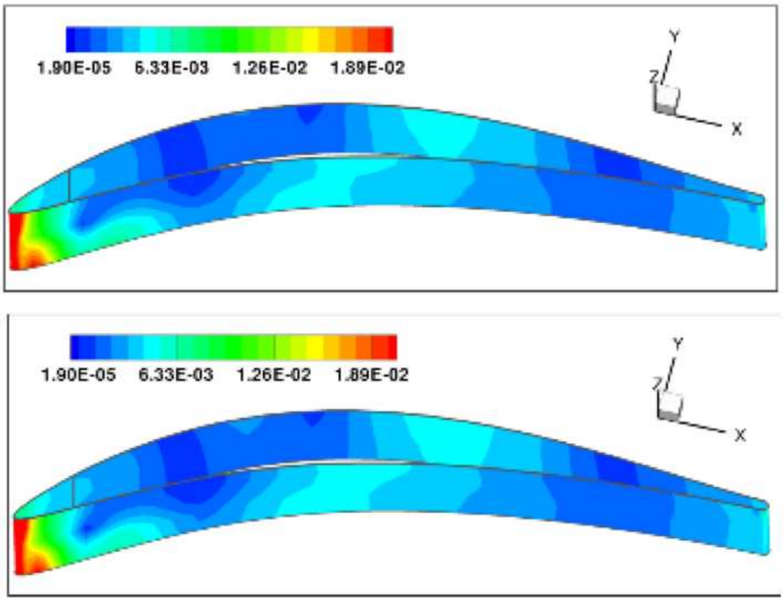


FIG. 3.9: Comparisons of URANS (up) and TSM (down) flow solutions in a subsonic compressor stage. Static pressure fluctuations correlated with the blade passing frequency on the stator wall.

3.2.6 Aerodynamic instabilities in a multistage compressor (F. Wlassow, N. Gourdain)

The objective of this study is to simulate and analyse the development of aerodynamic instabilities in a multistage compressor at near stall operating conditions. The analysis of these phenomena is not straightforward since the entire system has to be simulated with an unsteady flow method in order to capture low frequency phenomena. Under the leadership of CERFACS, and supported by its partners (SAFRAN, Ecole Centrale de Lyon, EDF), a flow simulation in the full annulus ($360°$ sector) of a 3-stage industrial compressor [1] was performed using an unsteady RANS approach with the *elsA* flow solver. This simulation was performed on 4096 computing cores of a massively parallel platform (IBM Blue Gene) [AAM5]. The flow unsteadiness was then analysed by means of sophisticated post-processing tools (based on a modal decomposition) which helped to understand the role of rotor-stator interactions in the development of massively separated flows.

[1] Ottavy, X., Trebinjac, I., Vouillarmet A. and Arnaud, D., *Laser measurements in high speed compressors for rotor-stator interaction analysis* Proceedings of 6th ISAIF, Shangha, China, 2003

4 Software engineering

4.1 Massively parallel CFD (M. Montagnac, N. Gourdain, F. Wlassow)

Parallel performance evaluations are performed on many different architectures, mainly clusters of nodes of multiprocessors but also vector machines, on complex CFD turbomachine and aircraft configurations [AAM18]. However, massively parallel computations are preferably tuned on the Cerfacs 4096-processor IBM BlueGene/L computer.

Before the upgrade of the Cerfacs BlueGene/L computer, EDF provided the CFD team with computational resources on their 8096-processor Blue Gene/P allowing a new step in the scaling of applications. After an initial important work of topology splitting and load-balancing, an unsteady flow simulation was performed in a full three-stage SNECMA compressor including 134M grid cells at the design operating point (Fig. 4.1). The major interest from the scientific point of view is to understand the development of aerodynamic instabilities and the impact of rotor-stator interactions in these systems. The computational time was 280,000 CPU hours to obtain a periodic solution at design conditions (with 512 computing cores) and 4,000,000 CPU hours at off-design conditions to simulate a rotating stall phenomenon (with 4096 computing cores) [AAM4, AAM5].

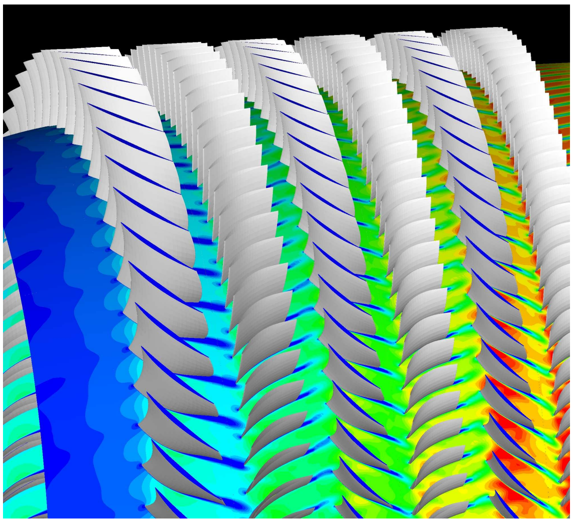


FIG. 4.1: Flow simulation of a full multistage compressor (134M cells grid) using up to 4096 computing cores.

4.2 Code coupling (M. Montagnac, J-F. Boussuge, N. Gourdain, F. Wlassow, A. Dechaume, S. Jauré)

A trend towards multidisciplinary simulations has clearly emerged in the previous decade. The common feeling is that a single simulation code can not provide all numerical features necessary for multiphysics calculations in most cases. Therefore, only the coupling of the best codes of each discipline will allow sufficient flexibility to understand the nature of interactions at reasonable cost. The coupling can be of different type, ranging from different numerical models (RANS/LES) to different physical models (heat transfer, structural displacement).

However, no solution has emerged so far in the coupling of simulation codes. Many technical solutions are available depending on the constraints imposed. Since the aerodynamic team interacts with various scientific centres, several possibilities have been studied.

4.2.1 Flow Simulation Data Manager (J-F. Boussuge, A. Dechaume)

In an industrial context, the experts in numerical calculations deliver multidisciplinary computational frameworks to their end-users so they can design their products. Obviously, these frameworks include many third-party tools and legacy codes, which exchange data between each other. Airbus France has developed a proprietary software architecture to enable the code coupling to perform multi-physics simulations. Since these numerical simulation scripts often include an aerodynamics solver, the *elsA* software was considered to be introduced as a python module in this framework. The purpose of the main module is to hold all the information about the simulation and it is therefore called the Data Manager. Each code that has to be included in this framework requires a proxy that converts the data in the Data Manager to the native format of the code and conversely.

Since the CFD team sometimes uses the Airbus tools to conduct numerical simulations, a proxy module was developed and successfully applied to simple scenarios. The steering application is written in python : the data manager module holds in particular all meshes and initial solutions read from a database, the *elsA* proxy module makes all these data comprehensible by the *elsA* module (aerodynamic solver). As a consequence, Airbus and Cerfacs can share Airbus databases and other python plugins.

4.2.2 *elsA*-AVBP coupling via PALM (M. Montagnac, F. Wlassow, N. Gourdain, S. Jauré)

Coupling numerical models is becoming a crucial issue in the Cerfacs CFD community especially for computations of full engines (compressor, combustion chamber, turbine). Indeed, different specialised and efficient solvers are used to compute very different physical problems. The coupling tool PALM, developed within Cerfacs by the Climate Modelling and Global Change team, has been chosen to exchange information in a synchronised way between the models.

To this end, a new version of the *elsA* software has been instrumented to be compliant with the PALM framework. In order to prepare the simulation of the entire hot part of the engine (*i.e.* the combustion chamber and the high pressure turbine), a tool has been developed to couple the AVBP code (reference code for flow simulation in combustion chambers) and the *elsA* code (reference flow solver for turbomachines). This tool is able to manage the transfer from an AVBP solution (unstructured mesh/LES) towards an *elsA* boundary condition (structured mesh, RANS) using linear interpolation. It is important to state that meshes do not need to have the same angular position or size, it is even possible to replicate a single AVBP angular sector into a fully 360 solution for *elsA* input without any mesh replication. The coupling application has been developed using the Python language.

4.2.3 Sequencing Strategy (F. Wlassow)

The most basic method corresponds to a code sequencing strategy. This method is based on a python driver that handles the submission of the different simulations and their synchronisation, the file exchanges and the generation of the boundary conditions files for each solver. The advantages of this method are that it is not code intrusive and it can be quickly set up from scratch. However if the frequency of exchange between the codes increases, the computational efficiency of the method can be affected since the exchange of data are managed through files.

4.3 JPOD chain : an adaptive POD/SVD surrogate model for aeronautic design (J.-C. Jouhaud and M. Ferrier)

Aerodynamic models are widely used in aircraft design and interdisciplinary process (loads, MDO, identification). A large variety of tools are available from empirical/handbook methods to flight-testing including numerical simulation. Progress made both in terms of computational resources and numerical algorithm improvement make the CFD to be efficient and accurate. Nevertheless full CFD often remains too costly and CFD based metamodels must be developed. These models give quickly the main features of the dynamic system and are well adapted to interdisciplinary exchange. Cerfacs developed a Proper Orthogonal Decomposition (POD) tool in order to build automatically metamodels for Aerodynamic data collection exchange. The main objective is to construct a model of the full aerodynamic field for a large number of parameters (flight points, Mach-alpha, altitude, shape parameters, actuator position) with the smallest number of CFD computations. The global process of the model generation is presented on figure 4.2. The amount of required full numerical flow simulations is minimised thanks to an automatic resampling technique based on error estimations with a leave-one-out strategy. Very good results have been obtained for space parameters creating exclusively subsonic or transonic configurations. However, the presence of the two physics (subsonic and transonic) in the same parameters space reduces the accuracy. To avoid this, we are currently working on the use of different POD database related to different physical zones ; these zones being defined with a Centroidal Voronoi Tessellation (CVT) approach. Despite this limitation, the JPOD tool was successfully evaluated at Airbus France on industrial configurations.

