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. 2010 – Dec. 2011

CERFACS
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Table des matières

Table des figures

Foreword

Welcome to the 2010-2011 Scientific Activity Report of CERFACS.

For CERFACS, this was a period of transition and transformation : a new director, a new building and several internal reorganizations.

The positioning of CERFACS is in applied research, as a bridge between academia and industry, with a constant requirement for excellence. But, CERFACS needs to face major transformations of his environment with global changes of its financing channels and arrivals of new players.

Through this period CERFACS has maintained its standard of scientific excellence with the yearly publication of over 50 articles in internationally-refereed journals. Training of new researchers has been intense with more than 25 theses defended over the period. And, CERFACS researchers and engineers have been very active in industry oriented research, with more than 50 grants per year.

Now, HPC is in the move with Exascale computing as an aim. CERFACS has responded through the definition of three challenges with a 2020 horizon. These willbring to CERFACS the knowledge for running its simulations on next generation supercomputers providing hundreds of thousands of cores.

But, with these new computers we need to rethink our HPC paradigm. Scalability cannot be the only measure of performance and justification of suitability for their use. Indeed, what we expect from HPC is not at all the same when the target is not running a single research code on a large number of processors, but rather handling legacy codes in parametric and/or statistical analysis on realistic configurations. This remark will forge the way we do science at CERFACS in the coming years.

I am sure that you will enjoy this detailed activity report, to pursue your collaboration with us and to initiate new ones.

Bijan MOHAMMADI
CERFACS Director

CERFACS Structure

CERFACS has 7 shareholders :	
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%

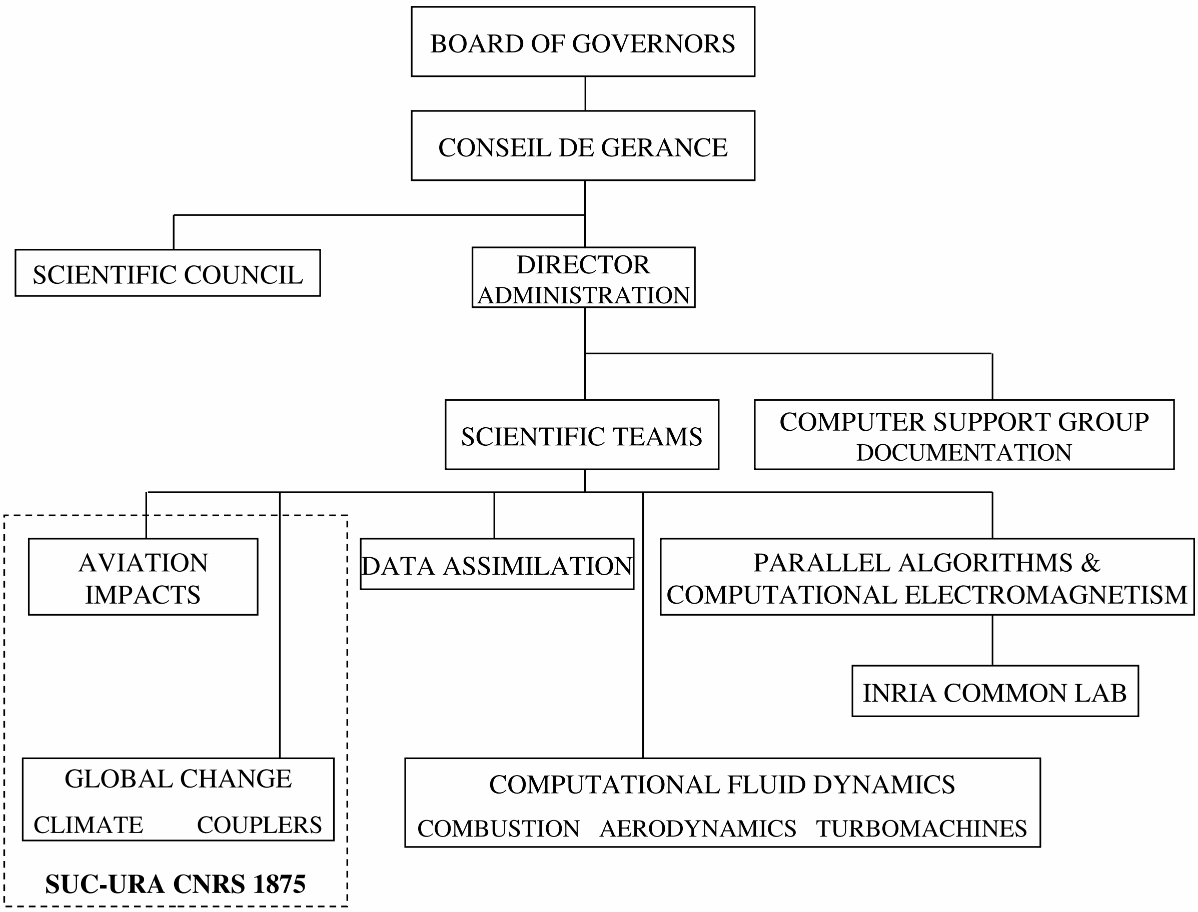
As a "Société Civile" CERFACS is governed by two bodies :
– Assemblé des Associés
– Conseil de Gérance.

The Board of Governors (Assemblée des Associés) is composed of representatives of CERFACS shareholders and of 3 invited personalities, including the Chairman of the Scientific Council. This board meets twice a year and validates the propositions of our Conseil de Gérance on CERFACS orientations and budget.

Conseil de Gérance is composed by7 managers (Gérants) each designated by one of the 7 CERFACS shareholders. These follow, on a quarterly basis, the activities of the center and its financial situation.

CERFACS Scientific Council has 16 members and is chaired by Professor Sébastien CANDEL.

CERFACS organization charts



CERFACS Staff

NAME	POSITION	PERIOD
GRATTON	Project Leader	2011/01
DUFF	Scintific Advisor	2011/01
VASSEUR	Senior	2007/05
BOITO	Post Doc	2010/06-2011/06
BYCKLING	Post Doc	2010/11
FUCHS	Post Doc	2009/06-2011/06
JIRANEK	Post Doc	2008/11
KAYA	Post Doc	2009/09-2011/08
MUCHERINO	Post Doc	2010/12-2011/08
PICHENY	Post Doc	2011/09
RINCON	Post Doc	2011/10
TROELTZCH	Post Doc Ph.D student	2011/11 2007/05-2011/04
AHIDAR	Ph.D student	2011/10
BERGOU	Ph.D student	2011/10
DIOUANE	Ph.D student Student	2011/10 2011/03-2011/09
FERREIRA LAGO	Ph.D student	2010/03
GENTILE	Ph.D student	2011/04-2011/08
GUROL	Ph.D student	2010/02
MURPHY	Ph.D student	2011/10
PINEL	Ph.D student	2006/10-2010/04
JOSLIN	Engineer	2011/10
TSHIMANGA	Engineer	2011/05-1011/07
BIARI	Student	2010/05-2010/09
VICENTE	Visitor	2010/04-2010/07

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

NAME	POSITION	PERIOD
POINSOT	Project Leader	1992/09
CUENOT	Senior	1996/10
DAUPTAIN	Senior Post Doc	2010/04 2008/04-2010/03
DENIAU	Senior	2006/11
DUFOUR	Senior	2009/06-2011/03
GICQUEL	Senior	2004/02
GOURDAIN	Senior	2008/02
JOUHAUD	Senior	2001/10
MONTAGNAC	Senior	2000/11
PUIGT	Senior	2005/12
RIBER	Senior Post Doc	2010/05 2008/05-2010/04
SICOT	Senior	2011/09
STAFFELBACH	Senior	2008/11
VERMOREL	Senior	2007/11
BOUSSUGE	Research Engineer	2002/02
AMAYA	Post Doc Ph.D student	2010/03-2011/03 2006/10-2010/02
CABRIT	Post Doc	2009/10-2011/03
CHENY	Post Doc	2009/09-2011/08
DECHAUME	Post Doc	2009/04-2011/03
ENAUX	Post Doc Ph.D student	2010/07-2011/03 2006/10-2010/06
GARCIA	Post Doc	2009/02-2010/09
GOUGEON	Post Doc	2008/07-2010/06
HALLEZ	Post Doc	2009/09-2010/08
KOLOMENSKIY	Post Doc	2011/05
KRAUSHAAR	Post Doc Ph.D student	2011/12 2008/10-2011/11
LAMARQUE	Post Doc	2009/07-2011/06
LAURENCEAU	Post Doc	2008/07-2010/06
LECOCQ	Post Doc	2010/04-2011/09
MOUFFE	Post Doc	2009/05-2011/04
NEOPHYTOU	Post Doc	2010/12
PINEL	Post Doc	2010/05
POITOU	Post Doc	2009/12-2011/11
ROUSSEL	Post Doc	2010/06-2010/10
URZAY	Post Doc	2010/05-2011/01
VASS	Post Doc	2011/10
WANG	Post Doc	2011/07
BARRE	Ph.D student Engineer	2010/06 2009/11-2010/05
BOCQUET	Ph.D student	2010/01
BODOC	Ph.D student	2007/07-2010/06
CHAUSSONNET	Ph.D student	2010/06
COLLADO	Ph.D student	2009/09

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

CREVEL	Ph.D student Engineer	2010/09 2010/04-2010/08
DURAN	Ph.D student Engineer Student	2011/01 2010/09-2010/12 2010/03-2010/08
EYSSARTIER	Ph.D student	2008/10-2011/10
FOSSO	Ph.D student	2007/10-2011/04
FRANCOIS	Ph.D student Engineer	2010/05 2010/01-2010/04
FRANSEN	Ph.D student	2010/01
FRANZELLI	Ph.D student	2008/01-2011/06
GALLARD	Ph.D student	2011/01
GIRET	Ph.D student Engineer Student	2011/03 2010/10-2011/02 2010/04-2010/09
GOMAR	Ph.D student Student	2010/09 2010/03-2010/08
GRANET	Ph.D student	2008/10-2011/12
GULLAUD	Ph.D student	2007/11-2010/11
GUEDENEY	Ph.D student	2008/11
HANNEBIQUE	Ph.D student	2009/10
HERMETH	Ph.D student	2009/03
HERNANDEZ VERA	Ph.D student	2008/11-2011/10
JAURE	Ph.D student	2009/04
LAPEYRE	Ph.D student	2011/10
LEGRAS	Ph.D student	2007/11-2011/04
LEONARD	Ph.D student Engineer	2010/06 2010/01-2010/05
LEYKO	Ph.D student	2006/09-2010/05
MAGLIO	Ph.D student	2007/07-2010/07
MARI	Ph.D student	2011/12
MISDARIIS	Ph.D student Engineer	2011/11 2011/10-2011/10
MOTHEAU	Ph.D student Engineer	2010/11 2010/07-2010/11
OZEL	Ph.D student	2007/09-2010/07
PAULHAC	Ph.D student Engineer Student	2011/12 2011/11-2011/11 2011/03-2011/09
PEDOT	Ph.D student	2008/10-2011/10
QUILLATRE	Ph.D student Student	2010/10 2010/03-2010/09
RICHARD	Ph.D student	2009/10
ROCCHI	Ph.D student	2009/11
RUIZ	Ph.D student	2008/10
SADOUDI	Ph.D student Engineer	2011/11 2011/02-2011/10
SENONER	Ph.D student	2007/01-2010/05
SIERRA SANCHEZ	Ph.D student	2008/10

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

SILVA GARZON	Ph.D student	2007/08-2010/12
WIECZOREK	Ph.D student	2007/06-2010/12
WLASSOW	Ph.D student	2009/03
WOLF	Ph.D student	2007/10-2011/11
ZUZIO	Ph.D student	2007/08-2010/07
BAUERHEIM	Engineer	2011/10
CAYOT	Engineer Student	2011/10 2011/02-2011/07
DOMBARD	Engineer	2011/10-2011/12
DOURNAC	Engineer	2010/03-2010/06
DUBUC	Engineer	2009/12-2010/12
ESTIVAL	Engineer	2009/04-2010/03
FRICHET	Engineer Student	2011/10 2011/03-2011/09
KOUPPER	Engineer	2011/10-2011/12
LIVEBARDON	Engineer	2011/11
PAPADOGIANNIS	Engineer	2011/11-2011/12
PARMENTIER	Engineer	2010/07-2011/05
ROBERT	Engineer	2011/01-2011/03
SAILLOFEST	Engineer	2008/11-2010/02
BENNANI	Student	2010/04-2010/09
BERGOTTI	Student	2010/04-2010/05
BURNAZZI	Student	2009/10-2010/05
BUSIELLO	Student	2011/05-2011/09
DAMIEN	Student	2011/04-2011/09
DEWANDEL	Student	2011/04-2011/09
KRUNEMACKER	Student	2011/04-2011/09
LEFORT	Student	2010/02-2010/09
NGUYEN	Student	2011/02-2011/09
NOLTE	Student	2011/02-2011/07
VUILLEMIN	Student	2011/07-2011/07
YABILI	Student	2010/04-2010/09
ZHU	Student	2010/07-2010/09
BIBRZYCKI	Visitor-PhD	2009/09-2010/02
BISSELING	Visitor	2010/05-2010/06
FRITZER	Visitor-PhD	2010/04-2010/06
FRU	Visitor-PhD	2010/05-2010/07
KOZOLUB	Visitor-PhD	2009/09-2010/02
KUBAN	Visitor-PhD	2010/10-2011/09
NAJAFIYAZDI	Visitor-PhD	2009/11-2010/04
ZIMMERMANN	Visitor	2010/09-2010/11
MOREAU	Formateur	2009/04
MULLER	Consultant	1997/11
NICOUD	Consultant	2001/10
RIZZI	Consultant	1987/10
SAGAUT	Consultant	2003/12
SCHONFELD	Consultant	2001/01

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

NAME	POSITION	PERIOD
THUAL	Project Leader	1991/09
DUCHAINE	Senior	2010/10
RICCI	Senior	2008/11
ROGEL	Senior	1998/10
TERRAY	Senior	1992/10
WEAVER	Senior	1999/11
BOURIQUET	Research Engineer	2006/08
MAISONNAVE	Research Engineer	2000/12
MOREL	Research Engineer	2000/03
PAGE	Research Engineer	2009/07
SANCHEZ	Research Engineer Engineer	2010/11 2009/05-2010/10
THEVENIN	Research Engineer	2008/09
VALCKE	Research Engineer	1997/02
MIROUZE	Post Doc Ph.D Student	2010/10-2011/12 2007/10-2010/09
MOINE	Post Doc	2008/12
MOUFFE	Post Doc	2011/09
PANGAUD	Post Doc	2009/12-2010/11
TITAUD	Post Doc	2010/06
CORRE	Ph.D Student	2008/10-2011/12
RUPRICH-ROBERT	Ph.D Student Student	2010/10 2010/02-2010/06
BRETONNIERE	Engineer	202011/02
FERNANDEZ	Engineer	2010/05-2011/10
LATOUR	Engineer	2009/05-2011/07
PIAZZA	Engineer Student	2010/10 2010/04-2010/09
TRESPEUCH	Engineer Student	2011/10 2011/02-2011/09
YAN	Engineer	2011/02
BERGER	Student	2011/06-2011/09
BLUHM	Student	2010/04-2010/05
DELMOTTE	Student	2011/02-2011/05
HARADER	Student	2011/02-2011/07
ICHARD	Student	2011/05-2011/08
KILICOGLU	Student	2010/03-2010/08
MALLET	Student	2010/03-2010/08
NINOVE	Student	2011/04-2011/09
PLANTE	Student	2011/04-2011/09
ROCHOUX	Student	2010/02
SOUCHU	Student	2011/06-2011/09
ARGAUD	EDF	2006/07-2011/07
BOE	CNRS	2010/10
CASSOU	CNRS	2002/11
COQUART	CNRS	2006/12
FERNANDEZ	CNRS	2011/11
PIACENTINI	Consultant	2007/06

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

NAME	POSITION	PERIOD
REMY	Senior	2003/12-2010/12
BOURDALLE-BADIE	Research Engineer	2001/01-2010/12
DERVAL	Research Engineer	2003/07-2010/12

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

NAME	POSITION	PERIOD
BONNET	Project Leader	2006/05-2011/12
FARES	Senior	1992/06
MILLOT	Senior	1995/11
PERNET	Senior	2007/03
COSSONNIERE	Ph.D student	2008/10-2011/09
PEYNAUD	Ph.D student	2009/10
STEIF	Ph.D student	2008/10
BART	Student	2011/07-2011/09
BERNARD	Student	2010/06-2010/09
BOURREL	Student	2010/06-2010/09
DECECCO	Student	2011/04-2011/07
MADIOT	Student	2011/08-2011/08
POPIE	Student	2011/07-2011/09
BENDALI	Consultant	1996/01
COLLINO	Consultant	1994/04

TAB. vi: List of members of the COMPUTATIONAL ELECTROMAGNETISM project fusioned with PARALLEL ALGORITHMS project in 2011

NAME	POSITION	PERIOD
GIRAUD	INRIA	2009/11
DUDOUIT	Ph.D student	2010/10
SALAS MEDINAS	Ph.D student	2010/03

TAB. vii: List of members of the HIEPACS team

NAME	POSITION	PERIOD
CARIOLLE	Project Leader	2003/08
MASSART	Senior	2004/12
PAOLI	Senior	2004/07
CRESPIN	Post Doc	2009/01-2010/03
JAUMOUILLE	Post Doc	2010/02
NYBELEN	Post Doc	2008/04-2010/03
THOURON	Post Doc	2010/10
PAJOT	Ph.D Student	2008/11-2011/12
PICOT	Ph.D Student	2009/10
POUBEAU	Ph.D Student	2011/10
PRAGA	Ph.D Student	2011/09
UNTERSTRASSER	Visitor	2010/10-2011/03
PIACENTINI	Consultant	2007/10

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

NAME	POSITION	PERIOD
CROS	Project leader	1997/04
JONVILLE	Engineer	2000/10-2010/12
MILHAC	Engineer	2004/01
OLIVEIRA	Technician	2007/06-2010/12

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

NAME	POSITION	PERIOD
MONNIER	Project Leader	1996/12
D'AST	Engineer	1996/10
JONVILLE	Engineer	2011/01
LAPORTE	Engineer	1988/04
CONTRERAS	Technician	2011/09
DEJEAN	Technician	1990/11
FLEURY	Technician	1999/10
BRUNEAU	Student	2010/02-2010/08
ETCHEVERRY	Student	2011/04-2011/09
GERS	Student	2010/04-2010/06
LEREDDE	Student	2010/02-2010/08
VANNIER	Student	2010/04-2010/06

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

CERFACS Wide-Interest Seminars

Peter Hanappe (Sony Computer Science Laboratory, Paris) : *Parallelisation of Edwards and Slingo's radiation algorithm on the CELL processor : results and perspectives.* (2010, March 3rd)

Thi Thu Huong Hoang (EDF R&D & Département de Mathématiques d'Orsay) : *Séries chronologiques non stationnaires non linéaires. Le cas des séries de températures en Europe.* (2010, March 5th)

Olivier Coulaud (Laboratoire commun INRIA-CERFACS) : *EPSN : a Computational Steering Environment for Legacy Parallel and Distributed Simulations.* (2010, March 16th)

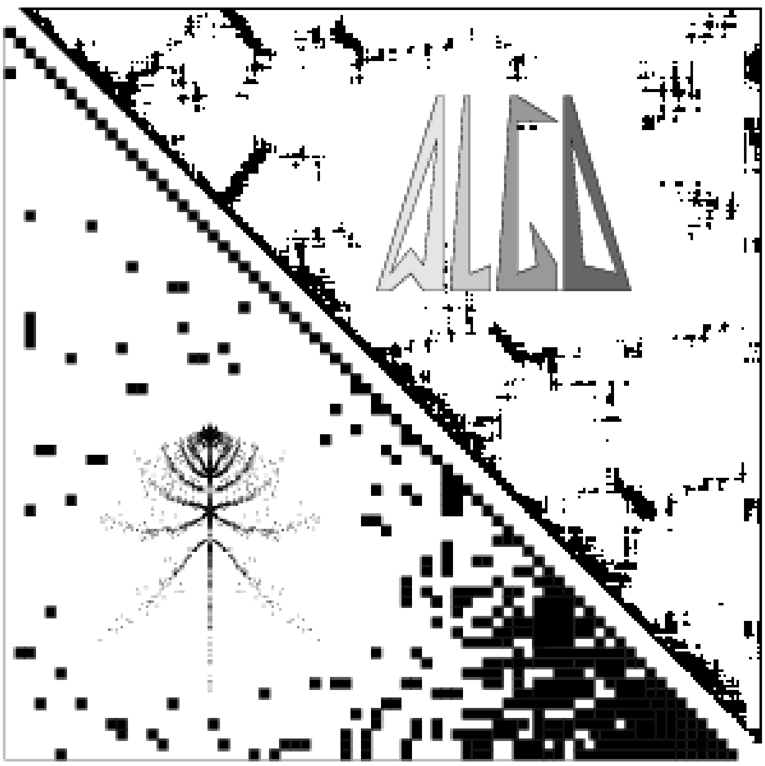
Ronan Paugam (King's College - London) : *Injection Height of Biomass Burning Emission.* (2010, September 8th)

Frédéric Alauzet (INRIA - Projet Gamma, Rocquencourt) : *Anisotropic Mesh Adaptation for CFD.* (2010, September 22nd)

NVIDIA - ATI - PGI - CAPS - Allinea : *Demi-Journée sur le thème du calcul hybride.* (2010, October 7th)

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, we can notice that 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.

As shown in Section 4, 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, ENS-Lyon, and INRIA-Bordeaux. The release currently being distributed is Version 4.10. Some research work that will most likely have an impact on future releases is discussed in the following sections, in particular in Sections 4.1, 4.2, 4.10. 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 electromagnetism. 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. The MUMPS is part of a set of codes considered as the best for solving general sparse linear systems. His performance is certainly due to a fruitful collaboration with persons from ENSEEIHT-Toulouse, and ENS-Lyon and INRIA-Bordeaux. This collaboration concerns the development of algorithms, and relies on theoretical results obtained from applications of graph theory to matrices. Year 2011 has been especially productive in this area, as presented in Sections 4.3, 4.5, 4.6, 4.8 and 4.9.

The development of robust and general purpose preconditioners and an analysis of their properties is discussed in many of the contributions to Section 5. 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. The results obtained during the year are very rich and can be sorted as follows. Some results are related to the development of new Krylov methods, that enable flexibility of the preconditioner, deflated restarting, inexact matrix-vector products or reuse of information as far as sequences of linear systems are considered. These results are presented in Sections 5.4, 5.7, 5.8 and 5.11. These methods have enhanced convergence properties, but the need for efficient preconditioning schemes remains very strong. Theoretical results related to generic preconditioners have been obtained in Sections 5.1, 5.5 and 5.6. Much of the work has been to extend these techniques so that they can be applied to a wider range of problems in different application areas. However, some preconditioners can be developed for a class of applications. The domain of geophysics proposes very important challenges around the preconditioning of the Helmholtz equation for which preconditioners have been proposed, making possible the solution of linear systems with billions of unknowns as presented in Sections 5.2, 5.3 and 5.14. The problem of efficiently solving large systems has also occurred in eigenanalysis for combustion, where a good choice of initial subspaces for eigensolvers has provided significant decrease in simulation time (see Section 5.9). Finally, iterative solvers are practically stopped before full convergence, and the control of errors, is essential. Progress has been made both for the solution of linear systems and least-squares problems, where closed formula and algorithms for computing these errors are presented, see Sections 5.10, 5.12 and 5.13. 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 into a book that will be published shortly (see Section 6).

These two years have seen a strong reinforcement of the team activities in the areas of nonlinear systems and optimization. This is the consequence of a growing interest of the CERFACS shareholders in this area, and has stimulated both fundamental and applied research activities. Most of the algorithms that are studied are formulated in a trust-region setting, an area in which the team is getting a growing experience, thanks in particular to the strong support of our consultant Philippe Toint from the University of Namur. A new ”retrospective” trust-region algorithm has been developed (see Section 7.2) that is a very natural variant of the most basic trust-region algorithm. We also worked on multigrid algorithms that can be considered as extensions of the full-multigrid algorithm (see Sections 7.12 or 7.15 for a Quasi-Newton variant). Large-scale least-squares techniques have also stimulated research in the area of preconditioning, model reduction, and duality see Sections 7.9, 7.11, 7.14, 7.19 and 7.20. These researchs have been made directly available to the ocean data assimilation community, thanks to our collaboration with the CERFACS Climate Modeling team. Derivative-free optimisation has also been a major research topic in the last five years. We proposed and developed the BC-DFO algorithm that is able to find first-order critical point of bound constrained optimization problems (see Sections 7.16, 7.17 and 7.24), and has shown good performance on real-life problems arising in shape optimization for aeronautics. The team also managed to extend its experience in error analysis to quadratic optimization problems giving in the case of total least-squares, truncated singular value decomposition, and bound constrained quadratic optimization useful formulas for sensitivity analysis and backward error (see Sections 7.1, 7.10, 7.13, 7.18 and 7.21). Activities have also been carried out in the domain of mixed-integer optimization as described in Sections 7.7 and 7.8, where real-life examples were successfully solved. We also mention the availability of a software tool for testing optimization algorithms that is described in Section 7.5 and that offers a lot of statistics for comparing optimization softwares. An important feature of the team is the constant involvement in applications that is illustrated in most of the pre-cited research topics, but which appears also clearly in Sections 7.3, 7.4, 7.6 and 7.23, where applications in electromagnetics, acoustics, aerodynamics have been tackled.

We continued our involvement into a large grant from RTRA-STAE to look into data assimilation problems 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. The fruitful collaboration with the foundation will continue even after year 2012, since the team has been given the responsibility to coordinate research on stochastic algorithms for Data assimilation in the framework of the MoMa group of discussion. This group is expected to select projects to be supported by the foundation in the area of complex physical systems.

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. 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 two stagiaires (Mohamed Biari and Youssef Diouane) from ENSEEIHT. 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. Xavier Pinel defended his thesis on preconditioned iterative methods for the Helmholtz problem in May 2010. Anke Tröltzsch completed her PhD thesis on active set techniques for bound constrained derivative free optimization in June 2011.

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.

We continue to have a "Sparse Days at CERFACS" meeting each year. On 15-17 June 2010, and 6-7 September 2011, these meeting were held with particular emphasis on sparse direct methods for the first and high-performance computing for the second. The 2010 Sparse Days included the final workshop of the ANR SOLSTICE project around direct methods for sparse matrices.

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.

We have continued the collaboration with Airbus on shape optimization for drag minimization under lift constraints (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 on gravity field determination. Our work is part of the RTRA-STAE ADTAO project and concerns regularization techniques for solving inverse problems using observations from the GRACE satellite.

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 finished in June 2010.
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 Modeling 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. These solvers are part of a broader project aiming at determining the velocity field of the Earth sub-surface. This latter problem is formulated as a nonlinear least-squares problem that exhibits many local minima. The PhD of Y. Diouane focuses on the use of appropriate techniques from global optimisation to tackle this situation.
We have also extended our collaboration with TOTAL in the direction of reservoir modeling, where we are expected to provide efficient solvers for solving problems issued from the discretization of coupled partial differential equations involving velocity, pressure and saturation variables.
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.

S. Gratton.

Visitors to Parallel Algorithm Project in 2010-2011

In alphabetical order, our visitors in the years 2010-2011 included :
MARIO ARIOLI (RAL, U.K.),
MICHELE BENZI (Emory University, U.S.A),
MIKE FISHER (ECMWF, Reading, U.K.),
ANDREAS FROMMER (University of Wuppertal, Germany),
JEAN-CHARLES GILBERT (INRIA Rocquencourt, France),
AZZAM HAIDAR (University of Tennessee, Knoxville, U.S.A),
MOHAMED HAMDAOUI (Ecole Centrale de Paris, France),
PATRICK LALOYAUX (The University of Namur, Belgium) ,
ANDREAS LANGER (University of Linz, Austria) ,
JULIEN LANGOU (The University of Colorado at Denver, U.S.A.),
SHERRY LI (University of California, U.S.A.),
SCOTT MACLACHLAN (Tufts University, U.S.A.),
GÉRARD MEURANT (CEA, Bruyères-le-Châtel, France),
KRISTIAN MOGENSEN (ECMWF, U.K.),
ESMOND NG (Lawrence Berkeley National Laboratory, Berkeley, U.S.A.),
CORNELIS OOSTERLEE (Delft University of Technology, The Netherlands),
DOMINIQUE ORBAN (Ecole Polytechnique de Montréal, Canada),
VICTOR PICHENY (Ecole Centrale de Paris, France),
MONSERRAT RINCON CAMACHO (University of Graz, Austria),
PHILIPPE SAMPAIO (The University of Namur, Belgium),
ANNICK SARTENAER (The University of Namur, Belgium),
CHARLOTTE TANNIER (The University of Namur, Belgium),
PHILIPPE TOINT (The University of Namur, Belgium),
BORA UCAR (CNRS and ENS, Lyon, France),
LUIS NUNES VICENTE (University of Coimbra, Portugal),

2 List of Members of the Algo Team

SERGE GRATTON - Scientific coordinator
XAVIER VASSEUR - Deputy project leader - Senior Researcher
IAIN DUFF - Scientific advisor
FRANÇOISE CHATELIN - Qualitative Computing group scientific advisor
PAOLA BOITO - Post. Doc., from June 2010 to July 2010
MIKKO BYCKLING - Post. Doc., from November 2010
MARTIN FUCHS - Post. Doc., until June 2011
PAVEL JIRANEK - Post. Doc., from October 2010
KAMER KAYA - Post. Doc., until August 2011
ANTONIO MUCHERINO - Post. Doc., from December 2010 to August 2011
VICTOR PICHENY - Post. Doc., from September 2011
MARIA MONSERRAT RINCON CAMACHO - Post. Doc., from October 2011
ANKE TRÖLTZSCH - Post. Doc., from November 2011 and Ph.D. Student, until April 2011
ADIL AHIDAR - Ph.D. Student, from October 2011
EL-HOUCINE BERGOU - Ph.D. Student, from October 2011
YOUSSEF DIOUANE - Ph.D. Student, from October 2011
SIMONE GENTILE - Ph.D. Student, from April 2011 to August 2011
SELIME GÜROL - Ph.D. Student, from February 2010
RAFAEL LAGO - Ph.D. Student, from March 2010
STEVEN MURPHY - Ph.D. Student, from October 2011
XAVIER PINEL - Ph.D. Student, until May 2010
GUILLAUME JOSLIN - Engineer, from October 2011
MOHAMED BIARI - Trainee, (May-September 2010)
YOUSSEF DIOUANE - Trainee, (March-September 2011)
BRIGITTE YZEL - Administration

3 List of Members of HiePACS

HiePACS stands for ”High-End Parallel Algorithms for Challenging Numerical Simulations” and is the first research action of the joint Inria-CERFACS Laboratory on High Performance Computing. It is also a Inria research team which scientific reports for 2010 and 2011 year can be found at the following URL address http ://www.inria.fr/equipes/hiepacs/(section)/activity. The initial core of the joint research activity lies in parallel linear algebra in collaboration with the Parallel Algorithms Project at CERFACS but it also extends to research activities related to parallel scalable numerical schemes as described in 3.2, 3.2 and 2.4.1.

Research Scientists
LUC GIRAUD [Inria, Team Leader since Oct. 2011, Senior Researcher (DR), HdR]
EMMANUEL AGULLO [Inria, Junior Researcher (CR)]
OLIVIER COULAUD [Inria, Senior Researcher (DR)]
JEAN ROMAN [Inria, Team Leader until Sept. 2011, Senior Researcher (DR on secondment), Professor at IPB, HdR]
XAVIER VASSEUR [CERFACS, ALGO Project, Senior Scientist]

Faculty Members
AURÉLIEN ESNARD [University of Bordeaux, Associate Professor (MdC)]
ABDOU GUERMOUCHE [University of Bordeaux, Associate Professor (MdC)]

External Collaborators
IAIN DUFF [CERFACS, ALGO Project, Senior Scientist, HIEPACS Scientific Advisor]
PIERRE FORTIN [Paris 6 University, LIP6, Assistant Professor (MdC)]
GUILLAUME LATU [Strasbourg University, LSIIT, Assistant Professor (MdC), on secondment at CEA Cadarache]

Technical Staff
MOHAMED ABDOUL ASIZE [CNRS, funding from ANR ARA CIS NOSSI, since Nov. 2010]
YOHAN LEE-TIN-YIEN [Inria, funding from ADT ParScaLi, ended Dec. 2011]
BÉRENGER BRAMAS [Inria, funding from ADT ScalFMM, since Dec. 2010]
MATTHIEU LECOUVEZ [Inria, funding from HiePACS, since Oct. 2011]

PhD Students
RACHED ABDELKHALEK [TOTAL, CIFRE, since Jan. 2008]
MATHIEU CHANAUD [Inria, funding from Inria and CEA, defended Oct. 2011]
YOHANN DUDOUIT [CERFACS, funding from TOTAL, since Oct. 2010]
ARNAUD ETCHEVERRY [Inria, funding from ANR-OPTIDIS, since Oct. 2011]
ANDRA HUGO [Inria, funding from Inria-Région Aquitaine, since Oct. 2011]
STOJCE NAKOV [Inria, funding from TOTAL, since Oct. 2011]
ALEXIS PRAGA [CERFACS, since Oct. 2011]
PABLO SALAS MEDINA [Inria, funding from Europe FP7/ITN (Marie Curie) MyPlanet, since June

2010]
JÉRÔME SOUMAGNE [CSCS, funding from Europe FP7/ICT/FET NextMuSE STREP, since Apr. 2009]
CLÉMENT VUCHENER [University of Bordeaux, funding from French Research Ministry, since Sept. 2010]
MAWUSSI ZOUNON [Inria, funding from ANR-RESCUE, since Oct. 2011]

Post-Doctoral Fellows

MIKKO BYCKLING [CERFACS, ALGO Project, since Oct. 2010]
YAN-FEI JING [Inria, since Oct. 2011]

Administrative Assistants

BARTA BENEDDINE [Inria, ended June 2011]
MARIE SANCHEZ [Inria, July-Oct. 2011]
CHRYSTEL PLUMEJEAU [Inria, since Nov. 2011]
BRIGITTE YZEL [CERFACS]

4 Dense and Sparse Matrix Computations

4.1 Analysis of the solution phase of a parallel multifrontal approach.

P. Amestoy : ENSEEIHT-IRIT, UNIVERSITY OF TOULOUSE, *France* ; **I. S. Duff** : RUTHERFORD APPLETON LABORATORY AND CERFACS, *UK and France* ; **A. Guermouche** : LABRI, UNIV. BORDEAUX 1 / INRIA BORDEAUX SUD-OUEST, *France* ; **Tz. Slavova** : CERFACS, *France*

In [ALG9], we study the forward and backward substitution phases of a sparse multifrontal factorization. These phases are often neglected in papers on sparse direct factorization but, in many applications, they can be the bottleneck so it is crucial to implement them efficiently. In this work, we assume that the factors have been written on disk during the factorization phase, and we discuss the design of an efficient solution phase. We will look at the issues involved when we are solving the sparse systems on parallel computers and will consider in particular their solution in a limited memory environment when out-of-core working is required. Two different approaches are presented to read data from the disk, with a discussion on the advantages and the drawbacks of each. We present some experiments on realistic test problems using an out-of-core version of a sparse multifrontal code called MUMPS (MUltifrontal Massively Parallel Solver).

4.2 On computing inverse entries of a sparse matrix in an out-of-core environment.

P. Amestoy : INPT(ENSEEIHT)-IRIT, UNIVERSITY OF TOULOUSE, *France* ; **I. S. Duff** : RUTHERFORD APPLETON LABORATORY AND CERFACS, *UK and France* ; **Y. Robert** : CERFACS, *France* ; **F.-H. Rouet** : INPT(ENSEEIHT)-IRIT, *France* ; **B. Uçar** : ENS LYON AND CNRS, *France*

The inverse of an irreducible sparse matrix is structurally full, so that it is impractical to think of computing or storing it. However, there are several applications where a subset of the entries of the inverse is required. Given a factorization of the sparse matrix held in out-of-core storage, we show how to compute such a subset efficiently, by accessing only parts of the factors. When there are many inverse entries to compute, we need to guarantee that the overall computation scheme has reasonable memory requirements, while minimizing the cost of loading the factors. This leads to a partitioning problem that we prove is NP-complete. We also show that we cannot get a close approximation to the optimal solution in polynomial time. We thus need to develop heuristic algorithms, and we propose : (i) a lower bound on the cost of an optimum solution ; (ii) an exact algorithm for a particular case ; (iii) two other heuristics for a more general case ; and (iv) hypergraph partitioning models for the most general setting. We illustrate the performance of our algorithms in practice using the MUMPS software package on a set of real-life problems as well as some standard test matrices. We show that our techniques can improve the execution time by a factor of 50. For more details, see [ALG33].

4.3 On the block triangular form of symmetric matrices.

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

In [ALG16], we present some observations on the block triangular form (BTF) of structurally symmetric, square, sparse matrices. If the matrix is structurally rank deficient, its canonical BTF has at least one underdetermined and one overdetermined block. We prove that these blocks are transposes of each other. We further prove that the square block of the canonical BTF, if present, has a special fine structure. These findings help us recover symmetry around the anti-diagonal in the block triangular matrix. The uncovered symmetry helps us to permute the matrix in a special form which is symmetric along the main diagonal while exhibiting the blocks of the original BTF. As the square block of the canonical BTF has full structural rank, the observation relating to the square block applies to structurally nonsingular, square symmetric matrices as well.

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

I. S. Duff : RUTHERFORD APPLETON LABORATORY AND CERFACS, *UK and France* ; **D. Mijuca** : UNIVERSITY UNION OF BELGRADE, *Serbia*

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. For more information, see [ALG15].

4.5 European exascale software initiative : numerical libraries, solvers and algorithms.

I. S. Duff : RUTHERFORD APPLETON LABORATORY AND CERFACS, *UK and France*

Computers with sustained Petascale performance are now available and it is expected that hardware will be developed with a peak capability in the Exascale range by around 2018. However, the complexity, hierarchical nature, and probable heterogeneity of these machines pose great challenges for the development of software to exploit these architectures. This was recognized some years ago by the IESP (International Exascale Software Project) initiative and the European response to this has been a collaborative project called EESI (European Exascale Software Initiative). This initiative began in 2010 and has submitted its final report to the European Commission with a final conference in Barcelona in October 2011. The main goals of EESI are to build a European vision and roadmap to address the international outstanding challenge of performing scientific computing on the new generation of computers.
The main activity of the EESI is in eight working groups, four on applications and four on supporting technologies. We first briefly review these eight chapters before discussing in more detail the work of

Working Group 4.3 on Numerical Libraries, Solvers and Algorithms. Here we will look at the principal areas, the challenges of Exascale and possible ways to address these, and the resources that will be needed. For more details, see [ALG50].

4.6 Push-relabel-based maximum cardinality matching algorithms for bipartite graphs.

K. Kaya : CERFACS, TOULOUSE, *France* ; **J. Langguth** : UNIVERSITY OF BERGEN, *Norway* ; **F. Manne** : UNIVERSITY OF BERGEN, *Norway* ; **B. Uçar** : ENS LYON, *France*

In [ALG64], we report on careful implementations of several push-relabel-based algorithms for solving the problem of finding a maximum cardinality matching in a bipartite graph and compare them with fast augmenting-path-based algorithms. We analyze the algorithms using a common base for all implementations and compare their relative performance and stability on a wide range of graphs. The effect of a set of known initialization heuristics on the performance of matching algorithms is also investigated. Our results identify a variant of the push-relabel algorithm and a variant of the augmenting-path-based algorithm as the fastest with proper initialization heuristics, while the push-relabel based one having a better worst case performance.

4.7 Maximum transversal algorithms

Iain S. Duff : CERFACS, TOULOUSE, *France,* RAL, OXFORDSHIRE, *UK* ; **K. Kaya** : CERFACS, TOULOUSE, *France* ; **B. Ucar** : CNRS AND ENS LYON, *France*

In [ALG49], we report on careful implementations of seven algorithms for solving the problem of finding a maximum transversal of a sparse matrix. We analyse the algorithms and discuss the design choices. To the best of our knowledge, this is the most comprehensive comparison of maximum transversal algorithms based on augmenting paths. Previous papers with the same objective either do not have all the algorithms discussed in this paper or they used non-uniform implementations from different researchers. We use a common base to implement all of the algorithms and compare their relative performance on a wide range of graphs and matrices. We systematize, develop and use several ideas for enhancing performance. One of these ideas improves the performance of one of the existing algorithms in most cases, sometimes significantly. So much so that we use this as the eighth algorithm in comparisons.

4.8 Elimination trees for sparse unsymmetric matrices

K. Kaya : CERFACS, TOULOUSE, *France* ; **B. Uçar** : CNRS AND ENS LYON, *France*

The elimination tree model for sparse unsymmetric matrices and an algorithm for constructing it have been recently proposed [Eisenstat and Liu, SIAM J. Matrix Anal. Appl., 26 (2005) and 29 (2008)]. The construction algorithm has a worst case time complexity $\mathcal{O}(mn)$ for an $n \times n$ unsymmetric matrix having m nonzeros. In [ALG63], we propose another algorithm that has a worst case time complexity of $\mathcal{O}(m \log n)$.

4.9 Integrated data placement and task assignment

Ü. V. Çatalyürek : THE OHIO STATE UNIVERSITY, COLUMBUS, *USA* ; **K. Kaya** : CERFACS, TOULOUSE, *France* ; **B. Uçar** : CNRS AND ENS LYON, *France*

In [ALG2], we consider the problem of optimizing the execution of data intensive scientific workflows in the Cloud. We address the problem under the following scenario. The tasks of the workflows communicate through files ; the output of a task is used by another task as an input file and if these tasks are assigned on different execution sites, a file transfer is necessary. The output files are to be stored at a site. Each execution site is to be assigned a certain percentage of the files and tasks. These percentages, called target weights, are pre-determined and reflect either user preferences or the storage capacity and computing power of the sites. The aim is to place the data files into and assign the tasks to the execution sites so as to reduce the cost associated with the file transfers, while complying with the target weights. To do this, we model the workflow as a hypergraph and with a hypergraph-partitioning-based formulation, we propose a heuristic which generates data placement and task assignment schemes simultaneously. We report simulation results on a number of real-life and synthetically generated scientific workflows. Our results show that the proposed heuristic is fast, and can find mappings and assignments which reduce file transfers, while respecting the target weights.

4.10 Partitioning problems with complex objectives

K. Kaya : CERFACS, TOULOUSE, *France* ; **F-H. Rouet** : ENSEEIHT-IRIT, TOULOUSE, *France* ; **B. Uçar** : CNRS AND ENS LYON, *France*

Hypergraph and graph partitioning tools are used to partition work for efficient parallelization of many sparse matrix computations. Most of the time, the objective function that is reduced by these tools relates to reducing the communication requirements, and the balancing constraints satisfied by these tools relate to balancing the work or memory requirements. Sometimes, the objective sought for having balance is a complex function of the partition. We describe some important class of parallel sparse matrix computations that have such balance objectives. For these cases, the current state of the art partitioning tools fall short of being adequate. To the best of our knowledge, there is only a single algorithmic framework in the literature to address such balance objectives. In this work [ALG8], we propose another algorithmic framework to tackle complex objectives and experimentally investigate the proposed framework.

5 Iterative Methods and Preconditioning

5.1 Parallel aspects of sparse factored approximate inverse

M. Byckling : CERFACS AND INRIA-CERFACS JOINT LABORATORY, *France*

Computation of approximate factors for the inverse constitutes an algebraic approach to preconditioning large and sparse linear systems as described in M. Byckling and M. Huhtanen, Numerische Mathematik, vol. 117, (2011). The aim is to combine standard preconditioning ideas with sparse approximate inverse approximation, to have dense approximate inverse approximations (implicitly). For optimality, the approximate factoring problem is associated with a minimization problem involving two matrix subspaces. This task can be converted into an eigenvalue problem for a Hermitian positive semidefinite operator whose smallest eigenpairs are of interest. Because of storage and complexity constraints, the power method appears to be the only admissible algorithm for devising sparse-sparse iterations. A specific focus on parallel aspects is considered now with application to preconditioning of indefinite problems.

5.2 Two-level preconditioned Krylov subspace methods for the solution of three-dimensional heterogeneous Helmholtz problems in seismics.

H. Calandra : TOTAL, CENTRE SCIENTIFIQUE ET TECHNIQUE JEAN FÉGER, *France*; **S. Gratton** : INPT-IRIT, UNIVERSITY OF TOULOUSE AND ENSEEIHT, *France*; **R. Lago** : CERFACS, *France*; **X. Pinel** : CERFACS, *France*; **X. Vasseur** : CERFACS AND HIEPACS PROJECT JOINT INRIA-CERFACS LABORATORY, *France*

In [ALG34], we address the solution of three-dimensional heterogeneous Helmholtz problems discretized with compact fourth-order finite difference methods with application to acoustic waveform inversion in geophysics. In this setting, the numerical simulation of wave propagation phenomena requires the approximate solution of possibly very large linear systems of equations. We propose an iterative two-grid method where the coarse grid problem is solved inexactly. A single cycle of this method is used as a variable preconditioner for a flexible Krylov subspace method. Numerical results demonstrate the usefulness of the algorithm on a realistic threedimensional application. The proposed numerical method allows us to solve wave propagation problems with single or multiple sources even at high frequencies on a reasonable number of cores of a distributed memory cluster.

5.3 Flexible variants of block restarted GMRES methods with application to geophysics.

H. Calandra : TOTAL, CENTRE SCIENTIFIQUE ET TECHNIQUE JEAN FÉGER, *France* ; **S. Gratton** : INPT-IRIT, UNIVERSITY OF TOULOUSE AND ENSEEIHT, *France* ; **J. Langou** : UNIVERSITY OF COLORADO DENVER, *USA* ; **X. Pinel** : CERFACS, *France* ; **X. Vasseur** : CERFACS AND HIEPACS PROJECT JOINT INRIA-CERFACS LABORATORY, *France*

In a wide number of applications in computational science and engineering the solution of large linear systems of equations with several right-hand sides given at once is required. Direct methods based on Gaussian elimination are known to be especially appealing in that setting. Nevertheless when the dimension of the problem is very large, preconditioned block Krylov space solvers are often considered as the method of choice. The purpose of this paper is thus to present iterative methods based on block restarted GMRES that allow variable preconditioning for the solution of linear systems with multiple right-hand sides. The use of flexible methods is especially of interest when approximate possibly iterative solvers are considered in the preconditioning phase. First we introduce a new variant of block flexible restarted GMRES that includes a strategy for detecting when a linear combination of the systems has approximately converged. This explicit block size reduction is often called deflation. We analyze the main properties of this flexible method based on deflation and notably prove that the Frobenius norm of the block residual is always nonincreasing. We also present a flexible variant based on both deflation and truncation to especially be used in case of limited memory. Finally we illustrate the numerical behavior of these flexible block methods on large industrial simulations arising in geophysics, where indefinite linear systems of size up to one billion of unknowns with multiple right-hand sides have been successfully solved in a parallel distributed memory environment. More details can be found in [ALG35].

5.4 A flexible generalized conjugate residual method with inner orthogonalization and deflated restarting.

L. M. Carvalho : RIO DE JANEIRO STATE UNIVERSITY, *Brazil* ; **S. Gratton** : INPT-IRIT, UNIVERSITY OF TOULOUSE AND ENSEEIHT, *France* ; **R. Lago** : CERFACS, *France* ; **X. Vasseur** : CERFACS, *France*

This work is concerned with the development and study of a minimum residual norm subspace method based on the generalized conjugate residual method with inner orthogonalization (GCRO) method that allows flexible preconditioning and deflated restarting for the solution of nonsymmetric or non-Hermitian linear systems. First we recall the main features of flexible generalized minimum residual with deflated restarting (FGMRES-DR), a recently proposed algorithm of the same family but based on the GMRES method. Next we introduce the new inner-outer subspace method named FGCRO-DR. A theoretical comparison of both algorithms is then made in the case of flexible preconditioning. It is proved that FGCRO-DR and FGMRES-DR are algebraically equivalent if a collinearity condition is satisfied. While being nearly as expensive as FGMRES-DR in terms of computational operations per cycle, FGCRO-DR offers the additional advantage to be suitable for the solution of sequences of slowly changing linear systems (where both the matrix and right-hand side can change) through subspace recycling. Numerical experiments on the solution of multidimensional elliptic partial differential equations show the efficiency of FGCRO-DR when solving sequences of linear systems. For more details, see [ALG13].

5.5 Preconditioners based on strong components.

I. S. Duff : RUTHERFORD APPLETON LABORATORY AND CERFACS, *UK and France* ; **K. Kaya** : CERFACS, TOULOUSE, *France*

In [ALG48], we propose an approach for obtaining block diagonal and block triangular preconditioners that can be used for solving a linear system Ax = b, where A is a large, nonsingular, real, $n \times n$ sparse matrix. The proposed approach uses Tarjan's algorithm for hierarchically decomposing a digraph into its strong subgraphs ["A hierarchical clustering algorithm using strong components", Information Processing Letters, 14 :26-29, 1982., "An improved algorithm for hierarchical clustering using strong components", Information Processing Letters, 17(1) :3741, 1983.]. To the best of our knowledge, this is the first work that uses this algorithm of Tarjan for preconditioning purposes. We describe the method, analyse its performance, and compare it with preconditioners from the literature such as ILUT and XPABLO and show that it is better than XPABLO and competitive with ILUT for many matrices with the advantage that a version of our preconditioner is fully parallelizable.

5.6 A FETI-preconditioned conjugate gradient method for large-scale stochastic finite element problems.

D. Ghosh : INDIAN INSTITUTE OF SCIENCE, *India* ; **Ph. Avery** : STANFORD UNIVERSITY AND CERFACS, *USA and France* ; **Ch. Farhat** : STANFORD UNIVERSITY, *USA*

In the spectral stochastic finite element method for analyzing an uncertain system, the uncertainty is represented by a set of random variables, and a quantity of interest such as the system response is considered as a function of these random variables. Consequently, the underlying Galerkin projection yields a block system of deterministic equations where the blocks are sparse but coupled. The solution of this algebraic system of equations becomes rapidly challenging when the size of the physical system and/or the level of uncertainty is increased. This paper addresses this challenge by presenting a preconditioned conjugate gradient method for such block systems where the preconditioning step is based on the dualprimal finite element tearing and interconnecting method equipped with a Krylov subspace reusage technique for accelerating the iterative solution of systems with multiple and repeated right-hand sides. Preliminary performance results on a Linux Cluster suggest that the proposed solution method is numerically scalable and demonstrate its potential for making the uncertainty quantification of realistic systems tractable. More information can be found in [ALG19].

5.7 Flexible GMRES with deflated restarting.

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

In many situations, it has been observed that significant convergence improvements can be achieved in preconditioned Krylov subspace methods by enriching them with some spectral information. On the other hand, effective preconditioning strategies are often designed where the preconditioner varies from one step to the next so that a flexible Krylov solver is required. In this paper, we present a new numerical technique for nonsymmetric problems that combines these two features. We illustrate the numerical behavior of the new solver both on a set of small academic test examples as well as on large industrial simulation arising in wave propagation simulations. For more information, see [ALG20].

5.8 Block Krylov subspace methods with deflated restarting.

L. Giraud : INRIA BORDEAUX SUD-OUEST AND INRIA-CERFACS JOINT LABORATORY, *France* ;
Y.-F. Jing : INRIA BORDEAUX SUD-OUEST AND INRIA-CERFACS JOINT LABORATORY, *France* ;
J. Roman : INRIA BORDEAUX SUD-OUEST AND INRIA-CERFACS JOINT LABORATORY, *France*

We investigate a variant of block-GMRES-DR (R. B. Morgan, Appl. Numer. Math., 2005, p. 222-236) method with inexact breakdowns (M. Robbé and M. Sadkane, Linear Algebra Appl., 2006, p. 265-285) for systems of linear equations with multiple right-hand sides. The new method keeps the efficiency of the block-GMRES-DR method by deflation of the targetted eigenvalues while it uses the technique of the block-GMRES method with inexact breakdowns to address the issue of breakdowns in the block-GMRES method. Properties of the new harmonic residual vectors as well as their relationships with the residual vectors from the minimum residual solutions of the linear equations problem are investigated. The block Arnoldi-like recurrence formulae still hold of the block-GMRES method with inexact breakdowns at each restart when refined information associated with a prescribed number new harmonic Ritz vectors are included. Some implementation details of the new algorithm are provided and the numerical behavior of the new solver is studied on a set of examples.

5.9 Nonlinear eigenvalue and frequency response in combustion problems.

L. Giraud : INRIA BORDEAUX SUD-OUEST AND INRIA-CERFACS JOINT LABORATORY, *France* ;
P. Salas : INRIA BORDEAUX SUD-OUEST AND INRIA-CERFACS JOINT LABORATORY, *France* ;
X. Vasseur : CERFACS AND INRIA-CERFACS JOINT LABORATORY, *France*

In the framework of an FP7 Marie Curie project (MyPlanet), we study parallel robust nonlinear quadratic eigensolvers for the solution of thermoacoustic instabilities in industrial gas turbine combustion chambers. The main numerical kernel is the solution of unsymmetric generalized linear eigenproblems. One of the objectives of this research activity is to improve the algorithms underlying in the 3D parallel code AVSP, developed by the CFD team at CERFACS (C. Sensiau, CERFACS PhD dissertation, TH/CFD/08/127, 2008).

Different algorithms for the solution of large-scale complex unsymmetric eigenproblems have been studied and/or developed : methods based on Jacobi-Davidson algorithms, which have shown themselves less efficient in this context than the methods based on the Arnoldi algorithm, such as the Implicit Restarted Arnoldi (IRA) method. The most successful and widely used implementation of the the IRA method is the package ARPACK (R.B. Lehoucq, D.C. Sorensen and C. and Yang, SIAM, 1998). It has been traditionally the choice done in AVSP. Improving the numerical performance of this package is a difficult task and today there is not yet a clear alternative to it. The research work of this Phd tries to deal with this challenge in order to develop an effective method adapted to the context of AVSP.

To do that, we intent to extract information from the solution of the symmetric problem (simulation without Flame Transfer Function) in order to accelerate the solution of the unsymmetric problem (simulation with FTF). A natural way to exploit this information is the use of block-methods. Classically, iterative methods such as ARPACK starts from a random vector. With block-methods it is possible to start the iterative process from a block of initial vectors. If this initial vector block contains useful *a priori* information, the number of iterations done before reach a converged solution can be reduced. This have been an important axis of the research work done till now. The first option consisted of implementing a block version of the Implicit Restarted Arnoldi method (R. Lehoucq and K. Maschhoff, Preprint MCSP6490297 Argonne National Lab, 1997). The need for a easier way to restart the method has led us to the study of a the Krylov–Schur approach, described by G. W. Stewart in (G.W. Stewart, SIAM J. Matrix Anal. Appl., p. 601–614, 2001).

We are currently working on this method and some variations as the block implementation or its use to compute the harmonic Ritz vectors (G.W. Stewart, SIAM J. Matrix Anal. Appl., 2002).

This work has been presented in conferences (e.g., P. Salas, L. Giraud, J. Muller, G. Staffelbach, T. Poinsot, ”Stability of azimuthal modes in annular combustion chambers”, INCA, November 2011) and a paper has been accepted for its publication in the journal of Combustion and Flame (CERFACS Technical Report, TR/CFD/11/35, J.-F. Parmentier, P. Salas, P. Wolf, G. Staffelbach, F. Nicoud and T. Poinsot, ”A simple analytical model to study and control azimuthal instabilities in annular combustion chambers”).

5.10 Minimizing the backward error in the energy norm with conjugate gradients.

S. Gratton : INPT-IRIT, UNIVERSITY OF TOULOUSE AND ENSEEIHT, *France* ;
P. Jiránek : TECHNICAL UNIVERSITY OF LIBEREC AND CERFACS, *Czech Republic and France* ;
X. Vasseur : CERFACS, *France*

In [ALG57], we derive backward error formulas for a linear system of equations in general norms induced by given symmetric positive definite matrices and consider a special case of a backward error induced by the energy norm when the system matrix is symmetric positive definite. We study the convergence of the conjugate gradient method (CG) with respect to this energy backward error. For that purpose we construct a hypothetical variant of CG called CGBACK which constructs the approximations that actually minimize the energy backward error over the associated Krylov subspaces and can therefore be considered as an analog of the GMBACK/MINPERT algorithms of Kasenally and Simoncini. We show that the optimal CGBACK approximation is a scalar multiple of the current CG approximation with the coefficient depending only on the weighting parameters appearing in the definition of the backward error and on the relative energy norm of the error of the current CG iterate. In addition when CG makes a moderate progress in terms of the energy norm of the error then the energy backward errors of the subsequent CG approximations start to be very close to the optimal energy backward errors of CGBACK approximations. In this way we deduce that CG approximations almost minimize the energy backward error.

5.11 Adaptive version of simpler GMRES.

P. Jiránek : TECHNICAL UNIVERSITY OF LIBEREC AND CERFACS, *Czech Republic and France* ;
M. Rozložník : ACADEMY OF SCIENCES OF THE CZECH REPUBLIC, *Czech Republic*

In [ALG29], we propose a stable variant of Simpler GMRES by Walker and Zhou (1994). It is based on the adaptive choice of the Krylov subspace basis at given iteration step using the intermediate residual norm decrease criterion. The new direction vector is chosen as in the original implementation of Simpler GMRES or it is equal the normalized residual vector as in the GCR method. We show that such adaptive strategy leads to a well-conditioned basis of the Krylov subspace and we support our theoretical results with illustrative numerical examples.

5.12 A posteriori error estimates including algebraic error and stopping criteria for iterative solvers.

P. Jiránek : TECHNICAL UNIVERSITY OF LIBEREC AND CERFACS, *Czech Republic and France* ; **Z. Strakos** : ACADEMY OF SCIENCES OF THE CZECH REPUBLIC, *Czech Republic* ; **M. Vohralík** : UPMC UNIV. PARIS VI AND CNRS, *France*

For the finite volume discretization of a second-order elliptic model problem, we derive a posteriori error estimates which take into account an inexact solution of the associated linear algebraic system. We show that the algebraic error can be bounded by constructing an equilibrated RaviartThomasNédélec discrete vector field whose divergence is given by a proper weighting of the residual vector. Next, claiming that the discretization error and the algebraic one should be in balance, we construct stopping criteria for iterative algebraic solvers. An attention is paid, in particular, to the conjugate gradient method which minimizes the energy norm of the algebraic error. Using this convenient balance, we also prove the efficiency of our a posteriori estimates ; i.e., we show that they also represent a lower bound, up to a generic constant, for the overall energy error. A local version of this result is also stated. This makes our approach suitable for adaptive mesh refinement which also takes into account the algebraic error. Numerical experiments illustrate the proposed estimates and construction of efficient stopping criteria for algebraic iterative solvers. For further details, see [ALG31].

5.13 Estimating the backward error in LSQR.

P. Jiránek : TECHNICAL UNIVERSITY OF LIBEREC AND CERFACS, *Czech Republic and France* ; **D. Titley-Peloquin** : MCGILL UNIVERSITY, SCHOOL OF COMPUTER SCIENCE, *Canada*

In [ALG30], we propose practical stopping criteria for the iterative solution of sparse linear least squares (LS) problems. Although we focus our discussion on the algorithm LSQR of Paige and Saunders, the ideas discussed here may also be applicable to other algorithms. We review why the 2-norm of the projection of the residual vector onto the range of A is a useful measure of convergence, and show how this projection can be estimated efficiently at every iteration of LSQR. We also give practical and cheaply-computable estimates of the backward error for the LS problem.

5.14 A perturbed two-level preconditioner for the solution of three-dimensional heterogeneous Helmholtz problems with applications to geophysics.

X. Pinel : CERFACS, *France*

The topic of [ALG66] is the development of iterative methods for the solution of large sparse linear systems of equations with possibly multiple right-hand sides given at once. These methods will be used for a specific application in geophysics - seismic migration - related to the simulation of wave propagation in the subsurface of the Earth. Here the three-dimensional Helmholtz equation written in the frequency domain is considered. The finite difference discretization of the Helmholtz equation with the Perfect Matched Layer formulation produces, when high frequencies are considered, a complex linear system which is large, non-symmetric, non-Hermitian, indefinite and sparse. Thus we propose to study preconditioned flexible Krylov subspace methods, especially minimum residual norm methods, to solve this class of problems. As a preconditioner we consider multi-level techniques and especially focus on a two-level method. This twolevel preconditioner has shown effcient for two-dimensional applications and the purpose of this thesis is to extend this to the challenging three-dimensional case. This leads us to propose and analyze a perturbed two-level preconditioner for a flexible Krylov subspace method, where Krylov methods are used both as smoother and as approximate coarse grid solver.

6 Qualitative Computing

Group member : Françoise Chatelin, CERFACS and Université Toulouse 1.

The main activity of the unique member in the Qualitative Computing group in 2010-2011 has been to continue the exploration of the multiplicative computing land presented in the book "Qualitative Computing : A computational journey into nonlinearity" to be published by World Scientific, Singapore in 2012. 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. The book proposes to explore radically 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 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 (i.e. vectors in nonassociative algebras $A_k, k \geq 1$ of dimension 2^k, recursively defined from $A_0 = \mathbb{R}$) 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 work of the years 2010-2011 is presented in detail in the five technical reports [ALG41, ALG46, ALG45, ALG43, ALG42]. In order to account for the phenomenon known as Special Relativity in Physics and that is found everywhere in Life Sciences, the classical addition of vectors can be generalized to define a *relativistic addition*, whose departure from commutativity and associativity is controled by an

automorphism called relator. This leads to the concept of an *organ* which broadens for Computation the classical notion of an additive abelian group in Mathematics. By framing an organ into a euclidean metric space, we obtain a metric cloth which allows us to perform *weaving* computations. This novel concept accounts for the emergence of meaning from a rich noneuclidean geometry. See [ALG46] for more information. The report [ALG42] shows how Einstein's relativistic addition (1905) in $\mathbb{R}^3$ is connected to and may modify computation in the quaternionic field $\cong \mathbb{R}^4$. We also indicate that the complex versions of Einstein's addition and Poincaré's hyperbolic translation (1880, 1907) are identical when they are based on the same reference value. With the choice of 1 as reference value, they both represent all automorphisms of the complex unit disk in $\mathbb{C}^n$ other than unitary maps.
In addition, some work has been done in 2010 for the book [ALG1]. An additional chapter has been prepared in 2011 for the republication of ”Eigenvalues of Matrices” (Wiley, 1993) in the SIAM Classics in Applied Mathematics Series to appear in 2012.

7 Nonlinear Systems and Optimization

7.1 A Contribution to the Conditioning of the Total Least-Squares Problem.

M. Baboulin : UNIVERSITY OF PARIS-SUD AND INRIA, *France* ; **S. Gratton** : INPT-IRIT, UNIVERSITY OF TOULOUSE AND ENSEEIHT, *France*

In [ALG10], we derive closed formulas for the condition number of a linear function of the total least-squares solution. Given an overdetermined linear system $Ax = b$, we show that this condition number can be computed using the singular values and the right singular vectors of $[A, b]$ and A. We also provide an upper bound that requires the computation of the largest and the smallest singular value of $[A, b]$ and the smallest singular value of A. In numerical examples, we compare these values and the resulting forward error bounds with the error estimates given by Van Huffel and Vandewalle [The Total Least Squares Problem : Computational Aspects and Analysis, Frontiers Appl. Math. 9, SIAM, Philadelphia, 1991], and we show the limitation of the first order approach.

7.2 A retrospective trust-region method for unconstrained optimization.

F. Bastin : UNIVERSITY OF MONTRÉAL, *Canada* ; **V. Malmedy** : FUNDP UNIVERSITY OF NAMUR, *Belgium* ; **M. Mouffe** : CERFACS, *France* ; **Ph. L. Toint** : FUNDP UNIVERSITY OF NAMUR, *Belgium* ; **D. Tomanos** : FUNDP UNIVERSITY OF NAMUR, *Belgium*

In [ALG11], we introduce a new trust-region method for unconstrained optimization where the radius update is computed using the model information at the current iterate rather than at the preceding one. The update is then performed according to how well the current model retrospectively predicts the value of the objective function at last iterate. Global convergence to first- and second-order critical points is proved under classical assumptions and preliminary numerical experiments on CUTEr problems indicate that the new method is very competitive.

7.3 Quasi-Newton methods for solving a two-dimensional acoustic waveform inversion.

M. Biari : ENSEEIHT AND CERFACS, *France*

We are interested in solving acoustic waveform inversion problem with the help of Quasi-Newton methods with application to geophysics. The theory is reviewed and we focus on the efficient solution of the adjoint problem with iterative methods. Two-grid methods are investigated as preconditioner of Krylov subspace methods, closely following strategies developed for the direct problem in X. Pinel's PhD thesis [ALG66]. Two-dimensional academic applications are considered. The master project has been supervised by S. Gratton and X. Vasseur.

7.4 Solving a two-dimensional full waveform inversion via global optimization methods.

Y. Diouane : ENSEEIHT AND CERFACS, *France*

The knowledge of Earth internal structures at different scales is of major interest for economy, humans, environment and science. Several methods have been developed for Earth imaging using seismic wave information (based on a model of the phenomenon propagation by the Helmholtz equation). The full waveform inversion attempts to build quantitative high-resolution images of the subsurface physical parameters using the full waveeld, solved as an optimization procedure.

Solving a full waveform inversion problem therefore leads to minimize a cost function corresponding to the norm of the gap between the observed data taken at the receiver positions and the data calculated from an initial model. It should be noted that such optimization problem has a lot of parameters in three dimensions (i.e the size of the velocity field) which prevents us to use directly global optimization methods. To overcome this constraint we have first decided to reduce the velocity field so as to be able to construct another field close to the original one using less parameters. During this internship, we first have tried to nd the best process to reduce the complexity of the velocity field using wavelet transform. Then and during the optimization stage (solving the inverse problem) we have tried to improve the global convergence of the algorithm based on an evolutionary strategy (CMA-ES of Hansen). The effectiveness and robustness of the algorithm have been tested on academic examples. The master project has been supervised by S. Gratton and L. N. Vicente.

7.5 The Optimization Test Environment.

F. Domes : UNIVERSITY OF VIENNA, FACULTY OF MATHEMATICS, *Austria* ; **M. Fuchs** : CERFACS, *France* ; **H. Schichl** : UNIVERSITY OF VIENNA, FACULTY OF MATHEMATICS, *Austria*

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. Further information is available in [ALG47]. Moreover, the planning for an extension to black box solvers has been completed and its implementation has started.

7.6 Fast regularized linear sampling for inverse scattering problems.

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

In [ALG17], a new numerical procedure is proposed for the reconstruction of the shape and volume of unknown objects from measurements of their radiation in the far field. This procedure is a variant and the linear sampling method has a very acceptable computational load and is fully automated. It is based on exploiting an iteratively computed truncated singular-value decomposition and heuristics to extract the desired signal from the background noise. Its performance on a battery of examples of different types is shown to be promising.

7.7 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. In [ALG18] we present a branching strategy for the case that 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.

7.8 Optimization in latent class analysis.

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

In latent class analysis (LCA) one seeks a clustering of categorical data, such as patterns of symptoms of a patient, in terms of locally independent stochastic models. This leads to practical definitions of criteria, e.g., whether to include patients in further diagnostic examinations. The clustering is often determined by parameters that are estimated by the maximum likelihood method. The likelihood function in LCA has in many cases (especially for sparse data sets) a complicated shape with many local extrema, even for small-scale problems. Hence a global optimization must be attempted. In [ALG51] we describe an algorithm and software for the global optimization of the likelihood function constrained by the requirement of a good fit of the data with a minimal number of classes. The problem is formulated in the algebraic modeling language AMPL and solved via state of the art optimization solvers. The approach is successfully applied to three real-life problems. Remarkably, the goodness-of-fit constraint makes one of the three problems identifiable by eliminating all but one of the local minimizers.

7.9 Preconditioning and globalizing conjugate gradients in dual space for quadratically penalized nonlinear-least squares problems.

S. Gratton : INPT-IRIT, UNIVERSITY OF TOULOUSE AND ENSEEIHT, *France* ; **S. Gürol** : CERFACS, *France* ; **Ph. L. Toint** : FUNDP UNIVERSITY OF NAMUR, *Belgium*

When solving nonlinear least-squares problems, it is often useful to regularize the problem using a quadratic term, a practice which is especially common in applications arising in inverse calculations. A solution method derived from a trust-region Gauss-Newton algorithm is analyzed for such applications, where, contrary to the standard algorithm, the least-squares subproblem solved at each iteration of the method is rewritten as a quadratic minimization subject to linear equality constraints. This allows the exploitation of duality properties of the associated linearized problems. This paper considers a recent conjugate-gradient-like method which performs the quadratic minimization in the dual space and produces, in exact arithmetic, the same iterates as those produced by a standard conjugate-gradients method in the primal space. This dual algorithm is computationally interesting whenever the dimension of the dual space is significantly smaller than that of the primal space, yielding gains in terms of both memory usage and computational cost. The relation between this dual space solver and PSAS (Physical-space Statistical Analysis System), another well-known dual space technique used in data assimilation problems, is explained. The use of an effective preconditioning technique is proposed and refined convergence bounds derived, which results in a practical solution method. Finally, stopping rules adequate for a trust-region solver are proposed in the dual space, providing iterates that are equivalent to those obtained with a Steihaug-Toint truncated conjugate-gradient method in the primal space. More details can be found in [ALG55].

7.10 On the accuracy of the Karlson-Waldén's estimate of the backward error for linear least squares problems.

S. Gratton : INPT-IRIT, UNIVERSITY OF TOULOUSE AND ENSEEIHT, *France* ; **P. Jiránek** : CERFACS, *France* ; **D. Titley-Peloquin** : UNIVERSITY OF OXFORD, *UK*

In [ALG56], we consider the backward error associated with a given approximate solution of a linear least squares problem. The backward error can be very expensive to compute, as it involves the minimal singular value of certain matrix that depends on the problem data and the approximate solution. An estimate based on a regularized projection of the residual vector has been proposed in the literature and analyzed by several authors. Although numerical experiments in the literature suggest that it is a reliable estimate of the backward error for any given approximate LS solution, to date no satisfactory explanation for this behavior had been found. We derive new bounds which confirm this experimental observation.

7.11 A reduced and limited-memory preconditioned approach for the 4D-Var data-assimilation problem.

S. Gratton : INPT-IRIT, UNIVERSITY OF TOULOUSE AND ENSEEIHT, *France* ; **P. Laloyaux** : FUNDP UNIVERSITY OF NAMUR, *Belgium* ; **A. Sartenaer** : FUNDP UNIVERSITY OF NAMUR, *Belgium* ; **J. Tshimanga** : INPT-ENSEEIHT AND IRIT, *France*

In [ALG22], we recall a theoretical analysis of the equivalence between the Kalman filter and the four-dimensional variational (4D-Var) approach to solve data-assimilation problems. This result is then extended to cover the comparison of the singular evolutive extended Kalman (SEEK) filter with a reduced variant of the 4D-Var algorithm. We next concentrate on the solution of the 4D-Var, which is usually computed with a (truncated) GaussNewton algorithm using a preconditioned conjugate-gradient-like (CG) method. Motivated by the equivalence of the above-mentioned algorithms, we explore techniques used in the SEEK filter and based on empirical orthogonal functions (EOFs) as an attempt to accelerate the GaussNewton method further. This leads to the development of an appropriate starting point for the CG method, together with that of a powerful limited-memory preconditioner (LMP), as shown by preliminary numerical experiments performed on a shallow-water model.

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

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

In [ALG24], we consider an implementation of the recursive multilevel trust-region algorithm proposed by Gratton et al. (A recursive trust-region method in infinity norm for bound-constrained nonlinear optimization, IMA J. Numer. Anal. 28(4) (2008), pp. 827-861) 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 with alternative optimization techniques such as mesh refinement and direct solution of the fine-level problem. It is also shown that its behaviour is similar to that of multigrid algorithms for linear systems.

7.13 Stopping rules and backward error analysis for bound-constrained optimization.

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

In [ALG23], 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.

7.14 On a class of limited memory preconditioners for large scale linear systems with multiple right-hand sides.

S. Gratton : INPT-IRIT, UNIVERSITY OF TOULOUSE AND ENSEEIHT, *France* ; **A. Sartenaer** : FUNDP UNIVERSITY OF NAMUR, *Belgium* ; **J. Tshimanga** : INPT-ENSEEIHT AND IRIT, *France*

This work studies a class of limited memory preconditioners (LMPs) for solving linear (positive-definite) systems of equations with multiple right-hand sides. We propose a class of (LMPs), whose construction requires a small number of linearly independent vectors. After exploring the theoretical properties of the preconditioners, we focus on three particular members : spectral-LMP, quasi-Newton-LMP, and Ritz-LMP. We show that the first two are well known, while the third is new. Numerical tests indicate that the Ritz-LMP is efficient on a real-life nonlinear optimization problem arising in a data assimilation system for oceanography. For more information, see [ALG25].

7.15 Approximate invariant subspaces and quasi-Newton optimization methods.

S. Gratton : INPT-IRIT, *France* ; **Ph. L. Toint** : FUNDP UNIVERSITY OF NAMUR, *Belgium*

In [ALG21], new approximate secant equations are shown to result from the knowledge of (problem dependent) invariant subspace information, which in turn suggests improvements in quasi-Newton methods for unconstrained minimization. A new limited-memory Broyden-Fletcher-Goldfarb-Shanno using approximate secant equations is then derived and its encouraging behaviour illustrated on a small collection of multilevel optimization examples. The smoothing properties of this algorithm are considered next, and automatic generation of approximate eigenvalue information demonstrated. The use of this information for improving algorithmic performance is finally investigated on the same multilevel examples.

7.16 An active set trust-region method for derivative-free nonlinear bound-constrained optimization.

S. Gratton : INPT-IRIT, UNIVERSITY OF TOULOUSE AND ENSEEIHT, *France* ; **Ph. L. Toint** : FUNDP UNIVERSITY OF NAMUR, *Belgium* ; **A. Tröltzsch** : CERFACS, *France*

In [ALG59], we consider an implementation of a recursive model-based active-set trust-region method for solving bound-constrained nonlinear non-convex optimization problems without derivatives using the technique of self-correcting geometry proposed by K. Scheinberg and Ph. L. Toint [Self-correcting geometry in model-based algorithms for derivative-free unconstrained optimization. SIAM Journal on Optimization, 20(6) :3512-3532, 2010]. Considering an active-set method in bound-constrained model-based optimization creates the opportunity of saving a substantial amount of function evaluations. It allows us to maintain much smaller interpolation sets while proceeding optimization in lower-dimensional subspaces. The resulting algorithm is shown to be numerically competitive.

7.17 A hybrid optimization algorithm for gradient-based and derivative-free optimization.

S. Gratton : INPT-IRIT, UNIVERSITY OF TOULOUSE AND ENSEEIHT, *France* ; **Ph. L. Toint** : FUNDP UNIVERSITY OF NAMUR, *Belgium* ; **A. Tröltzsch** : CERFACS, *France*

A known drawback of derivative-free optimization (DFO) methods is the difficulty to cope with higher dimensional problems. When the problem dimension exceeds a few tens of variables, a pure DFO method becomes rather expensive in terms of number of function evaluations. For this reason, using gradient information, if accessible, is highly useful in the context of efficient optimization in practice (even if it is expected to be noisy). This applies especially when working with real-life applications as in aerodynamic shape optimization. It is well known that when the gradient is known, the L-BFGS method is a very efficient method for solving bound-constrained optimization problems. Coming back to the derivation of the BFGS method, it is possible to see it as a way to correct the Hessian information using the so-called secant equation information. We would like to generate a set of Hessian updates, that would generalize the L-BFGS approach to situations where the function or the gradient are approximated. We propose a family of algorithms that will both contain the derivative-free approach and the L-BFGS method, and that would therefore be able to optimally take into account the error occurring in the cost function or gradient of the problem.

7.18 How much gradient noise does a gradient-based linesearch method tolerate ?

S. Gratton : INPT-IRIT, UNIVERSITY OF TOULOUSE AND ENSEEIHT, *France* ; **Ph. L. Toint** : FUNDP UNIVERSITY OF NAMUR, *Belgium* ; **A. Tröltzsch** : CERFACS, *France*

Among numerical methods for smooth unconstrained optimization, gradient-based linesearch methods, like quasi-Newton methods, may work quite well even in the presence of relatively high amplitude noise in the gradient of the objective function. We present some properties on the amplitude of this noise which ensure a descent direction for such a method. Exploiting this bound, we also discuss conditions under which global convergence can be guaranteed. More details can be found in [ALG59].

7.19 Inexact range-space Krylov solvers for linear systems arising from inverse problems.

S. Gratton : INPT-IRIT, UNIVERSITY OF TOULOUSE AND ENSEEIHT, *France* ; **J. Tshimanga** : INPT-ENSEEIHT AND IRIT, *France* ; **Ph. L. Toint** : FUNDP UNIVERSITY OF NAMUR, *Belgium*

The object of our work in [ALG26] is twofold. Firstly, range-space variants of standard Krylov iterative solvers are introduced for unsymmetric and symmetric linear systems. These are characterized by possibly much lower storage and computational costs than their full-space counterparts, which is crucial in data assimilation applications and other inverse problems. Secondly, it is shown that the computational cost may be further reduced by using inexact matrix-vector products : formal error bounds are derived on the size of the residuals obtained under two different accuracy models, and it is shown why a model controlling forward error on the product result is often preferable to one controlling backward error on the operator. Numerical examples finally illustrate the developed concepts and methods.

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

S. Gratton : INPT-IRIT, UNIVERSITY OF TOULOUSE AND ENSEEIHT, *France* ; **J. Tshimanga** : INPT-ENSEEIHT AND IRIT, *France*

In [ALG53], we consider parameters 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 the 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 behavior of PSAS algorithm when viewed in the model space, experimentally reported by some authors, can be fully suppressed in RPCG.
Moreover, since preconditioning and reorthogonalization of residuals vectors are often used in practice to accelerate convergence in high dimension 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.

7.21 The exact condition number of the truncated singular value solution of a linear ill-posed problem.

S. Gratton : INPT-IRIT, UNIVERSITY OF TOULOUSE AND ENSEEIHT, *France* ; **J. Tshimanga** : INPT-ENSEEIHT AND IRIT, *France*

The main result in [ALG54] is the investigation of an explicit expression of the condition number of the truncated least squares solution of $Ax = b$. The result is derived using the notion of the Fréchet derivative together with the product norm $\|[\alpha A, \beta b]\|_F$, with $\alpha, \beta > 0$, for the data space and the 2-norm for the solution. We also derive a lower and an upper bounds to estimate the condition number for the general case. Finally, we carry out numerical experiments and compare our results with respect to a finite difference approach.

7.22 Variable neighborhood search for robust optimization and applications to aerodynamics.

A. Mucherino : CERFACS, *France* ; **M. Fuchs** : CERFACS, *France* ; **S. Gratton** : INPT-IRIT, *France* ; **X. Vasseur** : CERFACS, *France*

Many real-life applications lead to the definition of robust optimization problems where the objective function is a black box. This may be due, for example, to the fact that the objective function is evaluated through computer simulations, and that some parameters are uncertain. When this is the case, existing algorithms for optimization are not able to provide good-quality solutions in general. We propose a heuristic algorithm for solving black box robust optimization problems based on the minimax formulation of the problem. We also apply this algorithm for the solution of a wing shape optimization where the objective function is a computationally expensive black box. Preliminary computational experiments are reported. For further information we report the reader to [ALG65].

7.23 Grace-derived surface mass anomalies by energy integral approach. Application to continental hydrology.

G. Ramillien : GRGS, DTP, CNRS, UMR 5562, OMP, *France* ; **R. Biancale** : GRGS, CNES, OMP, *France* ; **S. Gratton** : INPT-IRIT, *France* ; **X. Vasseur** : CERFACS, *France* ; **S. Bourgogne** : NOVELTIS, *France*

In [ALG32], we propose an unconstrained approach to recover regional time-variations of surface mass anomalies using Level-1 Gravity Recovery and Climate Experiment (GRACE) orbit observations, for reaching spatial resolutions of a few hundreds of kilometers. Potential differences between the twin GRACE vehicles are determined along short satellite tracks using the energy integral method (i.e., integration of orbit parameters vs. time) in a quasi-inertial terrestrial reference frame. Potential differences residuals corresponding mainly to changes in continental hydrology are then obtained after removing the gravitational effects of the known geophysical phenomena that are mainly the static part of the Earth's gravity field and time-varying contributions to gravity (Sun, Moon, planets, atmosphere, ocean, tides, variations of Earths rotation axis) through ad hoc models. Regional surface mass anomalies are restored from potential difference anomalies of 10 to 30-day orbits onto 1 degree continental grids by regularization techniques based on singular value decomposition. Error budget analysis has been made by considering the important effects of spectrum truncation, the time length of observation (or spatial coverage of the data to invert) and for different levels of noise.

7.24 An active-set trust-region method for derivative-free nonlinear bound-constrained optimization applied to noisy aerodynamic design problems.

A. Tröltzsch : CERFACS, *France*

Derivative-free optimization (DFO) has enjoyed renewed interest over the past years, mostly motivated by the ever growing need to solve optimization problems defined by functions whose values are computed by simulation (e.g. engineering design, medical image restoration or groundwater supply). In the last few years, a number of derivative-free optimization methods have been developed and especially model-based trust-region methods have been shown to perform well. In this thesis, we present a new interpolation-based trust-region algorithm which shows to be efficient and globally convergent (in the sense that its convergence is guaranteed to a stationary point from arbitrary starting points). The new algorithm relies on the technique of self-correcting geometry proposed by Scheinberg and Toint [Self-correcting geometry in model-based algorithms for derivative-free unconstrained optimization. SIAM Journal on Optimization, 20(6) :3512-3532, 2010]. In their theory, they advanced the understanding of the role of geometry in model-based DFO methods, in our work, we improve the efficiency of their method while maintaining its good theoretical convergence properties. We further examine the influence of different types of interpolation models on the performance of the new algorithm. Furthermore, we extended this method to handle bound constraints by applying an active-set strategy. Considering an active-set method in bound-constrained model-based optimization creates the opportunity of saving a substantial amount of function evaluations. It allows to maintain smaller interpolation sets while proceeding optimization in lower dimensional subspaces. The resulting algorithm is shown to be numerically highly competitive. We present results on a test set of smooth problems from the CUTEr collection and compare to well-known state-of-the-art packages from different classes of DFO methods. To report numerical experiments incorporating noise, we create a test set of noisy problems by adding perturbations to the set of smooth problems. The choice of noisy problems was guided by a desire to mimic simulation-based optimization problems. Finally, we will present results on a real-life application of a wing-shape design problem provided by Airbus. For more details, see [ALG67].

8 Conferences and Seminars

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

January

Seminar on Numerical Analysis and Winter School SNA'10, Nové Hrady, Czech Republic. 18-22 January 2010. P. JIRÁNEK, *A posteriori estimates and stopping criteria for iterative solvers*, contributed talk.

March

4th International Workshop on Reliable Engineering Computing (REC), Singapore, 3-5 March 2010. M. FUCHS, *Simulation based uncertainty handling with polyhedral clouds*, contributed talk.

16th Math. Programming Meeting, Blankenberge, Belgium, March 11-12, 2010. A. TRÖLTZSCH, *A recursive model-based trust-region method for derivative-free bound-constrained optimization*, contributed talk.

GAMM'10 Conference, Karlsruhe, Germany, 22-26 March 2010. M. FUCHS, *Cloud Based Robust Design Optimization*, minisymposia organizer.

SANUM, Stellenbosch, South Africa. 27-30 March 2010. I.S. DUFF, *The solution of really large linear systems arising from discretizations of three-dimensional problems*, invited talk.

April

CPSWEEK 2010 Workshop, Stockholm, Sweden, April 12-16, 2010. M. FUCHS, *Higher dimensional uncertainty modeling with polyhedral clouds*, invited talk.

MUMPS User Group Meeting, Toulouse, April 16, 2010 X. VASSEUR, *Null space computation of sparse singular matrices with MUMPS*, invited talk.

May

III Workshop G-HPC 2010 : High Performance Computing Applications, Vigo, Spain, 21 May 2010. I.S. DUFF, The solution of really large linear systems arising from discretizations of three-dimensional problems, invited talk.

June

3rd ”Scheduling in Aussois” Workshop, Aussois, France, June 2-4, 2010. K. KAYA, attendee.

The 16th Conference of the International Linear Algebra Society (ILAS), Pisa, Italy, June 21-25, 2010. P. BOITO, attendee.

9th International Conference on Unconventional Computation, Tokyo, Japan, June 21-25, 2010. F. CHATELIN, *A computational journey into nonlinearity*, invited speaker.

PMAA’10 - 6th International Workshop on Parallel Matrix Algorithms and Applications, Basel, Switzerland, June 29 - July 02, 2010. R. LAGO, *Solution of three-dimensional heterogeneous Helmholtz problems in geophysics*, contributed talk.

July

ICCOPT 2010, The International Conference on Continuous Optimization, Winter School, Santiago, Chile, 28 July 2010. A. TRÖLTZSCH, *An active-set trust-region method for derivative-free nonlinear bound-constrained optimization*, contributed talk.

August

TOGO10, Global Optimization Workshop, Toulouse, France, 31st August - 3rd September, 2010. M. FUCHS, *The Optimization Test Environment*, contributed talk.

September

2nd IMA Conference on Numerical Linear Algebra and Optimisation, University of Birmingham, UK, 13-15 September 2010. S. GÜROL, *Nonlinear least-squares problem minimization using subspace preconditioners with an application to data assimilation*, contributed talk.

EMG 2010, European Multi-Grid Conference, Isola d’Ischia, Italy, 19-23 September, 2010. X. PINEL, *Analysis of a perturbed two-grid preconditioner for indefinite three-dimensional Helmholtz problems*, contributed talk.

CNMAC 2010. XXXIII Congresso Nacional de Matematica Aplicada e Comptacional, Aguas de Lindoia, SP, Brazil. 20-23 September 2010, R. LAGO, *Augmentation and Truncation for Iterative Methods*, contributed talk.

CNMAC 2010. XXXIII Congresso Nacional de Matematica Aplicada e Comptacional, Aguas de Lindoia, SP, Brazil. 20-23 September 2010, I.S. DUFF, *Solving really large sparse linear problems from a range of applications*, invited talk.

October

CSDM 2010 Conference, Paris, France, October 27-29, 2010. M. FUCHS, *Discrete search in design optimization*, contributed talk.

December

IEEE BIBM 2010, International Conference on Bioinformatics & Biomedicine, Hong-Kong, December 18-21, 2010. A. MUCHERINO, *On the Solution of Molecular Distance Geometry Problems with Interval Data*, contributed talk.

January

The Second International Conference on Numerical analysis and Optimization. Sultan Qaboos University, Muscat, Oman. 3-6 January 2011. I.S. DUFF, *The use of direct methods in the solution of sparse linear equations from optimization and other applications*, invited talk.

February

Ateliers de Modélisation de l'Atmosphère, Toulouse, 8-10 février 2011, X. VASSEUR, *Architectures massivement parallèles : quelques questions algorithmiques ouvertes*, invited seminar.

March

ROADEF 2011, Saint-Etienne, France, March 2-4, 2011. A. MUCHERINO, *The Discretizable Molecular Distance Geometry Problem : from Ideal to Real Instances*, contributed talk.

Laboratoire Jean Kutzmann, Grenoble, 31 mars 2011. S. GRATTON, *Méthodes d'optimisation duales pour l'assimilation de données de grande taille*, invited seminar.