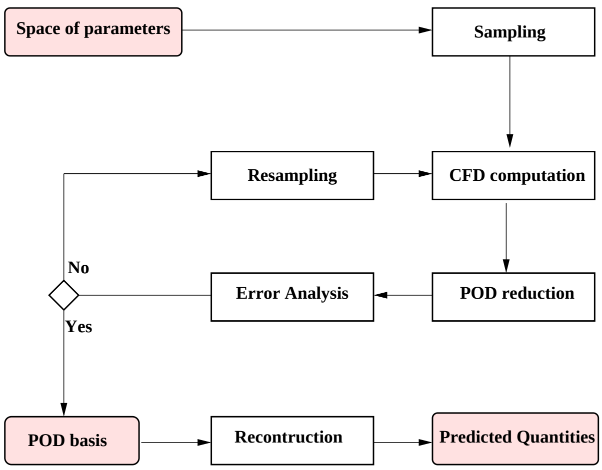


FIG. 4.2: A JPOD/SVD chain for aeronautic design.

5 Publications

5.1 Journal Publications

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[AAM12] J. Jouhaud, (2008), *Habilitation à Diriger la Recherche : Simulations Aérodynamiques et Aérothermiques Avancées pour la Conception et l'Amélioration des Avions - TH/CFD/08/48*, PhD thesis, Institut National Polytechnique de Toulouse, France.

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[AAM14] L. Nybelen, (2008), *Etude numérique d'écoulements tourbillonnaires de sillage d'avion - TH/CFD/08/60*, PhD thesis, Université Toulouse III - Paul Sabatier, Institut National Polytechnique de Toulouse, France - MEGeP - Dynamique des fluides.

[AAM15] F. Sicot, (2009), *Simulation efficace des écoulements instationnaires périodiques en turbomachines - TH/CFD/09/66*, PhD thesis, Ecole Centrale de Lyon - École Doctorale Mécanique, Énergétique, Génie civil et Acoustique.

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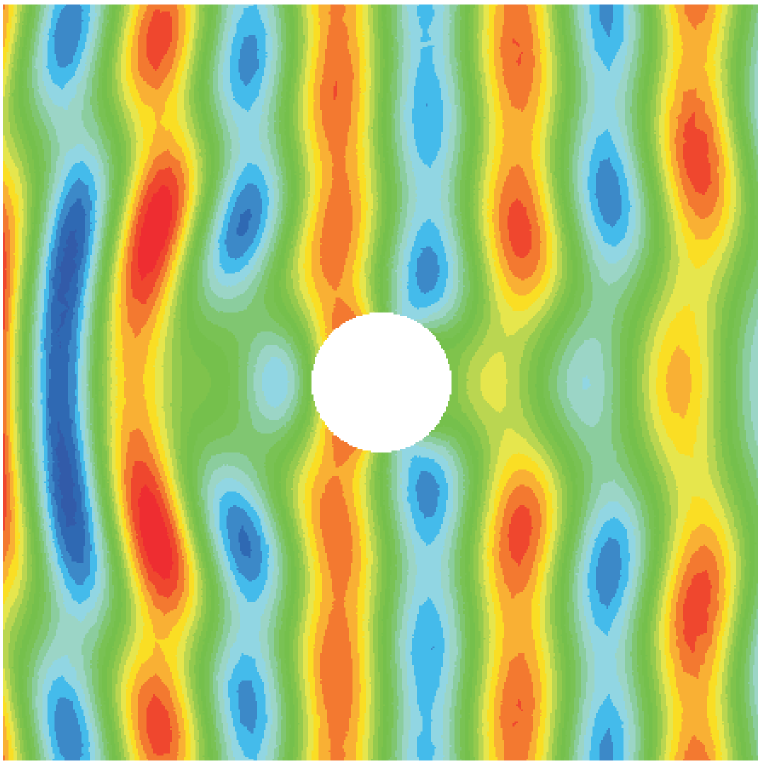
9

Electromagnetism and Acoustics Team



1 Overview presentation

The main expertise of the *Electromagnetic and acoustic* team concerns the numerical solution of problems related to the scattering of time-harmonic electromagnetic and acoustic waves.

In 3D electromagnetism, our efforts (in partnership with EADS and ONERA) are focused on the development of well-conditioned and accurate integral equation methods, which are implemented in the CESC code (CERFACS Electromagnetism Solver Code) and validated on realistic industrial cases (generally suggested by our partners MBDA and CNES).

A more recent activity concerns the numerical simulation of acoustic scattering in presence of an arbitrary mean flow : the method which couples continuous and discontinuous finite elements with Perfectly Matched Layers has been implemented in 2D. This activity is part of the ANR project AEROSON (in partnership with EADS and with POEMS and LAUM laboratories).

Our team has also produced, in collaboration with the INRIA Project DEFI, some contributions in the domain of electromagnetic imaging by the Linear Sampling Method (LSM). In partnership with the CERFACS Algo team, a very fast solution algorithm has been developed and tested. Some theoretical aspects are currently studied, which could help to image the interior of the scatterer.

Finally, the team contributes to the development of a high order Discontinuous Galerkin scheme for transient Maxwells equations which is implemented in the code FEMGD developped by the French Aerospace Lab (ONERA).

2 Integral equations for electromagnetism scattering

2.1 Intrinsically well-conditioned integral equations

F. Millot and S. Pernet

The pertinence of integral equation methods for solving electromagnetic scattering problems in harmonic regime requires no further proof. Using them in combination with a rapid multipole algorithm and an iterative solver makes them efficient and precise methods that can solve problems involving hundreds of thousands of unknowns.

However, the efficiency of iterative methods is strongly related to the conditioning of the linear systems. Thus in recent years, the preconditioning of large linear systems is becoming a crucial issue in order to enable the simulation and design of the complex electromagnetic systems of the future. Usually constructed after the discretization process, the preconditioners used in industry are purely algebraic.

In recent years, it appeared that the problematic of the preconditioning could be taken into account during the construction of equations ie at the continuous level of the formulation of the problem rather than after its discretization. Regularizing operators playing the role of preconditioners are constructed from the mathematical analysis of fundamental operators of electromagnetism ([1], [2], [3]).

During the last years, the EMA team has undertaken some works in this direction :

- We have proposed a new family of integral equations called GCSIE (Generalized Combined Source Integral Equation) to solve the scattering of an electromagnetic wave by imperfectly conducting objects [4]. These equations induce a linear system which is well conditioned by construction and whose inversion by an iterative solver requires no preconditioner. Moreover, the convergence rate of iterative solver is almost independent of the frequency and of the discretization used. The flexibility of use (no parameter to adjust in contrast to an algebraic preconditioner) and the robustness of this type of formulation gives rise to a good candidate for the resolution of future applications in electromagnetism.
- Within the context of applications for the MBDA company, we have extensively studied the performance of this type of approach for calculating the RCS of a perfectly conducting complex object. Two types of integral equations have been constructed [EMA11]. The first belongs to the source integral equation (GCSIE) methods where the unknowns are pure mathematical currents on the boundary. The second (GCFIE) belongs to the field integral equation methods where the unknowns have a clear physical meaning. We have proved that for a complex object with strongly singular parts, the GCSIE and the GCFIE are most robust than the CFIE which is generally the classical tool in the industry. The solution is usually obtained more rapidly (see fig 2.1). Moreover, concerning the accuracy of obtained solutions, we note that the GCSIE or GCFIE equation provide in some cases, more accurate solutions than those obtained with the CFIE equation (see fig 2.2). Finally, we note that the source equation seems to be the most efficient.
- In collaboration with the ONERA, we are working to extend the previous results to transmission problems in electromagnetism. A new integral equation type GCSIE has already been proposed [EMA20]. The integral equation obtained is well-posed for all frequencies and is a compact perturbation of the identity operator. The implementation of this approach is in progress.

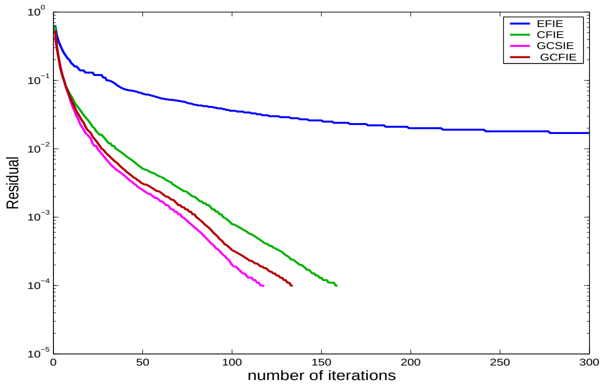


FIG. 2.1: Residual versus the number of iterations

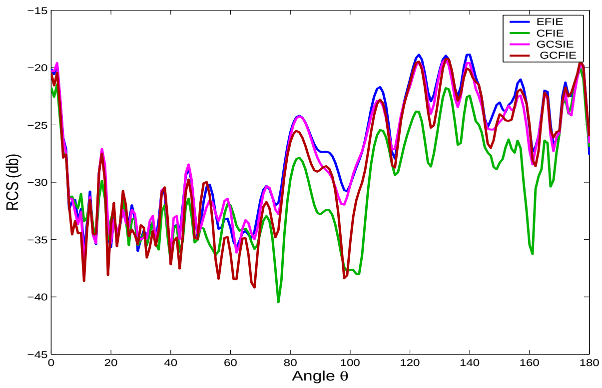


FIG. 2.2: Radar cross section versus the θ angle for an industrial case

[1] F. Alouges, S. Borel, and D. Levadoux, (2007), A stable well conditioned integral equation for electromagnetism scattering, *JCAM*, **204,2**, 440–451.

[2] F. P. Andriulli and E. Michielssen, (2007), Regularized Combined Field Integral Equation for Scattering From the 2D-perfect electrically Conducting objects, *IEEE Transaction on antennas and propagation*, **55**, 2522–2529.

[3] M. Darbas, (2006), Generalized CFIE for the Iterative Solution of 3-D Maxwell Equations, *Applied Mathematics Letters*, **19,8**, 834–839.

[4] S. Pernet, (2010, Published Online : 17 March 2010, DOI : 10.1051/m2an/2010023), A well-conditioned integral equation for iterative solution of scattering problems with a variable Leontovitch boundary condition, *Mathematical Modelling and Numerical Analysis*.

2.2 The current-charge formulation

A. Bendali, F. Collino, M. Fares and B. Steif

The combined field currents and charges formulation (C3IE) was devised by Taskinen and Yla-Oijala (see [5] and [6]) mainly as a tool for avoiding the instabilities that occur at very low frequencies when solving the time-harmonic electromagnetic equations by means of the usual boundary integral equations. After recalling some features of this formulation, we bring out the observations that led us to undertake its study.

We then give the results which have been obtained and some conclusions which have be drawn. This topic is the subject of the PhD thesis of Bassam Steif.

2.2.1 Main features of the currents and charges formulation

It is worth noting that low frequencies are met in electromagnetic scattering problems when dealing with geometries involving small details. The electric field integral equation (EFIE) or the combined field integral equation (CFIE) cannot be stated when the frequency is zero. As a result, these formulations may be not well-adapted at very low frequencies. However from several numerical experiments we have observed that if the EFIE gives rise to severe instabilities even at moderately low frequencies, the CFIE continues to be robust at very low ones.
The mathematical study which we have performed on the C3IE revealed the following feature which does not seem to have been already brought out. It is stable in the same framework than the magnetic field integral equation (MFIE) with the additional advantage that the solution it delivers cannot be damaged by the radiation of some possible spurious currents. Therefore it can be used when meshing various zones of the scatterer independently each from the other. This approach perfectly works for a smooth geometry, that is, in the parts of the scatterer with a continuous tangent plane. However we have observed that the currents and charges can be polluted by some spurious oscillations which concentrate on the elements of the mesh having a vertex or an edge on a singularity of the geometry (see 2.3a and 2.3b). We have hence been led to focus our study on understanding the cause of this flaw and finding the way to suppress it.

2.2.2 Mathematical study of the currents and charges formulation

We have performed an extension of the currents and charges formulation in the two following ways :
– a construction of this formulation in the two-dimensional case starting from the integral representation of the scattered wave in the TE case in terms of a double-layer potential,
– an extension of the formulation for a Neumann problem with an arbitrary boundary data.

This allowed us to bring out that the oscillations are not only due to the singularity of the geometry but also to the fact that the formulation amplifies highly oscillating evanescent modes. A thorough inspection of the formulation revealed that the instability is certainly due to one of the following features :
– the currents and charges formulation is in fact an instance of a system with a compatibility condition on the data ; the compactness property which ensures that the evanescent modes are not increased when solving the continuous problem are not preserved when passing to the discrete case ;
– even if the continuous problem owns good coerciveness properties, it behaves like a saddle-point problem ; it is well-known that the discretization of such kind of system must fulfill some compatibility conditions in order to preserve the stability properties of the continuous problem at the level of the discrete one.

We are presently exploring these two issues.

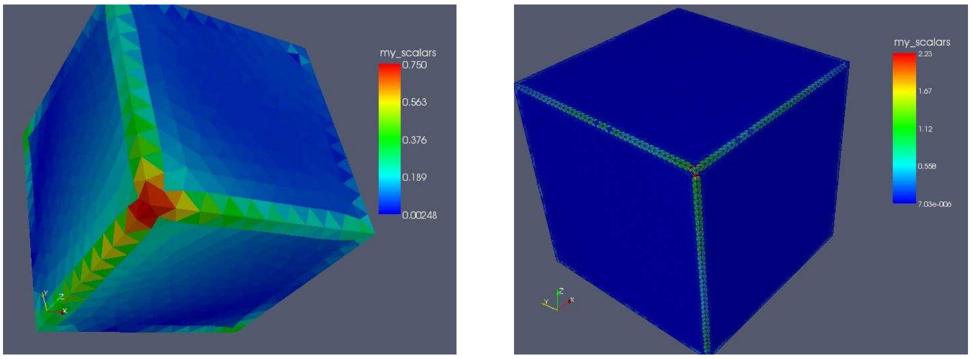
[5] M. Taskinen and P. Y. Oijala, (2000), Current and Charge Integral Equation Formulation, *IEEE Transactions on Antennas and Propagation*, **54,1**, 58–67.

[6] M. Taskinen and S. Vanska, (2007), Current and Charge Integral Equation Formulations and Picard's Extended Maxwell System, *EEE Transactions on Antennas and Propagation*, **55,12**, 3495–3503.

2.3 A weighted Combined Field Integral Equation

F. Collino, F. Millot and M. Fares

The *Combined Field Integral Equation* is the privileged formulation for solving large scale scattering problems. This is due to the (relatively) small number of iterations required to solve it by iterative methods.



(a) (b)

FIG. 2.3: currents spurious oscillations on a coarse mesh and a refined mesh

However, it is known, alghough not very well understood, that the precision of the numerical solution is sometimes low, especially when sharp edges or tips are present in the geometry of the scatterer. To circumvent this lost of precision, we have studied a modification of the `CFIE`.
The *Combined Field Integral Equation* consists in writing an impedance boundary condition for the interior electromagnetic total field. Usually, the value of the impedance is taken to be constant. What we propose is to consider the impedance as a variable and smooth function, vanishing in the vincinity of the singular edges or tips of the scatterer. We derived a mathematical framework for this ”new” equation, constructed a numerical code and made various numerical experiments. We have demonstrated that the new equation leads to a better numerical solution at the price of an increase of the number of iterations to solve the system.
Figure 2.4 aims at illustrating the method. The radiation pattern of a complex cavity (provided by `MBDA`) is computed by 3 differents integral equations : the *Electric Field Integral Equation*, the classical `CFIE` and the variable impedance `CFIE`. We can see that the `EFIE` and the `CFIE` with variable impedance solutions agree while the classical `CFIE` gives a poor solution. The number of iterations to obtain those solutions increases from 98 for the classical `CFIE` to 576 for the variable impedance `CFIE`. The obtention of the `EFIE` solution, which is known to be of good quality, requires a costly and sophisticated method (preconditionned flexible `FGMRES`). Thus, our new `CFIE` appears to be a good compromise beetwen cost and precision.

2.4 High order impedance conditions for coated scatterers

A. Bendali, M. Fares and S. Pernet

Dielectric thin coatings of metallic structures are usual in industrial applications : stealthiness technology in defense industry, protective covers, etc. We describe below the main difficulties arising in the numerical simulations of scattering problems involving such a setup and the efficient way with which we have handled this issue.
A full waves approach for solving scattering problems involving a thin dielectric layer may become inefficient mainly because of the two following drawbacks. The problem can become rapidly intractable since it involves as much as three times the number of unknowns corresponding to the case where the effect of the thin coating is neglected. Even if one resorts to a highly parallelized code capable of exploiting the by-now available massively parallel platforms, like the *Electromagnetic Solver Code* developed at CERFACS can do, the problem may behave singularly relatively to the small parameter describing the thickness so that the correctness of the results delivered by a direct numerical simulation becomes unpredictable.

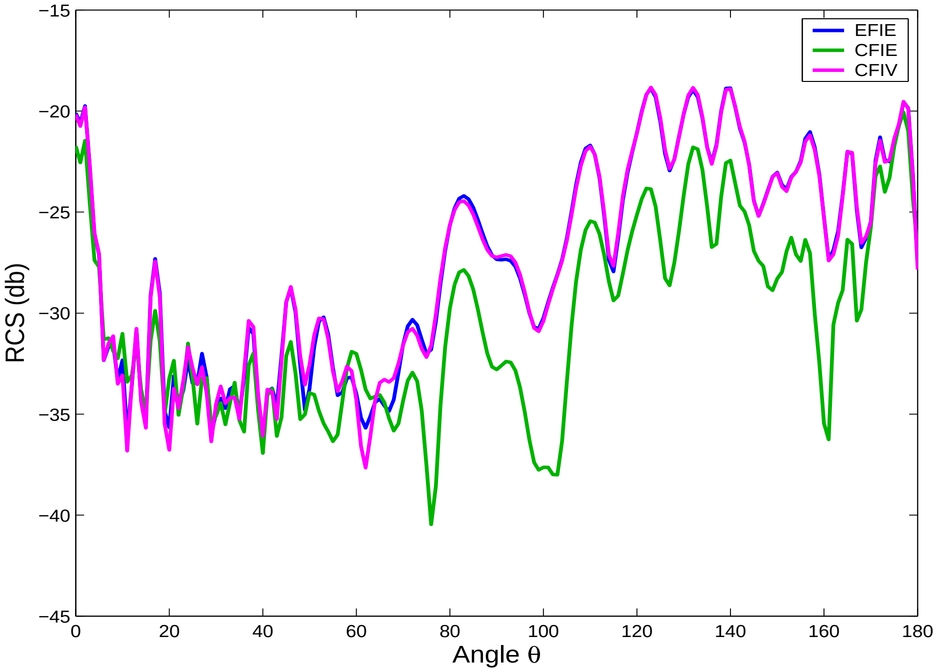


FIG. 2.4: `Mbda` Cavity at 6GH : radiation pattern in Db as a function of the observation angle θ.Comparison of the solutions provide by the `EFIE` in blue, the `CFIE`in green and the `CFIE` with variable impedance in pink.