April

17th Belgian mathematical programming meeting, La Roche-en-Ardenne, Belgium, April 7-8, 2011. S. GÜROL, *Preconditioning Krylov subspace methods in dual space for quadratically penalized nonlinear-least squares problem*, contributed talk.

May

Optimization Days, Montreal, Canada, 2-4 May 2011. M. FUCHS, *Simulated Polyhedral Clouds in Robust Optimization*, contributed talk.

SEA11 - International Symposium on Experimental Algorithms, Crete, Greece, May 5-7, 2011. A. MUCHERINO, *Influence of Pruning Devices on the Solution of Molecular Distance Geometry Problems*, contributed talk.

SIAM Conference on optimization, Darmstadt, Germany, May 16-19, 2011. S. GRATTON, *Preconditioning and Globalizing Conjugate Gradients in Dual Space for Quadratically Penalized Nonlinear-Least Squares Problems*, contributed talk.

SIAM Conference on optimization, Darmstadt, Germany, May 16-19, 2011. A. TRÖLTZSCH, *An Active Set Trust-region Method for Derivative-Free Nonlinear Bound-Constrained Optimization*, invited minisymposium.

SIAM Conference on optimization, Darmstadt, Germany, May 16-19, 2011. M. FUCHS, *Uncertainty Modeling for Robust Optimization*, contributed talk.

Preconditioning 2011 International Conference on Preconditioning Techniques for Scientific and Industrial Applications, Bordeaux, France, May 16-18, 2011. M. BYCKLING, *Numerical experiments on a Factored Approximate Inverse Preconditioner*, contributed talk.

Preconditioning 2011 International Conference on Preconditioning Techniques for Scientific and Industrial Applications, Bordeaux, France, May 16-18, 2011. K. KAYA, *Preconditioners based on Strong Components*, contributed talk.

Preconditioning 2011 International Conference on Preconditioning Techniques for Scientific and Industrial Applications, Bordeaux, France, May 16-18, 2011. X. VASSEUR, *A Multigrid Method for the Solution of Linear Systems with Multiple Right-Hand Sides*, contributed talk.

CSC11 - The SIAM Workshop on Combinatorial Scientific Computing, Darmstadt, Germany, May 16-19, 2011. I.S. DUFF, *On Hypergraph Partitioning based Sparse Matrix Ordering*, contributed talk.

CSC11 - The SIAM Workshop on Combinatorial Scientific Computing, Darmstadt, Germany, May 16-19, 2011. I.S. DUFF, *Preconditioners based on Strong Components*, contributed talk.

NWC'11 Second international workshop - New Worlds of Computation 2011, LIFO, University of Orléans, France, May 2324, 2011. F. CHATELIN, *The legacy of Fourier, Poincaré and Einstein about Relative Computation*, invited seminar.

4th "Scheduling in Aussois" Workshop, Aussois, France, May 29 - June 1st, 2011. K. KAYA, *On Constructing Elimination Trees for Sparse Unsymmetric Matrices*, contributed talk.

June

INRIA Summer School - Toward petaflop numerical simulation on parallel hybrid architectures, Sophia Antipolis, France, June 6-10, 2011. M. BYCKLING, attendee.

LSSC11 - 8th International Conference on Large-Scale Scientific Computations, Sozopol, Bulgaria, June 6-10, 2011. A. MUCHERINO, *Variable Neighborhood Search for Robust Optimization and Applications to Aerodynamics*, contributed talk.

Symposium on Eigenvalues, Model Order Reduction and Trust Regions in celebration of Danny Sorensen's 65th birthday, Reno, Nevada, USA. 11 June 2011. I.S. DUFF, *Partitioning Strategies for the Block Cimmino algorithm*, invited talk.

Householder Symposium XVIII, Tahoe City, California, U.S.A., June 12-17, 2011. P. JIRANEK, *A Posteriori Error Estimates Including Algebraic Error and Stopping Criteria for Iterative Solvers*, poster.

CTW11 - 10th Cologne-Twente Workshop on Graphs and Combinatorial Optimization, Frascati, Rome, Italy, June 14-16, 2011. A. MUCHERINO, *Sparsifying Distance Matrices for Protein-Protein Structure Alignments* & *Branch-and-Prune Trees with Bounded Width*, talks.

July

WCGO11 - The Second World Congress on Global Optimization in Engineering & Science, Crete, Greece, July 3-7, 2011.A. MUCHERINO, *The Discrete Side of Distance Geometry* and *Exploiting NMR Information for Solving Distance Geometry Problems*, talks.

Universidad Tecnica Federico Santa Maria, Valparaiso, Chile. July 16-24, 2011. A. MUCHERINO

Optimization 2011 Conference, Lisboa, Portugal, July 24-27, 2011. S. GRATTON, *An Active Set Trust-region Method for Derivative-Free Nonlinear Bound-Constrained Optimization*, contributed talk.

Minisymposium MS201 : The Linear Algebra of Optimization. Organizers : Michael Friedlander and Chen Greif. Invited minisymposium speaker. ICIAM 2011, Vancouver, Canada. 17-22 July, 2011. I.S. DUFF, *The use of direct methods in the solution of sparse linear equations for constrained optimization*.

August

COCOA11 - 5th Annual International Conference on Combinatorial Optimization and Applications, Zhangjiajie, China, August 4-6, 2011. A. MUCHERINO, *On the Number of Solutions of the Discretizable Molecular Distance Geometry Problem*, talk.

COPPE, Federal University of Rio de Janeiro, Brazil, August 16-29, 2011. A. MUCHERINO, *The Discretizable Molecular Distance Geometry Problem*, invited talk.

HPSS 2011, EuroPar 2011, Bordeaux, 29 August 2011. I.S. DUFF, *European Exascale Software Initiative : Numerical Libraries, Solvers and Algorithms*.

September

Tedx Session, Budapest, Hungary, September 23, 2011 F. CHATELIN, *Mathematics of Life*, invited seminar.

ESF OPTPDE Workshop, Fast solvers for simulation, inversion, and control of wave propagation problems, University of Wuerzburg, Germany, September 26-28, 2011. X. VASSEUR, *An Approximate Two-Level Preconditioner Combined with flexible Krylov Subspace Methods for the Solution of Heterogeneous Helmholtz Problems on Massively Parallel Computers*.

October

The Ninth International Workshop on Adjoint Model Applications in Dynamic Meteorology, Cefalu, Sicily, Italy, October 10-14, 2011. S. GÜROL, *Preconditioning of conjugate-gradients in observation space for 4D-VAR*, contributed talk.

RTRA-STAE Fall meeting, Toulouse, October 18, 2011. S. GRATTON, *L'assimilation de données : une approche générique pour la modélisation des systèmes complexes*, invited seminar.

Large-Scale Inverse Problems and Applications in the Earth Sciences, Workshop at RICAM, Linz, Austria, October 25, 2011. S. GRATTON, *Dual methods for data assimilation in Geosciences*, invited seminar.

10th Mathias Seminar, Workshop organized by TOTAL, Paris, France. 28-29 October 2011. S. GRATTON, *Globally convergent evolution strategies and CMA-ES*, invited talk.

November

Groupe de travail MIP at Univ. Paul Sabatier - Institut de Mathématiques, Toulouse, November 22, 2011. A. TRÖLTZSCH *An active-set trust-region method for bound-constrained nonlinear optimization without derivatives applied to noisy aerodynamic design problems,* invited seminar.

8.2 Conferences and seminars organized by the Parallel Algorithms Project

February

Advanced Methods and perspectives in nonlinear optimization and control (RTRA workshop) 3-5 February 2010 at ENSIACET, Toulouse, France.

June

Sparse Days Meeting at CERFACS 15-17 June 2010 at CERFACS, Toulouse, France.

September

Sparse Days Meeting at CERFACS 6-7 September 2011 at CERFACS, Toulouse, France.

8.3 Internal seminars organized within the Parallel Algorithms Project

May

A perturbed two-level preconditioner for the solution of three-dimensional heterogeneous Helmholtz problems with applications to geophysics., May 18, 2010. Ph.D. thesis defense. X. PINEL.

June

The Discretizable molecular distance geometry problem., June 24, 2010. A. MUCHERINO.

July

Further Optimization Interactions with Experts (FOIE) 7 July 2010 at CERFACS, Toulouse, France.

September

Multigrid preconditioning strategies for the Helmholtz equation., September 14, 2010. S. MACLACHLAN.
On the future of the HPC : How to think Exascale ? How the HPC community addresses this challenge, which direction they propose ?, September 15, 2010. A. HAIDAR.

December

An introduction to quantum graphs and their applications., December 9, 2010. M. ARIOLI.

January

Preconditioning for standard and two-sided Krylov subspace methods., January 13, 2011. M. BYCKLING.
Application of inverse problems and optimization techniques in aerospace problems., January 19, 2011. S. ALESTRA AND V. SRITHAMMAVANH.

February

A pressure-enthalpy coupling algorithm for CFD using AMG to solve mixed elliptic-hyperbolic systems., February 10, 2011. M. EMANS.

March

Energy preserving POD based ROMs., March 23, 2011. M. HAMDAOUI.
Domain decomposition for Total Variation Minimization., March 28, 2011. A. LANGER.

April

Optimization of noisy computer experiments using Gaussian processes., April 7, 2011. V. PICHENY.
Parallel Reduction to tri/bi-diagonal forms for symmetric eigenvalue problems using fine-grained and memory-aware kernels, April 7, 2011. A. HAIDAR.

May

An adaptive finite element method in L^2-TV-based image denoising., May 5, 2011. M. RINCON-CAMACHO.

June

An active-set trust-region method for bound-constrained nonlinear optimization without derivatives applied to noisy aerodynamic design problems., June 7, 2011. Ph.D. thesis defense. A. TRÖLTZSCH.

December

A stochastic inverse problem : identification of a distribution of a random variable under performance constraints., December 15, 2011. A. AHIDAR.

9 Publications

9.1 Books

[ALG1] F. Chatelin, (2011), *Spectral approximation of linear operators*, SIAM Classics in Applied Mathematics, 65, SIAM.

9.2 Conference Proceedings

[ALG2] U. V. Çatalyürek, K. Kaya, and B. Uçar, (2011), Integrated data placement and task assignment for scientific workflows in clouds, In *Proc. DIDC 2011, a workshop of HPDC 2011*, San Jose, California, 45–51.

[ALG3] F. Chatelin, (2010), A computational journey into nonlinearity, In *Unconventional Computation 2010, 9th International Conference, UC 2010, Tokyo, Japan, June 21-25, 2010, Proceedings*.

[ALG4] F. Chatelin, (2011), On the legacy of Euler, Fourier, Poincaré and Einstein about Computation, In *New Worlds of Computation 2011, NWC 2011, Orléans, May 23-24, 2011, Proceedings*.

[ALG5] F. Domes, M. Fuchs, and H. Schichl, (2010), The Optimization Test Environment, In *Proceedings of the Toulouse Global Optimization Workshop (TOGO)*, Toulouse, France, 39–42.

[ALG6] M. Fuchs and A. Neumaier, (2010), Discrete search in design optimization, In *Proceedings of the First International Conference on Complex Systems Design & Management (CSDM)*, Paris, France, 113–122.

[ALG7] M. Fuchs, (2010), Simulation based uncertainty handling with polyhedral clouds, In *Proceedings of the 4th International Workshop on Reliable Engineering Computing (REC)*, Singapore, 526–535.

[ALG8] F.-H. R. K. Kaya and B. Uçar, (2011), On partitioning problems with complex objectives, In *Proc. HPSS 2011, a workshop of Euro-Par 2011*, Bordeaux, France.

9.3 Journal Publications

[ALG9] P. Amestoy, I. Duff, A. Guermouche, and T. Slavova, (2010), Analysis of the solution phase of a parallel multifrontal approach, *Parallel Computing*, **36**, 3–15. Preliminary version available as CERFACS Technical Report TR/PA/08/82.

[ALG10] M. Baboulin and S. Gratton, (2011), A contribution to the conditioning of the total least-squares problem, *SIAM Journal on Matrix Analysis and Applications*, **32**, 685–699.

[ALG11] F. Bastin, V. Malmedy, M. Mouffe, P. L. Toint, and D. Tomanos, (2010), A Retrospective Trust-Region Method for Unconstrained Optimization, *Mathematical Programming*, **123**, 395–418.

[ALG12] C. Calude and F. Chatelin, (2010), A dialogue about Qualitative Computing, *Bulletin of EATCS (European Association for Theoretical Computer Science)*, **101**, 29–41. Preliminary version available as CERFACS Technical Report TR/PA/10/37.

[ALG13] L. Carvalho, S. Gratton, R. Lago, and X. Vasseur, (2011), A Flexible Generalized Conjugate Residual Method with Inner Orthogonalization and Deflated Restarting, *SIAM Journal on Matrix Analysis and Applications*, **32**, 1212–1235. Preliminary version available as CERFACS Technical Report TR/PA/10/10.

[ALG14] F. Chatelin, (2010), Numerical information processing under the global rule expressed by the Euler-Riemann ζ function defined in the complex plane, *Chaos, Focus issue : intrinsic and designed computation : information processing in dynamical systems*, **20**. Preliminary version available as CERFACS Technical Report TR/PA/10/49.

[ALG15] I. Duff and D. Mijuca, (2011), On accurate and time efficient solution of primal-mixed finite element equations in multiscale solid mechanics, *International Journal for Numerical Methods in Biomedical Engineering*, **27**. Preliminary version available as CERFACS Technical Report TR/PA/09/67.

[ALG16] I. S. Duff and B. Uçar, (2010), On the Block Triangular Form of Symmetric Matrices, *SIAM Review*, **52**, 455–470. Preliminary version available as CERFACS Technical Report TR/PA/09/57.

[ALG17] M. B. Fares, S. Gratton, and P. L. Toint, (2011), Fast regularized linear sampling for inverse scattering problems, *Numerical Linear Algebra and Applications*, **18**, 95–112.

[ALG18] M. Fuchs and A. Neumaier, (2010), A splitting technique for discrete search based on convex relaxation, *Journal of Uncertain Systems, Special Issue on Global Optimization and Intelligent Algorithm*, **4**, 14–21. Preliminary version available as CERFACS Technical Report TR/PA/10/5.

[ALG19] D. Ghosh, P. Avery, and C. Farhat, (2010), A FETI-preconditioned conjugate gradient method for large-scale stochastic finite element problems, *Int. J. Numerical Methods in Engineering*, **80**, 914–931. Preliminary version available as CERFACS Technical Report TR/PA/09/52.

[ALG20] L. Giraud, S. Gratton, X. Pinel, and X. Vasseur, (2010), Flexible GMRES with Deflated Restarting, *SIAM Journal on Scientific Computing*, **32**, 1858–1878. Preliminary version available as CERFACS Technical Report TR/PA/09/111.

[ALG21] S. Gratton and P. L. Toint, (2010), Approximate Invariant Subspaces and Quasi-Newton Optimization Methods, *Optimization Methods and Software*, **25**, 507–529. Preliminary version available as CERFACS Technical Report TR/PA/09/165.

[ALG22] S. Gratton, P. Laloyaux, A. Sartenaer, and J. Tshimanga, (2011), A reduced and limited-memory preconditioned approach for the 4D-Var data-assimilation problem, *Quarterly Journal of the Royal Meteorological Society*, **137**. Preliminary version available as CERFACS Technical Report TR/PA/09/98.

[ALG23] S. Gratton, M. Mouffe, and P. Toint, (2011), Stopping rules and backward error analysis for bound-constrained optimization, *Numerische Mathematik*, **119**. Preliminary version available as CERFACS Technical Report TR/PA/09/95.

[ALG24] S. Gratton, M. Mouffe, A. Sartenaer, P. L. Toint, and D. Tomanos, (2010), Numerical Experience with a Recursive Trust-Region Method for Multilevel Nonlinear Optimization, *Optimization Methods and Software*, **25**, 359–386. Preliminary version available as CERFACS Technical Report TR/PA/09/48.

[ALG25] S. Gratton, A. Sartenaer, and J. Tshimanga, (2011), On a class of limited memory preconditioners for large scale linear systems with multiple right-hand sides, *SIAM Journal on Optimization*, **21**, 912–935. Preliminary version available as CERFACS Technical Report TR/PA/09/99.

[ALG26] S. Gratton, P. L. Toint, and J. T. Ilunga, (2011), Inexact range-space Krylov solvers for linear systems arising from inverse problems,, *SIAM Journal on Matrix Analysis and Applications*, **32**, 969–986. Preliminary version available as CERFACS Technical Report TR/PA/10/141.

[ALG27] S. Gratton, P. Toint, and A. Troeltzsch, (2011), An active set trust-region method for derivative-free nonlinear bound-constrained optimization, *Optimization Methods and Software*, **26**, 875–896. Preliminary version available as CERFACS Technical Report TR/PA/10/70.

[ALG28] X. Guo and I. S. Duff, (2011), Semilocal and global convergence of the Newton-HSS method for systems of nonlinear equations, *Numerical Linear Algebra and Applications*, **29**, 299–315. Preliminary version available as CERFACS Technical Report TR/PA/10/14.

[ALG29] P. Jiránek and M. Rozloznik, (2010), Adaptive version of Simpler GMRES, *Numerical Algorithms*, **53**, 93–112. Preliminary version available as CERFACS Technical Report TR/PA/08/101.

[ALG30] P. Jiránek and D. Titley-Peloquin, (2010), Estimating the backward error in LSQR, *SIAM J. Matrix Analysis and Applications*, **31**, 2055–2074. Preliminary version available as CERFACS Technical Report TR/PA/09/77.

[ALG31] P. Jiránek, Z. Strakoš, and M. Vohralík, (2010), A Posteriori Error Estimates Including Algebraic Error and Stopping Criteria for Iterative Solvers, *SIAM J. Scientific Computing*, **32**, 1567–1590.

[ALG32] G. Ramillien, R. Biancale, S. Gratton, X. Vasseur, and S. Bourgogne, (2011), GRACE-derived surface mass anomalies by energy integral approach. Application to continental hydrology, *Journal of Geodesy*, **85**, 313–328.

9.4 Technical Reports

[ALG33] P. R. Amestoy, I. S. Duff, Y. Robert, F.-H. Rouet, and B. Ucar, (2010), On computing inverse entries of a sparse matrix in an out-of-core environment, Technical Report TR/PA/10/59, CERFACS, Toulouse, France.

[ALG34] H. Calandra, S. Gratton, R. Lago, X. Pinel, and X. Vasseur, (2011), Two-level preconditioned Krylov subspace methods for the solution of three-dimensional heterogeneous Helmholtz problems in seismics, Technical Report TR/PA/11/80, CERFACS, Toulouse, France.

[ALG35] H. Calandra, J. Langou, S. Gratton, X. Pinel, and X. Vasseur, (2011), Flexible variants of block restarted GMRES methods with application to geophysics, Technical Report TR/PA/11/14, CERFACS, Toulouse, France.

[ALG36] C. S. Calude and F. Chatelin, (2010), A dialogue about Qualitative Computing, Technical Report TR/PA/10/37, CERFACS, Toulouse, France.

[ALG37] L. M. Carvalho, S. Gratton, R. Lago, and X. Vasseur, (2010), A Flexible Generalized Conjugate Residual Method with Inner Orthogonalization and Deflated Restarting, Technical Report TR/PA/10/10, CERFACS, Toulouse, France.

[ALG38] L. M. Carvalho, S. Gratton, R. Lago, and X. Vasseur, (2011), A Flexible Generalized Conjugate Residual Method with Inner Orthogonalization and Deflated Restarting, Technical Report TR/PA/11/26, CERFACS, Toulouse, France. Revised version of CERFACS Technical Report TR/PA/10/10.

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9.5 Thesis

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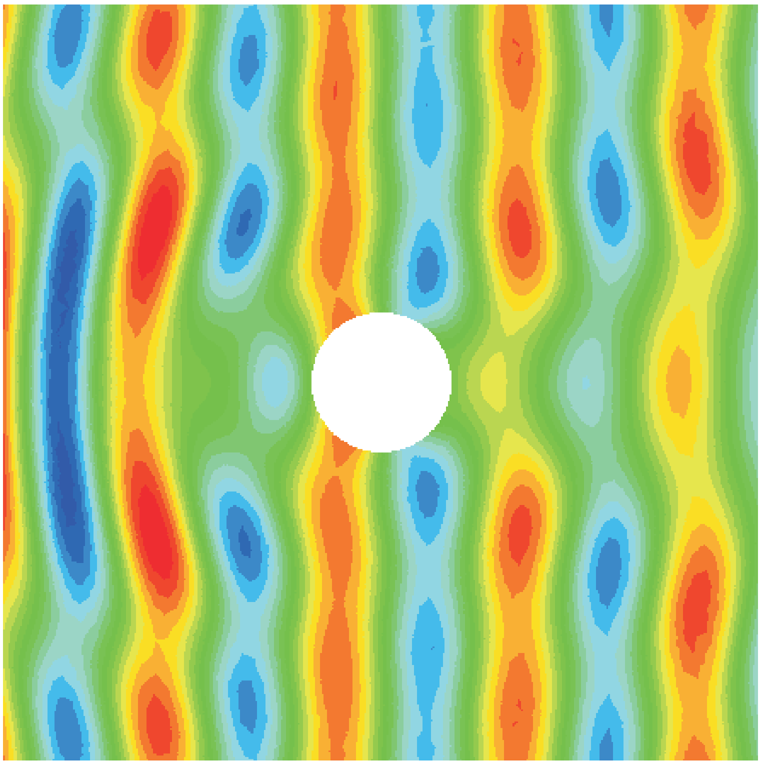
2

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 wave propagations. We study the scattering of time-harmonic electromagnetic and acoustic waves. But the transient regime in the case of electromagnetic and elastodynamic waves propagation is also analyzed.

In 3D electromagnetism, our efforts are focused essentially on integral equations method. First we have developed well-conditioned and accurate integral equation methods, which are implemented in the CESC code (CERFACS Electromagnetism Solver Code) . This work is done in collaboration with ONERA. And this activity is part of a ANR project ARTHEMIS (in partnership with ONERA and Polytechnique). Secondly, specific attention is led to the multipole algorithm in the case of low frequency or when the mesh is very refined.

A more recent activity concerns the numerical simulation of acoustic scattering in presence of an arbitrary mean flow : the method couples continuous and discontinuous finite elements with Perfectly Matched Layers. Two different approaches have been constructed and implemented. Several boundary conditions are analyzed. 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 Maxwell's equations, including local time-stepping and adaptative refinement strategy. This approach is implemented in the ONERA code.

2 Integral equations for electromagnetism scattering

2.1 Numerical simulation of a reflectarray antenna.

A. Bendali, F. Collino and M. Fares

The object of this study was to explore some modeling techniques for an efficient numerical simulation of reflectarray antenna. A reflectarray antenna is a skew finite grating of shallow rectangular waveguides enlighten by a small horn antenna. A electronic device inside each waveguide is designed to set up a phase shift locally for the reflected field. In this way, the direction of the main lobe of the antenna can be modified electronically without any mechanical move of the emitting device. We developed an impedance model based on an unimodal propagation in each cell taking into account the complicate phase shift process. All the remaining parts of the radiating system are dealt with using a direct numerical simulation approach. We derived a formulation of the problem in terms of a system of integral equations next discretized by means of the method of moments. We showed that this formulation provides a reliable method for computing the field radiated by the antenna. Moreover, it is well-adapted for providing a fast method for computing the variation in the direction of the main lobe resulting from a modification of the phase shift on each cell. The numerical method has been implemented within the CERFACS Electromagnetic Solver Code (CESC). Computed radiation pattern for a reflectarray designed by TSA-CNES showed an excellent agreement with experiments hence validating the accuracy of the approach as depicted in figure 2.2 and figure 2.3.

2.2 Extension to non-conforming meshes and stabilization of the combined current and charge integral equation.

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

An important issue in industrial applications in electromagnetism requiring the solution of a large scale boundary integral equation concerns the possibility of using meshes on different zones obtained independently each from the other, which thus do not comply with the usual matching requirement of finite element approximations. By bringing out some mathematical properties of the Combined Current and Charge Integral Equation (shortly C3IE) introduced by Taskinen and Yl-Oijala [2] when it is posed on a surface without geometrical singularities, we established that this equation can be solved by a Boundary Element Method (BEM) that requires no interelement continuity. This property is crucial when using meshes on different parts of the surface obtained independently each from the other. We showed how the C3IE can be implemented by slightly modifying a usual BEM electromagnetic solver code and that the numerical behavior of this method is very similar to the usual Combined Field Integral Equation (CFIE) when dealing with smooth surfaces. The extension to singular geometries showed that acute dihedral angles can lead to inaccuracies in the results. By considering a two-dimensional version of the formulation, we have brought out that the wrong results are due to spurious oscillations concentrating around the singular points of the geometry. Noticing that the system linking the current and the charge is a saddle-point problem, we have adapted a general procedure used for stabilizing the numerical approximation of mixed formulations as the Stokes system [1], consisting here in augmenting the approximation of the charge. This stabilization procedure, when coupled with a refinement of the mesh in the proximity of the geometrical singularities, obtained by a simple subdivision of the triangles, greatly reduces the effect of the spurious oscillations. This topic is the subject of Steif's PhD thesis which is planned to be defended before June 2012.

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

2.3 Model reduction for acoustic multi-perforated walls in aircraft engines.

A. Bendali, M. Fares, S. Laurens and S. Tordeux

To prevent them from being destroyed, the walls of the combustion chambers of aircraft engines are protected by injection of relatively cool air through a regular array of sub-millimeter holes. The designers of these engines are also faced with combustion instabilities due to excessive levels of noise which can destroy the engine. The properties of sound attenuation by perforated walls are reinforced when they are crossed by a bias flow. An additional advantage of cooling the walls is hence to avoid combustion instabilities due to the acoustics. Predicting these effects is of paramount importance in the process of developing new engines thus inducing a crucial need in numerical simulation. However, the submillimeter size and the number of perforations make prohibitive an approach by a direct numerical simulation which must be preceded by a model reduction. An example of such a perforated wall is depicted in figure 2.7.

A prohibitive discretization at the level of the perforations can be avoided by using a reduced model that brings about the effect of perforations by means an effective condition on the plate whose effective numerical simulation is thus affordable. These model reductions depend strongly on the porosity of the plate, defined as the open to total area ratio. Less than 4%, the porosity of the walls is considered as low. Usual walls involved in aircraft engines are of about 2% porosity. The model reductions for a low porosity plate are based on the calculation of the Rayleigh conductivity of an isolated perforation. This conductivity is defined as the ratio of the volume flux to the pressure across the perforation. This approach has a significant advantage : it makes it possible to couple the equations governing the propagation of acoustic waves outside a boundary layer near the plate with models of flows taking into account the dissipation by viscosity at the perforations.

The models are developed assuming that the size of the aperture of the perforation are small compared with the wavelength and that they constitute an infinite doubly periodic array. A systematic study, based on the availability in CERFACS of codes tailored to take advantage of massively parallel plateformes was conducted to accurately bring out the effect of the size of the orifices and the finite size of the lattice perforations. Figure 2.10, plotting the reflection coefficient for an infinite array of perforations, shows an agreement of the model with a direct simulation yielding an error less than 1%. The same simulation, but this once for a finite size array shown in figure 2.8, yielded an error of about 10% as reported in Figure 2.9. Several studies were also conducted in this framework. An attempt to give a mathematical justification to these models, based on intuitive approximations, led to the construction of second-order conditions for approximating the acoustic field. Figure 2.10 depictes the improvement gained by using these second-order conditions.

Some progresses have been also done in another direction. The thickness of the plate is usually taken into account by adding an inertial mass impedance term to the Rayleigh conductivity of the plate assued to be infinitely thin. This inertial impedance was formely determined by means of an intuitive reasoning only. A rigorous mathematical justification to these calculations made it possible to obtain it for an inclined perforation, which is the actual shape involved in realistic aircraft engines. This is an unprecedented result since no determination, even intuitive, was formely available in this case.

[3] A. Bendali, M. Fares, A. Tizaoui, and S. Tordeux, (2012), Matched asymptotic expansions of the eigenvalues of a 3-D boundary-value problem relative to two cavities linked by a hole of small size, *ommunications in Computational Physics*, **11 (2)**, 456–471.

[4] A. Bendali, A. Huard, A. Tizaoui, S. Tordeux, and J. P. Vila, (2009), Asymptotic expansions of the eigenvalues of a 2-D boundary-value problem relative to two cavities linked by a hole of small size, *C. R. Acad. Sci. Paris, Mathmatiques*, **347**, 1147–1152.

2.4 Electromagnetic imaging by the Linear Sampling Method

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

The theory of inverse scattering for acoustic and electromagnetic waves, is an active area of research with significant developments in the past few years. Inverse problems consist in getting informations on a physical object from measurement data. More specifically, the inverse scattering problem is the problem of finding characteristics of an unknown object referred to as scatterer (location, shape, material properties,...) from measurement data of acoustic or electromagnetic waves scattered by this object. The question is not only to detect objects like radar and sonar can do, but also to identify them.
Inverse problems are not easy to solve since they belong to the class of ill-posed problems as defined by Hadamard. Indeed, a solution may not exist but even if it is the case, the solution does not depend continuously on the data. Such problems require the use of regularisation schemes to be solved numerically.
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, the aim of the thesis of Anne Cossonnière (October 2008 - December 2011), under the supervision of Houssem Haddar (INRIA project-team DEFI), is to investigate the potential interest of the so-called interior transmission frequencies in order to image the interior of a penetrable scatterer and to answer some open problems on this subject.

2.5 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 fully 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 [EMA15].

2.6 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 study of transmission eigenvalues is closely linked to the study of the interior transmission problem which has been a subject of great interest in scattering theory for the past few years. This is due to the fact that transmission eigenvalues can give information on the properties of an obstacle, for instance on the index of refraction or if it contains a cavity or a crack. The interior transmission problem is defined by :

$$\operatorname{curl}\operatorname{curl}\mathbf{E} - k^2 N\mathbf{E} = 0 \text{ in } D \tag{2.1}$$

$$\operatorname{curl}\operatorname{curl}\mathbf{E}_0 - k^2\mathbf{E}_0 = 0 \text{ in } D \tag{2.2}$$

$$\nu \times \mathbf{E} - \nu \times \mathbf{E}_0 = 0 \text{ on } \partial D \tag{2.3}$$

$$\nu \times \operatorname{curl}\mathbf{E} - \nu \times \operatorname{curl}\mathbf{E}_0 = 0 \text{ on } \partial D \tag{2.4}$$

and transmission eigenvalues are values of k for which the interior transmission problem has a nontrivial solution. Although theoretical results about existence of transmission eigenvalues and the fact that they form a discrete set has been proven in many articles, a few papers consider the computation of transmission eigenvalues for general geometry and even less in electromagnetics.
The method we shall use here is based on the CESC code developped by the CERFACS which combines integral equations and finite elements. It first consists in expressing the solutions $(\mathbf{E}, \mathbf{E}_0)$ of the previous interior transmission problem with integral equations. Then the boundary conditions (2.3) and (2.4) lead to solve a system of the form $Z_k X = 0$ where $X = \begin{pmatrix} J \\ M \end{pmatrix}$ with $J = -\nu \times \operatorname{curl}\mathbf{E}$ and $M = \nu \times \mathbf{E}$. Transmission eigenvalues are values of k for which 0 is an engenvalue of Z_k. The main difficulty is that the operator Z_k is compact and therefore 0 is an accumulation point of its eigenvalues. As a consequence, the real eigenvalue 0 is “lost” numerically in the accumulation region. To get around this difficulty, we use a preconditioner B_k to shift the accumulation to 1 and we solve the generalized eigenvalue problem $Z_k X = \lambda B_k X$. We shall discuss proper choices of the operator B_k.
Another way to compute the transmission eigenvalues is to use far field data and the Linear Sampling Method. The Linear Sampling Method is based on solving an ill-posed far field equation using Tikhonov regularization. This method is usually used to determinate the shape of an obstacle. However, it can be shown that when k is a transmission eigenvalue for a sampling point $z \in D$ the norm of the regularized solution to the far field equation cannot be bounded as the parameter tends to zero. Thus this property provides us another method to find transmission eigenvalues as the location of the peaks on the plot of the regularized solution’s norm against k. Figures 2.11 and 2.12 demonstrate the concordance of the results provided by both methods.

2.7 Iterative solution of electromagnetic scattering

F. Collino, F. Millot and S. Pernet

Numerical solutions of problems related to the time-harmonic scattering are computed by using integral equation methods. The fast mutipole method allows us to obtain solutions of large size problems with for instance more than several millions of unknowns. We have focused our efforts in several items.

- In order to increase the capacity of our code to solve very large size problems, specific analysis of memory storage is investigated [EMA25].
- For iterative solution, the number of iterations is directly linked to the condition number. We develop well-conditioned integral equations in presence of dielectric bodies.
- The techniques of a posteriori error analysis and adaptative methods for the integral equations are investigated. In the 2D case, a posteriori error indicators are built and first results are very promising.
- It is well known that the algorithm of the fast mutipole method fails when the frequency decreases or when the mesh is very refined. Analysis of specific cases is investigated. We want to build a original method working at all frequencies and with all mesh steps.

2.7.1 A Generalized Combined Source Integral Equation for transmission problems

The success of FMM revealed a new limiting factor : the conditioning of linear systems. Indeed, due to the size of problems, one must use iterative solvers whose effectiveness depends crucially on the condition number of the linear systems to solve. Unfortunately, the main drawback of integral equations is the bad condition number of the linear system obtained from their discretization. This implies important computational costs when an iterative solution is used. This phenomena grows with the physical complexity and in particular, it becomes very problematic in the context of transmission problems. So the subject of preconditioning is at the heart of many researches. Nowadays, the best approach to address this problem is the pseudodifferential calculus. Indeed, contrary to the classical algebraic approach, it allows to construct either the preconditioners based on parametrers which contain physical informations (frequency dependence) or either new integral equations which are naturally well-conditioned (no preconditionner is needed). This kind of techniques has proven their superiority on their algebraic counterpart. We investigate this technique since some years. In particular, the results obtained for the impedance problems are very impressive [EMA5]. During the last two years, in collaboration with David Levadoux, we have proposed a new integral equation for the transmission problem [EMA17, EMA5]. These works are continuing in the project ARTHEMIS funded by the ANR (2011-2015).
In the following, we present a comparison of this new formulation with the well-known PMCHWT formulation [5]. The configuration chosen is a dielectric almond which is a relevant test-case in electromagnetism because of the presence of a tip. These results show the relevance of our approach.

Influence of the mesh step size

GCSIE formulation

k	$\frac{\lambda_o}{h}$	n_{iter}
4.715	14	23
4.715	28	27

PMCHWT formulation with SPAI preconditioner

k	$\frac{\lambda_o}{h}$	n_{iter}
4.715	14	40
4.715	28	$100(0.01)$

Influence of the frequency

GCSIE formulation

k	$\frac{\lambda_o}{h}$	n_{iter}
4.715	14	23
9.43	14	60
18.85	14	115

PMCHWT formulation with SPAI preconditioner

k	$\frac{\lambda_o}{h}$	n_{iter}
4.715	14	40
9.43	14	115
18.85	14	300(0.002)

[5] B.H. Jung and T.K. Sarkar and Y.S. Chung, *A survey of various frequency domain integral equations for the analysis of scattering from three-dimensional dielectric objets*, PIER, 36 :193-246,2002.

2.7.2 A posteriori error analysis for integral equations

In the field of electromagnetism, acoustics or elastodynamics, the ability of the methods of integral equations to solve large problems raised by the application has been widely proven. They are both less costly in degrees of freedom and less dispersive than methods based on the discretization of the entire domain (finite element method, finite difference method or discontinuous Galerkin method). In comparison with the finite element methods, integral methods remain insufficiently popularized and they are generally used by experienced specialists. We believe that one of the obstacles to wider use of these methods is the lack of automatic tools, to ensure the accuracy of the computed solution. Indeed, the techniques of an a posteriori error analysis and the adaptive methods are almost non-existent in the field of integral equations. Nevertheless, there are some theoretical results [6, 7] showing the possibility of constructing a posteriori error indicators for the integral formulations but these estimators do not seem to have been tried in practice. This is especially true in the fields of electromagnetism and acoustics for which we did not have find any result in the literature. The main technical difficulties to derive an a posteriori error indicator for integral equations are the nonlocal character of operators and the singularity of the Green kernel.
In 2011, we began this subject by a first trainee period [EMA27] in which we studied the possibility to use an a posteriori error indicator based on averaging techniques for the 2D acoustic problem. This first results are promising (see Fig. 2.15). In particular, the adaptive mesh refinement algorithm obtained allows to obtain the best rate of convergence of the numerical method when a singularity occurs. Moreover, the CPU time spent to obtain an accurate solution decreases.
As perspective, a project in collaboration with CNRS, EADS-IW, IMACS and THALES was submitted to the call for project MN of the ANR.

[6] C. CARSTENSEN and D. PRAETORIUS. Averaging techniques for the a posteriori bem error control for a hypersingular integral equation in two dimensions. SIAM J.SCI. COMPUT.,29 :782, 2007.

[7] C. CARSTENSEN and D. PRAETORIUS. Averaging techniques for the a posteriori error control in nite element and boundary element analysis. SIAM J.SCI. COMPUT., 2006.

FIG. 2.1: Reflectarray part of the TSA-CNES antenna at 9.65 Ghz including 12×24 cells.

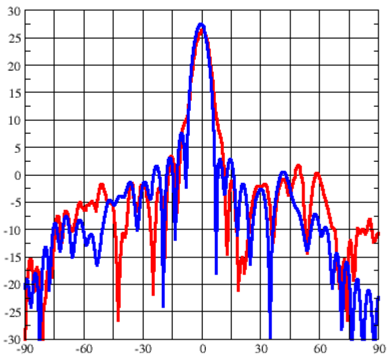

FIG. 2.2: Computed and measured radiation pattern when the main lobe is in the normal direction.

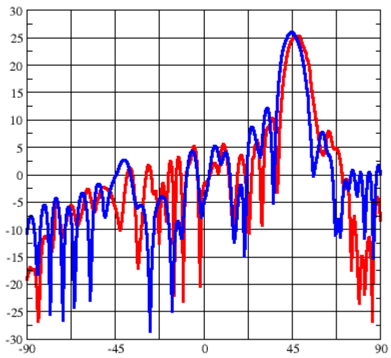

FIG. 2.3: Computed and measured modification of the main lobe resulting from a suitable data set of the impedance cells.

Mesh Size	10 pts/λ	20 pts/λ	40 pts/λ
C3IE	6.4	1.4	1.3
R-C3IE	4.7	1.9	–
S-C3IE	0.7	0.6	0.5
RS-C3IE	0.6	0.1	–

TAB. 2.1: Error in dB on the RCS for various versions of the C3IE, C3IE : plain C3IE, R-C3IE : C3IE with refined mesh around the sharp edges, S-C3IE : Stabilized C3IE, RS-C3IE : Stabilized C3IE with refined mesh around the sharp edges.

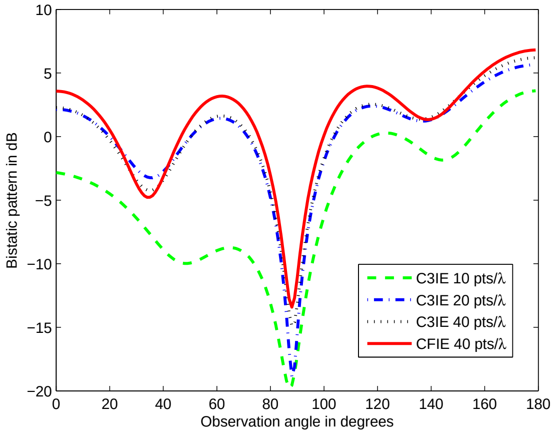

FIG. 2.4: Bistatic pattern of a rectangular brick obtained by solving the C3IE on usual and refined meshes and the CFIE on a very refined mesh.

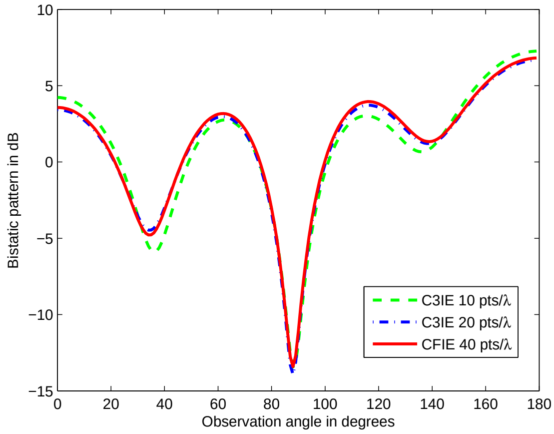

FIG. 2.5: Bistatic pattern obtained by the RS-C3IE.

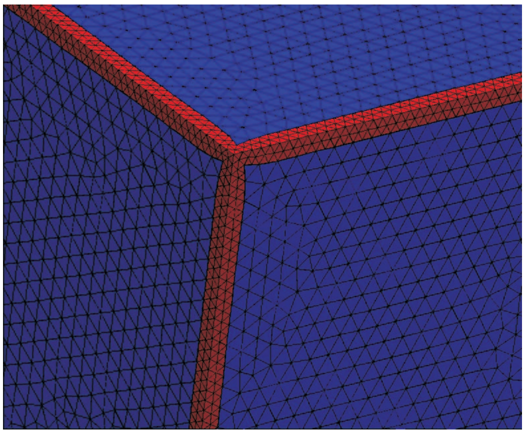

FIG. 2.6: A view of the refined mesh around the sharp edges of the geometry.

FIG. 2.7: View of a multi-perforated wall of the combustion chamber of an aircraft engine (Courtesy of SNECMA).

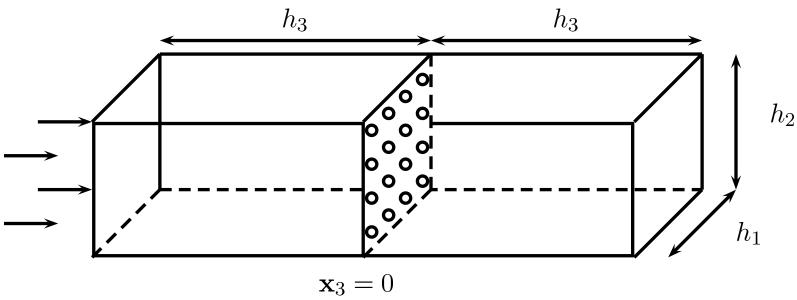

FIG. 2.8: Finite size array of perforations.

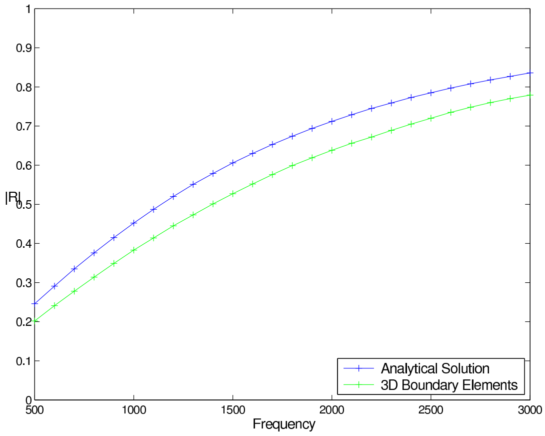

FIG. 2.9: Reflection coefficient corresponding to the finite size array.

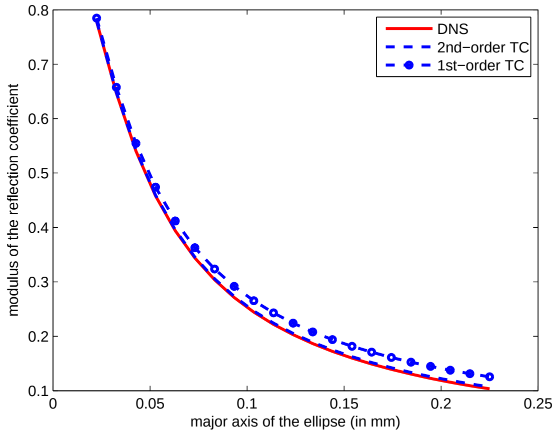

FIG. 2.10: Reflection coefficient corresponding to the infinite array.