This is why for a long time this kind of problems was tackled by means of an effective impedance boundary condition (IBC) taking into account the effect of the thin layer in an approximate way. Usually these IBCs are constructed by means of a Taylor expansion relatively to the small parameter. However, as for radiation conditions, such a way to design effective IBCs is suited only for low-order methods with a reduced accuracy. The way to improve the accuracy is to use IBCs based on Padé-like approximations. Such approximations were difficult to obtain and to solve for Maxwell equations. In collaboration with Professor Lemrabet of Algiers University, we succeeded in devising a general procedure which makes it possible to obtain stable IBCs up to the third-order and potentially even at higher orders. The related problems have then been solved using a novel procedure recently developed by the team to deal with IBCs (see section 2.1). We have then been able to solve some instances of this kind of scattering problems with a degree of accuracy not reached before. These results have been presented in a plenary conference at the previous international congress on mathematical and numerical aspects of waves phenomena WAVES-2009 held at Pau in June 2009.

2.5 Axisymmetric integral equation solver

A.S. Bonnet-Ben Dhia, S. Cambon and F. Collino

Sébastien Cambon carries out his `PhD` Thesis at `CEA-CESTA` on scattering problems in axisymmetric geometry under the supervision of A. S. Bonnet-Ben Dhia. The problem is to design an effective method for the computation of the Radar Cross Section of large size objects coated with dielectric and magnetic materials. The method under study rests on a formulation proposed by P. Lacoste which consists in coupling

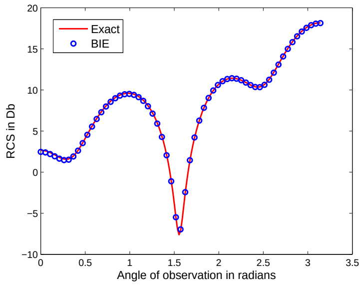
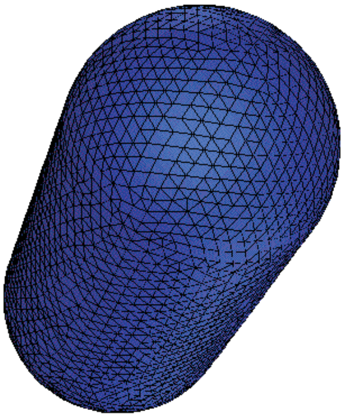
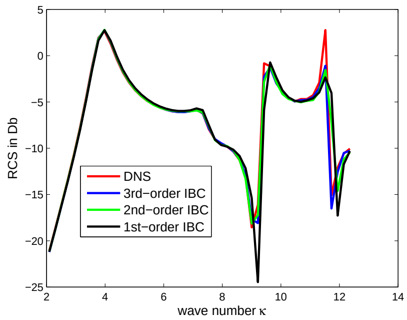


FIG. 2.5: Bistatic RCS related to the 3rd-order IBC obtained by Mie's series and numerical solution



(a) Cylinder with Half-spheres $\varepsilon = 1$, $\mu = 49$



(b) Monostatic RCS

FIG. 2.6: Test-case with a highly magnetic coating

integral equations and finite elements method. Its originality is in the choice of the degrees of freedom for the `FEM`. The first year was devoted to the implementation of the method.

3 Electromagnetic imaging by the Linear Sampling Method

A.-S. Bonnet-Ben Dhia, F. Collino, A. Cossonnière and M. Fares

The Linear Sampling Method is a technique which aims at reconstructing the shape of a scatterer from multi-static electromagnetic data at a given frequency : the scatterer, which may be a perfectly conducting body as well as a penetrable heterogeneity, is illuminated by harmonic plane waves in (almost) all possible directions and the resulting far-fields are recorded in all directions. These data are used to build the so-called LSM matrix whose (pseudo) inversion allows to discriminate between sampling points inside or outside the scatterer.
Our recent contributions on this topic concern on one hand algorithmic aspects : in collaboration with the ALGO team, a new approach has been developed leading to a significant acceleration of the whole imaging process. On the other hand, Anne Cossonnière started in October 2008 a PhD under the supervision of Houssem Haddar (INRIA project-team DEFI) : the objective is to investigate the potential interest of the so-called interior transmission frequencies in order to image the interior of a penetrable scatterer.

3.1 Fast solution algorithm : the SVD-tail

In the classical approach, a system involving the LSM matrix has to be inverted for each sampling point (and in practice, a large number of sampling points is required to get an accurate image). This system being ill-posed, a Tikhonov-Morozov regularization technique is used, which is quite costly since a full-SVD of the matrix is achieved and the Tikhonov regularization parameter has to be determined, using the Morozov discrepancy principle, for each sampling point.
The new approach that we have developed in collaboration with S. Gratton and P. Toint is both simpler and faster. The main point is that imaging the scatterer does not require the knowledge of the solution of the LSM system, but only the knowledge of whether this system has or has not a (pseudo) solution. This can be achieved by a full iterative algorithm : a small number of left singular vectors associated to the smallest singular values are first approximated (by the classical power method) ; then the orthogonality of the RHS to these vectors is simply tested. Let us emphasize that only few left singular vectors are needed thanks to the presence of noise in the data and in the discretized operator. In a typical application with 2252 incident directions and 125000 sampling points, a speed-up factor of 50 is obtained [EMA5].

3.2 The interior transmission eigenvalue problem

The Linear Sampling Method fails to image a penetrable scatterer for some exceptional frequencies, for which the LSM operator is not injective. These frequencies can be characterized as eigenvalues of a non-standard problem set inside the scatterer, referred in the literature as the interior transmission problem. These eigenvalues are directly related to the constitutive properties of the scatterer and they could be used to deduce from multi-frequency data some knowledge on this constitution.
The current efforts aim at better understanding the relation between the interior transmission eigenvalues and the properties of the scatterer.

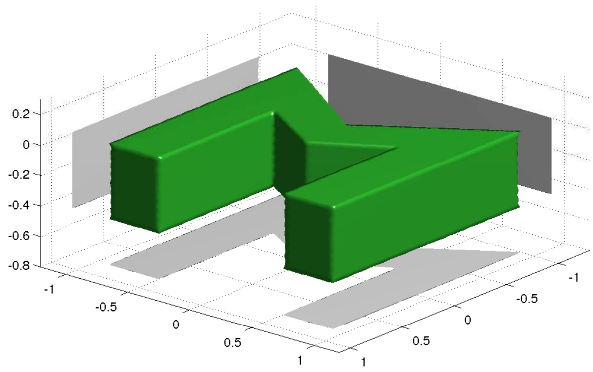


FIG. 3.1: The true Σ to be will reconstructed by different methods

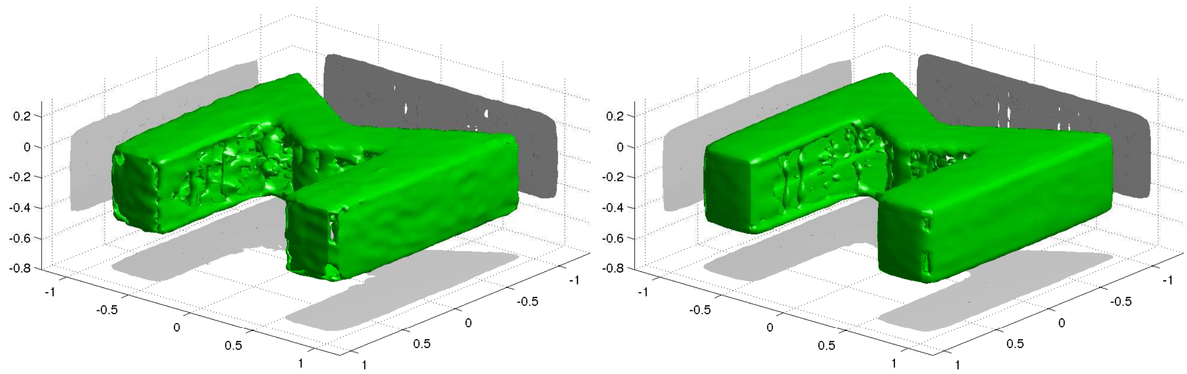


FIG. 3.2: The Σ reconstructed by SVD-tail(50) (left), and full-SVD (right)

During a three-months visit at Delaware University, Anne Cossonnière has obtained in collaboration with Fioralba Cakoni new theoretical results in the difficult situation where there are some void inside the scatterer.
Besides numerical tests have been performed for a spherically stratified scatterer. The objective is now to develop a general stable numerical approach for non spherical bodies.

4 A DG method for transient electromagnetism

S. Pernet

The discontinuous Galerkin methods have become a classical tool for the simulation of wave propagation in heterogeneous media and complex domains. The EMA team contributes to the development of a high order Discontinuous Galerkin scheme for transient Maxwell's equations in collaboration with the French Aerospace Lab (ONERA). The discretization used is based on a conformal hexahedral mesh of the computational domain and of a polynomial order of approximation which is the same for all cells [7]. Although this scheme has interesting performances, some improvements are required to accurately describe a complex scene. Indeed, the unstructured meshes used have inevitably over-refined zones and a great disparity in size between cells may occur. In this situation, the stability condition of the temporal scheme used implies a very small time step and a prohibitive calculation. These last years, we have investigated many ways to increase the performances of the scheme :

– We proposed and studied the introduction of dissipative penalization terms and an original local time-stepping strategy. It has been proved mathematically and confirmed by means of examples that the dissipative terms provide a new formulation which improves the quality of the solution for distorted meshes and ensures the convergence of our DG scheme for all spatial approximation orders. In particular, we have also the convergence of the order 1 approximation, whereas it was not the case without these penalization terms. To accelerate the DG method, we have also proposed a local time-stepping strategy defined by a recursive multi-class method based upon a leap-frog scheme. Some comparisons with other approaches have been done and show the advantages of the proposed method. The statement of an explicit stability condition for this local time-stepping strategy is still an open problem, but numerical examples validate this method and show that it can be applied without too many restrictions, even for cavity problems. This work has been published in [EMA6].
– An other improvement in terms of CPU-time and memory storage has been studied. We have coupled the previous local time-stepping strategy with a Local Spatial Order Approximation. This strategy consists in choosing for each cell of the mesh, the well-adapted spatial approximation to ensure an accurate solution. This choice is done by considering the size of the cell and the source given in the problem. This strategy allows us to obtain an important reduction of the costs in terms of CPU-time and memory. For example, the mixed method Q1-Q2 with local time step is 7 times less expensive than the Q2 method for a same accuracy (see fig. 4.1).
– The ultimate step to reduce the cost of numerical methods is the use of automatic space-time refinements. The flexibility of the Discontinuous Galerkin methods allows to naturally take into account this kind of approach. Nevertheless, their effectiveness requires an accurate localization of zones where they should be used. The most appropriate tool to accomplish this task is called an a posteriori error estimator. We have undertaken a number of actions to achieve this task. Firstly, within the context of the federating research project MAHPSO "Modèles d'Approximation de Haute Précision pour les Systèmes de propagation d'Ondes" organized by ONERA, we have extended our DG scheme to non-conforming meshes for an anisotropic polynomial approximation [EMA13]. The implementation of this scheme has not been yet realized. Secondly, we are being involved in the project funded by the plan REI "Recherche exploratoire et Innovation" of the DGA (Direction Générale de l'Armement) in which we try to construct

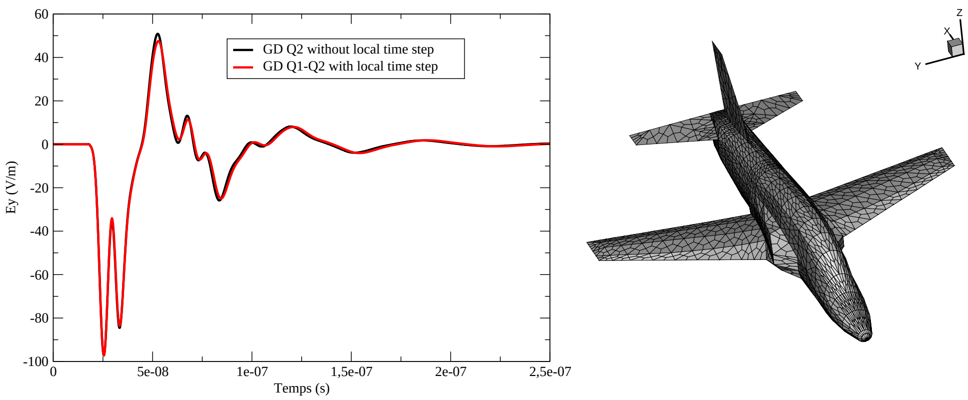


FIG. 4.1: Scattered field by an aircraft

an efficient a posteriori error indicator for our approximation of the transient Maxwell's equations. The first results can be found in [EMA14].

[7] G. Cohen, X. Ferrieres, and S. Pernet, (2006), A spatial high-order hexahedral discontinuous Galerkin method to solve Maxwell's equations in time domain, *J. Comput. Phys.*, **217**, 340–363.

5 Finite element simulation of acoustic scattering in a subsonic flow

As mentioned in the introduction, this activity is carried out in the framework of the AEROSON project, supported by the Agence Nationale de la Recherche, in partnership with EADS-IW, and the laboratories POEMS and LAUM. Part of this work is the object of the PhD of Emilie Peynaud.

5.1 A full coupling between acoustics and hydrodynamics

A.-S. Bonnet-Ben Dhia, F. Millot, S. Pernet and E. Peynaud

For the numerical simulation of time harmonic acoustic scattering in complex geometry, in presence of an arbitrary mean flow, the main difficulty is the coupling of two very different phenomena : acoustic propagation and convection of vortices.

Generally, these phenomena are modelized by using the Linearized Euler equations whose unknowns are the perturbation of velocity v and of pressure p. An alternative is to consider a less well-known equation called the Galbrun Equation where the unknown is the Lagrangian displacement u. These two approaches are equivalent and the classical quantities v and p can be easily recovered from u.

One difficulty is that a direct discretization of Galbrun equation by a Galerkin finite element method does not work, due to a lack of coerciveness [10, EMA2]. To overcome this difficulty and so to obtain a frame leading to a stable approximation, we have written an augmented equation by adding a term relative to a new unknown ψ. This term corresponds to the hydrodynamic phenomena and is obtained by solving a time-harmonic advection equation (see the next paragraph). To sum up, two coupled equations have to be solved : one is the augmented Galbrun equation and the other is a time-harmonic advection equation. We have proved that under some conditions for the mean flow, this coupled system is well-posed.

This work has allowed us to propose a stable approximation of the Galbrun Equation in 2D. For that, we use the Lagrange Finite Elements for the displacement u and a Discontinuous Galerkin scheme for the new unknown ψ. As an illustration of this approach, we present in fig. 5.2 the results obtained for a potential incompressible flow (see fig. 5.1) and for a source f such that $\nabla \times f \neq 0$ and $\nabla \cdot f \neq 0$. We observe that the method simulates correctly the physical phenomena : the acoustic waves particularly visible upstream and the hydrodynamic phenomena which can be seen downstream. The vortices are mainly produced by the source and are convected along the stream lines of the flow.

In the future, we will investigate more complex configurations, including flows coming from CFD codes and realistic wall conditions ....

5.2 The time-harmonic advection equation

A.-S. Bonnet-Ben Dhia, F. Millot, S. Pernet and E. Peynaud

As mentioned above, in the context of our research on modeling of sound propagation in a mean flow, we were led up to solve the following time-harmonic advection equation :

$$\begin{cases} -i\omega u + \mathbf{v_0} \cdot \nabla u = f \text{ on a bounded domain } \Omega \\ u \text{ given at inflow boundary} \end{cases} \tag{5.1}$$

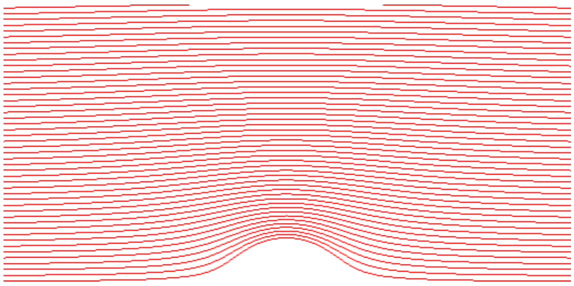


FIG. 5.1: Mean flow

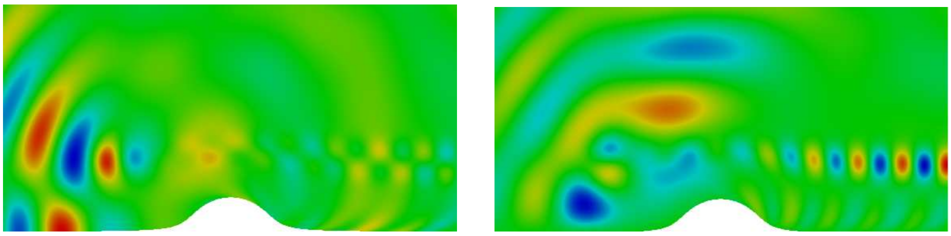


FIG. 5.2: Real part the components of u

Although the literature abounds in results on the analysis and resolution of this kind of equation in the time domain, there is, to our knowledge, no reference dealing with this problem in the frequency domain. One notes even that the analysis of the problem is not straightforward in spite of the simplicity of this equation. In a first time, we proved the well-posedness of this problem for the class of flows $\mathbf{v_0}$ which fill the bounded domain in the sense of Azerad [8], by establishing an inf-sup condition.
In a second time, we focused on developing a numerical method able to solve this problem. For this purpose, we studied and implemented two widespread methods commonly used to solve transport problems. The first approach is a finite element method based on a least-squares formulation [9] which has the advantage to yield a coercive hermitian bilinear form. The second approach is a Discontinuous Galerkin (DG) method [11] which turns out to be well-suited for advection equations as it naturally takes into account the transport phenomenon and for which we have proved a uniform discrete inf-sup condition. The analysis of these two approaches has led us to the following observation : the least-squares formulation has a widely dissipative behavior which makes it uncompetitive in comparison with the DG approximation (See fig. 5.3a where we have considered a uniform flow).
It may nevertheless be very interesting to have a finite elements method rather than a DG approach (costly in number of degrees of freedom). That's why, we have proposed an original method where the Galerkin approximation of the equation by using conformal H^1 finite elements is stabilized by a least-squares term. This last formulation turns out to be a good alternative to DG. The figures 5.3b and 5.3c show that the solution of the new formulation is more accurate for the same mesh.