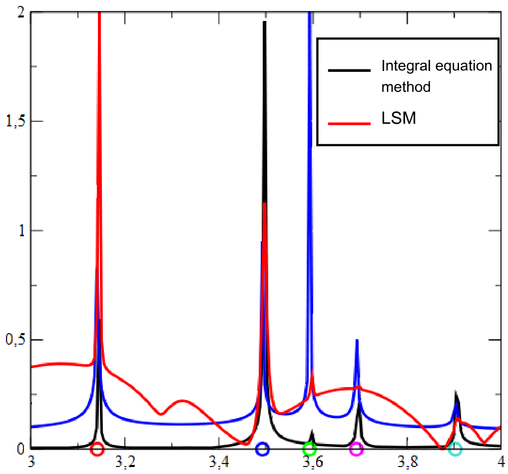

FIG. 2.11: Homogeneous sphere of radius 1 and index of refraction $n = 4$.

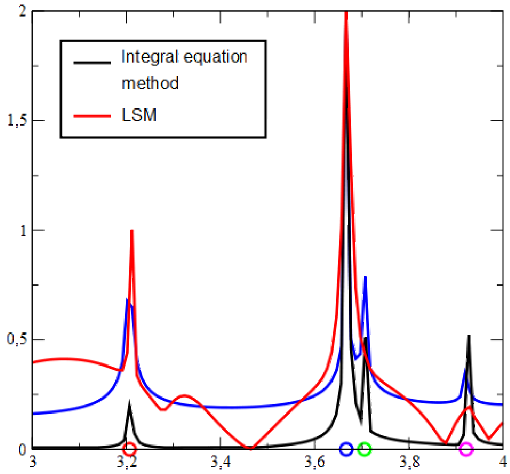

FIG. 2.12: Sphere D of radius 1 and index of refraction $n = 4$ containing a cavity D_0, a sphere of radius 0.25.

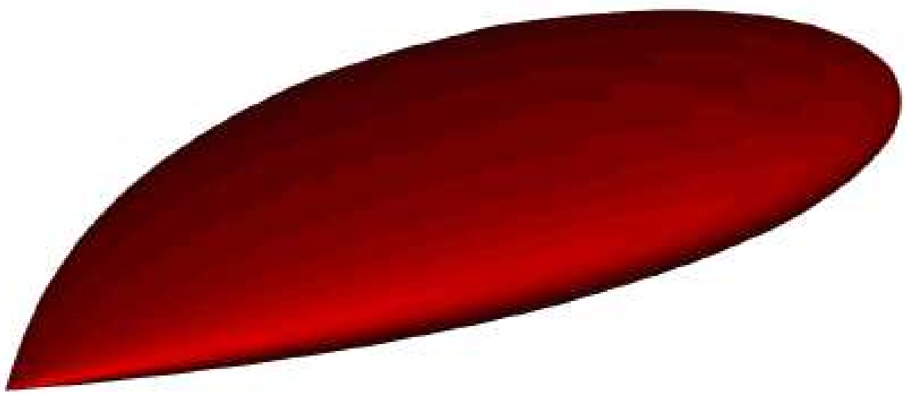

FIG. 2.13: Almond geometry.

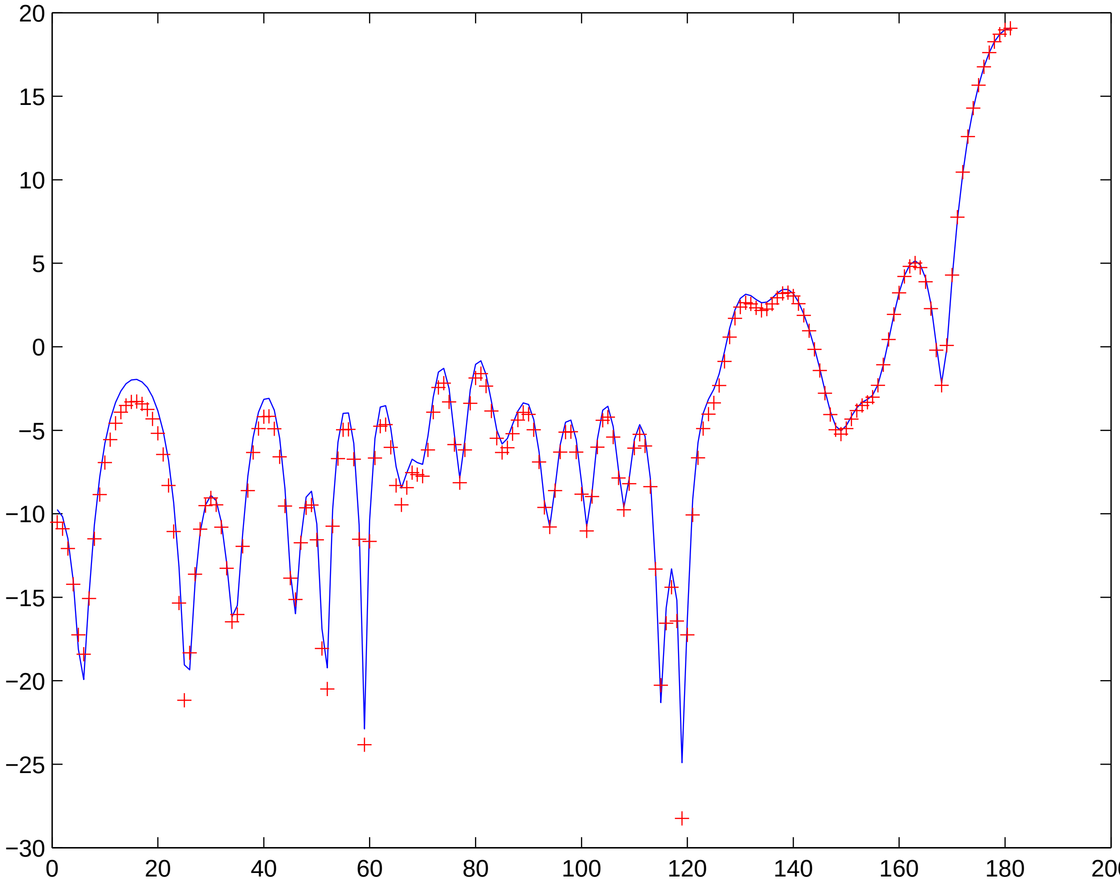

FIG. 2.14: Radar Cross Section of the dielectric almond : $\varepsilon_r = 4$, $k = 28\,m^{-1}$ and 200000 degrees of freedom

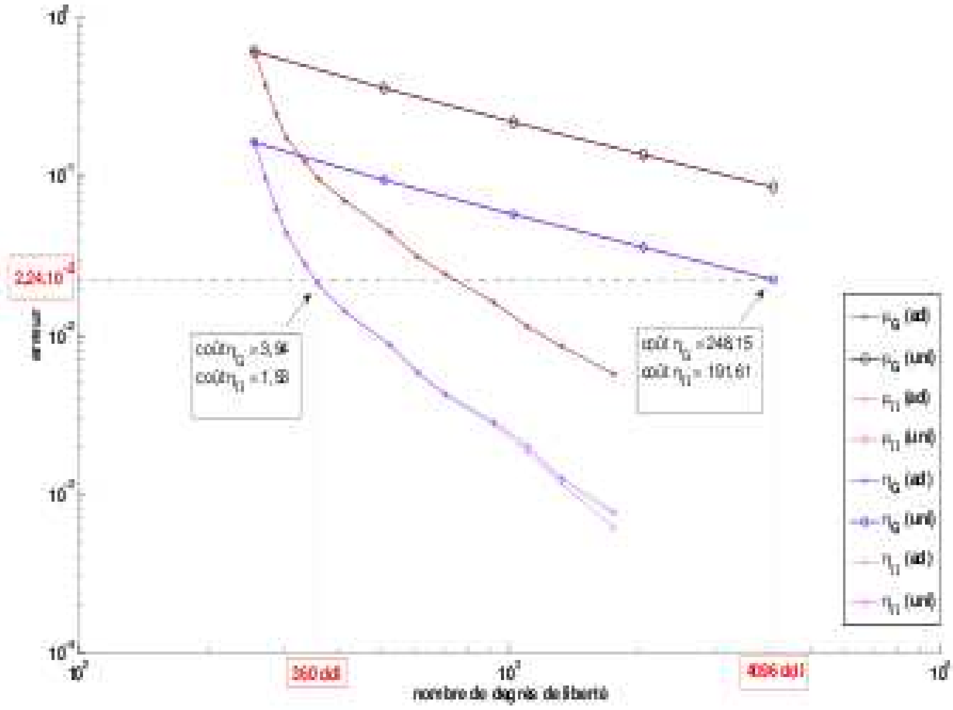

FIG. 2.15: Non smooth solution : behaviour of uniform (uni) and adaptive (adp) algorithms

3 Discontinuous Galerkin methods for time domain problems

3.1 A posteriori analysis for Maxwell equations

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).

Today, the a posteriori error analysis and automatic mesh adaptation have become important tools in numerical analysis of partial differential equations (PDE). Indeed, the quality of the solution is closely related to the quality of the mesh used. The automatic mesh adaptation has clearly proven its effectiveness. This technique allows to significantly reduce the computational cost (by reducing the number of degrees of freedom) and to achieve a numerical solution with the wanted accuracy. The quality of the solution is evaluated by using an a posteriori error estimator. The development of such tools remains a challenge in many situations. In particular, few results exist for the space-time adaptivity. This is especially true for Maxwell's equations for which there are only results in the frequency domain.

In the REI "Recherche exploratoire et Innovation" project DIGATOP funding by the DGA (Direction Générale de l'Armement), we have initiated a research on the derivation of a posteriori error estimates in the frame of the time domain Maxwell equations. In the first time, we have proposed a reliable and an efficient a posteriori error indicator (in sense of the a posteriori error analysis) of residual type in order to control the space discretization error for the energy norm. The construction is based on a reconstruction technique [8] which reduces the a posteriori error analysis to a "more simple" intermediate stationary problem. This reconstructed problem is based on the projector used to derive the optimal a priori error estimate of our scheme. One advantage of this type of estimator is the low computational cost. However, such an estimate involves many constants (not explicit) that can induce a pessimistic indicator. That is why, in a second step, we proposed estimators which do not involve undetermined constants. For that, we inspired of the approach established in [9, 10] : first, we give abstract error estimates which are independent of the numerical scheme used to obtain the approximate solution. These estimates then guide the construction of explicit estimators which are then scheme dependent. These are local reconstruction techniques which allow to obtain efficient error indicators.

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[9] A. Ern, A. F. Stephansen, M. Vohralik, *Guaranteed and Robust discontinuous Galerkin a posteriori error estimates for convection-diffusion-reaction problem*, J. Comput. Appl. Math., 234, 114–130 (2010).

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3.2 Space-time refinement for elastodynamic equation

Y. Dudouit, L. Giraud, F. Millot and S. Pernet

The numerical simulation of the propagation of seismic waves is a central concern for the seismic exploration. An important research activity is focused on finding fast and accurate numerical methods to solve the elastodynamic equation. In particular, the problematic of the software optimization by reducing the computational costs is crucial to our research.

For the solution of the elastodynamic equation on meshes with local refinements, we are currently collaborating with Total to design a parallel implementation of a local time refinement technique on top of a discontinuous Galerkin space discretization. This latter technique enables to manage non-conforming meshes suited to deal with multiblock approaches that capture the locally refined regions. This work is developed in the framework of Yohann Dudouit PhD thesis. A software prototype is currently developed to address these simulations.

4 Finite element simulation of acoustic scattering in a subsonic flow

4.1 A full coupling between acoustics and hydrodynamics

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

We focus now our attention on the acoustic scattering in a subsonic flow. Our objective is to develop a numerical method to solve linearized problem in time-harmonic regime in an unbounded domain and in a quite general case, in the sense that the geometry and therefore the mean flow can be complex. Contrary to the classical case when the fluid is at rest, the obtained problem is now vectorial since the presence of the mean flow generally couples two different phenomena : acoustic propagation and convection of vortices.

Up to our knowledge, only the potential case, which leads to a Helmholtz like scalar equation has been completely handled. But it is only available in specific cases when the flow and also the source are irrotational. This means that there is no coupling between acoustic and hydrodynamic pertubations. For more general cases for instance for an arbitrary flow, the problem is much more difficult to solve. Generally, it is modeling 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. Although the second is less usual, it has several advantages : in particular, it allows a very simple treatment of the boundary conditions, which are generally expressed with respect to the displacement (see paragraph 4.2).

One difficulty is that a direct discretization of Galbrun equation by a Galerkin finite element method does not work, due to the lack of coerciveness. We have proposed to write 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. Firstly, we have focused on this time-harmonic advection equation [EMA25]. We have proved the well posedness of this problem for a class of flows which fill the bounded domain [12]. Two different approachs have been studied to solve this kind of equation. The first method is a finite element method based on a finite element method based on a least-squares formulation. The second approach is a Discontinuous Galerkin (DG) method [15] which turns out to be well-suited for advection equations as it naturally takes into account the transport phenomenon. The analysis of these two approaches which can be found in [EMA23], has led us to choose the DG approach.

Secondly, we come back to the coupled system where the unknowns are u, ψ. For that, we use the Lagrange Finite Element for the displacement u and a Discontinuous Galerkin scheme for the new unknown ψ. When the flow and the source are irrotational,the potential approach can be done and is implemented. And the results obtained form the Galbrun coupled system are compared with those obtained from the potential method (see Fig. 4.2 in a complex flow).

4.2 Treatment of the lined walls

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

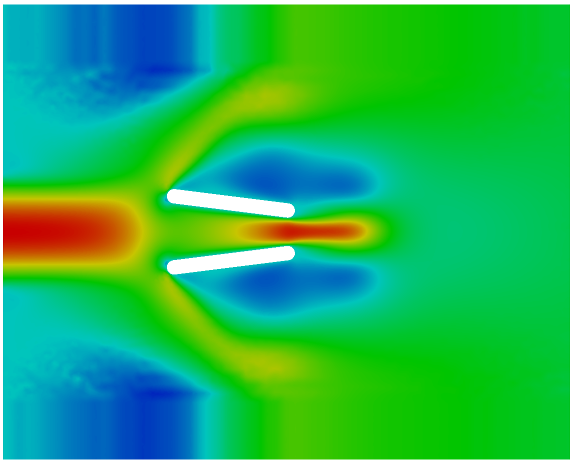

FIG. 4.1: Mean flow.

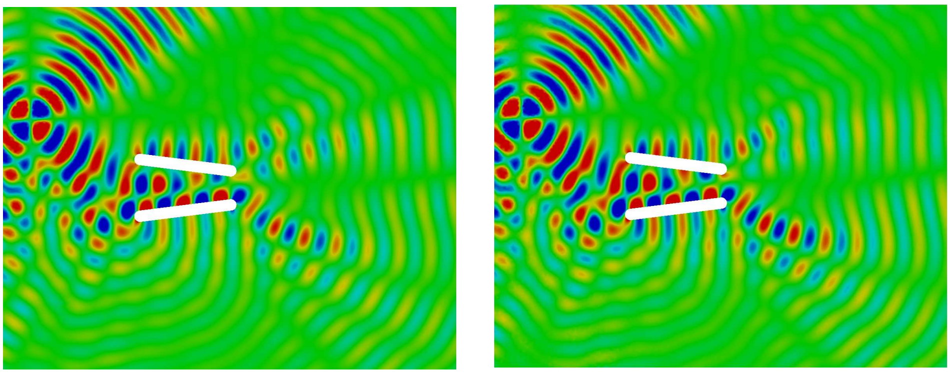

FIG. 4.2: Real part the components of Euler velocity (on left obtained form the Galbrun system, on right with the potential approach.

One main advantage of the Galbrun's model is that the unknown is well adapted to write boundary conditions. Indeed boundary conditions are naturally expressed with the displacement rather the pressure or the velocity. In particular, in presence of lined walls, it is simple to write a condition on the displacement, defined by $divu = ikZu$ where Z is the dimensionless impedance. Now , in this case, the proof of well-posedness is not straightforward with this boundary condition even if the flow is uniform. Some work has been done in order to clarify this situation. We have proposed an other boundary condition depending on a small parameter β. We have proved that in this case, the new problem is well-posed and when β tends to zero, the boundary condition tends to the condition of lined walls. Numerical results are in progress [see Figure 4.3).

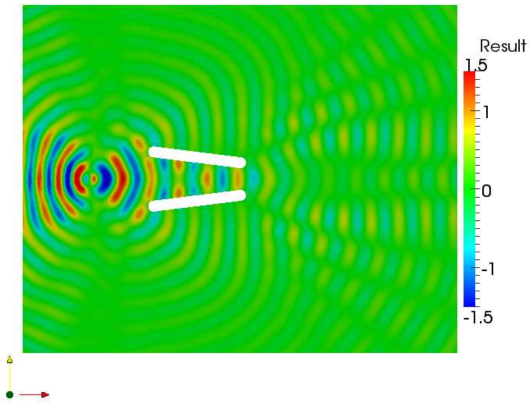

FIG. 4.3: Real part of the displacement component for a value Z.

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

[13] P.B. BOCHEV AND M.D. GUNZBURGER, *Least-Squares Finite Element Methods*, Springer, Applied Mathematical Sciences, Vol. 166.

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4.3 A new model called the Goldstein-Visser model

Let us come back to the potential case. Contrary to the Galbrun case, only a scalar equation has to be solved, which is very attractive. But this potential equation is only available in specific case in particular when the flow is irrotational, so when the coupling between acoustic and hydrodynamic effects are neglected. We have extended this approach in more general cases. We have proposed to write an augmented equation by introducing a new variable ξ. This latter is directly linked to the vorticity of the flow and for example is equal to zero when the flow is irrotational. Again, this variable is obtained through a time harmonic advection equation. Remark that this equation is very similar to that obtained in the Galbrun system . So we obtain a coupled system where there are a scalar unknown the potential ϕ and a vector unknown ξ. So we use the Lagrange Finite Elements for the displacement ϕ and a Discontinuous Galerkin scheme for the new unknown ξ. This approach is implemented and first results are obtained (see Fig. 4.4.

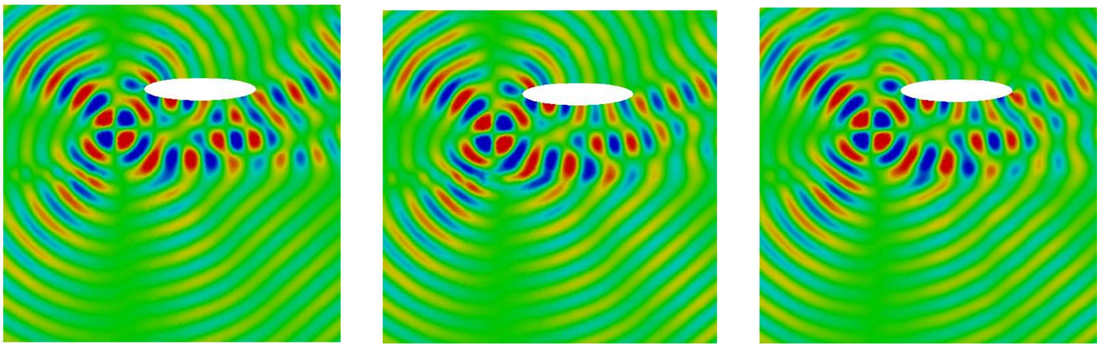

FIG. 4.4: Real part the components of the Euler velocity (on left obtained form the potential approach system, at middle form the new model, on right with the Galbrun system.

4.4 Domain Decomposition Method

The Galbrun or Golstein-Visser models used to compute the time harmonic acoustic perturbations in the mean flow yield indefinite linear systems after discretization. Indeed, the principal part of the operators are Helmholtz type. This drawback comes problematic when an iterative solver is used to invert the system because the convergence of the method is very slow. Two types of approaches exist to circumvent this. First, a preconditioning technique can be used. Unfortunately, for the Helmholtz-like equations, the construction of an efficient algebraic preconditioner is still an open problem. An other approach is the Domain Decomposition Method (DDM) [EMA19]. This approach allows to replace the solution of the entire problem by the solution of a succession of smaller problems which can be solved by using a direct solver. The effectiveness of the method depends on the choice of appropriate transmission conditions. For the Helmholtz equation, the good conditions have been proposed by Bruno Despres in his Phd thesis. We extended the DDM proposed in [16] for acoustic problems in presence of a mean flow. In particular, by using the Lorentz transformation, we have proposed efficient transmission conditions [EMA19] which allows to obtain a convergent method by using an algorithm based on a Jacobi method (see Fig. 4.5 and 4.6) . These first results are very encouraging.

[16] Francis Collino, Souad Ghanemi, Patrick Joly. *Domaine decomposition method for harmonic wave propagation : a general presentation* , 1999.

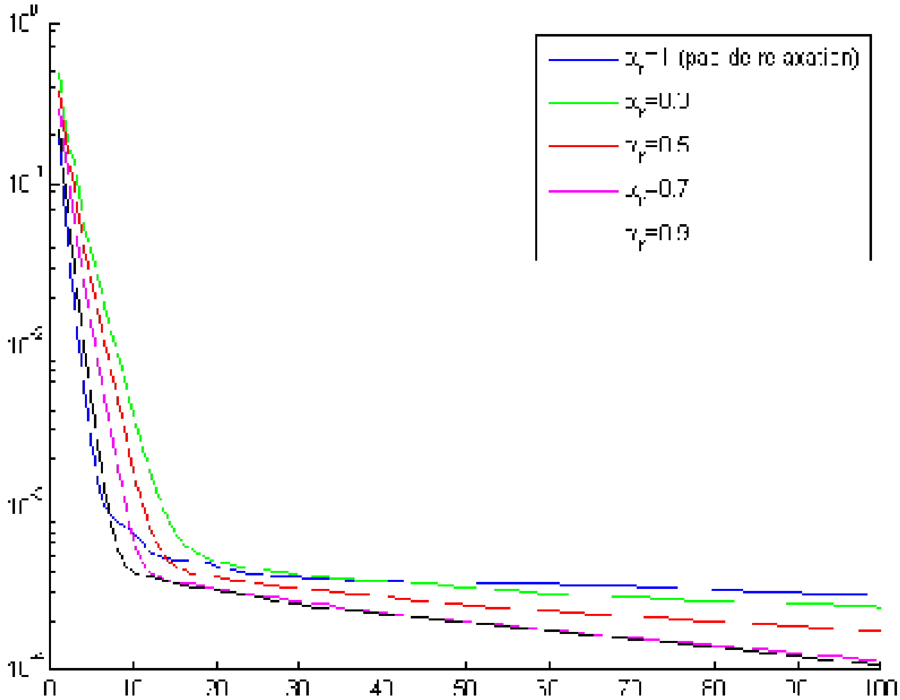

FIG. 4.5: Relative error versus the number of iterations for different relaxation coefficients

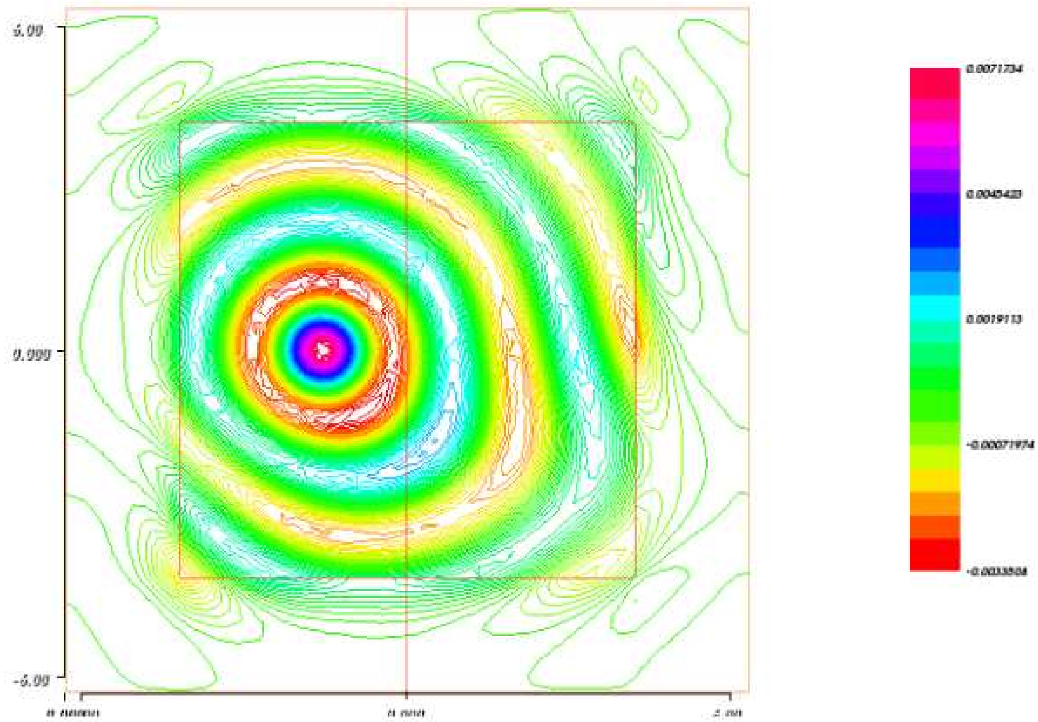

FIG. 4.6: DDM solution for a non uniform mean flow

5 Publications

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[EMA2] A. BONNET, J. MERCIER, and F. MILLOT, (2011), Time harmonic acoustic scattering in presence of a shear flow and a Myers impedance condition, Portland, 32nd AIAA Aeroacoustics Conference.

[EMA3] J. LAURENT, V. MOUYSSET, S. PERNET, and X. FERRIERES, (2011), Development of an adaptive mesh in a discontinuous Galerkin method for time Maxwells equations, Vancouver, Waves.

[EMA4] D. LEVADOUX, F. MILLOT, and S. PERNET, (2010), Comparison between the Classical Integral Equations and a Well Conditioned Integral Equation, Cambridge, USA, PIERS.

[EMA5] D. LEVADOUX, F. MILLOT, and S. PERNET, (2010), Intrinsically well-conditioned integral equations for scattering by homogeneous bodies, Toulouse, France, SCEE.

[EMA6] E. PEYNAUD, F. MILLOT, S. PERNET, A. BONNET, and J. MERCIER, (2011), A mixed continuous/discontinuous finite element method for acoustics in an arbitrary flow, Vancouver, Waves.

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[EMA12] A. BONNET-BEN DHIA, J. MERCIER, E. REDON, and S. POERNOMI SARI, (2011), Non-reflecting boundary conditions for acoustic propagation in ducts with acoustic treatment and mean flow, *Int. J. Numer. Methods Eng.*, **86**, 1360–1378.

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[EMA14] A. COSSONIÈRE and H. HADDAR, (2011), The electromagnetic interior transmission problem for regions with cavities, *SIAM J. Math. Anal.*, **43**, 1698–1715.

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[EMA16] M. FARES, J. HESTHAVEN, Y. MADAY, and B. STAMM, (2011), Reduced Basis Method for the parametrized Electric Field Integral Equation, *J. Comput. Phys.*, **14**, 5532–5555.

[EMA17] D. LEVADOUX, F. MILLOT, and S. PERNET, (2010), New Trends in the Preconditioning of Integral Equations of Electromagmetism, *Mathematics in Industry*, **14**, 383–394.

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5.4 Thesis

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3

Data Assimilation

1 Introduction

Data assimilation is a strong research theme at CERFACS. The GLOBC team is developping links between numerous applications, such as oceanography or hydrology, and theoretical progresses, such as the one developed in the ALGO team. Applications of data assimilation to atmospheric chemistry, developed by the PAE team, are also reported in this chapter. This is also the case for applications to the modelling of forest fire, performed in collaboration with the CFD team, as well as applications to nuclear core modelling, performed in collaboration with EDF, a CERFACS partner. The following research actions are reported in the chapter :

1. Data assimilation for oceanography
2. Data assimilation for atmospheric chemistry
3. Data assimilation for hydraulics and hydrology
4. Data assimilation for forest fire
5. Data assimilation with EDF neutronic models

During the 2010-2011 period, there has been as strong collaboration between the oceanography and atmospheric chemistry research axes, through the joint development of data assimilation methods (3D-FGAT and 4D-Var) based on the modeling of the background errors with an anisotropic diffusion operators. Both axes has converged towards operationnal models, since the NEMOVAR oceanographic system is used by ECMWF and the Valentian atmospheric system is used by Météo-France :

The domain of data assimilation for hydraulics and hydrology has started at the begining of the 2010-2011 to become a flourishing research axis inside the GLOBC team. Various collaborations have been established and numerous PhD thesis have started. The activity on forest fire modelling is a smaller project, but the obtained results are intersting.

At last, the activity on neutronic models and their application to nuclear core management has become a real research activity during the 2010-2011 period with the publication of several paper in highly ranked journals.

2 Data assimilation for oceanography

The ocean data assimilation project has aimed at furthering the scientific and technical development of NEMOVAR, a multi-incremental variational assimilation system for the NEMO ocean model. The development of NEMOVAR is a collaborative project involving different partners, including CERFACS who pioneered the development of the OPAVAR system on which NEMOVAR is based. NEMOVAR is used for both research and operational applications. CERFACS plays a leading and unique role in the development of the assimilation driver and minimization algorithms, as well as the covariance models used for representing background and observation error. This activity is supported by the European project COMBINE (FP7), the ANR-COSINUS project VODA, the RTRA project ADTAO, and LEFE-ASSIM. A summary of the main results obtained during the period 2010–2011 is given below.

2.1 Global ocean analysis and reanalysis (A. Weaver)

The recent operational implementation of NEMOVAR for ocean analysis at ECMWF has been a major milestone. It is the first time that NEMOVAR is used operationally. The system is based on a 3D-Var version of NEMOVAR. CERFACS has made significant contributions to its development, documentation and evaluation [3]. Multi-decadal global ocean reanalyses produced by the ECMWF NEMOVAR system have been used by several partners, including CERFACS and CNRM, for initializing decadal forecasts in the context of the COMBINE project.

2.2 Background-error correlation modelling using diffusion operators (I. Mirouze, A. Weaver)

There was continued work on improving the diffusion-based spatial correlation models used for representing background error. A new formulation based on implicitly-formulated diffusion operators was developed as part of the PhD work of [DA36]. [DA7] described the theoretical basis of the method, focussing on the one-dimensional (1D) diffusion problem. Particular attention was given to the specification of appropriate boundary conditions (especially important in oceanography where the land geometry is complex) and to the estimation of the normalization factors required to ensure that the implied correlation functions have correct (unit) amplitude. The 1D implicit diffusion operator has been used as a building block for constructing correlation operators in higher dimensions. [DA36] described the implementation of the method in NEMOVAR and the computational savings that have resulted in comparison with an existing scheme based on an explicitly-formulated diffusion operator.

Extensions of the method to represent anisotropic correlations have recently been proposed by [DA18]. The fundamental parameter of the anisotropic correlation model is the diffusion tensor which controls the spatial scale and directional response of the diffusion operator. A practical method for estimating the elements of the diffusion tensor from a sample of background-error estimates was described and its effectiveness illustrated in a simplified framework. This work has formed the basis for future developments of the correlation model and for combining it with an ensemble data assimilation system to provide flow-dependent estimates of the background-error covariances.

2.3 Calibrating observation- and background-error variances using assimilation statistics (T. Pangaud, A. Weaver)

The difficulty in defining background- and observation-error statistics means that they are likely to be incorrectly specified in a practical data assimilation system. [1] discuss how the innovations and analysis increments generated by a data assimilation system can be used to diagnose *a posteriori* the covariances of observation error and the covariances of background error in observation space. Here we have attempted to use these diagnostics, known as the Desroziers method, to calibrate the *variances* of background and observation error. Innovations and increments were collected from a 5-year assimilation experiment from January 1, 2004 to December 31, 2008 with a pre-operational version of NEMOVAR [3] and used to diagnose the temperature and salinity observation- and background-error variances (σ_o^2 and σ_b^2) on a regular $5^\circ \times 5^\circ$ global grid. The method produces largest σ_o and σ_b in boundary current regions where the variability is dominated by mesoscale eddies which are unresolved in the global (ORCA1) configuration considered. The parameterized σ_o and σ_b that were specified in NEMOVAR do not capture this important source of error.

The assimilation experiment was then repeated using the diagnosed (tuned) σ_o and σ_b in place of the parameterized ones. The left panel in Figure 2.1 shows the globally averaged vertical profiles of the specified σ_b (solid curves) and diagnosed σ_b (dashed curves) for salinity, before tuning (red curves) and after tuning (blue curves). Before tuning, the specified σ_b is largely overestimated compared to the diagnosed values, especially in the upper 250m. After tuning, there is greater consistency between the specified and diagnosed σ_b as one might expect. The right panel in Figure 2.1 shows the impact of using the tuned variances on the globally averaged root-mean-square of the innovations. The rms errors are systematically reduced below 100 metres, while in the upper 100 metres the impact is neutral. These results illustrate that, as well as being a useful diagnostic, the Desroziers method can be an effective tool for objectively tuning covariance parameters.

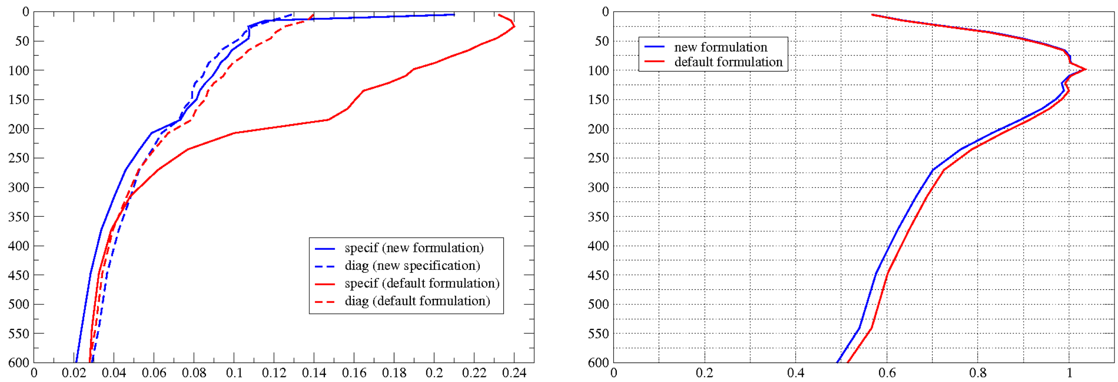

FIG. 2.1: Left panel : vertical profiles of the 2004-2008, globally averaged specified (solid curves) and diagnosed (dashed curves) standard deviations of background salinity error before tuning (red curves) and after tuning (blue curves). Right panel : globally averaged root-mean-square salinity errors (background-minus-observations) before and after tuning of the background-error standard deviations (red and blue curves, respectively). The horizontal axis is in psu ; the vertical axis is depth in metres.

2.4 Representation of correlated observation error (A. Piacentini, O. Titaud, A. Weaver)

The initial implementation of NEMOVAR has employed a very simple formulation of the observation-error covariances. All data (T and S profiles, SST, altimeter) are assumed to be uncorrelated. This assumption is common in data assimilation systems even if it is known to be incorrect for certain data-sets. An important example is satellite altimeter data. Altimeter data are available as anomalies with respect to a long-term mean in order to remove the poorly known geoid from the altimeter measurement. For assimilation, a Mean Dynamic Topography (MDT) must be added to the sea-level anomalies (SLA) to produce measurements of Absolute Dynamic Topography (ADT), which can then be related to the sea-surface height variable in the ocean model. The MDT used in NEMOVAR is based on a gridded product derived from the model itself in a long-term integration that assimilates only T and S profiles. Uncertainty in the MDT is a major source of error in the ADT and this uncertainty must be carefully taken into account in the assimilation method. By construction, errors in gridded MDT products are correlated in space. Furthermore, the stationary nature of MDT errors induces a time-correlated component in the ADT, which cannot be neglected. An ADT correlation model that accounts for both of the aforementioned components of correlated error has been developed for NEMOVAR. The full ADT error covariance matrix depends on the altimeter observation network as well as the individual error covariance matrices for SLA and MDT. Preliminary results with NEMOVAR illustrate that ADT error correlations can significantly reduce the weight given to the altimeter data in regions where the MDT correlation scales are large and the measurements are densely distributed. Further work is needed to assess their impact in NEMOVAR. Methods are also currently being developed to account for correlated error in gridded SST products used by NEMOVAR.

2.5 Conjugate gradient minimization (S. Gratton, S. Gurol, A. Piacentini, A. Weaver)

The conjugate gradient (CG) algorithm initially implemented in NEMOVAR was based on a close variant of the ECMWF CONGRAD software. While CONGRAD has efficient minimization properties, it requires large memory storage, particularly with applications involving high-resolution configurations. In collaboration with the ALGO team, two alternative CG algorithms, CGMOD and RPCG [2], have been implemented in NEMOVAR. CGMOD and RPCG have identical convergence properties to CONGRAD but require substantially less memory in general. This is particularly true for RPCG, which performs the minimization in observation space, contrary to the other two CG algorithms which perform the minimization in model (control) space. In ocean data assimilation, observation space is typically one order of magnitude smaller than control space. Experiments with RPCG applied to the global 3D-Var system used at ECMWF have resulted in a significant reduction ($\sim$3 GB) in memory compared to that required by CONGRAD and CGMOD. This result is impressive and will become even more significant with future high-resolution NEMOVAR configurations currently in development.

2.6 References

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[2] S. Gratton and J. Tshimanga, (2009), An observation-space formulation of variational assimilation using a restricted preconditioned conjugate-gradient algorithm, *Quart. J. Roy. Meteor. Soc.*, **135**, 1573–1585.

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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.

To combine all the measurement types within the models in an optimal manner using data assimilation techniques, we have been developing and using at CERFACS for several years the data assimilation suite built upon the Météo-France/CNRM chemistry transport model (CTM) MOCAGE. The develpment started with the EC-FP5 ASSET European project in January 2003 in close collaboration with Météo-France/CNRM. As the assimilation algorithm was developed under the CERFACS PALM (research) environment, the resulting assimilation system was first called MOCAGE-PALM. But since the assimilation modules are independent from the development of the PALM software and can be adapted to other models than MOCAGE, we named later Valentina the reassembly of all the assimilation modules. This also corresponded to the objectives of the ADOMOCA project of the PNCA (latter replaced by the LEFE program) which promote Valentina as a common collaborative tool for the whole French community involves in the ADOMOCA project. Starting in 2005, ADOMOCA made Valentina a more flexibility tool in particular to be coupled with other models than MOCAGE (on regular or Gaussian global grid, on regional grids, with various vertical grids and resolution) and to be able to assimilate a large range of atmospheric composition data.

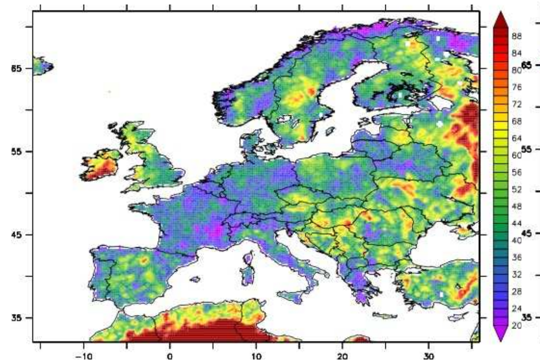
In parallel of the development work, we have improved Valentina in order to increase the quality of the analysis it could provide. The most noticeable improvement came from the characterisation of the forecast error and its model. This work was conducted in synergy with CERFACS assimilation studies in the area of oceanography. To improve the analyses, several other directions were explored : four dimensional assimilation method, a re-linearization iterative process and a control in the spectral space. Moreover, we have developed linear chemical schemes for other species than ozone that prove to be very computationally efficient for data assimilation.

Until recently, all scientific studies conduced with Valentina used MOCAGE in its global configuration. But being involved in the regional cluster of the EC-FP7 MACC European project, we had to develop for Météo-France/CNRM mi-2009 a system that is able to analyse daily ozone measurements from ground-based station at the surface over Europe. The system was delivered to be operational mi-2010 with an adapted version of Valentina able to assimilate data in the European domain of MOCAGE. Then we began to conduce scientific studies with this new assimilation system.

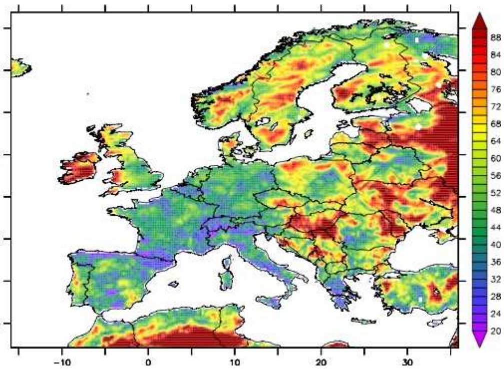
3.1 Toward operational analyses and reanalyses of European air quality (S. Massart, A. Piacentini, E. Jaumouillé)

Up to recently, the Valentina assimilation system has been involved in programs dealing with the global atmospheric chemical composition, from the upper troposphere to the lower mesosphere. In the framework of the EC-FP7 collaborative MACC project and the POGEQA (RTRA/STAE) national project, we had to

address the monitoring of air quality with MOCAGE-Valentina. The MOCAGE model has the advantage of offering the possibility to work on four nested domains, from global to local 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. The Valentina system has thus been further developed to produce chemical analyses on the limited area covered by the regional version of MOCAGE.
The first requirement of the MACC project was to produce analyses of the concentration at the surface of several key atmospheric components. The analyses had to use the surface measurements from ground-based stations available each day for the day before. As Valentina is able to assimilate only one chemical component, we selected the ozone molecule. This choice was driven by the fact that ozone is one of the most observed species and because ozone is actively involved in air pollution. We decided to use the full chemical scheme of MOCAGE to obtain values for all the key atmospheric components of MACC. Because even if only ozone is assimilated, modifying the ozone concentration produces modifications in the concentration of other species due to the chemical links between them.
The version of MOCAGE-Valentina that assimilates the surface ozone measurements was delivered to Météo-France/CNRM in mid-2010 for a pre-operational daily production of the ozone surface analysis of the day before. We intensively used this pre-operational production to evaluate our analyses. In particular we have developed a monitoring suite that produces each day and each week some plots that are displayed on a web site to easily follow the evolution of the products. This monitoring allowed us to detect that we had to periodically update the error statistics both for the forecast and for the observation. We have then developed tools based on a posteriori diagnostics to automatically update the forecast and the observation error covariances matrices. The monitoring was also useful to point out the stations where the measurements were repeatedly not coherent with the model. This has lead to the creation of a blacklist for such stations, the blacklist being also automatically updated.



(a) West-East length-scales



(b) North-South length-scales

FIG. 3.1: Diagnosed length-scales (in km) of the horizontal correlation of the forecast error, averaged on the period between 1^{st} and 10^{th} July 2010 : West-East (left) and North-South (right) length-scales.

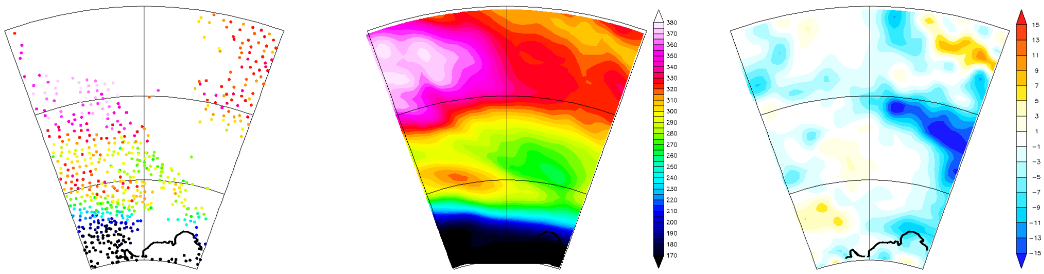
Among the work to ensure a good quality of the daily analysis of the surface ozone, we had begun a thorough investigation on the background error covariance matrix (BECM). In the operation suite, the background error variances comes from a posteriori diagnostics. The background error correlations are fixed in time and had never changed. We first diagnosed the BECM using an ensemble method with a methodology similar to the one we used for the global scale (see section 3). We have found that there are strong space and time variations in the background error covariances (Fig. 3.1), the use of constant values for the correlations as in the pre-operational suite is therefore not a good option [4]. We then derived several configurations of the

BECM using or not the ensemble-diagnosed values for each of its components. This allowed to measure the effect on the analysis and on the forecast of using an ensemble-diagnosed BECM compared to the one used in the pre-operational suite.
We have also participated within MACC to the reanalyses of the ozone concentration at the surface with the regional version of MOCAGE-Valentina. The aim was to produce reanalyses for the years 2008 and 2009 using more validated surface ozone measurements. This gave another opportunity to work on the background and observation error covariances. For example we tried to evaluate the benefit from monthly averaged statistics for these errors, and the benefit from hourly statistics. Seven assimilation systems participated to the reanalysis exercise, and MOCAGE-Valentina was ranked second for the scores in comparison to independent validation data. The huge potential of Valentina was further stressed by the fact that the stand alone simulation of MOCAGE did not compared well with the validation data.