[8] P. Azerad, (1996), *Analyse des équations de Navier-Stokes en bassin peu profond et de l'équation de transport*, phd thesis, Université de Neuchâtel (Suisse).

[9] P. B. Bochev and M. D. Gunzburger, (1996), Least-Squares Finite Element Methods, *Applied Mathematical Sciences, Springer*, **166**.

[10] A.-S. Bonnet-BenDhia, E. M. Duclairoir, G. Legendre, and J. F. Mercier, (2007), Time-harmonic acoustic propagation in the presence of a shear flow, *J. of Comp. and App. Math.*, **204,2**, 428–439.

[11] A. Ern and J. L. Guermond, (1996), Theory and Practice of Finite Elements, *Applied Mathematical Sciences, Springer*, **159**.

(a) The least-squares method : error= 25.4% for 13 568 dof

(b) The discontinuous Galerkin method : error= 4.34% for 19 998 dof

(c) The stabilized method : error= 0.33% for 13 568 dof

FIG. 5.3: Solutions obtained by the three methods for a uniform flow and corresponding L^2 errors

6 Publications

6.1 Journal Publications

[EMA1] A. Bendali and K. Lemrabet, (2008), Asymptotic Analysis of the Scattering of a Time-Harmonic Wave by a Perfectly Conducting Metal Coated with a Thin Dielectric Shell, *Asymptotic Analysis*, **57**, 199–227.

[EMA2] A.-S. Bonnet-BenDhia, J. Mercier, F. Millot, and S. Pernet, (2009), A low Mach model for time harmonic acoustics in arbitrary flows, *J. Comput. Appl. Math.*, **doi :10.1016/j.cam.2009.08.038**.

[EMA3] Y. Boubendir, A. Bendali, and M. Fares, (2008), Coupling of a non-overlapping Domain Decomposition Method with a Boundary Element Method, *International Journal for Numerical Methods for Engineering*, **73,11**, 1624–1650.

[EMA4] F. Collino, F. Millot, and S. Pernet, (2008), Boundary-integral methods for iterative solution of scattering problems with variable impedance surface condition, *PIER*, **80**, 1–28.

[EMA5] M. Fares, S. Gratton, and P. L. Toint, (2009), Svd-tail : a new linear-sampling reconstruction method for inverse scattering problems, *Inverse Problems*, **25,9**.

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10

Technology Transfer

1 Introduction

Pierre-Henri Cros

TT Group is aiming at making use of CERFACS results and/or competencies to explore new application domains. The activity programme of these two last years has been mainly defined to reinforce TT Group reputation in the sectors chosen for exploring these new application domains.

For ”Flow Modeling” team, the wealth of subjects successfully treated, highlight the ability of this team to open new application domains in CFD. As large companies of the building sector have paid attention to these results, discussions are on-going to team-up with them to answer to call for tenders in which flow modeling competencies in buildings are required.

For ”Computer Supported Collaborative Work” (TC) team, most of their time has been developing, integrating and testing the web and tailored release of N’S^3 collaborative solution called ColSol. Prototype benchmarks have been performed thanks to some CERFACS shareholders. Results analysis has been focused on understanding their skill concerns when using ColSol. Final objective was to collect enough information to get a tool box allowing TC team to adapt quickly ColSol to user requirements. Like for ”Flow modelling” team, there are on-going discussions with EADS service companies to team-up with them to answer to call for tenders about collaboration workspaces.

This activity should have reached a new development level at the end of the next period.

2 Flow Modeling

G. Jonville, consultants T. Schönfeld, C. Garrigue

The group has carried out simulations using of predictive computational fluid dynamics software to study and analyse the flow in buildings having heating, ventilating and air conditioning systems. The group has also transferred the data assimilation mock-ups in hydrology towards operational environment and brought out the use of PALM for the fluid-mechanic coupling in solid propulsion simulation.

2.1 Designing a ventilation system with CFD in a painting hall

In 2008 an upstream study on the design of the ventilation system for a new aircraft workshop has been realised for AIRBUS in the frame of a long range painting hall project. The aim of the study was to evaluate several technical solutions and to show the impact of the technical choices (Fig 2.1).
Numerous of 2D operating conditions have been numerically tested and some 3D configurations have been evaluated, regarding the efficiency of the ventilation system, by the use of Fluent CFD software. For each configuration, some quantitative criteria have been computed as angular deviation field, direct extraction rate and extraction efficiency of a weighted particles cloud around the aircraft. These simulations and the quantitative criteria allowed to analyse each ventilation flow and to identify an optimal solution for a correct pollutant extraction.

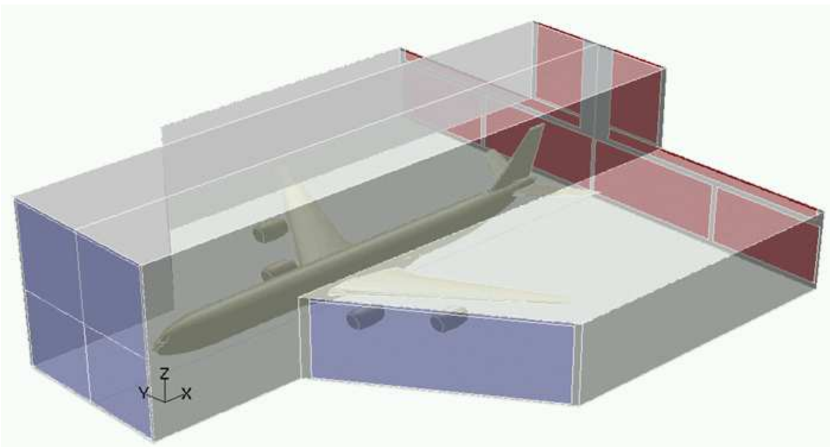


FIG. 2.1: Blowing and extracting vents in the painting hall geometry.

2.2 Checking the ambient temperatures with CFD in a data center

To study the temperature distribution in the data center of METEO-FRANCE, a simulation study has been conducted in 2009 with the specialised CFD software Flovent dedicated to the ventilation in building. The aim was to have at one's disposal a numerical tool to improve the air cooling system of computing rooms and to test the installation of new supercomputers.

The first step was to realise the numerical mock-up of the data center composed of two computing rooms for a total surface of 900m^2. A large number of components are represented : supercomputers, disks and switches racks, air conditioning units, perforated slab, floor grids, ceiling grids and cable ways in the plenum. A structured hexahedral mesh has been generated in the plenums and the rooms.

The second step was to choose the right grid refinement and the right boundary conditions. The air flow of each air conditioning unit is imposed. A blowing temperature value is imposed up to the unit's maximum power in relation to the extracting temperature.

The numerical results (Fig 2.2) have been compared to temperature measurements in order to tune the model. The use of CFD permitted a better understanding of the cooling system and allowed us to evaluate its operation in case of air conditioning unit breakdown or extreme climatic situation. The simulations showed that the air conditioning system is sufficient regarding the present machine load and that the thermal conditions are still acceptable even in extreme situations.

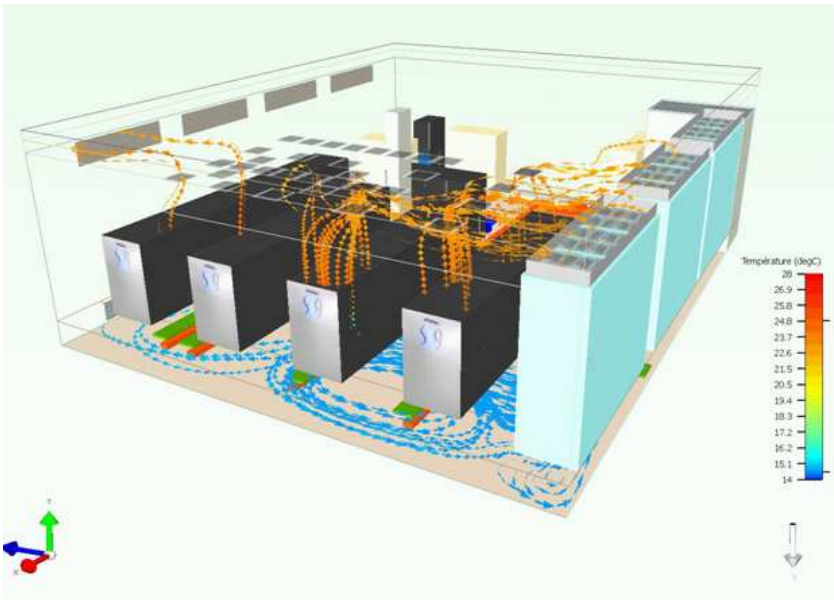


FIG. 2.2: Path lines from one air conditioning unit colored by temperature.

2.3 Data assimilation in hydrology

In collaboration with the GlobC team (see 2-4.2 Data assimilation applications in hydrology), the group participated in 2008-2009 to the research agreement between the Service Central d'Hydrologie et d'Aide aux Prévisions des Inondations (SCHAPI) and CERFACS, aiming to improve the flood forecasting by the use of data assimilation.
A classical BLUE (Best Linear Unbiased Estimate) assimilation algorithm has been used to tune some relevant parameters of the direct models. A case study used the rain-discharge model of the ATHYS platform to simulate the flash floods of the Gardon d'Anduze river. A second one used the fluvial model MASCARET for the real-time simulation of the course of the Adour river and of its tributaries.
The flood forecast scores obtained with this technique showed a considerable improvement if compared to other classical approaches in hydrology and hydraulics. The use of the PALM coupler allowed to be less intrusive in the models and will allow to easily replace a model by another for the application of different flood model systems.
The group has implemented evaluation criteria of flood simulations and has validated the results of data assimilation methods. The data assimilation mock-ups have been adapted to the operational environment of SCHAPI and have been installed.

2.4 Code coupling with PALM for solid propulsion

A fluid-mechanic coupling with the PALM software tool has been conducted in the frame of a contract with SAFRAN (SPS) during 2009. The aim was to develop a coupling application which is efficient, flexible and easy to handle and maintain.
The MPI-2 parallel library was used to assemble the fluid code and the mechanic code in PALM. The coupling application was designed to run the fluid code in parallel. The mechanical code was connected to PALM by the implementation of user subroutines only. An explicit algorithm was used to enable the exchange of physical quantities between the two codes (Fig. 2.3).
This new coupling solution has a better performance with a factor 8 compared to the present solution. It allows easy evolution to the coupling algorithm.

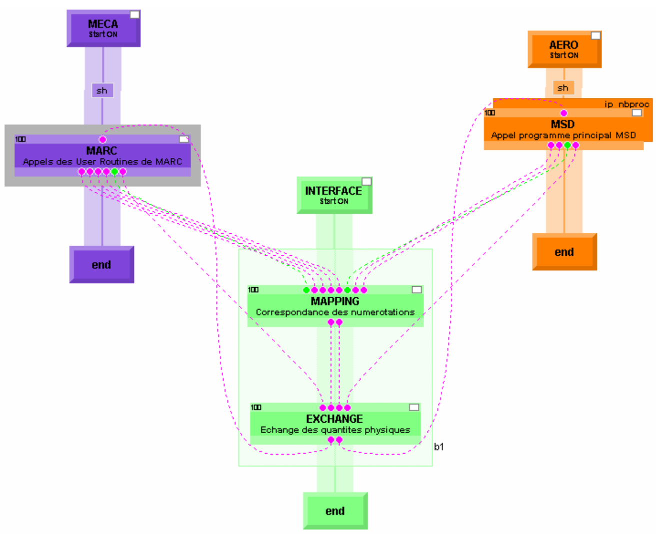


FIG. 2.3: PrePALM framework of the MSD-MARC coupling.

3 Development of collaborative working solutions

S. Milhac, F. Oliveira, consultant D. Vincent

3.1 Introduction

TT-TC team works on the development of a synchronous collaborative tool allowing distant people to work in real time as if they were in the same place. It means the possibility to access to a collaborative space and see and hear each other, use a common whiteboard, share and discuss documents and co-manipulate data (office or numerical simulation results).
The first version, called N'S^3 Package, was a hardware/software solution with 3 screens, 2 PCs and dedicated network lines.

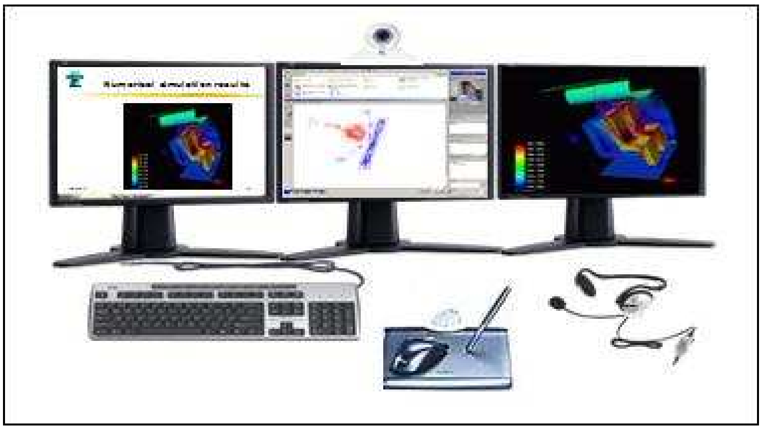


FIG. 3.1: N'S^3 Package.

The tool was considered as a meeting room where the users had to come in to attend a meeting. To achieve a good ergonomic, we used 3 screens where each screen had a specific role to reproduce a meeting space :
– First one to display the office documents ;
– Second one to communicate (via audio, video and whiteboard) and manage the meeting ;
– Third one to manipulate the 3D data.

With the evolution of new technologies and to answer the users' requirement to attend a meeting from their workstation, the N'S^3 package was replaced by a web version, called ColSol, giving access to a collaborative space on Internet from a common computer.

ColSol implied developments in Java, HTML, javascript and PHP to produce a web application using a client/server architecture. The dedicated network lines were no longer required allowing the connection from anywhere.

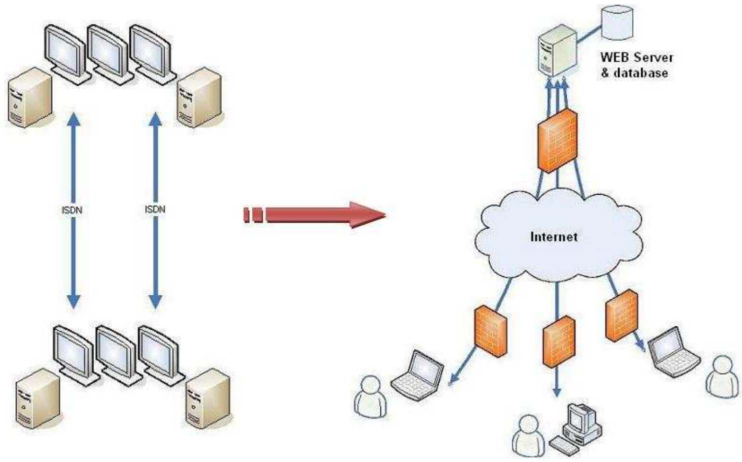


FIG. 3.2: To a web application.

All the collaborative functionalities proposed by the N'S^3 package were redeveloped to be available with CoSol which also provides meeting management functionalities (cf. Figure 34). The user can plan, hold and archive the meetings. He can explore previous meetings with a related topic agenda in order to come up with a suitable agenda that covers all the relevant issues.

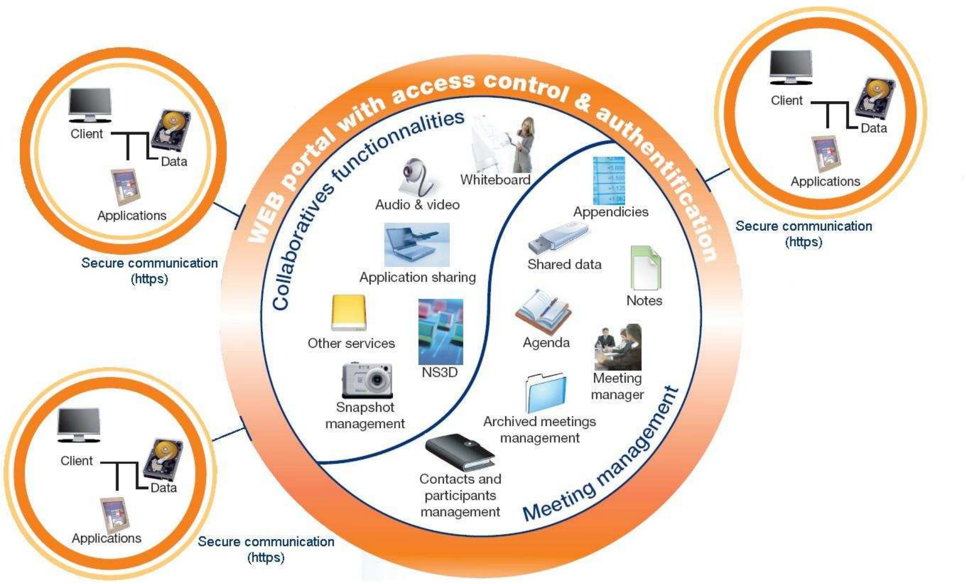


FIG. 3.3: ColSol.

ColSol	
WEB Application	YES
MEETING PREPARATION PHASE	
Invitation	YES
Data exchange	YES
HOLDING PHASE	
Audio-Video, Chat	YES
Application sharing	YES
Multi-applications sharing	YES
Synchronised viewer	YES Ensight, Catia
Remote control	YES
STORING PHASE	
Meeting storing	YES
Meeting data	YES
ATTRIBUTE/RIGHTS	
Meeting invitation	YES
Meeting data	YES
Stored data	YES
SECURITY	
Tools	VPN + SSL
COMPATIBILITY	
OS	Windows
Navigator	IE 6 and more

FIG. 3.4: ColSol functionalities.

3.2 ColSol

3.2.1 R&D

During the year 2008, the team continued the developments of ColSol to make it robust and more and more intuitive.
Despite the fact of having to use only one screen, ColSol gets an intuitive GUI by using tabs and a central area updated regarding the selected tab.