3.2 Toward the global assimilation of atmospheric data from new generation instruments (B. Pajot, S. Massart, A. Piacentini)

With Valentina coupled with the global version of MOCAGE, we were pioneer in the assimilation of atmospheric composition retrievals from the Infrared Atmospheric Sounding Interferometer (IASI) remote sensor launched in 2006 onboard the first European meteorological polar-orbiting satellites, METOP-A. The specific problem raised was that the pixel size of IASI is much smaller than the horizontal grid size of most of the global CTMs like MOCAGE. In order to assimilate the maximum of information from the IASI retrievals, we could increase the horizontal resolution of MOCAGE to be consistent with the IASI pixel size. But this would significantly increase the numerical cost (in terms of memory and computational time) of the assimilation process. Rather, we have made steps toward a multi-scale assimilation strategy in the spectral space. The assimilation process is 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).
The first steps toward this multi-scale assimilation strategy were performed, i.e. the outer loop, the assimilation in the spectral space and the assimilation at different resolutions as the T170 one. The outer loop proved to be unappropriated combined with the 3D-FGAT in particular situations [DA6] that made us move toward an incremental 4D-VAR. Conducing the 4D-VAR assimilation process in the spectral space, despite that MOCAGE is discretized in the physical space, allows the size of the control vector to be reduced by a factor four, and allows to save computational time without loosing quality in the analysis. We then measured the effect on the global ozone simulation of the MOCAGE horizontal increase with and without assimilation before going toward the multi-scale assimilation strategy.
Experiments were carried out using as horizontal grid for MOCAGE a standard T42 Gaussian grid and a higher resolution T170 Gaussian one [DA15]. We assimilated combined data from the IASI instrument and from the Microwave Limb Sounder (MLS). The latter dataset allows the information to be spread through the whole atmospheric columns at a low computational cost. Two datasets of ozone super-observations have been constructed by averaging the IASI data on the two model grids. Direct model simulations without data assimilation showed that the increase of the horizontal resolution modifies the ozone smallest scale structures as well as the ozone meridional distribution. This modification probably results from a better representation of the vertical velocity with the T170 configuration. When the ozone assimilation is performed there is less influence of the horizontal resolution of the model. Nevertheless, in a general way, comparisons with independent data show large reductions of the ozone standard deviations when the resolution is increased.
However, we also showed that when the ozone assimilation is performed with the highest resolution of MOCAGE and the high resolution dataset, the ozone analysis is not improved compared to the one obtained when assimilating the low resolution dataset. This result is due to the combination of the IASI data and MLS

data. To assimilate the IASI data at their highest resolution, the horizontal correlation length-scale of the forecast error had to be decreased to match the small scale structures present in the dataset (Fig. 3.2). By doing so the influence of the coarser resolution MLS data is decreased and part of the information brought on the vertical shape of the ozone profile is lost. This result highlight that it is essential to add information on the vertical distribution of ozone column when the IASI data are assimilated at a resolution close to the pixel size. Using IASI averaging kernels would likely improve the simulations, but the computational cost would be much higher. This will be tested in the near future before the implementation of the multi-scale assimilation strategy. Nonetheless, a mock-up of MOCAGE-Valentina has been derived and provided to the CERFACS algo team to introduce the outer loop (that is a requirement of the multi-scale assimilation strategy) and to test their minimisers and pre-conditioners.



(a) IASI total columns between 00 :00 and 12 :00 (DU).

(b) 12 :00-forecast of the total ozone columns (DU).

(c) 00 :00 increment in terms of total ozone columns (DU).

FIG. 3.2: Zoom over the South Pole between 70°S–40°S and 20°E–60°E of the situation for the 30th September 2008.

3.3 Background error covariance matrix (S. Massart, A. Piacentini, E. Jaumouillé)

Since the early beginning of the Valentina assimilation suite, important scientific effort were made on the key-component background error covariance matrix (BECM) modelling and determination. First because it gives to the analysis the respective weights between the background information and the observational information. Moreover, the background matrix determines the spatial distribution of the correction around the measurement location and the balance between the controlled variables of the system. An optimal state can only be obtained by the assimilation process if this matrix and the observation error covariance matrix are correctly specified. But direct determination of the BECM requires information that is not directly available. It is thus important to find the appropriate way to estimate the BECM. Especially because the BECM is known to strongly influence the assimilation results.

The BECM is a statistical information that cannot be directly obtained since the true state is unknown. To get around this problem, in most atmospheric chemistry applications only the variance part of the BECM is considered. Some assimilation systems use the Kalman Filter approach to advect background error variances. Fewer systems consider the correlation part of the BECM, and its modelling is generally simplified. For instance, it is sometime taken flow dependent and is specified in terms of distance using

the potential vorticity field. But even if the BECM is a key-component, its evaluation has not yet been the object of thorough investigations for atmospheric chemistry assimilations.
Meanwhile, in meteorology background (and analysis) errors were successfully assessed with ensemble data assimilation systems. Outputs of in a cycled assimilation system can produce an estimate of a flow-dependent BECM. The ensemble approach is not restrained to Kalman Filter methodologies. Useful information can statistically be extracted from an adequately perturbed ensemble variational data assimilation system. Up to now, the use of ensembles in combination with a variational assimilation scheme is relatively unexplored in atmospheric chemistry data assimilation. We have thus performed two studies to investigate the potential of an ensemble of atmospheric chemistry analyses to provide useful flow-dependent estimates of the background error variance and correlations, the first one with the four-dimensional variational assimilation global MOCAGE-Valentina suite [DA13] and the other with the three-dimensional variational assimilation regional MOCAGE-Valentina suite [4].

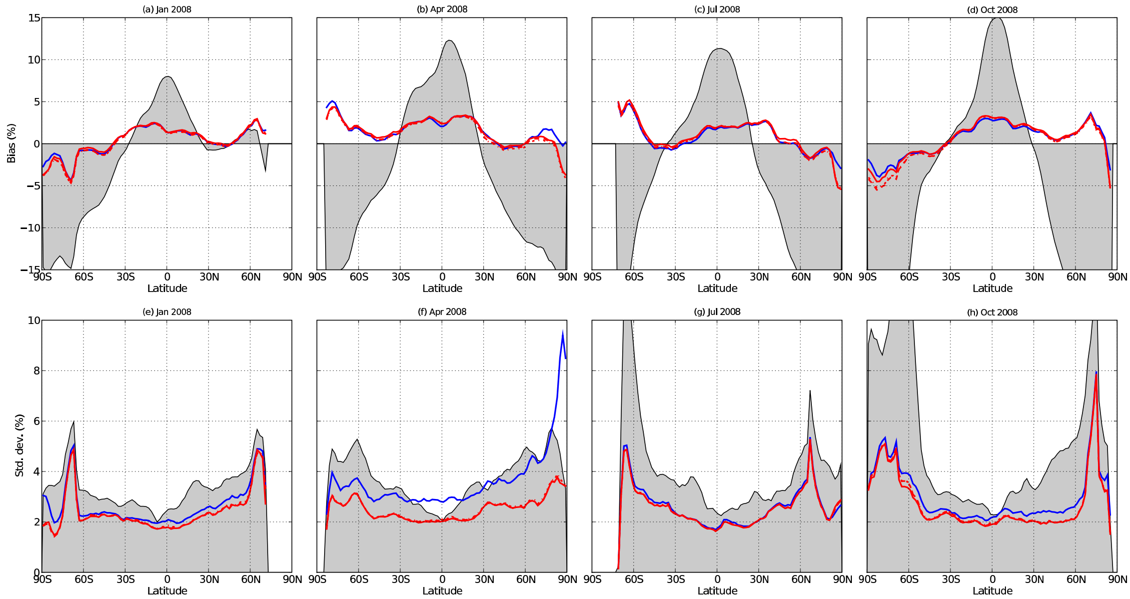


FIG. 3.3: Mean (top) and standard deviation (bottom) of the difference in terms of total ozone column (in %) between the OMI (independent) data and the model without assimilation (grey shaded area) or the analyses as a function of latitude, for January, April, July and October 2008. For the top panel, positive (negative) values stand for an underestimation (overestimation) of the model or the analyses compared to OMI data. The analyses differ from the modelling of the BECM : simple formulation (blue line) or from ensemble-based diagnostics (red line).

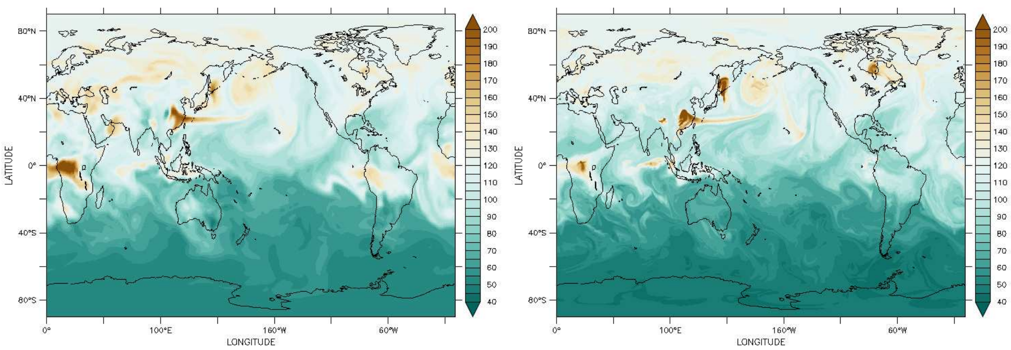
The study with the global MOCAGE-Valentina suite showed that the analysis of the MLS ozone profiles (from the upper troposphere to the lower mesosphere) using all the components of the ensemble-estimated BECM produces ozone concentrations with a low biases and errors (Fig. 3.3). But estimating the BECM with ensemble methods has an important cost that could become unaffordable. We thus tried to use simpler methods to calculate the BECM. Replacing the estimated standard deviation by a standard deviation proportional to the background value is one of them. This simplification does not modify significantly the analysis quality. Replacing the estimated length-scales by a constant value is the second simplification we tried. This dramatically deteriorates the analysis quality for a few time periods. This simplification is thus irrelevant for analysing the stratospheric ozone.

In the regional version of MOCAGE-Valentina, we have performed several experiments assimilating surface ozone measurement. The experiments also differ by the choice of the BECM configuration, in which the correlations and standard deviations matrices come from the ensemble-based diagnostics or from a posteriori diagnostics. All the analyses from these experiments are very well correlated to the observations, what assimilated or validation stations. Comparisons of the analyses with the validation stations show that the use of a BECM with time-dependent length-scales gives the largest correlation. All the analyses have a better correlation with the observations than the direct MOCAGE simulation, but the differences between them are small and we cannot conclude which BECM formulation is the most appropriate to the ozone simulation over Europe. The impact of the BECM formulation has been also difficult to evaluate because the model MOCAGE shows systematic bias in situation with low ozone concentration. So the impact of the analysis process is mostly to remove this bias.

3.4 Development of linear chemistry schemes (S. Massart, D. Cariolle J. Flemming)

During those past years a linearised ozone photochemical scheme has been developed for use within GCMs and CTMs. 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 had therefore extended the methodology to treat other chemical species, in particular a linearised scheme has been derived for CO and was implement in MOCAGE [DA3, DA12, DA4]. CO is one of the most important tropospheric trace gases. In particular because it affects the concentrations of the OH radical. Moreover the main sources of CO are incomplete fossil fuel and biomass burning, which lead to enhanced surface concentrations. And with a lifetime of a few months CO can serve as a tracer for regional and inter-continental transport of polluted air.

Within MACC a major development effort of the Global Reactive Gases sub-project is the on-line integration of the chemistry in the IFS (known as C-IFS). C-IFS aims at a modular implementation of the chemical scheme used in several global CTMs including MOCAGE. To complement the complex schemes, linear scheme are explored in C-IFS for their potential in computational demanding application such as high resolution simulations and data assimilation. So, in parallel with the comprehensive detailed chemical schemes, we implemented in C-IFS the linearised parameterisation for CO.



(a) GEMS reanalysis

(b) High resolution simulation

FIG. 3.4: CO concentration (in ppbv) at 500 hPa for the 19th January 2008.

A two years simulation within C-IFS shows that the linear carbon monoxide chemical scheme produces similar tropospheric concentrations of CO than a more complete tropospheric chemical scheme available in C-IFS. But it underestimates the tropospheric concentrations by 10 to 50 ppbv both compared to the GEMS reanalysis and measurements from the Mozaic dataset. To reduce this tropospheric bias, we adjusted the production minus loss rate term of the linear scheme in order to obtain a similar evolution in the CO total mass than the one extracted from the GEMS reanalysis [5]. This allowed us to run another two years C-IFS simulation that produces global CO fields at a resolution of about 25 km (Fig. 3.4). The evaluation of this simulation in under progress.

3.5 References

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[5] S. Massart, J. Flemming, D. Cariolle, V. H. Peuch, and L. Jones, (2012), Implementation of the linear carbon monoxide chemical scheme in the European Centre for Medium Range Weather Forecast's Integrated Forecast System, *Geosci. Model Dev.* to be submitted.

4 Data assimilation for hydraulics and hydrology

In 2007, CERFACS started investigating the use of data assimilation techniques with hydrology and hydraulic models. This activity was conducted as part of a contractual framework with SCHAPI (Service Central d'Hydrométéorologie et d'Appui à la prévision des inondations) and led to the developement of two data assimilation prototypes : one built on top of the hydrological model ATHYS and the other on top of the 1D hydraulics model MASCARET.
During the course of these studies, it has been shown that data assimilation is a promising approach for the forecast of flood events and more generally for the study of continental water dynamics. Building on the expertise in data assimilation for oceanography and atmospheric chemistry and encouraged by the success of the existing collaboration between CERFACS and EDF R&D on data assimilation for nuclear core modeling, actions were taken at CERFACS to expand data assimilation to hydraulics and hydrology.
As of today, the scope of the project still covers flood forecasting, it also widens to the study of hydrodynamics for rivers and lakes as well as to the use of future missions satellite data such as SWOT data. This project relies on the collaboration between CERFACS and its shareholders, especially EDF (Laboratoire National d'Hydraulique et Environnement -LNHE), CNES and CNRM as well as partners such as SCHAPI, LEGOS, HSM (Hydro Sciences Montpellier). It fits into the dynamics of assimilation studies at CERFACS in the fields of oceanography, atmospheric chemistry and nuclear engineering. It also benefits from CERFACS's expertise in the use of coupling softwares, such as Open-PALM, to build assimilation systems.
The major results for data assimilation in the field of water ressources stand in the following outline :

- Flood forecasting improvement : data assimilation applications in hydrology for short time scales at regional scale.
- Simulation and forecast of the hydraulic state of a river using data assimilation with the 1D hydraulic model MASCARET.
- Investigation for the use of data assimilation techniques to improve the modeling of the hydrodynamics of the Berre lagoon with TELEMAC 3D.
- Investigation of the use of satellite measurements in conjunction with in situ data to improve water ressources studies in the framework of data assimilation in hydrology and hydraulics.

4.1 Flood forecasting improvement : data assimilation applications in hydrology for short time scales at regional scale (S. Ricci, O. Thual, in collaboration with HSM)

A data assimilation (DA) prototype was developed at CERFACS on top of the rainfall-runoff, event-based, spatial, parsimonious hydrological model ATHYS. This prototype was used for a PhD at HSM (Mathieu Coustau), in collaboration with CERFACS, on the modeling of the flooding dynamics in the context of the "Lez project" ("Lez Gestion Multi Usages" financed by the city of Montpellier and the

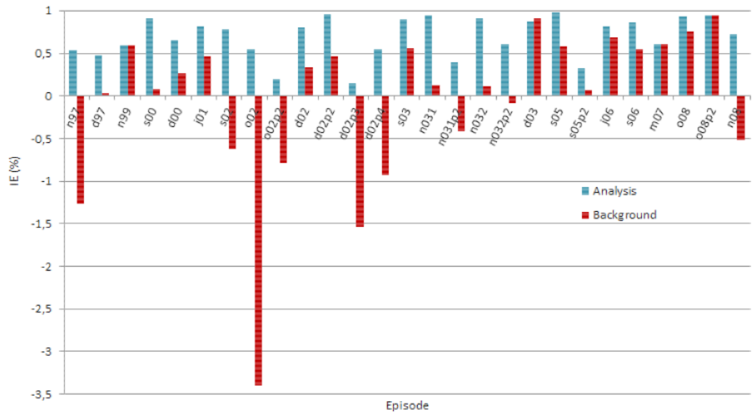

FIG. 4.1: Reduction of the uncertainty in the rainfall data using data assimilation. Comparison of Nash criteria before (background) and after (analysis) data assimilation.

region Languedoc Roussillon). This project gathers experts in hydrology, hydraulics, biology and geology to improve the knowledge of the Lez hydrosystem. The uncertainties on the hydrological model are related to simplified physics in the equations, to approximations on hydrological and hydrogeological parameters as well as errors in rain fall data. In this application, discharge observations are assimilated to correct model parameters such as the initial water deficit in the soil reservoir, the velocity of travel in the routing model or rain fall data.

In the framework of M. Coustau PhD, it was shown that discharge observations can be used to correct initial soil deficit and consequently improve flood simulation on the Lez catchemnt. A simplified kalman filter algorithm, as presented in [DA8] and [DA9], was built on top of the rainfall-runoff ATHYS model to assimilate discharge observations at the catchment outlet. The study site is the 114 km^2 Lez Catchment near Montpellier, France. This catchment is subject to heavy orographic rainfall and characterized by a karstic geology, leading to flash flooding events. The hydrological model uses a derived version of the SCS method, combined with a lag and route transfer function. It was shown that the correction of the initial water deficit in the soil reservoir leads to an improvement of 12% for the flood peak forecast in 75% of the simulated events. The results of this study were presented at AGU (2010) and are described in M. Coustau PhD manuscript [DA37].

Further study, in the framework of E. Harader's Master2 internship at CERFACS (in collaboration with HSM), explored the application of the data assimilation procedure to correct the radar rainfall inputs of the hydrological model. The rainfall inputs came exclusively from the HYDRAM rainfall radar product provided by Météo-France. Because it depends on geographic features and cloud structures, the radar rain fall input to the model is particularily uncertain and results in significant errors in the simulated discharges. The DA analysis was applied to estimate a constant correction to each event hyetogram. The analysis was carried out for 19 events, in two different modes : re-analysis and forecast. In both cases, it was shown that the reduction of the uncertainty in the rainfall data leads to the reduction of the error in the simulated discharge as presented in Fig. 4.1. The resulting correction for the radar rain fall data was then compared with the mean field bias (MFB), a corrective coefficient determined using ground rainfall measurements. It was shown that the radar rain fall corrected using DA leads to improved discharge simulations and Nash criteria, over MFB correction as presented in Fig. 4.2. This work is being pursued in the framework of E. Harader's PhD (started in October 2011), funded by Ecole Doctorale SDU2E, at CERFACS. The results of this study were presented at AGU (2011) and are currently being detailed in a submitted scientific publication([6]).

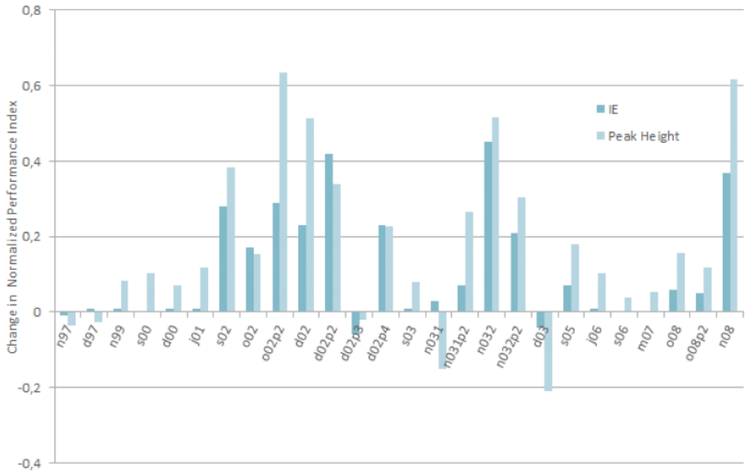

FIG. 4.2: Improvement of Nash criteria (IE) and peak height with rain fall data correction computed with MFB and data assimilation, by event (the event label is month-year-peaknumber).

4.2 Simulation and forecast of the hydraulic state of a river using data assimilation with the 1D hydraulic model MASCARET (S. Ricci, A. Piacentini, G. Jonville, O. Thual, in collaboration with LNHE, SCHAPI, CNRM, CEMAGREF)

The aim of the Hydraulics Data Assimilation project is to open the way for the improvement of river streamflow forecasting. This is a challenging issue for the security of people and infrastructures as well as for the exploitation of hydroelectic plants and the management of water ressources. This project started in 2010 within the framework of the collaboration between CERFACS, LNHE (EDF R&D), SCHAPI and CETMEF ([DA35], [DA26],[DA27]). Over 2010-2011, a collaborative relationship between CERFACS and LNHE, along with SCHAPI and CETMEF, consisted in furthering the scientific and technical development on the existing prototype, leading to the present prototype named DAMP (Data Assimilation with MASCARET Prototype).
The DAMP was developped with Open-PALM, a coupling software developped at CERFACS and particularly convenient to design data assimilaiton applications. It allows the assimilation of river water level and discharge observations and enables to improve flood forecasting. The water level and discharge data were assimilated using a Kalman Filter algorithm to control the upstream flow and dynamically correct the hydraulic state. The first step of the analysis was based on the assumption that the upstream flow can be adjusted using a simple three-parameter correction. These three control parameters were adjusted over a two-day time window after one day of free run. The second step of the assimilation consisted of correcting the hydraulic state every hour (the observation frequency) during one day. The simulation was then integrated in forecast mode for an additional day. With this algorithm, the background error covariance matrix is not explicitly propagated by the dynamics of the system. Still, a particular effort was made to model background error covariance functions which were coherent with the dynamics of the hydraulic model. Anisotropic functions were used to represent the background error spatial correlations for the water level and the discharge, respectively. The justification for this choice was made by applying a full Kalman Filter algorithm on a diffusive flood wave propagation model. It was shown that the analysis turns a Gaussian correlation function into an an anisotropic correlation function where the correlation length scale

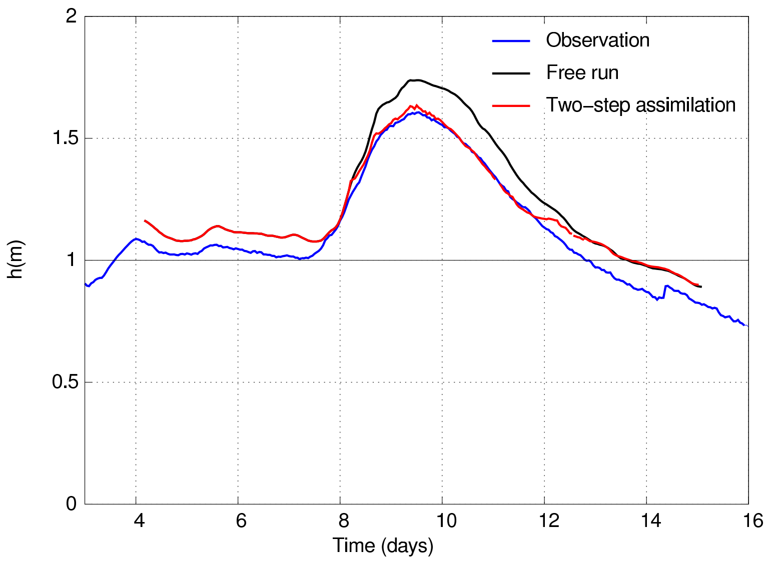

FIG. 4.3: April 2006 event, Marne Vallage catchment. Two-hour forecasted water level at Joinville for the Free run (black curve), the observation (blue curve) and the analysis of the Assim run with the two-step assimilation (red curve).

is shorter downstream of the observation point. This approach enabled a realistic modeling of the spatial error correlations for the data assimilation algorithm with MASCARET.

It was shown that the correction of the hydraulic state is not as predictive as the upstream flow correction and is not sufficient to constrain the simulation over an interesting forecast period. This justifies the need for the two-step data assimilation approach. This two-step procedure was applied to the Adour and Marne catchments (France) and the results were interpreted for several events in each catchment. The two-hour forecasted water levels in the Marne Vallage catchment, at Joinville, for the April 2006 event are presented in Fig. 4.3 As the Free run (no assimilation) significantly overestimates the flood peak at Joinville, the simulated discharge was improved by 35% at Joinville with the two-step data assimilation procedure. On the Adour catchment, it was shown that, on average, the Nash-Sutcliffe criteria is improved by 60 % for short time scale and 35% for 12 hours forecast. This work was accepted for publication in HESS in 2011 [DA16].

Complementary studies were carried out with the DAMP, on other catchments in France ([DA32]). It has also been noted that the 2 approaches here do not allow for all necessary corrections and that the extension of the control space could be useful as other sources of uncertainties or model errors (for example the simplification of the flood plain representation) result in errors in the hydraulic state. Indeed, the correction of the Strickler coefficients or of the bathymetry will be investigated in the framework of J. Habert's PhD at CERFACS/SCHAPI (started Oct. 2011). Finally, theoretical issues regarding the data assimilation algorithm, especially the dynamics of the background error covariances matrices were conducted at CERFACS in the framework of a Master2 internship ([DA31],[DA34]), in collaboration with CNRM (Olivier Panneckouke). This study carried out on a diffusive flood wave propagation model opens the way for the understanding and the implementation of advanced techniques such as Ensemble Kalman Filter that will be applied to the DAMP in the framework of a PhD (S. Barthélémy) at CERFACS, founded by SCHAPI and the Région Midi-Pyrénées.

4.3 Investigation for the use of data assimilation techniques to improve the modeling of the hydrodynamics of the Berre lagoon with TELEMAC 3D (S. Ricci, A. Piacentini, O. Thual, in collaboration with LNHE)

The Berre lagoon, located in the South East of France, is one of the largest lagoons in the Mediterranenan area. It is located in the South East of France. It is a receptacle of $1000 Mm^3$ where salty sea water meets fresh water discharged by the hydroelectric plant at Saint-Chamas and by natural tributaries (Arc and Touloubre rivers). EDF fresh water discharge can reach up to 1200 Mm^3 per year and has a strong seasonal variability. To better qualify and quantify the relationships between the salinity of the lagoon, the fresh water inputs (from the powerplant and from the rivers), the water exchanges with the sea and the wind mixing, EDF started an in-situ continuous monitoring of the lagoon and built a 3D hydrodynamic model with the TELEMAC software. EDF R&D at LNHE aims at maximizing the benefits of this numerical tool by simulating new scenarios of exploitation and optimizing the operation of the hydroelectric production while preserving the lagoon ecosystem.
The objectif of the project at CERFACS is to investigate the use of data assimilation techniques in the context of the Berre lagoon study, especially to improve the representation of the salinity field using CTD salinity profiles. The developement of the 3D-FGAT algorithm is on-going at CERFACS : it consists in correcting the salinity state at the beginning of an assimilation window. This approach is the same as the one used in meteorology, oceanography and atmospheric chemistry. The successul achievement of this project partly relies on the good use of the expertise at CERFACS in other applicative fields [DA7],[7], [9],[8], available at CERFACS, for variational data assimilation and optimization.
The implementation of the algorithm for the prototype is currently being done using the Open-PALM software. Some of the technical aspects for this part have already been solved in close collaboration with the Open-PALM team at CERFACS. This choice was made to ease the development and the use of the assimilation prototype. Still, this collaborative project should fit into EDF R&D dynamics regarding the use of the SALOME platform. The project benefits from CERFACS's expertise with this coupling software, as well as from LNHE involvement with the use of this tool (1D/2D hydraulic coupling, data assimilation for 1D hydraulic).

4.4 Investigate the use of satellite measurements in conjunction with in situ data to improve water ressources studies in the framework of data assimilation in large scale hydrology (M. Mouffe, S. Ricci, in collaboration with LEGOS/CNES, CNRM)

About 73% of global water ressources is provided by continental waters. Understanding and forecasting these ressources is then a crucial issue that can only partly be addressed with in situ observations. Hydrodynamics modeling plays a major role in this study but as data are required to initialize and force these models, modeling can also partly adress this question and major uncertainties remain on estimation of water levels and discharges. Observation from space, especially altimetry can notably help reducing uncertainties. The joint mission SWOT (CNES and NASA) to be launched in 2020, will provide wide swath (120 km) altimetry data with a global coverage over oceanic and continental waters. These data will enable the observation of middle size rivers (from 50 m wide) with a temporal frequency of at most 22 days. In the framework of a post-doc funded by CNES (Mélodie mouffe, started in September 2011), at CERFACS, a study on the use of SWOT data for large scale hydrology was initiated. The HYMAP hydrological model was developped at CNRM in the framework of a CNES post-doc. This model is forced by a surface model (surface run off and drainage) such as ISBA. The routing model solves the cinematic flux to describe the water level and discharge, it also takes into account the evaporation and floodind processes. Uncertainties in model parameters such as Manning coefficient, river depth and width results in errors in water level and discharge estimation. In order to provide a better estimate of these model parameters, an optimization procedure was set up using ENVISAT data, on the Amazon basin. Currently, synthetical SWOT data are being generated and integrated within the optimization process [DA33]. Finally, alternative optimization solutions are under investigation to reduce the computational cost for the calibration process.

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5 Data assimilation for forest fire

5.1 Flame speed correction using airborne fire observations (S. Ricci, M. Rochoux, B. Cuenot in collaboration with UMD)

An innovative project on the use of data assimilation for wildfire propagation modeling was initiated in 2010 by three teams at CERFACS (GLOBC, AE, CFD) together with University of Maryland (Pr. A. Trouvé). This study was mostly carried out in the framework of a Master 2 internship in 2010 ([DA29],[DA28]) and in 2011 ([DA30]). It aims at demonstrating that some of the limitations of wildfire modeling can be overcome by coupling information coming from both observations and models using data assimilation techniques. A simplified model of premixed combustion represents the flame as a discontinuity between burnt and fresh fuel, through a progress variable in which the local flame speed is the main physical quantity. This formulation links the local flame speed with the local fuel characteristics and flow conditions. The front propagation is based on the Level-Set front tracking method. The data assimilation algorithm is aimed at correcting the input parameters, which are significant sources of uncertainties in the estimation of the flame speed. Observations of the front positions are assimilated using a simplified Kalman Filter algorithm : the data assimilation approach is applied over a time window, where several observations of the front are available and where the model parameters are assumed to be constant. The data assimilation methodology was first applied in the framework of OSSE (Observing Simulation System Experiment) then on a real case of wildfire propagation (data from a controlled burning experiment provided by [10]). It was shown that data assimilation is a highly satisfactory strategy to integrate airborne fire observations into fire models. The estimation of optimal vegetation input parameters involved in the estimation of the rate of spread enabled to provide an accurate simulation and forecast of the fire propagation as presented in Fig. 5.1. These study results are presented in an article submitted to the INCA conference and was presented in AGU 2011.

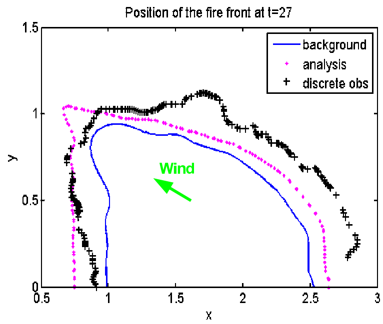

FIG. 5.1: Improvement of fire front propagation with fire front position data assimilation

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6 Data assimilation with EDF neutronic models

The collaboration between the department SINETICS of EDF/R&D and CERFACS on data assimilation has started in 2003 with the ADONIS project (2004-2007). This first collaboration was followed by the ARTEMIS project (2008-2010) aimed at using data assimilation schemes to improve the modelling of the neutronic state of power plants nuclear cores as well as the estimation of model parameters. The various results provided during this period led to an extension of those researches within the ARTEMIS 2 project (2011-2014). Making the most of this collaborative work, data assimilation is becoming a constitutive part of neutronic studies and several prototypes were already built on top of the new neutronic model COCAGNE.

6.1 Data assimilation for field reconstruction (B. Bouriquet, O. Thual)

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 ([23]). These results were presented in [24, 21] and corroborate the previous studies carried out on the neutronic model COCCINELLE. This work have been extended to the new COCAGNE code for various detailed studies in [15, DA21]. This work was improved using an extensive study on the modelling of the covariance matrix reported in [16].

6.2 Robustness of data a assimilation respect to the number of measurements (B. Bouriquet, O. Thual)

Knowing the quality of the field reconstruction through data assimilation study the robustness of the method when the amount of measured information decreases. We then study the influence of the nature of the instruments and their spatial repartition on the efficiency of the field reconstruction. It was shown that the slopes of the reconstruction quality is mainly governed by the repartition of the instruments. Depending on the chosen repartition, the decrease consists in two or three distinct phases. The behaviour with two phases within the decreasing quality of the reconstruction as a function of the number of instruments removed is understood in term of repartition effect, but not quantified yet. Those studies have been reported in [15] and have been published in Nuclear Instrumentation and Method A [DA11].

6.3 Determination of the most important instrument for nuclear core reconstruction (B. Bouriquet, O. Thual)

The previous studies prove that global activity fields of a nuclear core can be reconstructed using data assimilation and that robustness is depending on the instrument network design. We present and apply a specific procedure which evaluates this influence by adding or removing instruments in a given measurement network (possibly empty). That procedure using the Schur complement have been detailed in [DA22]. The study of various network configurations of instruments in the nuclear core establishes that the influence of the instruments depends both on the independent instrumentation location and on the chosen network.

It was proven also that results are very different when instruments are added to a non instrumented system than to a partially (half) instrumented one. Such a non equivalence respect to starting point proves that building a complete instrumental system cannot be done iteratively. Such a system will have limited efficiency as each step is dependant upon the previous and not of the global situation. This implies that, in order to build an optimal measurement network in a nuclear core, it is necessary to be able to take into account all the instruments globally.

Those results have been reposted in [DA22] and published in Nuclear Instrumentation and Method A [DA2].

6.4 Optimisation of the instrument network for the nuclear core (B. Bouriquet, O. Thual)

Knowing that an optimal network cannot be constructed iteratively we focused on solving the inverse problem of determining an optimal repartition of the measuring instruments within the core, to get the best possible results from the data assimilation reconstruction procedure. The position optimisation is realised using Simulated Annealing algorithm [22], based on the Metropolis-Hastings one. Moreover, in order to address the optimisation computing challenge, algebraic improvements of data assimilation have been developed and are presented here. Two main conclusions arises from those studies. The first one is that the standard PWR900 instruments repartition is characterized by an excitingly good quality. This instruments repartition is *a priori* the best we know, even if it was not originally designed using a data assimilation framework background. The second point is that the simulated annealing method can always find a ameliorated instrument locations set. Those results have been reported in [DA19] and was accepted for publication in Nuclear Instrumentation and Method A.

6.5 Sensitivity of the data assimilation (B. Bouriquet, O. Thual)

Some studies have been carried out on sensitivity of the analysis obtained by data assimilation. In order to obtain this sensitivity it has been determined the values that are conditioning the evolution of the analysis respect to a small change if the data assimilation component. Studies have been done for PWR900 and PWR1300. In order to synthesise sensitivity information as well as data assimilation sub product matrix (as analysis error matrix) several method of information reduction are used. Specially we focused on the MMSE (Minimal Mean Square Error) that allow to evaluate the extra diagonal information in a covariance matrix. Those results are reported in [DA21].

6.6 Parameter estimation through data assimilation (B. Bouriquet, O. Thual)

Another important point on data assimilation usage is the parameter adjustment. The aim is to find the best estimation of the parameter using the available data. Such studies have already done in [13] on one parameter with the COCCINELLE code. Then they have been extend with the use of COCAGNE in [14]. In that report the first test on estimation of several parameter at one have been tried. From that experience some detail research on the assimilation of several parameter together have been performed. Those studies demonstrate that only parameter that show some kind independence can be estimated together. Moreover the independence conditions have been pointed out through a detail sensitivity study of the parameters.

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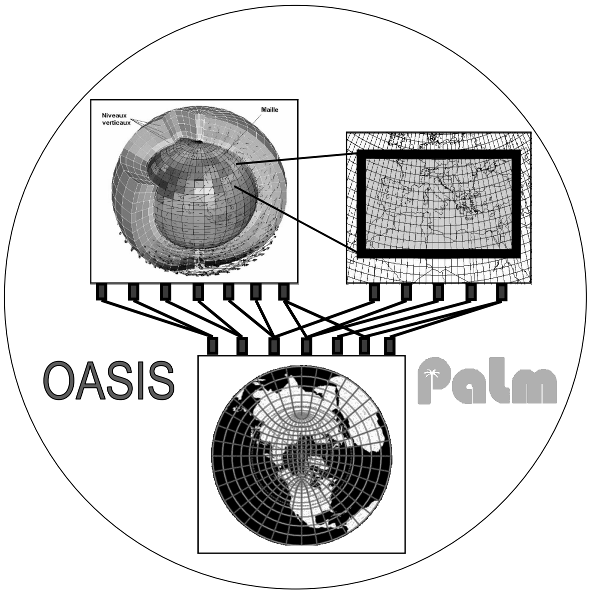
4

Coupling tools and HPC Climate Modeling



1 Introduction

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

Coupling numerical models, i.e. implementing synchronized exchanges of information between models, is a central issue in many research fields such as climate modelling, data assimilation, or computational fluid dynamics. Since about 20 years, CERFACS specializes in developing coupling software tools, also called "couplers", and in setting-up coupled systems using these couplers.

The following research actions are reported in the chapter :

1. The OASIS coupler
2. The OpenPALM coupler
3. HPC Climate modelling

During the last two years, the Global Change team has continued to ensure the maintenance, support and development of the OASIS and OpenPALM couplers. 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. OASIS, used by about 35 research groups around the world, specializes in coupled climate modelling while OpenPALM, developed in collaboration with ONERA, is a dynamic coupler currently used in more than 40 industrial applications or data assimilation suites. Thanks to these activities, the Global Change team plays a central role in the adaptation of coupled applications to the new and future massively parallel platforms, in particular for HPC climate modelling.

2 The OASIS coupler

The OASIS coupler is an open source software developed at CERFACS since 1991, used to couple numerical codes modelling the different components of the Earth System (ocean and atmosphere 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, which performs the exchange of data.

2.1 OASIS development

OASIS is used by about 35 climate modelling groups in France and in other countries world-wide. In Europe for example, OASIS is used by : the European Centre for Medium range Weather Forecasts (ECMWF) for their operational seasonal prediction suite, the EC-Earth consortium gathering 25 ECMWF member states in which ECMWF seasonal forecast system is developed into an Earth System Model, the Max-Planck Institute for Meteorology (MPI-M) in Germany in the framework of the Community Earth System models (CMOS) project, the National Centre for Atmospheric Science (NCAS) and the MetOffice in the UK, the Swedish Meteorological and Hydrological Institute (SMHI) in Sweden, the “Koninklijk Nederlands Meteorologisch Instituut” (KNMI) in the Netherlands, the “Istituto Nazionale di Geofisica e Vulcanologia” (INGV) and the “Ente Nazionale per le Nuove tecnologie, l’Energia el Ambiente” (ENEA) in Italy, etc. Five of the seven European climate coupled models participating to the international 5^{th} Coupled Model Intercomparison Project (CMIP5), that will be the basis of the next Intergovernmental Panel on Climate Change (IPCC) report due in 2013, use the OASIS3 version of the coupler [2] [3] [5] [4]. For example, CNRM-CM5 is an Earth System model developed jointly by Météo-France/CNRM and CERFACS for the CMIP5 decadal and centennial simulations [CC12], into which OASIS3 is used to couple the ARPEGE-Climat V5 atmosphere model (including the new Météo-France surface module SURFEX), the NEMO V2.2 ocean model (developed at the Laboratoire d’Océanographie et du Climat -LOCEAN, into which the GELATO sea-ice model developed at CNRM has been interfaced), and TRIP, a runoff model from University of Tokyo. OASIS is also used in the USA (Oregon State University, Hawaii University), in Canada (Environnement Canada, Université du Québec à Montréal), in Peru (Instituto Geofisico del Peru), in Japan on the Earth Simulator super computer (the Japan Marine Science and Technology Center), in China (Meteorological National Centre, China Academy of Sciences), in Australia (the Bureau of Meteorology Research Center -BMRC, the Commonwealth Scientific and Industrial Research Organisation -CSIRO, and the University of Tasmania), etc.

CERFACS, devoting one person full time to OASIS, provides the services needed to maintain a strong community network around the coupler : development, maintenance, integration, user support, etc. This has been possible up to now thanks to numerous collaborations on specific developments and to temporary but important funding streams (projects PRISM in 2002-2004, CICLE in 2006-2009, METAFOR[1] in 2008-2011, and IS-ENES[2] in 2009-2013). The investment of the French Centre National de la Recherche

[1] www.metaforclimate.eu
[2] https ://verc.enes.org

Scientifique (CNRS), also devoting one full time engineer for OASIS since 5 years, is in that respect particularly valuable.

During the last two years, active user support was provided to the OASIS users. Within IS-ENES, OASIS Dedicated User Support was offered to IPSL (1 person-month), SMHI (2 persons-months) and ETH Zurich (2 persons-mponths) (see [CC16], [CC24]). In addition, a new web site[3] is now open to the community through the IS-ENES portal and offers different services such as on-line documentation, user guides, tutorial, FAQs, user forum and tips for best practices. The central position of CERFACS in the coupled climate modelling community was also confirmed by the success of the workshop "Coupling Technologies for Earth System Modelling : Today and Tomorrow"[4] organised in collaboration with the Georgia Institute of Technology in December 2010. Forty-five participants from around the world (20 from France, 12 from other EU countries, 11 from the US, and 2 from China) explored the trade-offs involved in the different approaches to coupling in use throughout the climate modeling community and laid out a vision for coupling Earth System Models (ESMs) in the year 2020 (see also [CC1]).

2.2 OASIS3

Although it is foreseen that it will become a bottleneck for high resolution ESMs running on massively parallel platforms, OASIS3 is still being used successfully in different high resolution ESMs with a reasonnable overhead, thanks to its field-by-field "pseudo-parallelism".

For example, the EC-Earth model, which underlying atmospheric model IFS, was increased to T799 (25km, or 843,000 points) and 62 levels, along with a 0.25-degree (1.5M points), 75 depth-level configuration of the NEMO ocean model, was run on the Ekman cluster at the PDC Centre for High-Performance Computing on Sweden (1268 nodes of dual-sock quad-core AMD Opteron processors, i.e. a total of 10144 cores) with different numbers of cores for each component and OASIS3. Different combinations were tested. A coupling overhead of about 3% was observed with the 512-128-10 configuration (i.e. when 512, 128 and 10 cores are respectively used for IFS, NEMO, and OASIS3) and an overhead of about 1.3% was observed for the 800-256-10 configuration, which in both cases are still reasonnable overheads.