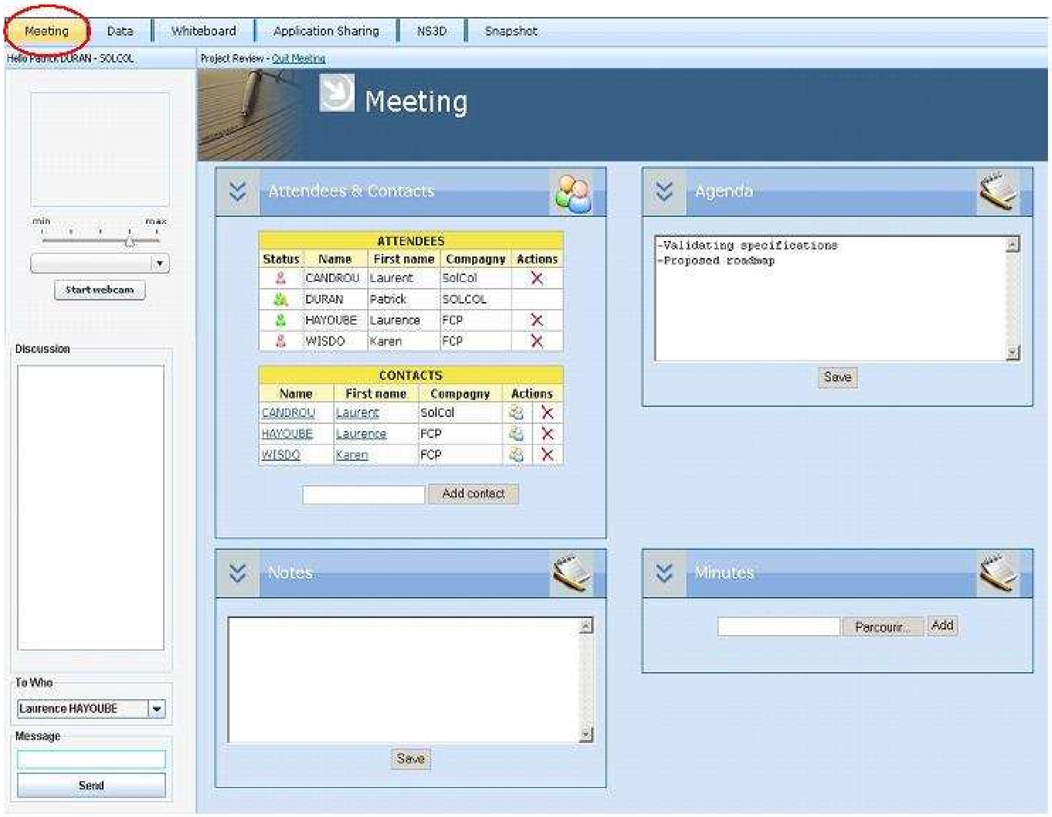


FIG. 3.5: ColSol GUI.

A multi-language version was also developed to allow the use of ColSol through a German, Spanish, French or English interface. The installation and user guides are available in the 4 languages. It made it possible to carry out test sessions with voluntary colleagues from various European countries.

R&D activities continued throughout the years 2008-2009 with SAFRAN Group and CNES support.

3.2.2 Deployment

Two types of architecture are available for deployment :

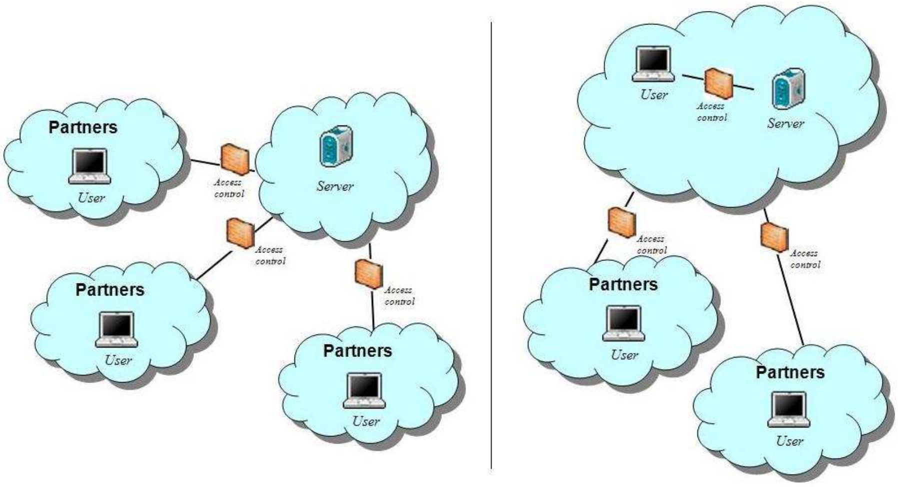


FIG. 3.6: Hosting at a third party (A1) ; In-house hosting (A2)

For A1, the access to the collaborative workspace is protected via the setting up of a VPN (Virtual Private Network) SSL (Secure Sockets Layer).
Two technologies could be used :
– a hardware solution with a firepass VPN SSL from F5 ;
– a software solution with OpenVPN, open source application.

For A2, the server must be installed on the company network and the required ports must be opened :
– TCP 1935 for audio/video module ;
– TCP 4561 and TCP 2050 to 2049+X for meeting management. X represents the maximum of concurrent meetings started in the server ;
– TCP 3306 for database access ;
– TCP 80 and 8080 for web pages loading.

Both architectures were tested in a working environment with the help of some stakeholders :

A1 :
– Distant follow up by Turbomeca of numerical simulation results realized by Cerfacs ;
– Distant Cimpa RCO[1] meetings ;
– Organize between CoWI, University of Koln and Cerfacs testing of different collaborative components in the framework of CoSpaces projects.

A2 :
– Colamed project (CNES) : organize, from a server installed at Institute Claudius Regaud for Institute Claudius Regaud, distant RCP[2] between doctors from the Institute Claudius Regaud and those from Hôpitaux de Toulouse ;

[1]Research Chief Officers
[2]Runion de Concertation Pluridisciplinaire (Multi-specialty consultation meetings)

– MPEG project (Groupe SAFRAN) : hold, from a server installed at Snecma, distant meetings between Turbomeca and Snecma ;
– Virtual Testing project (Seed companies) : perform different tests, from a server installed at Théogone, for specifying the collaborative workspace expected by this sector.

3.3 Prototype of ColSol v2

During the year 2009, a new version, called ColSol2, was developed. The benefit of this version is the possibility to preconfigure some meeting templates using the required functionalities only. For example the user would be able to choose between a simple presentation meeting, a workshop or a conference call.

This version is based on modules to activate or not during the meetings depending on the users' needs.

FIG. 3.7: Modular version.

The team continued to work on the GUI to take into account feedback from users. One of the most significant developments was to add the possibility to change the dimensions of the windows of the functionalities.

3.4 2010 program

In 2010, R&D activities on ColSol2 will address the different specifications coming from 2008-2009 evaluation phase :

- A version not requiring the administrator rights ;
- A multi-language version and the corresponding installation and user guides will be produced ;
- An integrated version to an information system ;
- An integrated version with a Data Management tool.

In 2010, with the contribution of the SAFRAN Group and CNES, ColSol2 will be tested in a real working environment. It would be the opportunity to set up and assess the support team.

11

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 ;
- 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 support activity is the responsability of a five people team.

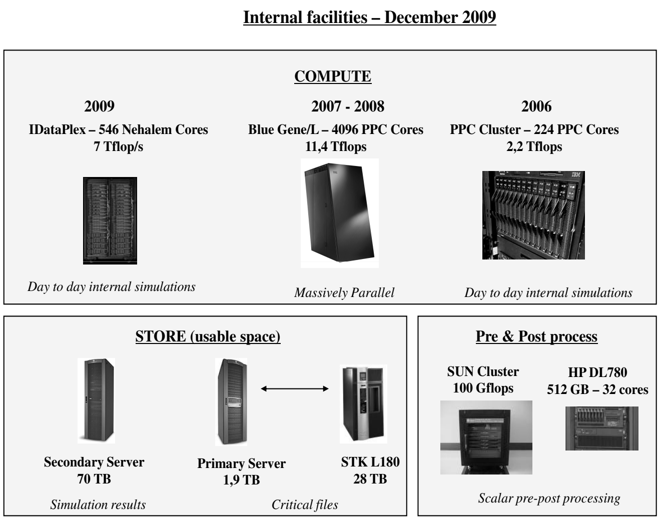
1.2 General strategy

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.

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

2.1 CERFACS' computing resources (As of Dec 09).



During the period CERFACS' computer resources have seen main improvements :

- Computing power : 2.5 times faster with two new configurations.
  - An IBM iDataPlex cluster, installed in august 2009, offers a peak performance of 7 Tflop/s with 656 Intel Nehalem cores. This new cluster increase significatively our day-to-day simulation power.
  - One of major issue is to prepare codes to petaflop resources needs adapting them on massively parallel servers. The IBM Blue Gene/L installed in july 2007 has been upgraded one year later. The new configuration offers a peak performance of 11.4 Tflop/s with 4 096 PowerPC cores to help researchers to adapt their codes on this kind of supercomputer and deliver an efficient power to large simulation problems.

  These two servers shares a 60 TB parallel filesystem based on a GPFS solution.
- Storage : The capacity of our fileserver dedicated to the storage of large simulations has been upgraded from 45 TB to 70 TB. This new storage capacity is mainly dedicated to climate results generated on Meteo-France's Supercomputers.
- Pre and Post processing : The increase of our computing power asked us to set up more powerfull solutions to visualize bigger data sets and generate bigger meshes. A new HP server has been installer with 32 cores AMD shangai and 512 TB of shared memory to prepare and exploit some of the Blue Gene/L bigger data sets.

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 (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 A Management Server, MatLab servers) or an integral part of CERFACS' infrastructure (Web servers, Mail server, printer server, NIS, ...).