It has to be noted however that in these configurations there is some imbalance between the components elapse times, which allows OASIS3 to interpolate the fields when the fastest component waits for the slowest. For other coupled models, this may not be possible. A high-resolution version of CNRM-CM5 (50 km-atmosphere, 0.25 degree-ocean) has been compiled and run on more than 1000 cores on the PRACE tier-0 "curie" Bullx supercomputer to study regional scale / large scale interactions. The ocean model is used in a mixed layer mode (a configuration called NEMIX) to simplify and better understand coupled processes. In this configuration, the component models run sequentially and OASIS3 cost is directly added to the component elapse times. On 1024 cores (500 for the atmosphere, 512 for the ocean, 12 for the coupler), it was observed that OASIS3 takes up to 20% of total elapsed time to perform interpolations and communications between coupled components, which becomes an overhead barely acceptable.

Two approaches are currently followed to introduce true parallelism into OASIS and remove the observed bottleneck. The first one relies on the OASIS4 version of the coupler using its "user-defined" interpolation, and the second one is based on the modification of OASIS3 to use the Model Coupling Toolkit (MCT).

[3]https ://verc.enes.org/models/software-tools/oasis

[4]https ://verc.enes.org/models/software-tools/oasis/general-information/events

2.3 OASIS4

Since the beginning of the IS-ENES project in March 2009, CERFACS, CNRS and DKRZ (Deutsches Klimarechenzentrum GmbH, in Hamburg, Germany) have been collaborating on the development and evaluation of a new fully parallel version of the coupler, OASIS4. In particular, OASIS4 includes a library performing a fully parallel calculation of the source neighbour weights and addresses needed for the regridding of the coupling fields between the source and target grids (hereafter called the "neighbourhood search library") originally developed by NEC Laboratories Europe - IT Research Division (NLE-IT). This work resulted in June 2011 in the release of the latest OASIS4 version, OASIS4_1beta ([CC29], [CC10]).
OASIS4 was used by Météo-France, KNMI (Netherlands), and MPI-M (Germany) in the framework of the EU GEMS project (lead by ECMWF) for 3D coupling between atmospheric dynamic and atmospheric chemistry models and is currently used by SMHI (Sweden), the Alfred Wegener Institute for Polar and Marine Research (AWI in Germany), the BoM in Australia for ocean-atmosphere 2D regional or global coupling. In the framework of the METAFOR project, OASIS4 was adapted so to allow the use of the Common Information Model standard to configure the coupling exchanges ([CC28]).
However, this work also lead us to conclude that OASIS4 parallel neighbourhood search library, originally developed by NEC, presents some fundamental weaknesses in its design. In particular, the support of unstructured grids was not originally included and it would be very difficult to add it in the current code. Also, it is now very clear that it was developed with efficiency as the prime criteria, leaving aside readability and ease of development.
Therefore we decided to retrofit OASIS4 for pre-computed regridding weights, thereby circumventing its parallel neighbourhood search library, and use what we call the OASIS4 "user-defined" interpolation ([CC23]). To use this functionality, the user has to describe the links associating specific source grid points with specific target grid points in a separate NetCDF file. For each link, the index of the source point, the index of the target point and the weight associated to that link have to be provided. The OASIS4 communication library reads these indices and weights and automatically defines on each side a non-geographical grid with one point for each link. The multiplication of the source field values by the appropriate weights is done in parallel on the source side and a parallel redistribution of the results is done directly between the source and the target processes by the OASIS4 communication library. The user-defined regridding has been validated with simple toy models. It now has to be validated for real grids and in real coupled ESMs.

2.4 OASIS3-MCT

The second solution is based on the modification of OASIS3 to use the Model Coupling Toolkit[5] (MCT) developed by the Argonne National Laboratory in the USA. MCT requires that the regridding weights are pre-computed offline, but then implements fully parallel regridding and exchanges of the coupling fields and has proven parallel performance. MCT embodies a generic approach for creating coupled applications. Its design philosophy, based on flexibility and minimal invasiveness, is close to the OASIS approach. MCT uses distributed objects to store the coupling data and pre-computed regridding weights as well as a domain decomposition descriptor (DDD) to describe the parallel decomposition of the component models. Parallel communication patterns are computed automatically from the source and target DDDs. To use MCT, one has to load the coupling data into MCT data types and call MCT parallel matrix multiplication (for regridding) and communication methods. Parallel data transfer is then accomplished by pairs of send/receive methods with coupling data and communication pattern as inputs. MCT is, most notably, the underlying coupling software used in National Center for Atmospheric Research Community Earth System Model 1 (NCAR CESM1) [1]. Interfacing MCT in OASIS3 will provide a valid and efficient solution to remove current OASIS3 bottleneck ; in this case, the coupling fields will be regridded in parallel in the source

[5] http ://www.mcs.anl.gov/research/projects/mct/

communication library and directly redistributed between the source and target parallel distribution without the need to gather the whole coupling field onto one OASIS3 process. One advantage of this solution is that it will be totally transparent for the OASIS3 user, in the sense that the current OASIS3 communication library API (Application Programming Interface) will not change.

Technically, the two solutions described above, i.e. the OASIS4 user-defined regridding and the interfacing of MCT in OASIS3, are in principle equivalent. It will therefore be interesting to compare the two solutions and choose the most efficient one if they both prove to be valid options for massively parallel coupled simulations.

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3 The OpenPALM coupler

3.1 Introduction

OpenPALM is a software tool codeveloped by CERFACS and ONERA based on the PALM library (from CERFACS) and the CWIPI library (from ONERA). OpenPALM is distributed under the open source license LGPL since the first of January 2011. The distribution is done via a download from the website of OpenPALM (http ://www.cerfacs.fr/globc/PALM_WEB/EN/BECOMEAUSER/download/). After one year of open access, about 80 downloads have been registred.
This software allows for 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 OpenPALM is that it allows the components to be launched at any point during the run ; in this sense, OpenPALM is a dynamic coupler. The main characteristics of OpenPALM 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 OpenPALM allows for 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 current available version, OpenPALM 4.0.0, 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 addition, 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), an MPI-1 version of OpenPALM has been developed. Still in this scope, a brand new communication scheme is being implemented.

In order to provide performant coupling solutions for the aerospace and aeronautic communities either for the research and industry, CERFACS, ONERA, SAFRAN, EADS and CNES have shared in 2010 an intensive reflexion on the definition of the next generation coupling tool. A confrontation between existing tool like Salomé (EDF), CWIPI (ONERA) and PALM (CERFACS) have led to the conclusion that the existing tools CWIPI and PALM are a very good basis for the development of such an ultimate coupler. Thus, a collaboration between CERFACS and ONERA is born from this reflexion in order to develop the open source coupler OpenPALM based on the complementary tools CWIPI and PALM. Current and future developments of the OpenPALM coupler are based on the tender specifications resulting from the common

2010's reflexion. Financial support is provided by CERFACS and ONERA completed by projects as the FLUI project COSMOS+.

More and more users would like to couple commercial codes like Fluent or Abaqus with OpenPALM. The standard use of OpenPALM 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. This last protocol is a very promising path and will allow to couple solvers that run on distinct architectures connected on a network.

In parallel the OpenPALM team has granted the maintenance of the previous versions and has provided extensive user support, including training sessions (at least 4 per year) both on the use of the coupler itself and on its application to parallel coupling and data assimilation suites ([CC6]).

Today, the OpenPALM 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 OpenPALM website :
http ://www.cerfacs.fr/globc/PALM_WEB/index.html

3.2 Usage of OpenPALM

3.2.1 Data assimilation with OpenPALM

As a data assimilation framework, the OpenPALM 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. CNRM, CNES, IPSL and LA use OpenPALM in the French project ADOMOCA for atmospheric chemistry data assimilation. CNRM also takes advantage of OpenPALM to build a hydro-meteorological data assimilation suite based on the Safran-Isba-Modcou chain. In the same field the SCHAPI uses OpenPALM to assemble two data assimilation suites in hydrology and hydraulics for the river floods forecasting. The hydraulic data assimilation suite is currently being tested in their real time operational forecasting system, while different research actions, including a PhD thesis constantly improve the suite.
EDF used OpenPALM in the ADONIS project to design a data assimilation methods in neutronics simulation that was eventually implemented within the prescribed operational environment based on Salomé. From this experience and from the results obtained at SCHAPI, another research department in EDF, the LNHE got interested in the use of OpenPALM for hydraulics application, namely for a data assimilation suite for the complete 3D modelling of the salinity evolution in a salted water basin where fresh water is discharged from production plants.

3.2.2 Code coupling with OpenPALM

As a code coupler, OpenPALM has started to be used at CERFACS by the CFD TEAM in RANS (N3S-Natur) and LES (AVBP) coupled applications ([17]). 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 OpenPALM in CFD coupled applications. The CFD-Team of CERFACS uses intensively the OpenPALM coupler for multiphysics and multi-composant simulations [7, 8, CC3, 21, 28, 27, 29, 31, 30]. The main codes of the CFD-Team are interfaced with the coupler (AVBP, AVTP, PRISSMA and elsA).

In the NitroEurope research project, INRA (Rennes, Grignon, Avignon), AARHUS UNIVERSITET, FZK, RWTH and the Technical University of Madrid use OpenPALM to couple models in order to study the flows and transformations of nitrogen at the landscape scale. The LNHE research department of EDF uses OpenPALM to couple 1D global river flow modelling with detailed 2D representations of larger and more complex river portions. IFREMER is coupling a coast model with a waves' one with PALM. Other users are MINES Paris, IFP (Institut Francais du pétrole), MINES Albi, ECP, CORIA, IMT (Institut mathématique de Toulouse), SCHAPI, BRGM, LMTG, LEGOS, UMR CNRS 5805 EPOC, DRM (Environnement Canada), LMMC (Algérie) and FUNDP (Faculté Univesitaire Notre-Dame de La Paix, Belgium). The German Science Foundation is funding a PhD student from the Karlsruher Institut für Technologie to work on the improvement of the parallel data distribution dynamic evolution, in order to efficiently use OpenPALM to couple a local weather forecast and/or hydrology model with a point based 2D biology model, capable of self adjust the data distribution to achieve the best load balancing.
In the framework of the French RTRA/STAE funded project, PALM is used to build an interdisciplinary modelling platform devoted to study the impact of city expansion modes on local climate. Up to five models are integrated on the platform : the ENM-CIRED (Ecole Nationale de la Meteorologie - Centre International de Recherche sur l'Environnement et le Developpement) socio-economical model, the GEODE (Geographie de l'Environnement) geographic model, the LRA (Laboratoire de Recherche en Architecture) urban morphology model, the CNRM-LA (Centre National de Recherches Meteorologiques - Laboratoire d'Aerologie) MESONH and SURFEX models for atmosphere and land surface respectively.

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4 HPC Climate modelling

4.1 General context

Based on recent findings and thanks to new observational products (mostly satellite) traditional spatial grid scales used for climate (on the order of 100-200 km) appear to be insufficient to adequately resolve physical processes such as those involved in air-sea interaction which are critical if one wants to assess the true predictability and associated mechanisms of the climate system. Higher resolution is also necessary (but not sufficient) to generate more reliable extreme event probabilities that are critical for impact assessment. The current and future high-end computational power will likely enable soon climate prediction at the regional (10-25km) and later local (less than 10 km) scales. These scales are required to make further progress : (1) for evaluation of processes at the cloud and eddy scale (air-sea coupling, aerosol activation, cloud microphysical and dynamical interactions) that affect regional and global climate sensitivity and drive climate biases and (2) for estimation and assessment of impacts using self-consistent models to produce more accurate statistics of climate variability (e.g., intensity of precipitation) and extreme events (e.g., hurricanes) to drive impact assessment models (e.g., of the hydrological cycle).

This scientific context has led us in 2011 to a project of a Grand Challenge for the next decade. Our 2020 HPC Grand Challenge is to develop, in close relation with our national, (Météo France, IPSL, DRAKKAR group) and international partners, a global climate model system at very high atmospheric and oceanic resolution (horizontal 10-25 km, vertical 70-90 levels) on various massively parallel computers (with O(10^4-10^5) processors). The considered climate variability and predictability temporal scales are from interannual to decadal.

Many challenges, both scientific and technical, need to be adressed along the path of our 2020 Grand Challenge. Among them, our initial focus in 2011 was on the development and evaluation of an intermediate high resolution configuration of our ARPEGE-NEMO climate model (atmospheric resolution of 50 km or spectral truncature T359, oceanic resolution of 0.25 ^{o}). This intermediate configuration is necessary to prepare and ease the on going and widespread vector to scalar computing migration and the optimal use of ultra-high resolution climate models on the new generation of high performance computers.

4.2 Development and implementation of the ARPEGE-NEMIX model

In 2011, a simplified version of this intermediate ARPEGE-NEMO coupled model (called ARPEGE-NEMIX) has been developed and evaluated in the framework of the ANR funded project SPADES (08-ANR-SEGI-025). This simplification deals with disabling of any ocean horizontal motion and the coupling of the atmospheric model with a mixed layer ocean. The mean effect of the tracer advective transport is then represented by a flux correction methodology (NEMIX, [CC17]). This configuration has been widely used within the international community for a wide range of studies going from climate sensitivity to greenhouse forcing to influence of air-sea coupling upon tropical to midlatitude intraseasonal variability, including the representation of tropical cyclones (for our own recent science applications, see 2.1.2 in paragraphe "Climate Variability and Global Change" and [CC21]).

Another asset of this simplified configuration is its lack of climate biases of large amplitude due to the flux corection implementation. The energetic balance of the model, both at the top of atmosphere and air-sea interface, is quickly reached without the need of exhaustive parameter sensitivity experiments. This allows a quick and robust estimation of the similarity of simulated climates on different architectures which is a necessary condition in a machine to machine porting context.

In the framework of the FP7 European project IS-ENES, the ARPEGE-NEMIX model has been successfully implemented and tested on a broad selection of scalar supercomputers, from which a PRACE tier-0 machine ([CC8]). Efficient weak scaling of both ARPEGE and NEMIX models allows the use of more than 1000 cores. The performed benchmarks suggest that decadal-scale climate experiments at such resolution can now be realistically processed on such machines (less than 5 days necessary to simulate 10 years of climate).

4.3 Coupling technical aspects and fault tolerance compliance

Preliminary simulations showed the lack of performance of the OASIS3 coupling implementation : measured on a set of European coupled GCMs, from 1 to 20 percent of the total duration could be spend on coupling exchanges ([CC16], [CC24]). First, an OASIS4 alternative has been explored, using our model and several other CGCMs, revealing other incompatibilities ([CC25]). At the moment, a newly developed OASIS3-MCT solution is tested, to try to enhance coupler scalability. Furthermore and based on the practical IS-ENES funded exercice of coupler interface coding and performances analysis ([CC26]), a testbed for a comparison of the NCAR(flux coupler) and CERFACS(OASIS) coupling environment has been suggested, revealing the strong and necessary interaction between OASIS development and beta testing during OASIS model interface implementation on HPC configurations.

The performed intermediate high resolution experiments revealed new bottlenecks such as :
- Output speed decrease
- Data storage capabilities
- Runtime environnement unstability

which can strongly impact the overall performance of our climate numerical laboratory. New data production paradigms are currently tested by CERFACS partners (IPSL) and started to be included within our own HPC configurations. In parallel, we investigated the reduction of the amount of produced climate data using traditional (interpolation) and new (reduction) schemes.

Concerning runtime environment stability and to start exploring fault tolerance compliance of existing climate models, a study with the NEMO code has started on how to adapt an error handling that could reorganize MPI communications after failure and keep calulating on the remaining process. This work is part of code adaptation for HPC, developed in the framework of ANR SPADES jointly with INRIA Saclay laboratory (LRI).

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5

Climate Variability and Global Change

1 Introduction

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

- To improve the understanding and simulation of climate processes underlying the variability of the main climate natural modes, such as the Northern and Southern Annular Modes (NAM and SAM), the Atlantic Meridional Overturning Circulation (AMOC) and the El Nino Southern Oscillation (ENSO) (and its decadal counterpart, the Pacific Decadal Oscillation (PDO)) and of the response of the NAM/SAM, AMOC, ENSO and PDO to anthropogenic climate change.
- To detect, attribute and describe anthropogenic climate change on global to regional scales using high resolution climate models, statistical methods and long-term high quality observations.
- To assess the impacts of anthropogenic climate change at regional to local scale with specific interest in the changes of the hydrological cycle and to provide reliable uncertainty bounds in future climate projections.
- To study the potential of decadal predictability due to both external forcing (from both natural and anthropogenic sources) and low frequency ocean fluctuations.
- To explore the influence of small-scale phenomena upon ocean-atmosphere coupling and their impact on intra-seasonal to interannual predictability

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. As an example, we have recently achieved a very large ensemble of decadal hindcasts and forecasts simulations in the framework of the Coupled Model Intercomparison Project version 5 (CMIP5) exercise which will provide the modelling results for the next Intergovernmental Panel on Climate Change (IPCC) assessment report planned in 2013. The climate model is the CNRM-CM5 model developed jointly with the Centre National de Recherches Météorologiques (CNRM). More than 5000 years of simulated climate have been performed requiring 200 000 CPU hours on the Météo-France NEC supercomputer and generating 120 Terabytes of data. This first achievement is the first step of a 10-year program devoted to the study of decadal variability and predictability and its impacts.
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 7, FP7 : COMBINE, IS-ENES ; Agence Nationale de la Recherche ANR : SCAMPEI, ASIV ; Ministère de l'écologie, du Développement Durable, du Transport et du Logement (MEDDTL) : DRIAS, EPIDOM ; Fondation BNP-Paribas : PRECLIDE.

2 Climate variability and predictability

The weather/climate system exhibits considerable variability on a wide range of spatial and temporal scales. Those are characterized by strong interactions that must be taken into account to better understand and predict the atmosphere from daily variability to climate change. Interest in weather/climate fluctuations have been rapidly growing over the last few years following the recent recurrence of extremes and the more pressing evidence for anthropogenic influences on climate. In such a context covering a large spatio-temporal spectrum, demand for predictability of weather/climate variability over the next decades is strongly emerging.

The activities of the “Climate variability and predictability” project directly take place within this framework. Based on a process-oriented approach, our goal is to better understand the physical origin of the low-frequency variability of the climate system and its interaction with weather-type events, with the underlying objective to eventually improve their prediction over a wide range of timescale. Our grand challenge is to tackle the issue of decadal variability and predictability using a hierarchy of numerical tools. This activity has been at the forefront of our research in 2010-2011 and will be so for many years due to the numerous complex scientific and technical issues remaining to be solved. In line with these objectives, the key step was our participation to the current international decadal prediction exercise which is coordinated by the World Climate Research Program (WCRP) to fulfill the IPCC requirements for their next assessment report (AR5) to be delivered in 2013.

Fundamental research activities, in line with traditional and historical expertises, are first presented, followed by a more detailled description of the decadal forecast initiative.

2.1 Interaction between the North Atlantic-Europe atmospheric dynamics and the local surface conditions (J. Boé, C. Cassou, E. Maisonnave, S. Bielli)

Previous studies realized at Cerfacs have shown that weather regimes can be considered as elementary bricks for North Atlantic-Europe (NAE) atmospheric dynamics whose seasonal-to-decadal variability can be interpreted to the first order as the time integration of their anomalous occurrence. In addition to occurrence, transitions between regimes also appear a relevant criterion especially to link large-scale variability and extreme events. Finally, evidence has been provided that the internal characteristics of the regime (strength, spatial departure to mean etc.) are also crucial to interpret climate variability accross timescales. Interaction between the atmosphere and the continent on one hand, and the ocean on the other hand, have been investigated in 2010-2011.

2.1.1 Soil-moisture-precipitation interactions

How soil moisture affects precipitation is an important question – with far reaching consequences, from weather prediction to centennial climate change –, albeit a poorly understood one. Thanks to observations and the results of an high resolution hydro-meteorological analysis over France, we have studied how previous soil moisture conditions affect precipitation and surface water budget over France during summer, for different weather regimes (Boé 2011).

Soil moisture-precipitation coupling has been shown to be highly dependent on large scale circulation, even simply in terms of sign. If dry soil conditions always lead to an increase of the lifted condensation level, which is unfavorable to precipitation, the sign of the effect of previous soil moisture conditions on atmospheric stability depends on large scale circulation. In the end, for two weather regimes, dry soil conditions lead to less precipitation. However, this should not be interpreted as the sign of a positive soil moisture-precipitation feedback, because drier soils also lead to a decrease of subsequent evapotranspiration. As soil moisture effect on evapotranspiration is larger than its effect on precipitation independently of large scale circulation, the total soil moisture-precipitation feedback over France has therefore been found to be negative.

2.1.2 Ocean-atmosphere coupling

Within the ANR-IRCAAM project, a dedicated study of the 2003 climate dynamics has been carried out using a suite of GCM configurations based on the ARPEGE AGCM. Tropical-limited atmospheric nudging towards observed circulation in ARPEGE confirms that tropical-extratropical connections are important to explain the 2003 NAE anomalous atmospheric circulation (Cassou et al 2005). We demonstrated that the anomalous convective activity over a broad tropical Atlantic basin is at the origin of a Rossby wave train which propagates northeastward towards Europe and alters in fine the occurrence/strength statistics of the NAE weather regimes. We then set up a simplified coupled model configuration where ARPEGE is coupled to NEMIX, acronym for the NEMO model transformed into independant single column ocean models. NEMIX has been developed at Cerfacs in 2010 : the full vertical ocean physics of NEMO is retained while horizontal exchanges are cast off and compensated by a flux correction term. Targeted simulations for 2003 using the ARPEGE-NEMIX configuration highlight that the ocean-atmosphere extratropical coupling is important to reinforce the primary tropical-extratropical atmospheric signal. The mechanism is based on the so-called water wapor feedback at work over the continent due to the advection of moister air from the ocean when the coupling is activated. This is associated with a strong positive feedback on the anomalous NAE atmospheric circulation leading to enhanced northward advection of warm air from North Africa towards Europe, as well as local enhanced subsidence over Europe and excessive solar radiation at the surface. All together, the retroaction when the ocean-atmosphere coupling activated, is such that the warmer conditions over Europe are amplified by a factor of two.

2.2 Decadal prediction (C. Cassou, E. Sanchez, Y. Ruprich-Robert, E. Maisonnave, E. Fernandez, P. Rogel, L. Terray, C. Pagé, S. Valcke, M.-P. Moine, L. Coquart)

2010-2011 has been almost entirely devoted to the setup, the realization and the basic evaluation of the so-called decadal or “near term” coupled experiments performed within the Coupled Model Intercomparison Project (CMIP5) further used for AR5. A new version of the general circulation model CNRM-CM (Voldoire et al 2011) has been developed jointly by Météo-France (CNRM-GMGEC) and the Cerfacs Global Change team. The exact same model, named CNRM-CM5, is used in both centennial (carried out by CNRM) and decadal exercises that consequently differ only by the initialization step (same binaries and same namelists), . The use of the exact same code in the two centers is the concrete result of strong colloborations that have been reinforced to pool the limited resources devoted to the development of the new Earth system for CMIP5. This very demanding project absorbed most of our human ressources over the 2010-2011 period and required a full investment from all the team members, leaving little room, compared to previous years, for other fundamental research activities.

The CORE experiments of CMIP5 considered as the “entry ticket” for model intercompararison studies, have been completed and are available on the local CNRM-Cerfacs Earth System Grid (ESG) node.

Additional experiments have also been carried out and published. Additional members have been added leading to a total of 10 for each forecast date. 2 additional dates per decade have been also integrated, namely 1959, 1964, 1969, ..., 2004, as a supplement to the mandatory 1960, 1965, 1970, ..., 2005 suite. Finally, a fake 2010-pinatubo eruption has been introduced in an additional set of forecasts for the 2005-2035 timeslot. The decadal forecast activity at Cerfacs is also part of the ongoing EC-FP7 COMBINE project coordinated by MPI, the GICC EPIDOM project started at the beginning of 2011 and coordinated by Cerfacs and the ANR CECILE coordinated by BRGM. The two main preliminary results are listed below.

2.2.1 Ocean initialization

In order to minimize the initial shocks and drifts during the forecasts, initial conditions are obtained from a coupled simulation of CNRM-CM5 integrated from 1958 to present where the sole ocean is nudged in temperature and salinity towards the NEMOVAR-COMBINE (Balmaseda et al. 2010) ocean reanalysis. Within this simulation, the other components (atmosphere, sea-ice, continents etc) are thus freely coupled and do not contain any observational data. The NEMOVAR-COMBINE reanalysis has been produced using a multivariate 3D-var data assimilation method (Weaver et al. 2005, Daget et al. 2009) applied to the NEMO model running on the same ORCA1 configuration as CNRM-CM5, and with the physical parameterizations as close as possible. The surface temperature and salinity are restored towards NEMOVAR using a flux derivative term while the subsurface ocean nudging is based on a 3D Newtonian damping in temperature and salinity (see Madec et al. 2008 for details) which is function of depth and space. No 3D damping is applied between the surface and the thermocline thus leaving the mixed layer free to evolve ; the damping is equal to 10 days below the thermocline and to 360 days for the deep ocean (below 800m depth). There is no nudging near the coasts to avoid spurious effects on boundary currents, neither within the tropical band.

The latter choice tends to account for the fact that tropical subsurface ocean and tropical surface wind should be consistent to minimize the excitation of tropical Kelvin and Rossby waves when one lets the model go at the beginning of the forecast. We performed two sets of experiments where nudging is excluded either within 1^oN-1^oS (hereafter GLOB) or within 15^oN-15^oS (hereafter EXTROP). We show that GLOB has a much stronger initial shock than EXTROP ; it is characterized by a systematic excitation of an El Niño events in the Pacific leading, by teleconnection, to enhanced drift in the entire Northern Hemisphere. We found that such a disruption affects the mean drift of the model up to about 4 year leadtime stressing out the importance of the initialization step (Sanchez et al 2011).

2.2.2 Skill score

Decadal predictability arises from two sources : anomalous states assimilated in the initial conditions of the climate system (here the NEMOVAR ocean, -first kind predictability) and so-called external forcings linked to natural (volcanoes and solar activities) events or anthropogenic influences (e.g. GHGs increase, aerosols emission, land use etc. -second kind of predictability). Skill scores have been computed for global temperature as a function of leadtime. Data have been debiased following the CMIP5 linear protocol. Very high positive scores (from 0.93 to 0.98) are found whatever the leadtime. At global scale, the predictive skill is mostly explained by the warming trend and the interannual cooling events associated with the external forcings, respectively the increase of GHG concentrations and the volcanic aerosols that are prescribed in the model (Figure 2.1).

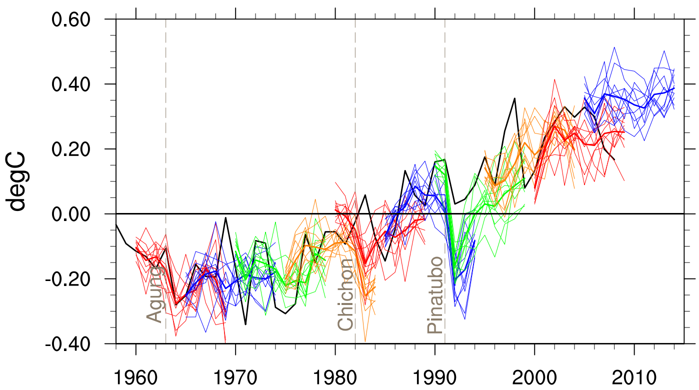

FIG. 2.1: Anomalous global SST from observation (black) and for decadal forecasts (colors) initialized on Jan 1, 1960, 1965, 1970, ..., 2005. Each spaghetti corresponds to one member. The reference period is 1970-1990. Major volcanic eruptions are mentionned

More interestingly, skill scores are computed for the Atlantic Sea Surface Temperature anomalies to evaluate the ability of the model to predict the so-called Atlantic Multidecadal Oscillation (AMO). In line with pionner studies about the thermohaline predictability (Pohlmann et al., 2011), preliminary results (Figure 2.2) suggest that the ocean initialization is a clear added-value for leadtime up to 10 years. Correlations skill ranges from 0.41 to 0.72 as function of leadtime when trends linked to external forcings are removed prior to the statistical computation, while there is no skill in the so-called historical experiments (carried out by CNRM) where the ocean is not initialized. .

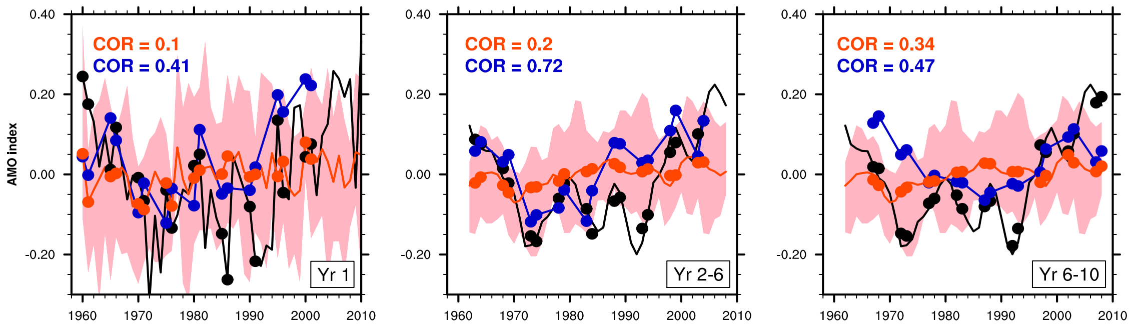

FIG. 2.2: AMO predictability for 1 year (left), 2-6 years (middle) and 6-10 years (right) leadtime from decadal forecasts (blue) and historical simulations (red). Correlations between ensemble mean and observation (black) are given in the upper-left corners of the panels. The pink shading stands for the ensemble spead of the historical experiments.

2.2.3 Decadal internal variability in CNRM-CM5 and its potential predictability

A 1000-yr control integration of CNRM-CM5, hereafter PIctrl, has been carried out by CNRM for CMIP5. Within EPIDOM and with the support of EDF, we started to analyse this simulation where external forcings are set to constant (pre-industrial 1850 values), in order to document and understand the low-frequency intrinsic (or internal) variability simulated by the model. Emphasis is laid on the Atlantic Meridional Overturning Circulation (AMOC), the AMO as well as the Pacific Decadal Oscillation (PDO) that could potentially lead to decadal signals over the adjacent continents like in observations. The realism of the simulated modes has been first quantified. The mechanisms at the origin of their excitation have been then investigated based on classical statistical lead-lag analysis. We show that in CNRM-CM5, a maximum of AMOC is preceeded, about 30-yr before, by an anomalous cyclonic circulation off Europe leading to enhanced meridional ocean heat transport into the subpolar gyre as well as into the GIN seas. Excess of heat there induces a strong sea-ice response leading to salinity anomalies that are advected into the subpolar gyre through the Denmark Strait, thus further reinforcing the direct acceleration of the subpolar gyre due to overlying atmospheric forcing. This dominant mode for AMOC is damped by the northward advection of subtropical fresher water along the subtropical gyre. Predictability studies within the so-called “prefect model framework” has been started for the AMO and will be completed in 2012.

2.2.4 The decadal signature of sea-level changes

The ANR CECILE project started in 2010. It aims at evaluating the impact of sea level variations, including future sea level rise, on erosion and the coast lines. In collaboration with CNRM, Cerfacs provides expertise and decadal forecast simulations to make this evaluation both retrospectively and prospectively. The work done during this first phase of the project was directed towards evaluation of the different experiments produced so far. First comparison to the reanalyses, including NEMOVAR, have been compared to quality controled, long tide gauge time series and sea level reconstructions. Second, a first order predictability evaluation of the sea level regional anomalous patterns in both retrospective decadal hindcasts, hereafter DEC, and historical XXth century simulations, hereafter HIST, has been conducted using the reliability approach. First results show that the DEC ensemble spatial spread is smaller than HIST which is itself underestimated compared to NEMOVAR. Second, preliminary analyses suggest that the predictability at regional timescale in both DEC and HIST ensemble can barely be demonstrated using single model 10-member ensemble hindcasts.

3 Climate change and impact studies

3.1 Detection and attribution of climate change

The world climate is currently changing due to the human-induced increase in the atmospheric concentrations of CO_2 and other greenhouse gases. Global warming is also very likely to increase in the 21st century with a range of 1.5 to 6.4 degree Celsius as estimated from the last Intergovernmental Panel for Climate Change (IPCC) fourth assessment report (AR4). However, there are still large uncertainties related to the fate of the global or regional evolution of other variables such as those related to the hydrological cycle (precipitation and evaporation), in particular over the world oceans. Our objective for this period was thus first to quantify the influence of anthropogenic causes upon recent marine hydrological changes climate versus the role of intrinsic variability (the detection and attribution question). We have also revisited the question of the detection of upper ocean temperature changes in the last 50 years using a new approach and recent ocean reanalyses and observed datasets.

3.1.1 Detection of changes in the marine hydrological cycle (L. Terray, L. Corre)

Changes in the global water cycle are expected as a result of anthropogenic climate change, but large uncertainties exist in how these changes will be manifest regionally. This is especially the case over the tropical oceans, where observed estimates of precipitation and evaporation disagree considerably. We have used an alternative approach, namely to examine changes in near-surface salinity. To first order, large-scale salinity changes reflect the variations in the precipitation minus evaporation balance. Data sets of observed tropical Pacific and Atlantic near-surface salinity combined with climate model simulations were used to assess the possible causes and significance of salinity changes over the late twentieth century (Terray et al. 2012). We have then applied two different detection methodologies to evaluate the extent to which observed large-scale changes in near surface salinity can be attributed to anthropogenic climate change. Basin-averaged observed changes were shown to enhance salinity geographical contrasts between the two basins : the Pacific is getting fresher and the Atlantic saltier. While the observed Pacific and inter-basin averaged salinity changes exceed the range of internal variability provided from control climate simulations, Atlantic changes are within the model estimates. Spatial patterns of salinity change, including a fresher western Pacific warm pool and a saltier subtropical North Atlantic, are not consistent with internal climate variability. They are similar to anthropogenic response patterns obtained from transient 20th and 21st century integrations therefore suggesting a discernible human influence on the late 20th century evolution of the tropical marine water cycle. Changes in the tropical and mid-latitudes Atlantic salinity were not found to be significant compared to internal variability. These results are important as it is the first time that a significant change due to anthropogenic forcing is detected in the observed tropical marine hydrological cycle.

3.1.2 Detection of changes in upper ocean temperature (L. Corre, L. Terray, A. Weaver)

A multivariate analysis of the upper ocean thermal structure was performed to examine the recent long-term changes and decadal variability in the upper ocean heat content using both a set of ocean reanalyses and a model-independent objective analysis (Corre et al. 2011). Several variables were used : the mean temperature above the 14^{o}C isotherm, its depth and a fixed depth mean temperature (250 m mean temperature). This choice of variables provides information about the local heat absorption, vertical distribution and horizontal redistribution of heat, this latter being suggestive of changes in ocean circulation. Use of the mean temperature above the 14^{o}C isotherm is a convenient, albeit simple, way to isolate thermodynamical changes by filtering out dynamical changes related to thermocline vertical displacements. We have found that the global upper ocean observations and reanalyses exhibit very similar warming trends (0.045^{o}C per decade) over the period 1965-2005, superimposed with marked decadal variability in the 1970s and 1980s. The spatial patterns of the regression between indices (representative of anthropogenic changes and known modes of internal decadal variability), and the three variables associated with the ocean heat content are used as fingerprint to separate out the different contributions. Two robust findings result from our analysis : (1) the signature of anthropogenic changes is qualitatively different from those of the internal decadal variability associated to the Pacific Interdecadal Oscillation and the Atlantic Meridional Oscillation, and (2) the anthropogenic changes in ocean heat content do not only consist of local heat absorption, but are likely related with changes in the ocean circulation, with a clear shallowing of the tropical thermocline in the Pacific and Indian oceans.

3.2 Statistical downscaling and impact studies

The downscaling activities have been aimed toward application of the previously developed statistical downscaling methodology, using it for diversified climate change impact studies and research at regional to local scales. Some studies have also taken place to better understand the characteristics and the stochastic aspects of the methodology. In parallel, work has begun regarding the standardization of downscaled data, along with the development of user guidance aimed at the impact communities, as well as the development of new collaborative web portals to help dissemination.
A summary of the main activities during the period 2010-2011 is given below.

3.2.1 Impact of climate change on mountainous areas in France (C. Pagé, L. Terray, M. Piazza, E. Sanchez, J. Boé)

Our main objective was to adapt the DSCLIM statistical downscaling methodology to study the impacts of climate change on the mountainous areas in France, in the context of the ANR/SCAMPEI project led by Météo-France CNRM. Several geographical domains for the large-scale circulation have been evaluated by comparing the performance of downscaled precipitation to the original configuration used previously, as well as the relevance of the generated weather types. The configuration has also been standardized among the different seasons (number of weather types, mask to use only data exclusively over France, random selection of analog day within closest days). After evaluation, it has been decided to keep the original geographical domain. This result is also confirmed by the thesis results of M. Lafaysse (Lafaysse, 2011), which also stated the importance of taking into account the stochastic aspects of the methodology when working on quite small geographical domains. A new dataset have been generated given this new configuration, called SCRATCH2010, which improves DSCLIM results especially over southern Alps and along the Mediterranean coast (except for Roussillon). DSCLIM downscaled scenarios have also been compared to dynamically downscaled ARPEGE scenarios by Météo-France CNRM (using a bias correction quantile-quantile methodology). Surface feedbacks have also been studied for the present climate, and also in dynamically downscaled (non-corrected) scenarios, over the Alps and Pyrenees. Two hypothesis have resulted from this study : a) In the south, feedbacks between snow cover and temperature occur mainly in April (with a 2-month time lag), caused mostly by the generation of mist and fog which limits the solar radiation. b) In the north and east, the correlation time lag is of 6 months, and the physical process is related to the soil water content.

3.2.2 French and European collaboration for dissemination of downscaled scenarios for impacts (C. Pagé)

Two main actions have taken place for the dissemination of downscaled scenarios to the climate change impact communities in France and in Europe. The first action is the GICC/DRIAS French project, in collaboration with Météo-France and IPSL, while the second is the EU FP7 European project IS-ENES, in collaboration with more than 20 partners throughout Europe (including Météo-France and IPSL) and coordinated by IPSL. Many links were put in place between the two projects. The GICC/DRIAS project will end at the first semester of 2012, and the main outcome is a web portal to make available downscaled climate scenarios by Météo-France , IPSL and CERFACS to the French impact communities. The portal will include guidance, discovery, and data access with support. It is now included in the main objectives of Météo-France. The IS-ENES project embraces larger objectives, but one of the work package deals with bridging the gap between the climate modelling community and the impact communities. An impact interface portal is currently being designed and coded, but with somewhat different objectives than the DRIAS project portal. The main objectives of this portal is to develop standards for describing downscaled data (with links to the EU FP7 METAFOR project), as well as to develop basic data access and processing interoperable tools based on OGC and upcoming standards. The portal development is being done in close collaboration with KNMI, while the guidance documentation work is lead by SMHI and CMCC partners with CERFACS. In 2010-2011, Use Cases have been constructed, along with common tools specifications. These are the basis of the portal development, which has begun in August 2011.

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

We have used the DSCLIM software to produce an updated set (of SCRATCH08) of multi-model high resolution climate scenarios for France (at a horizontal resolution of 8 km). The DSCLIM configuration used in the ANR/SCAMPEI project have been used for this update. We have performed an updated downscaling of 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. Other scenarios have been downscaled, such as PRUDENCE ARPEGE scenarios (for application in the ANR/SCAMPEI project), and work has begun to also downscale all the GCM scenarios from the EU FP7 ENSEMBLES project. This set of regional scenarios, named SCRATCH10, has been primarily used for a number of applications linked to climate change impact assessment through our participation to funded projects, ranging from agronomy (ANR/ORACLE, ANR/CLIMATOR, ANR/VALIDATE), mountainous areas (ANR/SCAMPEI), hydrogeology (BRGM/LEZ), insurance (MAIF/CLIMSEC), forestry (GICC/FAST). Furthermore we have also provided SCRATCH10 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. Several new research collaborations have been initiated, notably with Estuary Researchers (Boulogne-sur-Mer), different themes (vineyards ANR/TERVICLIM-GICC/TERADCLIM, agroclimatology, urban climatology) with the COSTEL Laboratory at Université Rennes 2 (4 thesis), hydrogeology at Université Rennes 1 (Géosciences Rennes - UMR CNRS 6118), hydrology at Université d'Orléans (INSU), biology at Université de Pau, urban pollution at CEREA, seasonal prediction at Météo-France/DCLIM, most of them being related to thesis work. Those also implies giving one two or three days training.

3.2.4 Further improvement of the DSCLIM software functionalities (C. Pagé)

Given feedbacks from thesis students M. Lafaysse and S. Singla, as well as some previously identified needed functionalities, DSCLIM has been refined by adding more control in its behavior, adding new configuration parameters. Some previous technical dependencies have also been eliminated. Extensive use by M. Lafaysse has further validated DSCLIM, notably by using several different large-scale variables and geographical domains. Its stochastic aspects have been studied in more details, leading to a reconsideration of these aspects when producing scenarios for very small geographical areas. Consequently a new set of post-processing scripts have been developed, starting from M. Lafaysse work, to modify how the analog day is selected within the DSCLIM methodology to take into account these stochastic aspects, while preserving the standard deviation of the results.

4 Publications

4.1 Journal Publications

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[CM2] J. Cattiaux, R. Vautard, C. Cassou, P. Yiou, V. Masson-Delmotte, and F. Codron, (2010), Winter 2010 in Europe : A cold extreme in a warming climate., *Geophys. Res. Letters*, **37**, L207704.

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[CM9] C. Cassou, M. Minvielle, L. Terray, and C. Périgaud, (2011), A statistical-dynamical scheme for reconstructing ocean forcing in the Atlantic. Part I : weather regimes as predictors for ocean surface variables., *Clim. Dyn.*, doi :10.1007/s00382–010–0781–7.

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[CM21] E. Sanchez-Gomez, S. Somot, S. A. Josey, C. Dubois, N. Elguindi, and M. Déqué, (2011), Evaluation of Mediterranean Sea Water and heat budgets simulated by an ensemble of high-resolution regional climate models., *Clim. Dyn.*, **37**, 2067–2086.

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4.2 Thesis

[CM23] L. Corre, (2011), *Evolution récente des Océans Tropicaux : le rôle de l'influence humaine.*, PhD thesis, Université de Toulouse (UPS).

6

Computational Fluid Dynamics

1 Introduction

The CFD (Computational Fluid Dynamics) team is the largest team of CERFACS. It gathers 60 to 70 researchers and more than half of them are PhD students. The team is organized around three main themes and the present text is organized in the same way :

– combustion (leader : Bénédicte Cuenot),
– turbomachinery (leader : Nicolas Gourdain),
– aerodynamics (leader : Jean Francois Boussuge).

The CFD team develops codes in these fields for CERFACS shareholders and academic partners. To build codes which are both efficient in terms of computer science and physics, the CFD team is not only developing these codes but also applying them directly to multiple real-life CFD problems in aircraft, engines, furnaces...

Important actions at CERFACS in 2012 are the consequences of the definition in 2011 of 'CERFACS challenges' for 2020. The two CFD challenges are COUGAR (the computation of a full gas turbine engine) and PUMA (the computation of a full aircraft). After defining what the targets were, the team has prepared these actions and many themes described below participate to this effort. At the same time, present actions must be continued and the support for users of CERFACS codes on a daily basis must be improved because more and more partners use CERFACS codes. This has also lead CERFACS to recognize that, in addition to developing the codes themselves, preparing interfaces for users to utilize these codes efficiently is one of the new missions of CERFACS.

The two CFD challenges correspond to multiphysic / multiscale projects. They will drive the CFD team activity in the next years but also require significant collaborations with other CERFACS teams : typically ALGO and PAE for the codes themselves and GLOBC for the coupler OpenPalm. Indeed the 2020 challenges can be met only by leading two simultaneous actions : (1) preparing CFD codes for exaflop machines (with the ALGO team anda the HIEPACS INRIA/CERFACS laboratory) and (2) preparing coupling methodologies to run multiple codes on a given exaflop machine (with the GLOBC team which has a long-term expertise in the field of code coupling).

Massively parallel computing is and will still remain a central activity of the CFD team. Staying at the forefront of HPC research in CFD is one of our goals. This is achieved by developing our own codes for all new architectures but also by working at the European level to ensure that CFD needs are taken into account in future projects. The CFD team is present for example in the EESI project (www.eesi-project.eu) which prepares the European FP8 directions in the field of massively parallel computing and in the scientific committe of PRACE (www.prace-project.eu) where scientists can have access to Tier0 machines. CERFACS is one of the few non american groups having access to the US super computers through the INCITE project (www.alcf.anl.gov/collaborations/incite10.php). CERFACS also works with machine vendors, for example Bull in 2011 to use the Curie Machine for AVBP or IBM for the BlueGene platforms.

Inside CERFACS, AVBP remains one of the world most efficient Large Eddy Simulation codes on parallel machines while elsA now allows aerodynamic simulations on thousands of processors. However, the CFD team has started thinking about 2020 along a simple question : will these codes still be our workhorses in ten years or should we start to work on a new code generation ? This work has lead to different initiatives : one of them is the collaboration with CORIA (CNRS Rouen, Dr Vincent Moureau) to work for SAFRAN on a new solver called YALES 2. Other paths are being discussed and this discussion is important because it controls the team long term evolution.

Formation and teaching is becoming an increasingly larger part of CERFACS mission. The CFD team has initiated and is now using a site dedicated to eLearning (www.cerfacs.fr/elearning) where students following courses given by CERFACS can have access to all documents. CERFACS is organizing multiple courses every year, on LES, acoustics or couplers, for researchers, partners and for laboratories. CERFACS will also collaborate to the Equip@meso project starting in 2011.
In terms of academic research and visibility, CERFACS remains very active :

– The CFD team has organized the MUSAF meeting (Multiphysics Unsteady Simulation for Aerodynamic Flows) in Toulouse on Sept 27-29, 2010 with the support of Airbus, Safran, Onera and the European commission : this meeting has gathered more than 250 world experts in the field of multiphysics applied to simulations around the aircraft and within engines. With the support of the Toulouse RTRA and the Marie Curie project COPA-GT (coordinated by the CFD team) , this workshop will be repeated in 2013.
– CERFACS is invited to meetings like SCIDAC (Scientific Discovery through Advanced Computing), QLES (Quality in LES, Pisa 2009), DEISA-PRACE symposium (Helsinki 2011) for invited plenary lectures. At SuperComputing 2010 in Hamburg, an invited talk was given on HPC and CFD by Dr Staffelbach. Young seniors of the team are also teaching, for example at the Von Karmann Institute where Dr N. Gourdain gave a course on High Performance Computing for CFD. This effort will continue.
– CERFACS distributes codes to research centers and laboratories : AVBP is available in CNRS laboratories in France (IMF Toulouse, IRPHE Marseille, EM2C Centrale, CORIA Rouen), Institut Francais du Pétrole, ONERA Toulouse and Paris. Within France, CERFACS and CORIA will collaborate within a GIS (Groupement d'Interet Scientifique) managed by CORIA to distribute AVBP and YALES 2 to all CNRS laboratories interested by these technologies. In Europe, AVBP is available at Universities of Munich, Belfast, Madrid, Zaragozza, Twente, Graz, Eindhoven ; etc. CERFACS and IFPEN (the owners of AVBP) re integrate developments coming from those partners. CRCT (Centre de Recherche sur la Combustion Turbulente) keeps working as well as ever and gathered more than 100 scientists in IFPEN in March 2010 and in Ecole Centrale Paris in March 2011.
– Outside Europe, CERFACS promotes multiple collaborations. The most active is the Stanford / CERFACS work in the field of turbulent combustion. After the post doc stays of V. Moureau, T. Lederlin, A. Roux, a new PhD (J. Dombard from IMFT) has joined CTR in 2012 to work on UQ (Uncertainty Quantification) with Pr. Iaccarino. During the 2010 Summer Program at Stanford, seven members of the CFD team spent one month at CTR to work on thermoacoustics and coupled LES/heat transfer computations (see www.stanford.edu/group/ctr/Summer/SP10).

2 Combustion

The research activity of the combustion team at CERFACS is continuously adapting to face new challenges, and is now structured in three main domains : (1) fundamentals of turbulent combustion remain an important topic to continue to improve simulation capabilities for gas turbines, rocket engines and piston engines ; other phenomena exist in such burners, such as (2) acoustics and combustion instabilities, which are another major subject, and (3) heat transfer, and more generally multi-physics, is becoming also an important topic. Such simulations require highly efficient and accurate numerical and computational methods, a central and crucial topic for the team, and imply to test solvers on all computational platforms. Multi-physics add a new dimension to parallel computing, as it includes the simultaneous coupling of different solvers. Target applications remain mainly in the domain of transportation (aircrafts, helicopters, rockets and piston engines), and has been recently extended to furnaces and explosion under the impulse of CERFACS shareholder TOTAL.

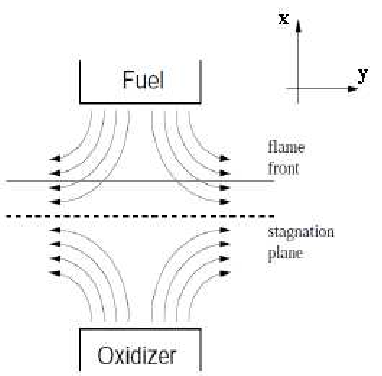
2.1 Turbulent Combustion

2.1.1 Chemistry (B. Franzelli, E. Riber, B. Cuenot, T. Poinsot)

A growing need for simulations based on reliable chemistries has been underlined in the last years to improve the prediction of flame-turbulence interactions as well as pollutant emissions. Two approaches have been proposed to overcome this problem. On the one hand, reduced chemistry consists in simplifying a detailed mechanism to obtain the main features (flame structure and species concentrations) using fewer species and reactions. CERFACS has developed a methodology to build two-step mechanisms valid over a wide range of pressure, temperature and equivalence ratio. It has been applied to kerosene-air flames [CFD70] and methane-air flames [CFD33]. These reduced schemes are systematically tested in academic laminar configurations (freely propagating premixed flames and strained premixed counterflow flames) to anticipate their behavior in three-dimensional turbulent configurations. The methodology has been tested for methane-air flames, comparing five reduced mechanisms from a two-step scheme to a more complex scheme comprising 13 resolved species and 73 elementary reactions [CFD90, CFD178]. On the other hand, tabulated chemistry is a promising technique based on the idea that tabulated information from academic laminar flames may be used for turbulent calculations. This method is still difficult to handle when heat losses, dilution by recirculating gases or several streams feeding combustion must be accounted for. CERFACS collaborates with IFPEN, CORIA and EM2C to develop tabulation methods in AVBP and apply them to complex geometries [CFD25].

2.1.2 Pollutant emissions (G. Lecocq, I. Hernandez, D. Poitou, E. Riber, B. Cuenot)

In parallel to chemistry modelling, CERFACS has started to develop soot models. Soot particles contribute to the thermal balance of a combustion chamber and can notably affect the burnt gas temperature seen by the turbine blades [CFD1]. At a larger scale, soot particles are suspected to trigger contrail formation in the wake of planes during cruise flight. Such contrails may modifiy the cloud coverage and, through altered radiative balance, affect the local climate. Soot is the product of complex processes, starting by nucleation (formation of the first particles) that occurs through collision of polycyclic aromatic hydrocarbons (PAHs), for which chemical paths are still to be understood and modeled. This step is followed by particle size increase due to mass addition on the surface, either C2H2 addition or condensation (PAHs addition). Simultaneous oxidation by both O2 and OH may counteract particle growth and even lead to particle size decrease. Finally, soot particles aggregate to form nano-size particles. Accounting for all these physical and chemical features is very demanding in terms of modelling and computing resources. Soot models are semi-empirical [20], or use sectional approaches [22], stochastic models or methods of moments [6]. As a first step, the Leung et al. [16] semi-empirical model which considers acetylene as the precursor species of soot has been chosen. Two conservation equations are solved for the soot mass fraction and the number density of soot particles, including several source terms. A tabulation method is used to predict acetylene and OH [CFD48]. The model was tested on ethylene-air flames [28], and reasonable agreement with measurements was obtained. Ethylene/oxygen/nitrogen counterflow diffusion flames with varying oxygen content [10] have been also calculated (Fig. 2.1), where soot production processes have been coupled to radiation using PRISSMA [CFD181]. The model has been finally applied to a staged helicopter combustion chamber.



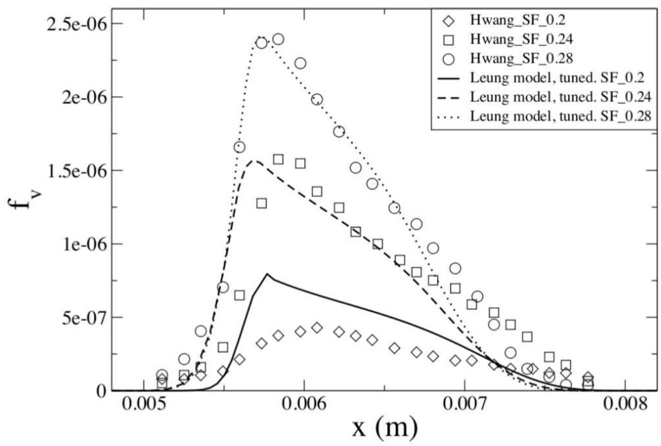


FIG. 2.1: Left : counterflow diffusion flame configuration ; Right : spatial profiles of soot volume fraction in the ethylene/oxygen/nitrogen counterflow diffusion flame with varying oxygen content in the oxidizer stream. Comparison between calculations (lines) and experiments (symbols).

2.1.3 Eulerian two-phase simulations (P. Sierra, A. Vié, 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 [8] has been developed and implemented in the code AVBP in collaboration with IMFT since 2003. The approach is based on the decomposition of the droplet velocity into a correlated and an uncorrelated contribution (RUM), this latter becoming negligible for droplet with low inertia. 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. Euler-Euler simulations in particle-laden decaying Homogeneus Isotropic Turbulence have shown reasonable agreement with reference Euler-Lagrange simulations [12] but failed in a particle-laden jet flow due to an overestimation of the uncorrelated velocity in mean-sheared flows. In collaboration with Pr O. Simonin and Dr E. Masi from IMFT, several new models have been first proposed, then a priori tested in a particle-laden turbulent planar jet flow and finally a posteriori tested with AVBP in the same configuration. The non-linear model assuming local weak equilibrium and based on an eigenvalue of the deviatoric particle rate-of-strain tensor shows very good results in Direct Numerical Simulations (DNS) of the particle-laden slab configuration (Fig. 2.2), on a wide range of particle inertia and Reynolds numbers [19]. Meanwhile, Euler-Euler LES have been performed without any RUM model in a combustion chamber and compared with Euler-Lagrange simulations. A fuel injection model has been developed for both approaches to mimic liquid fuel injection using experimental measurements and atomizer characteristics [CFD106].

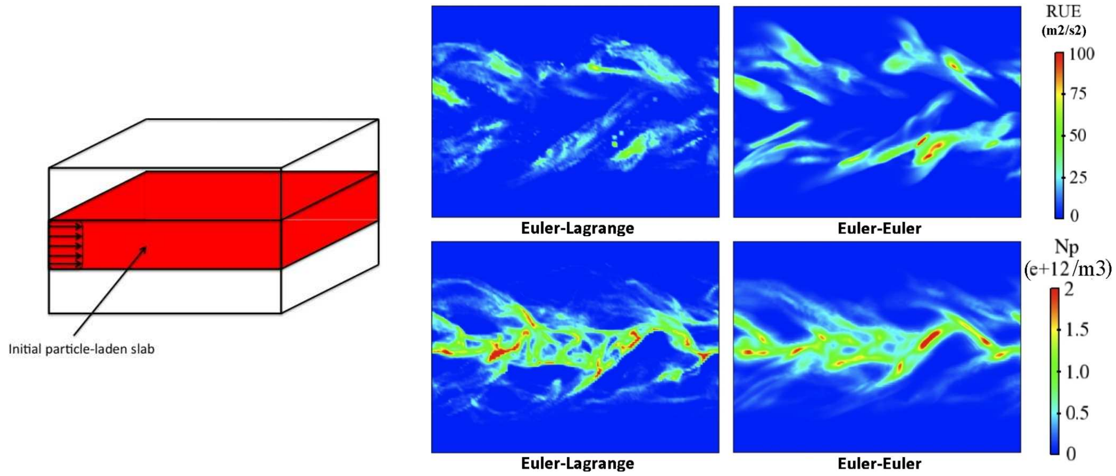


FIG. 2.2: Left : sketch of the particle-laden slab configuration. Right : instantaneous fields of Random Uncorrelated Energy (top) and droplet number density (bottom) in the vertical cut plane of the particle-laden slab configuration. Comparison between Euler-Lagrange simulations projected on the Eulerian grid (left column) and Euler-Euler simulations (right column).

Another important development was also performed during the PhD of A. Vié [CFD174], in collaboration with IFPEN (S. Jay) and EM2C Lab. (M. Massot), to extend the Eulerian formulation to polydisperse sprays.

2.1.4 Lagrangian two-phase simulations (M. Garcia, JM. Senoner, G. Chaussonnet, D. Paulhiac, E. Riber, B. Cuenot)

In parallel to the Eulerian two-phase solver, a Lagrangian solver has been built in AVBP by M. Garcia. Particular attention was put on the parallel efficiency of the solver, leading to a new partitioning algorithm which allows to take into account both the gaseous and liquid computational load. The Lagrangian solver was tested in an aeronautical burner by JM. Senoner [CFD172], showing a good behavior of the model. This work is now continued with two PhD thesis. G. Chaussonnet started in 2010 to develop a model for droplet-wall interactions, from full rebound to splashing and liquid film formation. The latter phenomenon is crucial in the injection system, as in most cases, the spray issuing from the pilot central injector impacts the surrounding diffuser walls and forms a liquid film, which flows towards the diffuser tip where it atomizes again. This means that the spray characteristics inside the chamber are not controlled by the pilot spray but by the liquid film. This work is realized in the framework of the European project FIRST. In 2011, D. Paulhiac started his PhD (CIFRE Safran/Turbomeca), with the objective to apply the Lagrangian solver to the combustion in real industrial geometries and to compare the results and performances with the Eulerian two-phase solver. Figure 2.3 shows an example of Lagrangian solution for the Mercato configuration of ONERA [15].

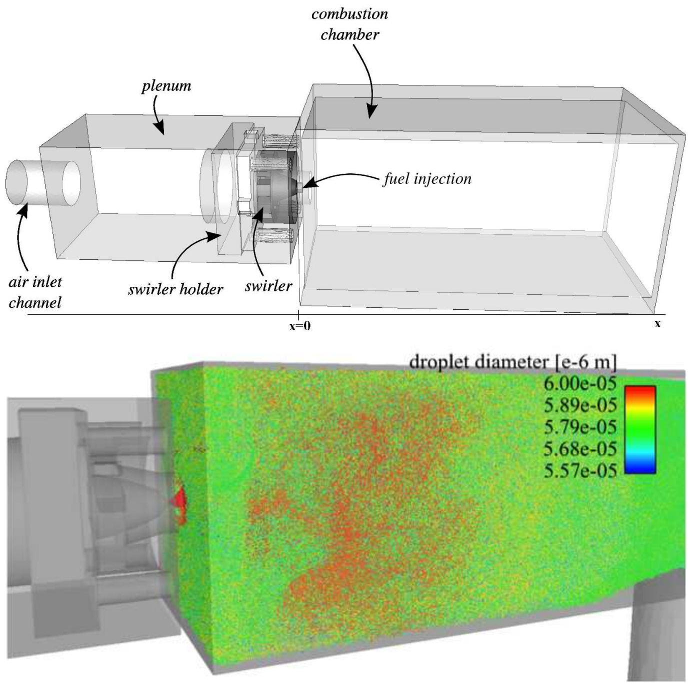


FIG. 2.3: Top : geometry of the Mercato configuration of ONERA. Bottom : Instantaneous field of droplet diameter in the Mercato configuration.

2.1.5 Ignition (D. Paulhiac, L. Esclapez, D. Barré, A. Eyssartier, G. Hannebique, A. Neophytou, B. Cuenot, L. Gicquel, T. Poinsot)

Ignition of combustion systems is a recurrent problem where multiple phenomena are at play in a fully transient process. First, the ignition of one single sector, where the ignitor is placed, is studied by depositing of energy in an unsteady cold flow. Within the Ph.D. work of A. Eyssartier [CFD29, CFD30], a first attempt to generate a probability map of ignition has been developed (Fig. 2.4), using only non-reacting LES snapshots. Results are compared to transient LES of ignition and validated against experimental data. After the ignition of the first sector, the flame must propagate to ignite neighbouring sectors and finally lead to full burner ignition.This phase controls the time needed to establish full burning, as well as the maximum distance between two sectors, above which the flame can not propagate anymore. This problem is currently studied by G. Hannebique in a multipoint burner of Snecma, by L. Esclapez (PhD started in 2011 in the LEMCOTEC european project) in a burner experimentally studied at CORIA (in the framework of the KIAI european project), and by A. Neophytou (post-doc) in a LPP configuration of Turbomeca installed at ONERA (Fauga).

2.1.6 Transcritical combustion and rocket liquid propulsion (A. Ruiz, J.-P. Rocchi, R. Mari, B. Cuenot, L. Selle)

Liquid-burning rocket engines burn cryogenic fluids, injected in the burner in a supercritical or transcritical state, ie. at either a pressure or a temperature (or both) above their critical values, so that real gas thermodynamics must be included in simulations. Since 2005, CERFACS is developing a version of AVBP for such transcritical flows, using a cubic equation of state and associated thermodynamics. These developments are performed in collaboration with EM2C lab. in Paris. Validations are usually obtained

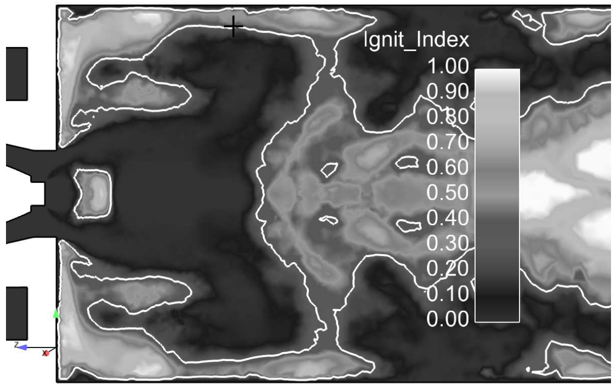


FIG. 2.4: Typical probability map for the success rate of ignition after energy deposit by a sparking device obtained in the Mercato configuration of ONERA, through the statistical analysis of non-reacting LES predictions.

[15](see Fig. 2.3),[CFD30]

on the Mascotte experiment of ONERA. A first version was available in 2008, which has been since consolidated (in terms of numerics and physics) by A. Ruiz (PhD, CIFRE Snecma), who performed DNS of transcritical mixing layers (Fig. 2.5). The next step is to couple such simulations with heat transfer, to study the impact on flame stabilization and heating of the solid parts (PhD of R. Mari, CNES fellowship).

The solver is now sufficiently mature for industrial applications : it is used to study the highly unsteady flow issuing from the coaxial injectors of the VINCI engine. The solver is installed at Snecma, under the C3S application, for direct use by engineers. Training sessions have been organized to ensure a fast and correct use of the code.

A second important aspect of liquid propulsion for rockets is ignition. It must be reliable, to guarantee 100% success, but not "violent" to avoid destructive pressure waves. However H2-O2 chemistry is very fast and powerful, therefore delicate to control for smooth ignition. LES is helpful to study mixing and combustion of both reactants in the exact real injector geometry. In this context, the initial work of Lacaze [14], studying the ignition of one injector, has been continued in the PhD of JP. Rocchi to address the ignition of a set of injectors and the driving mechanism of flame propagation from one injector to the other.

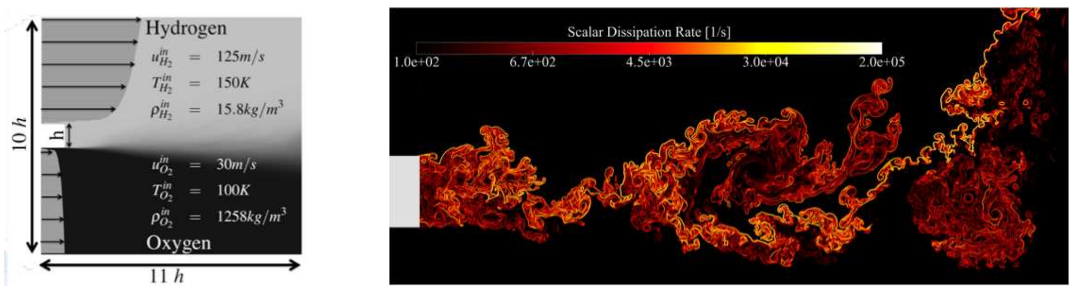


FIG. 2.5: Direct Numerical Simulation of a transcritical mixing layer.

[CFD60]

2.1.7 Two-phase reacting flows in aeronautical engines (G. Hannebique, L. Esclapez, A. Neophytou, E. Riber, B. Cuenot)

LES is now currently used to help for the design of new combustor geometries for aeronautical engines. Today's preoccupations of engineers are to decrease the NOx and CO production, while keeping high combustion efficiency and stability. This reflects in a number of past and present european projects, such as TLC, TECC or LEMCOTEC. In these projects, LES of multi-point burners of Snecma (PhD of G. Hannebique and L. Esclapez), and LPP (Lean Premixed Pre-vaporized) burners of Turbomeca (A. Neophytou) are performed to characterize the two-phase flame structure, ignition behavior, pollutants emission and combustion efficiency.

2.1.8 Piston engines (V. Granet, B. Enaux, A. Misdariis, O. Vermorel, T. Poinsot)

In piston engines, cycle-to-cycle variations (CCV) affect combustion efficiency, and must be understood and controlled to optimize engines. 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. Moreover the simulation of CCV remains a computing challenge today, which only a few groups in the world have tried to tackle.
The multi-cycles LES performed during the PhD thesis of B. Enaux [CFD89, CFD88] and V. Granet [CFD95] have confirmed the high potential of LES to reproduce cyclic combustion variability in spark ignition engines (Fig.2.6). Thanks to the LES database, which includes more than 150 individual cycles, and to the experimental database of IFPEN created during the SGEMAC ANR project, different scenarii have been proposed to explain why and how a specific operating point can generate high CCV levels. In the present case, it was shown that CCV are essentially due to aerodynamic fluctuations at the spark plug, which induce variations of the early flame kernel growth and of the overall combustion duration.

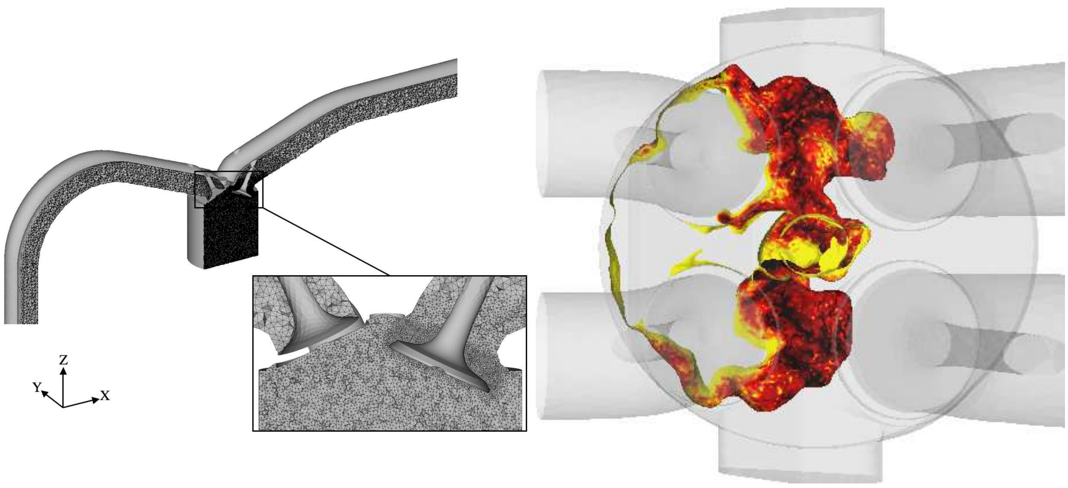
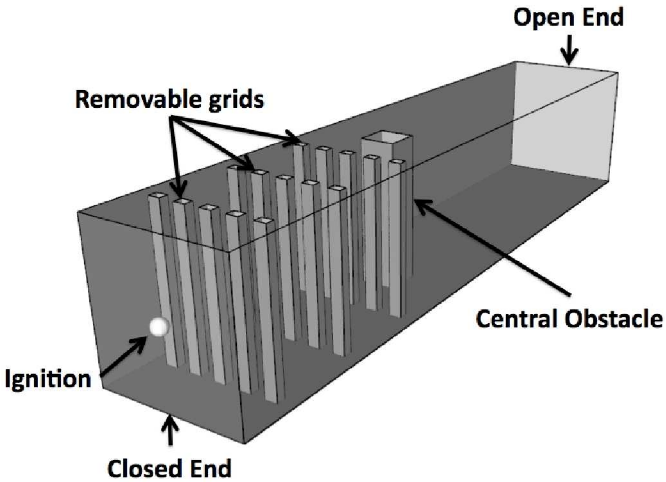


FIG. 2.6: Combustion variability in a four-valve spark ignition engine : iso-surface of temperature for 4 consecutive LES cycles (same crank angle).

2.1.9 Explosion phenomena (P. Quillatre, O. Vermorel, T. Poinsot)

Accidents due to gas explosions are a major concern for oil or chemical industries. Being able to locate precisely the hazardous areas in industrial buildings, typically offshore oil and gas producing platforms is an issue of prime importance. Thanks to the growing computational power, LES appears as an interesting alternative to experiments which are expensive and to URANS (Unsteady Reynolds Averaged Navier Stokes) approaches which are classically used to simulate gas explosion configurations nowadays. In this context, a first application of LES in a combustion venting chamber with obstacles [13] has been performed. Figure 2.7 displays a typical example of the turbulent propagation of the flame in this semi-confined configuration. The first results showed the ability of LES to capture accurately the peak over-pressure in the chamber, which is the critical parameter in industrial safety. A sensitivity analysis revealed that chemistry and molecular transport modeling play an important role in the pressure history and its peak value.



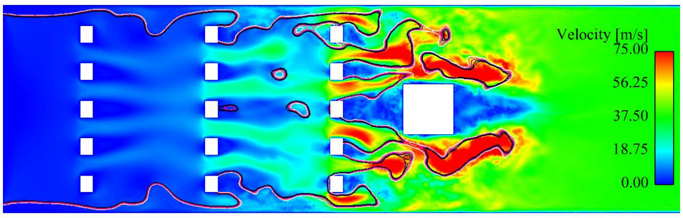


FIG. 2.7: Visualization of the flame propagation past repeated obstacles (AVBP results). Velocity field and iso-surfaces of reaction rate in the combustion venting chamber of Sydney.
[13]

2.2 Acoustics and combustion instabilities

CERFACS studies both the noise created by combustion and the instabilities induced by combustion when it gets coupled to acoustics. Most applications are dedicated to gas turbines. Studies are performed in close collaboration with the top European laboratories working in this field (TU Berlin, EM2C Paris, TU Munich, Un. Twente, Cambridge) : in most collaborations, CERFACS takes care of the large scale computations. Simulation methods for noise and instabilities have common elements. Both rely heavily today on LES of the combustion chamber. For combustion noise studies, LES is coupled to analytical methods to propagate the noise through the turbine stages. For combustion instabilities (CI), two methods are used :
(1) Brute force LES : recent progress in LES of reacting flows allows simulation of full combustion

chambers and theoretically of CI. This is an attractive method made possible by recent progress in HPC technologies on machines using 10 000 to 300 000 processors and demonstrated by various groups in the last years, many of them using the AVBP code developed at CERFACS [23, 27].
(2) Thermo-Acoustic (TA) codes coupled to forced response LES : in most CIs, acoustics are the dominant resonant mechanism and a proper method to decompose the physics of CIs is to use TA codes which can track the propagation of waves in the combustor. In this approach, the mean flow is frozen and the solver only tracks the acoustic modes of the system. The flames are replaced by active components (which can be compared to complex loud speakers). If the action of these active elements is properly represented, the global stability of the combustor can be predicted.

Both methods are required to understand CIs. A major interest of TA codes is to isolate the elements leading to CIs into different blocks (something a brute force LES cannot do) : a) the acoustics of the combustor, b) the outlets and inlets impedances and c) the response of the flame which is quantified by a function called the Flame Transfer Function (FTF) describing how much unsteady heat release is produced by a flame when it is submitted to an acoustic velocity fluctuation.

2.2.1 Combustion noise (M. Leyko, I. Duran, C. Silva, C. Lapeyre, T. Livebardon, F. Nicoud, S. Moureau)

The noise generated by unsteady combustion in a gas turbine is becoming a significant source for aircraft and helicopter engines. CERFACS is studying combustion noise with SNECMA (PhD of M. Leyko and I. Duran), TURBOMECA (PhD of T. Livebardon) and through national or European projects like BRUCO, DISCERN or ECCOMET (PhD of C. Silva and C. Lapeyre). This work is performed in close collaboration with Pr. Nicoud (Montpellier) and Pr. Moreau (Un. Sherbrooke, Canada). Evaluating the noise generated by combustion in a gas turbine requires to compute the noise sources (due to unsteady combustion) but also their propagation through the turbine stages. For the generation, CERFACS performs LES of combustion chambers. For propagation, CERFACS analyzes the waves leaving the combustor outlet in the LES and computes their transmission and reflection through the turbine stages using the compact nozzle analytical theory [17, CFD99] proposed initially by Marble and Candel [18] and extended by Cumpsty and Marble [5]. In 2012, these methods will be applied to two new combustors : a lab-scale burner installed at EM2C Paris (DISCERN) and a full helicopter engine at TURBOMECA instrumented in the European TEENI project.

2.2.2 Brute force LES of combustion instabilities (I. Hernandez, S . Hermeth, P. Wolf, G. Staffelbach, T. Poinsot)

CERFACS explores brute force LES of combustion instabilities (CIs) in different configurations : in laboratory burners during the LIMOUSINE Marie Curie project, I. Hernandez performed an LES of self-excited oscillation modes in a lab-scale combustor installed at U. Twente and showed that LES was able to capture the first two unstable modes observed experimentally and to predict that these modes would disappear when the equivalence ratio would decrease. S. Hermeth, working in the MYPLANET Marie Curie project, studied the forced response of another lab-scale combustor installed at TU Berlin before simulating one sector of a real industrial burner for the Ansaldo company. Finally, P. Wolf (PhD for TURBOMECA) has performed the largest LES ever done for combustion in a 360 degrees combustion chamber. This work initiated during the 2010 Summer Program of CTR at Stanford has lead to various publications [CFD64, CFD110], providing new insights into the nature of the azimuthal turning or standing modes in full annular chambers. For all these brute force LES, companion simulations using acoustic solvers (TA codes, see Section 2.2.3) have been performed to compare the output of the TA code to the LES data. A workshop organized at CERFACS on Nov. 22, 2011 with most European experts (Alstom, Siemens, Safran, TU Berlin, TU Munich, EM2C Paris) has allowed to identify the paths to follow to combine experiments and high fidelity simulations to study CIs.

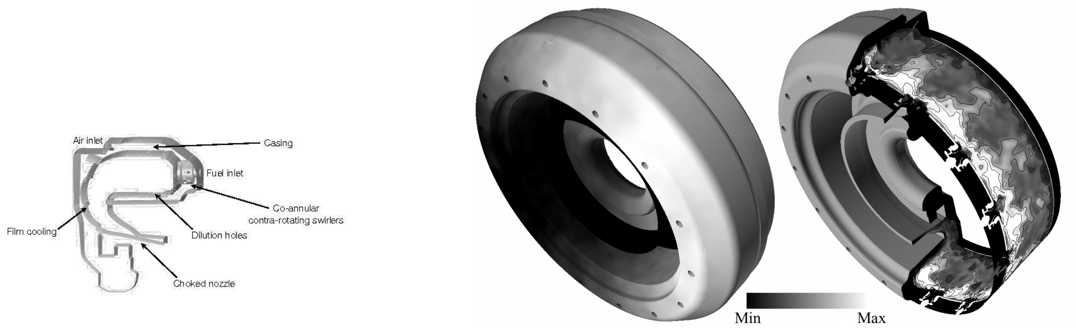


FIG. 2.8: Large Eddy Simulation of azimuthal unstable modes in a full annular burner. Left : configuration of a single sector. Center : instantaneous pressure field on combustor skin. Right : isosurfaces of velocity colored by temperature. PhD of P. Wolf.
[CFD184]

Fig. 2.8 shows an LES of a self-excited CI in a gas turbine combustion chamber [CFD110] : this high resolution LES (40 to 330 million cells) running on a BlueGene machine (16 000 proc.) captures the instabilities which appeared for certain regimes in the first prototypes of the real engine. Acoustic waves interact with combustion, leading to a strong unstable mode characterized by periodic flashback through the swirling systems used to inject and mix fuel. For the fine grid (330 million cells), 1000 CPU years were used.

2.2.3 Acoustic solvers (TA codes) (E. Gullaud, C. Silva, K. Wieczorek, P. Salas, E. Motheau, JF. Parmentier, L. Giraud, T. Poinsot,F. Nicoud)

The efforts to build a powerful TA code have been intensified at CERFACS with the development of a new branch dedicated to combustion noise. The TA and LES computations of the CESAM experiment of EM2C [CFD173, CFD108] will be pursued during DISCERN ANR project started in october 2011. Different models for the acoustic dissipation induced by perforated liners were also implemented [CFD170] and were used for large scale computations of full engines. Such computations are now easier thanks to the improvement of the numerics of AVSP made by L. Giraud (HIEPACS project) and his PhD student (P. Salas) supported by the MYPLANET Marie Curie project lead by the CFD team (Dr. T. Schönfeld). The required boundary conditions are also computed by a new dedicated tool (SNozzle which took over Nozzle in 2011) which solves the full Linearized Euler Equations for nozzle flows under the quasi-1D approximation. Thanks to SNozzle, the acoustic-entropy waves interactions in the accelerated regions and the contribution from the rotor stages are now accounted for properly when computing the effective impedance of compressors and turbines [CFD173]. A consistent way to use these equivalent upstream/downstream boundary impedances in the framework of a Helmholtz solver such as AVSP was also established by E. Motheau [CFD52]. At last, several theoretical works were conducted to support the AVSP development : an original quasi-analytical model for instability modes in an annular combustion chamber fed by N burners was proposed by J-F. Parmentier [CFD103]. This model was used to demonstrate the ability of AVSP to perform the modal analysis of annular geometries where standing modes can combine to produce rotating modes as observed in actual systems. The impact of the zero-Mach number assumption on the modal analysis was also studied in details by K. Wieczorek [CFD175]. Theoretical assessments of the non-zero Mach number effects on the frequency of oscillation and growth rate of the thermo-acoustic modes of a quasi-1D academic configuration [21] were obtained. A methodology to predict the transient growth generated when several non-normal stable modes combine was also derived [CFD109].

2.3 Heat transfer and multi-physics

2.3.1 Radiation (J. Amaya, D. Poitou,T. Pedot, F. Duchaine, B. Cuenot, M. el Hafi)

Radiative heat transfer has a non-negligible impact on flames. In small burners, the radiated energy is small compared to the combustion energy, and can be neglected in the energy balance, but it may locally modify the gas temperature and the subsequent production of pollutants such as NOx or soot. In large burners or fires, radiation becomes the main heat transfer process and controls the flame. In combustors, the radiative heat transfer is not limited to wall exchanges, as hot products such as water vapor or CO2 have the capacity to both absorb and emit thermal radiation. As a consequence, radiation calculations in combustors must solve the Radiative Transfer Equation (RTE) in the gas, taking into account their spectral behavior.

In collaboration with M. el Hafi from EMAC, a radiation solver (PRISSMA) has been developed, using the Discrete Ordinate Method (DOM) and several spectral models for the gas [CFD105]. This solver has been used in the PhD of J. Amaya [CFD168] to study the impact of radiation on the temperature distribution at the exit of the combustion chamber of a helicopter engine [CFD1]. A similar work was started by D. Poitou (post-doc) in the framework of the STRASS project (FNRAE), and is now continued by F. Duchaine. Finally, PRISSMA was also used by T. Pedot (PhD, defended in Feb. 2012) to calculate heat transfer in a refinery furnace, in order to predict the occurrence of coking in the heating tubes (Fig. 2.9).

In all these problems, one critical parameter is the wall temperature, usually unknown. To determine this wall temperature, coupling of the radiative, convective and conductive (in the solid wall) heat transfer is performed (see Section 2.3.3).

Due to the non-local nature of the RTE and the complexity of gas spectra, radiation calculations are extremely demanding in terms of CPU costs. Important efforts have been already made to reduce this cost, mainly directed towards simplified spectral models and increased parallelism over the discrete directions of the RTE and the frequencies of the spectra. Recently a significant step has been made, with the successful implementation of parallel domain decomposition, which raises particular difficulties due to the sequential nature of the RTE solving algorithm.

2.3.2 Fluid-structure interaction in Solid Rocket Motors (J. Richard, F. Nicoud)

Solid Rocket Motors (SRM) may be subjected to thrust oscillations which might jeopardize the integrity of the payload due to vibrations. The phenomenon has been investigated extensively over the last decades. This mechanism arises from a coupling between the acoustic mode and the hydrodynamic perturbation, as represented in Fig. 2.10(left). An unstable shear layer in the mean flow produces vortices which are convected until they impact the head of the nozzle. The acoustic wave generated by this impact can move back upstream since the mean flow is subsonic. It then perturbs the unstable shear layer, intensifying the generation of vortices. Such an aero-acoustic mechanism can lead to high amplitude fluctuations when the underlying frequency is close to the frequency of an acoustic mode of the whole geometry. A numerical chain was built in order to assess to what extent the coupling between the fluid flow and the engine structure (Fig. 2.10 (right)) influences the amplitude of the aeroacoustic oscillations within the combustion chamber. A particular attention was paid to the coupling algorithm between the fluid and the solid solvers (AVBP and MARC respectively, coupled with Open-PALM) in order to ensure energy conservation through the interface [CFD56, CFD57].

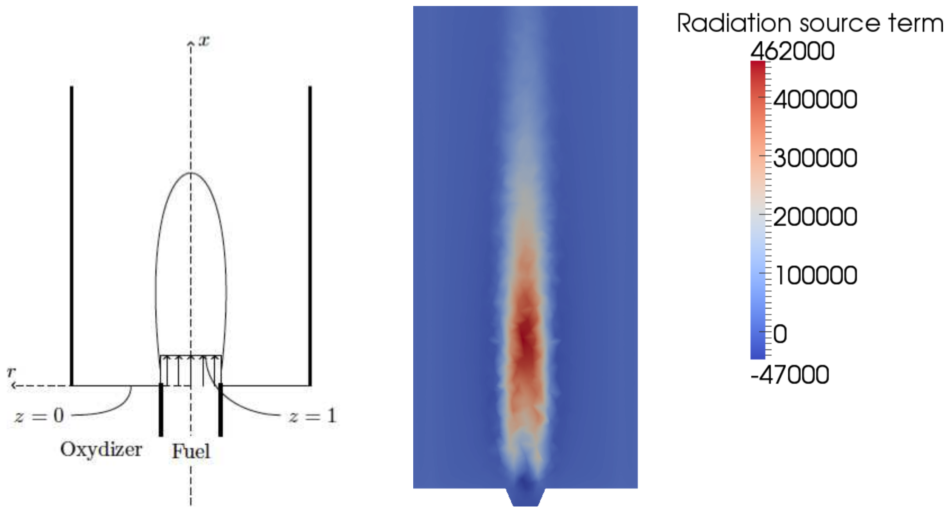


FIG. 2.9: Radiation source term of one refinery furnace burner (W/m^3).

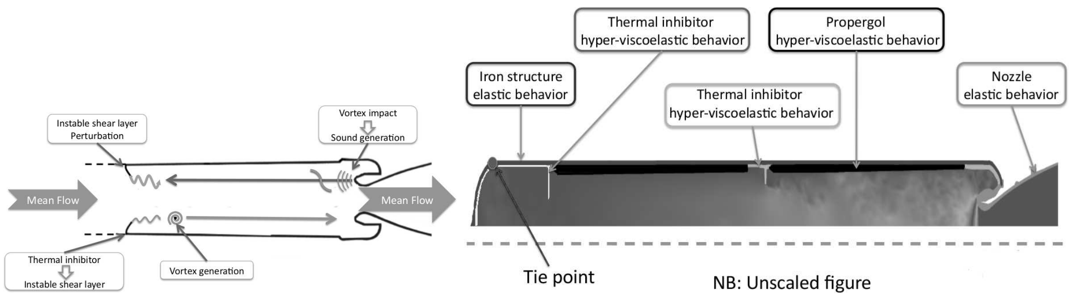


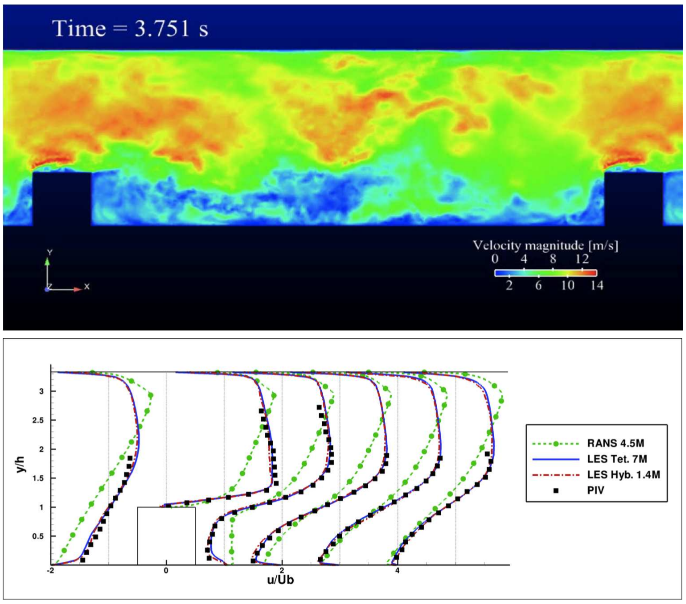
FIG. 2.10: Instabilities mechanism (left) and fluid-structure interaction (right) in the rocket configuration. The thermal inhibitor vibrates and creates vortices which impact on the nozzle.

2.3.3 Coupled simulations (J. Amaya, D. Poitou, Y. Hallez, T. Pedot, G. Wang, R. Fransen, E. Collado, S. Jauré, L. Gicquel, F. Duchaine, B. Cuenot, T. Poinsot)

The optimization of many industrial devices such as gas turbine and electronic components are complex multi-physics and multi-component problems that have long been based on engineer intuition and expensive experiments with trial and error tests. Being able to include for example thermal transfer in combustion simulations makes the result much closer to reality and allows to better understand the behavior of the complete system. This is part of the objectives of the ”2020 Grand Challenges” of the CFD team. Multi-physics and multi-component simulations imply not only to master different physics and their associated solvers, but also the way they are coupled. This raises the questions of when, where and which variables should be exchanged between the solvers.
Determination of heat loads, as wall temperatures and heat fluxes, is a key issue in combustion : the interaction of hot gases and reacting flows with colder walls is an important phenomenon in combustion chambers and a main design constraint in gas turbines. In 2010, Hallez *et al.* [CFD96] demonstrated the importance of conjugate heat transfer for the prediction of thermal efficiency in hot jets in cross-flow over cold plates. Similarly, by taking into account conjugate heat transfer, R. Fransen has worked on the

prediction and dimensionalisation of cooling channels in aeronautical applications (Fig. 2.11). Amaya *et al* [CFD1] showed interesting results on the thermal environment of a combustion chamber by coupling three solvers (Combustion-AVBP, heat conduction-AVTP and radiation-PRISSMA) with the coupler PALM. Such coupled simulations have been also run by D. Poitou and F. Duchaine in the framework of the FNRAE-funded STRASS project.

(a)



(a)

FIG. 2.11: (a) Transversal instantaneous view of the LES velocity field prediction for ribbed cooling channel typical of turbine blade cooling systems and (b) validation of the predictions obtained with several grid resolution and modeling tools.

[CFD32]

Thanks to a collaboration with ONERA, PALM has evolved to an open source code called OpenPALM in 2011 with among other new features an enhancement of massively parallel coupled simulations based on mesh exchanges. With the clear intent of producing reliable solutions for real gas turbine burners, issues of efficiency and code implementation of massively parallel coupled conjugate heat transfer solutions are at the center of the work of S. Jauré, Fig. 2.12 [CFD46]. A part of the activity focuses on the determination of methodologies to ensure the stability and the precision of the coupled schemes with the lowest restitution times. The aerothermal chain AVBP/AVTP/PRISSMA uses these new functionalities which opens the door to a wide range of new problems and applications based on LES.

Finally studies have started in 2011 to analyze the interaction between the combustion chamber and the turbine, using LES with AVBP for the combustors and RANS/URANS with elsA for the turbine. Ongoing solutions investigate the interface needed for the one-way and two-way coupling (feedback of elsA predictions to be imposed back to the AVBP computations), in the framework of the PhD of E. Collado and the post-doc of G. Wang.

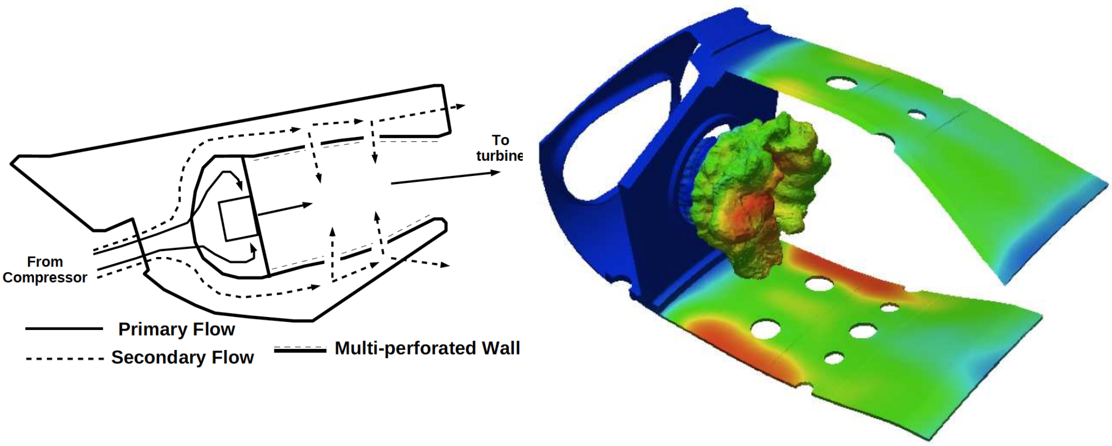


FIG. 2.12: Conjugate heat transfer prediction obtained by use of a massively parallel solution applied to a gas turbine combustor : field of wall temperature complemented by an iso-surface of temperature, allowing to visualize the flame position in the LES instantaneous prediction used in the coupled solution.

2.4 Methods

2.4.1 Numerics (M. Kraushaar, L. Gicquel, V. Moureau, G. Wang, F. Duchaine, L. Giraud)

Numerical schemes for LES require certain properties, i.e. low-diffusion schemes of high-order of accuracy so as not to interfere with the turbulence models. To meet this purpose in the context of fully unstructured solvers, a new family of high-order time-integration schemes with adjustable diffusion has been proposed by M. Kraushaar in his thesis, in collaboration with CORIA (V. Moureau) [CFD182].

Another aspect is the comparison of compressible and incompressible formulations. Being fully unsteady by nature, LES is very consuming in terms of CPU time and a possible way to decrease this cost for low-speed flows is to use low-Mach or incompressible formulations, allowing much larger convective time-steps. This is of particular interest for the simulation of combustors, where the flow velocities stay often low. The impact of the incompressibility assumption and the different nature of the numerical algorithms have also been addressed in the PhD of M. Kraushaar, where detailed comparisons of a fully explicit compressible solver and an incompressible solution developed at CORIA (YALES2 code) are proposed for an experimental swirled configuration representative of a real burner.

Work has also been done on the AVTP solver, for heat conduction in solid media. In order to relax the time step constraint imposed by the Fourier condition on the explicit scheme implemented in AVTP, an unconditionally stable implicit scheme has been implemented . Using the mesh partitioning parallelism of AVTP and adapting the existing numerical kernels, matrix-free parallel linear solvers were designed for the linear systems involved in implicit schemes. These linear solvers are based on Krylov subspace techniques, namely un-preconditioned Conjugate Gradient and un-preconditioned GMRES. Even though implicit schemes enable significant decrease of the parallel elapsed time for AVTP, up-to a speed-up of 200, further improvement will be gained by preconditioning techniques. To this purpose, scalable preconditioners will be designed, having a convergence behaviour independent of the number of subdomains and weakly dependent on the subdomain size.

2.4.2 HPC (G. Staffelbach, P. Wolf, L. Kuban)

Following the global trend to ever more powerful computers, CERFACS has continued optimizing and pushing the limits of its solvers on new architectures. For example the scalability of the AVBP solver has been pushed up to 92% of the ideal performance on 16384 cores on the BlueGene P at Argonne. This activity has been a continued effort along scientific projects on the national project calls by GENCI and National Grand Challenges at CINES [CFD64] and CEA but also on international initiatives such as INCITE and PRACE. CERFACS has been one among only three european project holders under the American Department of Energy INCITE program in 2010 and in 2011 focusing on HPC applied to combustion instabilities and two-phase flows. In parallel CERFACS was awarded 8.5 million CPU hours in the 2nd call of PRACE, to study high frequency jet interaction under transcritical conditions with EM2C (Paris). The ANR COSINUS project SIMTUR has also enabled CERFACS to simplify the workflow, leading to even more challenging simulations such as the extinction mechanisms of an aeronautical engine performed by L. Kuban (Fig. 2.13). This shows that HPC is of direct interest to applications and that HPC technology transfer towards industry is effective.

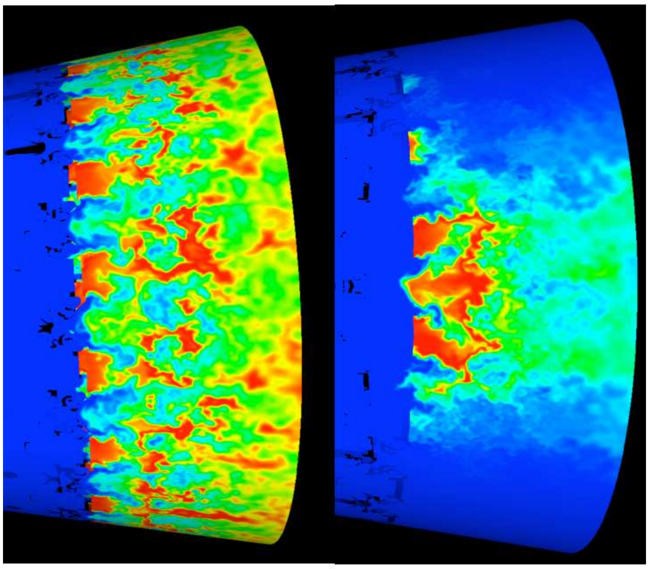


FIG. 2.13: Combustion in a full aeronautical engine : temperature field on a cylinder passing through the axis of the swirlers when all of them (left) or only one of them (right) are fed with fuel (ANR SIMTUR)

2.4.3 ”Interface Homme-Machine” (IHM) C3S (A. Dauptain, E. Riber, G. Frichet)

CERFACS believes that developing interfaces for LES runs is as critical today as developing the LES tools themselves. The C3S project is dedicated to the construction of this interface and is continuously using two to four researchers/engineers at CERFACS. C3S is now used on a daily basis at CERFACS, IMFT, SNECMA and Turbomeca. In april 2011, an industrialized version of AVBP-Gaz Réels has been included and made available to SAFRAN-Vernon, for rocket engine liquid propulsion simulations. In July 2011, a tool to directly and simply plug AVBP results into other engineering tools of the ”Bureau d’Etudes” has been delivered to Turbomeca. This last step places our numerical tools at the center of the design methodology, and increases the link between Cerfacs and its partners.
In parallel, the C3SM project started in april 2011. C3SM is a first prototype of IHM of second generation,

designed to alleviate the work of the developing teams while significantly improving the user perception of the interface. A detailed analysis of the underlying concepts has been presented at the last colloque INCA [CFD26]. As a first step, C3SM will include the YALES2 code developed at CORIA (Rouen). This will be followed by the inclusion of most numerical tools developed by the combustion group (AVBP, AVSP, AVTP, PRISSMA). The C3SM project has received a very positive response from Cerfacs partners, confirmed by several requests to use it : SAFRAN for N3S-Natur, ONERA for the code CEDRE. This success goes beyond CFD, with a request from CNES to use C3SM for the electromagnetism code CESC developed at Cerfacs. SAFRAN will continue to support C3SM in 2012, for the first time together with automotive industry via the ”Groupement scientifique moteurs (GSM)”, for LES solutions for IC engines.

3 Turbomachinery

The turbomachine group is the most recent component of the CFD team and gathers around 12 people. The main effort of the group has been put on the development and the application of methods to simulate unsteady flows in compressor and turbine components. Recent breakthroughs include the successful implementation of the harmonic balance method in *elsA* and the application of LES (both with *elsA* and AVBP) to address complex flow phenomena (such as shock/boundary layer interaction and laminar-turbulent transition) in turbomachine configurations. Another promising work is the code coupling activity : coupling methods are developed in cooperation within the CFD team (COMB and AAM groups) and with the GLOBC team (which develops the code coupling tool Open-PALM). The target is to prepare techniques for the 2020 challenge ”COUGAR” (for which the objective is to perform an unsteady flow simulation in a whole gas turbine). The work of the turbomachinery group also led to industrial applications, supported by SAFRAN, Airbus and EDF. The group is involved in European Projects (*e.g.* COPA-GT, a Marie-Curie program, and FACTOR). The cooperation with research partners (VKI, LMFA, ONERA) has also been strengthened through the co-direction of Phd students and the definition of common test cases (CREATE, LS89, etc.).

3.1 Numerical methods and software

The development of numerical methods for turbomachinery focuses on three main topics : the reduction of the computational cost for unsteady flows, the quantification of the solution to unknown/uncertain parameters and the code coupling activity.

3.1.1 Spectral methods : development of the Harmonic Balance Technique (T. Guedeney)

Some flows are controlled by a strong periodic forced activity : for turbomachinery flows for example, developing a method which includes this information allows computations that are more efficient than classical unsteady CFD approaches (Dual Time Stepping, etc.). The Time Spectral Method (TSM) has been implemented in the code *elsA* following this philosophy. Thanks to Fourier spectral analysis, the unsteady Navier-Stokes equations can be read as $2N + 1$ steady problems coupled by a source term (with N the number of harmonic of a frequency given by the user). The phase-lagged functionality [7] has been also implemented in the spectral method to reduce the computational domain to only one single blade passage per blade row.

The TSM is able to deal with only one frequency and its harmonics (for example the blade passing frequency) and is therefore limited to a single stage computation. To extend the method to multistage turbomachines, it is mandatory to take into account several frequencies which are not necessarily multiples of a base frequency. This new method is called the Harmonic Balance Technique (HBT). To implement the HBT, all features developped for TSM were adapted to a multifrequential formulation. However, while the position of the time instants with TSM was simply equally distributed along the flow period, the same approach with HBT led to serious conditioning problems, especially for multifrequential test cases. To circumvent this issue, different methods such as the APFT algorithm (which stands for Almost Periodic Fourier Transform) or genetic algorithms have been implemented. The development of the HBT is now completed and the validation step has already started [CFD42].

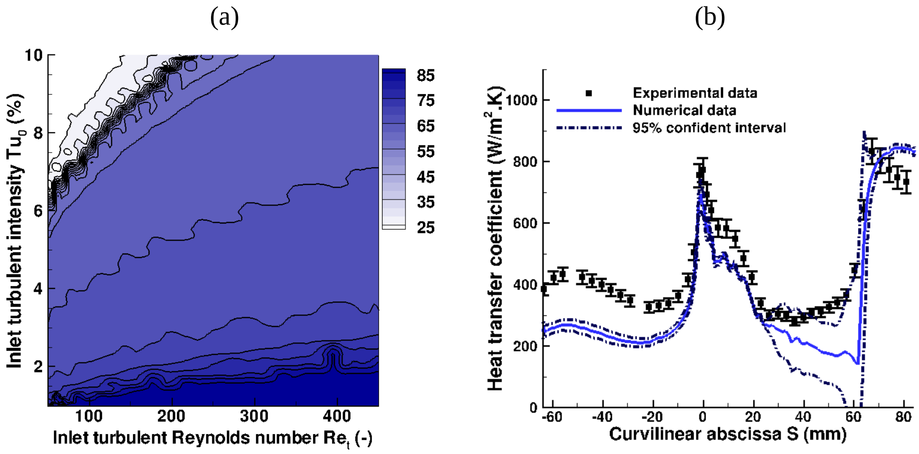


FIG. 3.1: Application of a UQ method to turbomachine configurations : influence of inlet turbulent Reynolds number Re_t and turbulent intensity Tu on (a) the transition abscissa in a turbine guide vane (the leading edge, resp. the trailing edge, is located at $S = 0$mm, resp. $S = 85$mm) and (b) the wall heat flux.

3.1.2 Uncertainty quantification : development of a stochastic collocation method (K. Dewandel, N. Gourdain)

The simulations of flows in real gas turbine configurations usually consider geometries and flows that are different from the reality (ill-defined boundary conditions, inaccuracy of the geometry, etc.). These differences can significantly affect the accuracy of the numerical solution. The aim of this work was thus to apply a method to turbomachinery test cases, in order to estimate the influence of unknown/uncertain parameters on the numerical solution. The approach is based on a Stochastic-Collocation (SC) method, based on Clenshaw-Curtis sampling points.
This method is validated against the classical Monte-Carlo (MC) method (that uses random sample points to describe the space of parameters) [CFD38]. The computational cost required to evaluate the sensitivity to two parameters is reduced by a factor 30 with the SC method compared to MC. The SC method is then applied to an inlet guide vane of a high-pressure turbine (shown in Fig. 3.7) and a three and a half stage compressor (shown in Fig. 3.4). For the turbine case, the results quantify the sensitivity of the wall heat transfer to inlet turbulent intensity, inlet turbulent Reynolds number and outlet Mach number. For the compressor case, the study shows the dependence of the overall performance (pressure ratio, efficiency and stability) to the size of the rotor tip clearances. An example of how such methods can provide useful information is reported for the turbine test case in Fig. 3.1(a) (dependency of the transition abscissae to inlet turbulence) and Fig. 3.1(b) (dependency of wall heat fluxes prediction to inlet turbulence).

3.1.3 Code coupling methods : application to *elsA* / *AVBP* (E. Collado Morata, F. Duchaine, M. Montagnac)

CFD for turbomachinery usually focuses only on isolated components while real systems involve interactions between different components and physics (aerodynamics, heat transfer, combustion, etc.). The goal of this research topic is to enable large-scale integrated simulations of unsteady turbulent flows in gas turbines. The study is a preliminary mandatory work to achieve the objective of other ambitious projects, such as FACTOR (flow simulation in a combustion chamber simulator coupled with the high-pressure turbine) and COPA-GT (flow simulation in the compressor/combustor module). Due to the specificity of each component, the flow is not necessarily solved with the same numerical method in the whole system. For example, previous works indicate that LES is a very efficient method for predicting reactive flows in a combustion chamber while RANS based approaches are more convenient for turbomachines. Based on a literature review, the first step towards integrated simulations is to develop a framework to exchange information between the combustion chamber (LES with the unstructured code AVBP) and the high-pressure turbine (RANS with the structured code *elsA*). The coupling between AVBP and *elsA* has been developed using the Open-PALM code coupling tool. The technique is based on the exchange of the conservative variables from AVBP to *elsA* with a method similar to the Chimera approach while *elsA* sends the pressure information to define the outlet non-reflective boundary condition of AVBP. This coupling process is done at each iteration of the flow solver until convergence is achieved. It was validated in a simple test case : a laminar Poiseuille channel flow. The technique needs now to be validated and tested with more complex test cases.

3.1.4 Code coupling methods : application to *elsA* / *elsA* (F. Crevel, M. Montagnac)

For some specific applications the use of different time steps can be helpful to reduce the cost of an unsteady flow simulation. For example, to describe a surge cycle in a gas turbine, it is mandatory to simulate both high frequencies (generated by the blade passing frequency, o(10,000)Hz) and low frequencies (due to the surge phenomenon, o(1)Hz). A simulation with a unique time step would need very large computing resources to describe the low frequency phenomenon. In that context, a simulation that uses a large time step in parts where only the description of low-frequency is important, coupled with a simulation that uses small time steps (where high-frequencies must be computed) is an attractive approach. This method has been tested by coupling two *elsA* simulations (considering two different time steps) with the Open-PALM coupling tool.

The coupling developed here is based on the exchange of conservative fields on an interface defined by the user. The simulations are time accurate, which means that if N is the ratio between the time steps used in the two simulations, the large-time-scale simulation does one time step while the small-time-step simulation does N time steps. The small-time-step simulation sends to Open-PALM N fields while the large-time-step simulation only sends one. Open-PALM allows to exchange fields after calculating a moving average in order to smooth the solution over a coupling period. The application was tested on a turbulent channel. The channel is split in two parts and a wake is injected in the upstream part. As shown in Fig. 3.2, the wake is well transmitted in the downstream channel by the coupling method.

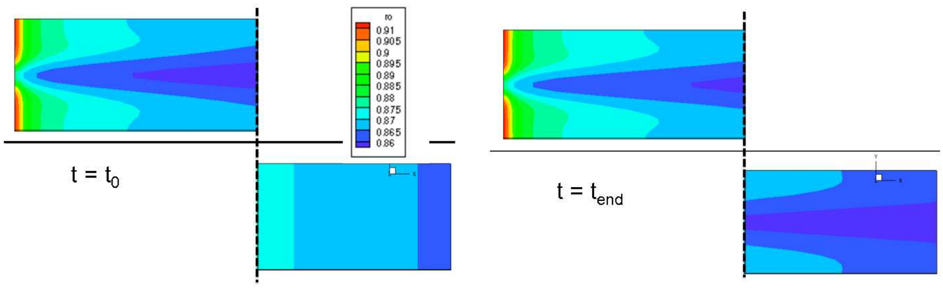


FIG. 3.2: Coupling of two *elsA* simulations with the code coupling tool Open-PALM. The fields, colored with the density, show that the wake generated at the inlet of the upstream channel (up) is transmitted to the downstream one (bottom).

3.1.5 Post-processing methods : development of the MARS tool (G. Legras, F. Wlassow)

An original post-processing tool called MARS ("Module d'Analyse du ReSidu") has been developed to analyze the results of aerodynamic simulations, originally for casing treatment applications [CFD183]. MARS is dedicated to the budget analysis of terms of all important terms in (U)RANS equations on control volumes. The tool can be used to analyzed the momentum conservation as well as the entropy production equation to determine the source and the location of entropy production. For example, Fig. 3.3(a) shows that the main contribution to entropy production in a high pressure turbine rotor passage is turbulent dissipation. Figure 3.3(b) allows to identify the main regions of entropy production in the control volume by presenting the entropy production along the axial distance at 95% of the blade span (close to the casing). Three areas are identified : the stagnation point region where entropy production is associated with friction losses, the near wall region along the blade where entropy production is also associated with friction losses and the aft part of the blade where the tip leakage vortex and passage vortex interaction increase the production of entropy (at about 50% of the blade chord). MARS has a great potential to investigate complex 3D flow fields and provide intelligible information, useful both for the analysis of profile performance and the understanding of the flow topology.

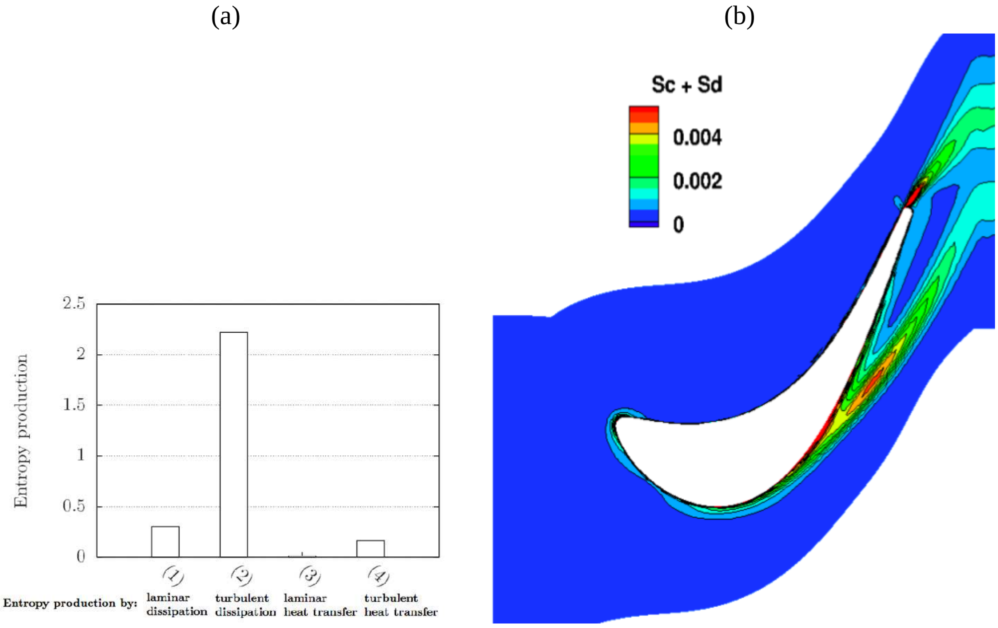


FIG. 3.3: Application of MARS to a high-pressure turbine test case : (a) source of entropy production and (b) view of the entropy production at 95% of the blade span.

3.2 Applications

The applications to turbomachinery flows deal with purely aerodynamic simulations (*e.g.* aerodynamic instabilities, shock/vortex interaction, etc.) as well as multi-physics simulations (aero-elasticity, aero-thermics, etc.). A strong emphasis is put on LES for complex flows, using both structured and unstructured solvers.

3.2.1 Application of spectral methods to aero-elasticity (F. Sicot, G. Dufour)

Aeroelasticity studies the impact of a flow on a flexible structure. Fluid/structure interactions can potentially be destructive (*e.g.* the flutter phenomena) and therefore must be thoroughly investigated. One way to assess the sensitivity of a turbomachinery to flutter is the so-called weak-coupling approach where the response of the fluid to a forced harmonic motion of the structure is simulated. Correlated to the lag (*i.e.* advance or delay) of the fluid with respect to the excitation, a stability analysis can tell if the fluid is damping or exciting the structure vibrations. CERFACS is developing a harmonic balance method in the *elsA* solver. This method is well suited for weak-coupling simulations [CFD68] and the CFD team was involved in many projects concerning the aeroelasticity of turbomachinery with harmonic balance methods :

- the MACAO project [CFD149] studied an isolated axial compressor. This first successful application was made possible thanks to a collaboration with the aeroelasticity department of ONERA [CFD63],
- the Aerovista project (with ONERA and Safran [CFD166]) encompasses several configurations :
  - an isolated centrifugal compressor [CFD167],
  - an isolated axial compressor with technological effects [CFD165]. This requires the use of overset grids (*i.e.* Chimera technique) to represent complex geometry,
  - a counter-rotating fan [CFD164] : the blade passing frequency and vibration frequency can be different and this configuration requires a non-uniform harmonic balance using an arbitrary set of frequencies and a non-uniform time sampling to capture all phenomena,
  - open rotors (CROR) will also be investigated in this project.
- the validation against experimental data has been assessed for the 11$^{\text{th}}$ standard configuration for aeroelasticity (namely the STCF11) which is a turbine blade oscillating in its first bending mode. The results have been submitted to the AIAA journal in January 2012,
- Finally Cerfacs is involved in the FUTURE (Flutter-Free Turbomachinery Blades) FP7 European project.

3.2.2 Application of spectral methods to multistage turbomachines (T. Guedeney, Y. Sadoudi)

The Harmonic Balance Technique (HBT), presented in section 3.1.1, is used to predict the unsteady flow induced by the relative motion between rotating and non-rotating blades. The main interest is to reduce the cost of unsteady RANS simulations. For example, in the case of a 3.5 stage compressor (CREATE, Fig. 3.4), HBT presents a gain of 4 for the same level of accuracy compared to the classical approach based on a Dual Time Stepping algorithm. Since the periodicity of this test case is $2\pi/16$, the gain expected for other configurations should be of one order of magnitude higher (the usual periodicity for a turbomachinery is 2π, which corresponds to primary blade numbers). Other complex 3D test cases have also been successfully performed, such as a transonic 1.5 stage compressor (ECL4) and a multistage turbine (HTLC). These results show that HBT is a efficient method to reduce the cost of unsteady flow simulations in turbomachinery. The evaluation of the influence of the frequency set on the HBT results is now under progress as well as the quantification of the computational speedup compared to classical unsteady RANS simulations.

3.2.3 Compressor flows : control with casing treatment (G. Legras, N. Gourdain)

Passive control devices based on casing treatments have already shown their capability to improve the flow stability in axial compressors. Among many geometries that have been investigated, axisymmetric (axial grooves) and non-axisymmetric (slots, etc.) geometries have shown a good ability to enhance stall margin. However their optimization remains complex due to a partial understanding of related flow mechanisms. The objective of this work was to numerically investigate different compressor configurations equipped with casing treatments, such as a transonic axial compressor rotor with slot-type casing treatment or a multistage compressor with axial grooves or honey-comb (Fig. 3.5).

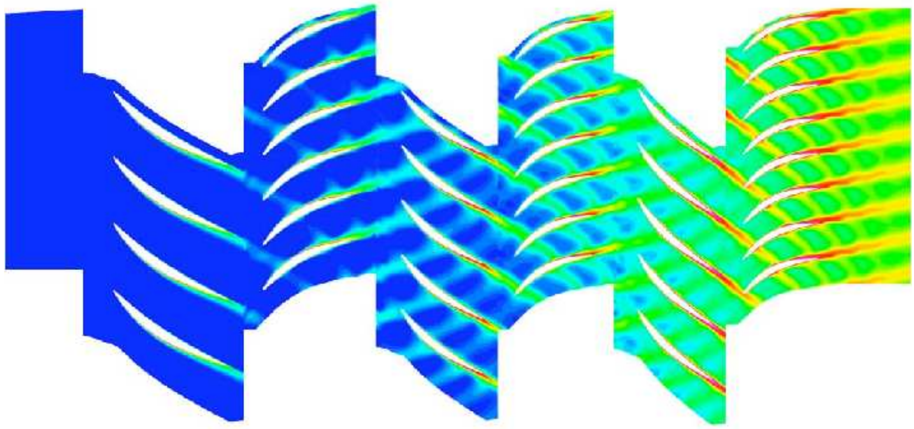


FIG. 3.4: Application of HBT to compressor CREATE. Entropy field at 50% of the compressor span.

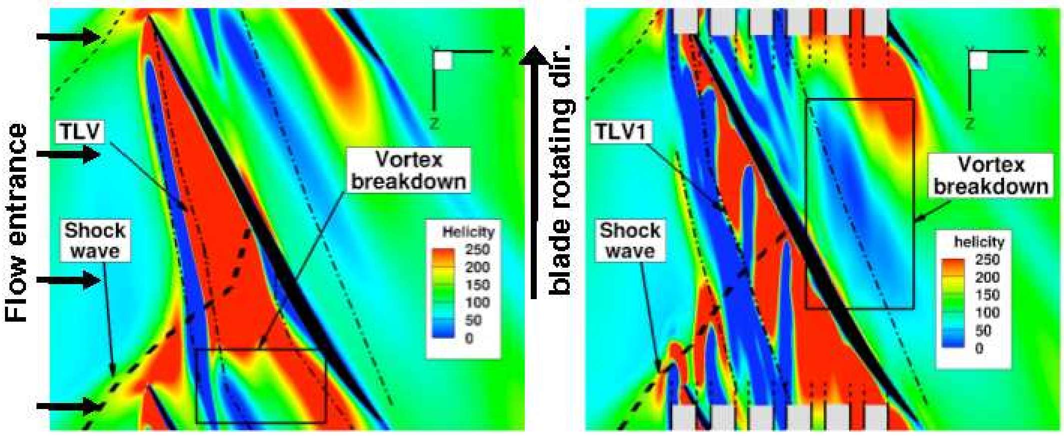


FIG. 3.5: Influence of the casing treatment on the tip leakage vortex (TLV) in a transonic compressor. Left : smooth wall and right : casing treatment case.

Unsteady flow simulations of casing treatments are performed using *elsA*. Control devices are connected to the main compressor grid using either a Chimera technique or a sliding mesh method. Numerical results obtained with and without casing treatment are compared and validated with experimental data [CFD78]. In order to understand the influence of casing treatment on the flow, a budget analysis of the unsteady axial momentum equation is performed on a control volume located in the rotor tip region (the so-called MARS tool [CFD50]), following the idea proposed by Shabbir and Adamczyk [24].

3.2.4 Compressor flows : simulation of turbulent flow patterns (A. Gomar, T. Leonard, G. Dufour, N. Gourdain)

Flows in turbomachines are very complex : turbulence, relative motion between rotating and non rotating parts, 3D blade geometry and technological effects are among the difficulties encountered by flow solvers. While the overall performance of turbomachinery elements in nominal conditions is usually well estimated (efficiency, pressure ratio, etc.) by classical RANS simulations, it is no longer true when an accurate description of the flow unsteadiness is necessary, especially at off-design conditions. In that context, LES could give a better understanding of the flow and thus allow considerable breakthrough in the machine design. LES has thus been performed with *elsA* on a whole 3D passage of a single transonic rotor of an axial compressor (the so-called NASA rotor 37 [26]). This test case is close to an industrial configuration (high Reynolds number 5×10^6, supersonic tip Mach number, etc.). The results obtained with different "classical" numerical schemes (both upwind and centered schemes, second and third order) have been compared. A mesh convergence has also been conducted, considering from 10 to 100M cells to represent the blade passage. Results shows that a 3^{rd} order upwind scheme on a 100M cells mesh is necessary to obtain a correct description of the flow unsteadiness, such as the interaction between the boundary layer and the shock at the leading edge, Fig. 3.6(a). Moreover, the prediction of the efficiency by LES (that remains challenging in this configuration) is largely influenced by the grid density, Fig. 3.6(b).

(a)

(b)

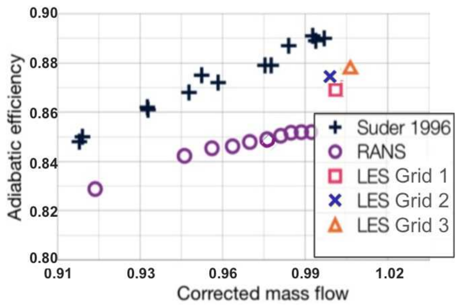


FIG. 3.6: LES results with *elsA* in NASA rotor 37 : (a) Instantaneous flow field shaded with the density gradient and (b) comparison of efficiency curves (grid 1 : 10M cells, grid 2 : 25M cells, grid 3 : 100M cells).

The understanding of the route leading to unstable behaviors in centrifugal compressors is also of primary interest. Since most RANS flow solvers usually exhibit poor predictive capability at near stall conditions (especially regarding the physical phenomena that lead to surge), a study is currently under progress to apply and compare different approaches in *elsA* in a centrifugal compressor. The configuration is a high-pressure single stage compressor (Pi9), experimentally investigated at Ecole Centrale Lyon, which is representative of the SAFRAN Turbomeca engines.

(U)RANS and hybrid RANS-LES (DDES type) have been tested on a centrifugal compressor complex flow. RANS simulations were performed using various turbulence model (Smith, Spalart and EARSM) on two grids of different refinement levels. The comparison with experiments shows a good agreement on a large range of mass flow, but some discrepancies appear on the prediction of the surge line position. DDES are currently investigated on the isolated rotor to study the effect of turbulence and secondary flows (such as the tip clearance flow) on the compressor stability.

3.2.5 Turbine flows : influence of the environment on aerothermal performance (F. Wlassow, N. Gourdain)

The prediction of blade temperatures for high-pressure turbines is challenging because of the complex environment that interacts with the turbine : hot-streak migration, unsteady flow phenomena, fluid/solid thermal coupling and technological details (squealer tip, coolant ejections, fillets, etc.). Several unsteady RANS simulations have been performed with *elsA* in a single stage high-pressure turbine to investigate these points. The baseline simulation takes into account a squealer tip and an inlet condition representative of a hot streak generated by the combustion chamber.

Other technological details (coolant ejections and fillets) and fluid/solid thermal coupling on the rotor blade were also studied. The Chimera technique is used to ease the integration of technological details. The conjugate heat transfer (CHT) problem is solved by means of a code coupling where fluxes and temperatures are exchanged at the blade surface between the fluid dynamics solver (*elsA*) and the solid thermal code (AVTP). Coupling has been done with two different techniques : first a Python loop has been developed to achieve a steady-state convergence (codes are run independently and boundary condition are updated at some meeting points), then the code coupling tool Open-PALM has been used to obtain a time-dependent coupling solution. Both techniques provide identical results.

Results shows that rotor blade fillets have a limited impact on both the blade temperature and the turbine efficiency (less than 1%). On the contrary, taking into account external cooling leads to a modification of radial distribution of loss and loading coefficients and reduces the efficiency by 2%. The blade temperature is also impacted, mainly on the suction side where differences of several per cent with the base-line case are observed. Fluid/solid coupling mainly affects the blade temperature prediction by homogenizing and inducing differences of around 3% with the base-line case.

3.2.6 Turbine flows : aerothermal prediction with wall-resolved LES (E. Collado Morata, L. Gicquel, N. Gourdain)

Recent developments for the prediction of turbulent flows around blades point LES as a very promising tool. While LES of wall bounded flows are now well mastered in academic test cases, the use of LES in configurations close to industrial applications is not yet well established. To partly address this important issue, a structured multi-block flow solver (*elsA*) and an unstructured code (AVBP) are used to perform LES of the flow in a high pressure turbine vane cascade at high Reynolds number (about 10^6). The predictions obtained with both solvers are compared to measurements obtained by Arts *et al.* [1] and to RANS simulations [CFD39], Fig. 3.7(a). Results show that LES is about 10,000 times more costly than RANS. However only LES is able to estimate the wall heat transfer, which is mainly driven by boundary layer transition on the vane suction side. For example, Fig.3.7(b) shows a comparison of the wall heat transfer coefficient with measurements. The agreement is very good on the pressure side and the location of the transition point on the suction side is also correctly predicted with both solvers. Detailed analysis of the flow predictions also underlines the role of long streamwise streaky structures, responsible for the increase of wall heat transfer.

3.2.7 Turbine flows : aerothermal prediction with wall-law LES (S. Bocquet)

LES with a wall law formulation is applied to the VKI high pressure turbine vane cascade [1] at high Reynolds number (2×10^6). The use of such an approach on this test case is motivated by two reasons. One is the need to assess LES with wall law on a configuration representative of industrial applications, implying both complex physical effects and geometry. Second, while very expensive in terms of computational cost, wall-resolved LES [CFD39] is available on this configuration to validate the results obtained with a wall law LES.

(a) (b)

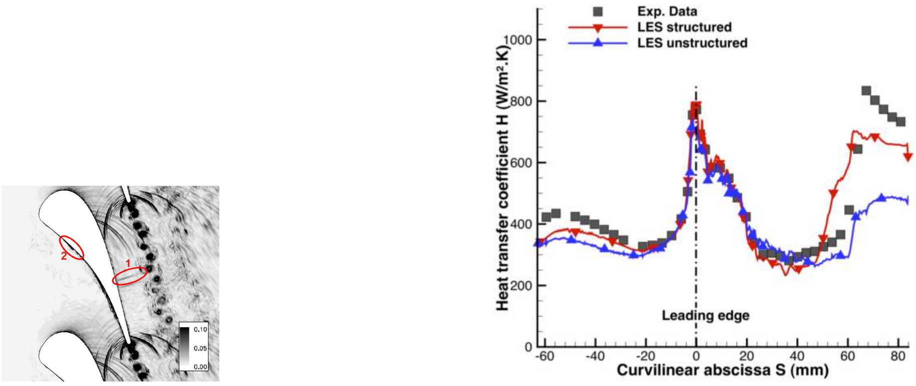


FIG. 3.7: Application of LES to the MUR235 test case : (a) instantaneous flow field colored by density gradient $grad\rho/\rho$ (mark 1 is related to the normal shock and mark 2 to vortices produced by the impact of freestream turbulence) and (b) wall heat transfer coefficient predicted with structured (*elsA*) and unstructured (AVBP) flow solvers.

LES with wall laws is expected to decrease the computational cost by about one order of magnitude, making the computation of the whole blade feasible. A first attempt of LES with wall law around the turbine vane was performed with *elsA*. The same domain as for the wall-resolved LES is computed and simple wall laws, namely the logarithmic law and Kader law, are used respectively for the velocity and temperature fields. The computational cost is decreased by a factor close to 5. However, this conclusion needs further investigations since several meshes and wall laws still need to be evaluated. Despite this simple modelling, reasonable results are obtained on the second half of the pressure side and suction side. One difficulty raised by this configuration is the laminar to turbulent transition of the boundary layer on the suction side : wall laws, derived for fully turbulent flow, overpredict the wall heat flux in laminar regions.

3.2.8 Turbine flows : simulation of internal blade cooling devices (R. Fransen, L. Gicquel, N. Gourdain)

The efficiency of aeronautical engines can be increased by raising the combustor outlet temperature, but this rise in temperature can decrease the blade life duration if the cooling system is poorly designed. Today, for the fluid in the main vein and within the cooling ducts, RANS modeling is routinely used. In that context, LES can greatly improve the predictive capability of flow solvers.
LES of blade cooling ribbed channels have been computed with AVBP and compared with *elsA* RANS results. PIV measurements performed by Casarsa [2] allow validations in several planes in the channel. Comparison with experiment shows that LES gives very good agreement with experimental data, Fig. 3.8. In contrast, RANS is not able to capture large-scale unsteadiness of the flow produced by the ribs in the cooling channel. The thermal efficiency on the wall of the channel has also been computed yielding to better LES predictions of cooling than RANS. Interestingly, the methodology developped here will be used in 2012 to compute heat transfer and pressure losses in ribbed ducts for petrochemical applications (partnership with Total).

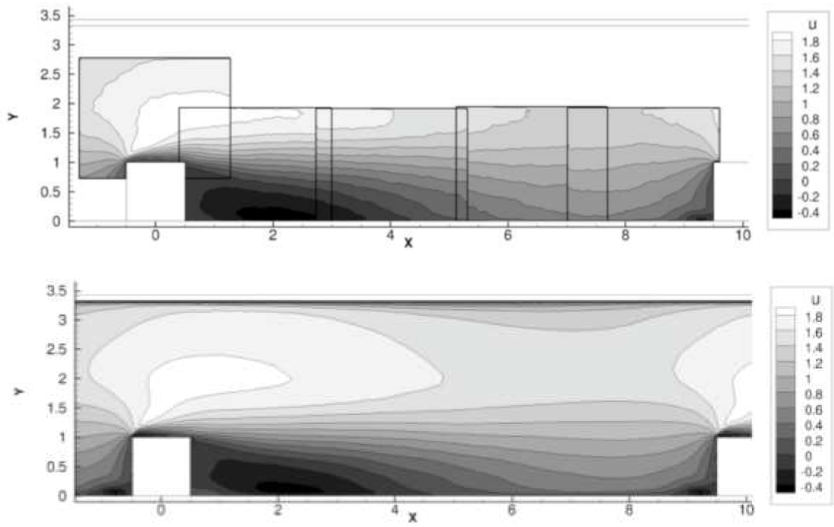


FIG. 3.8: Comparison of PIV measurements (up) with LES predictions (down) in a ribbed channel configuration.

4 Advanced Methods and Multiphysics

The ”Advanced Aerodynamics and Multiphysics” group is a component of the CFD Team. Around 15 researchers (seniors, PhD and Post Doctoral students) are involved in aerodynamics activities. The objective of the group is to develop, maintain and use efficient numerical solvers related to academic and industrial CFD simulations. Most of our efforts focus on the elsA software (owned by Onera) but we also use in-house solvers : AVBP for unstructured Large Eddy Simulation (LES) and NTMIX for Direct Numerical Simulation.

During the past two years, LES activities have grown significantly, especially in unsteady simulations (aeroacoustics or aerothermal) where RANS is not sufficient. To be able to deal with accurate LES in elsA, several developments have been done (high order scheme, non reflexive boundary conditions, wall laws, turbulence injection) leading to new applications : jet, airfoil and landing gear noise but also aerothermal jet in cross flow.

In addition to advanced turbulence methods, the team (in collaboration with Onera) continues the extension of elsA to the unstructured world. This will allow more flexibility to deal with complex geometries and help us to answer the 2020 challenge ”PUMA” defined by CERFACS in 2011, which ambitions to compute a fully unsteady aircraft.

To finish, the activity concerning design optimization is also growing in collaboration with the Algo team.

The work presented in the next sections has been done in close collaboration with our industrials partners (Airbus, Snecma, Turboméca) but also with research centers among which Onera, Paris VI, KTH, ECL.

4.1 Numerical methods

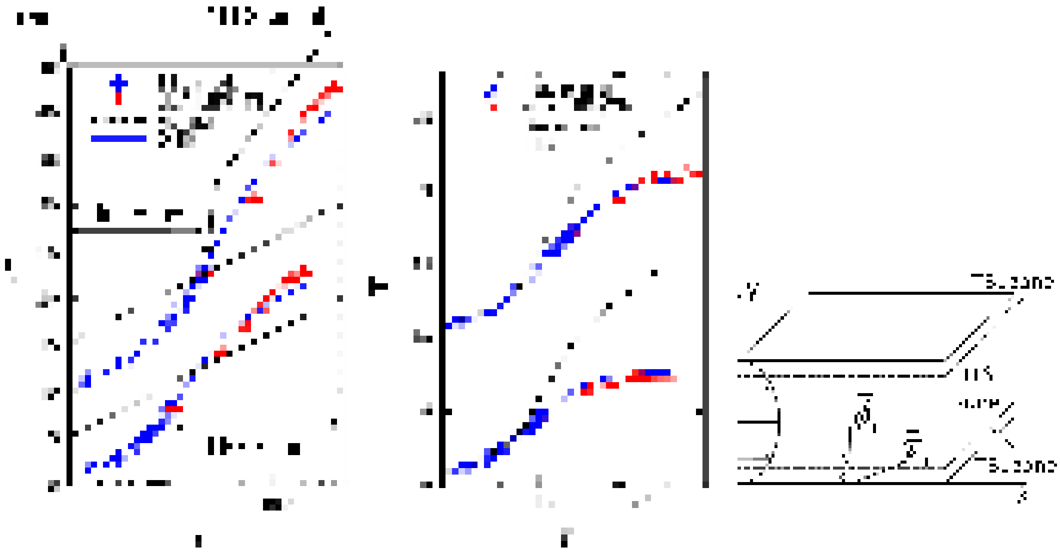
4.1.1 Improve LES capabilities (S. Bocquet, J-C. Jouhaud)

Large-Eddy Simulation (LES) of industrial high-Reynolds number flows is still far from being practical on a daily basis. Various methods have been proposed to reduce the computational cost of LES. These last years, the team has investigated two approaches : Thin Boundary Layer models and embedded LES.

Thin boundary layer laws

The cost of LES is mainly due to the resolution of the small but dynamically important structures present in the inner layer of the boundary layer. The LES with wall model approach is one technique to reduce the computational cost of such computations. A coarse mesh is used close to the wall so that the inner layer of the boundary layer is not captured. In the coarse cells adjacent to the wall, the wall fluxes need to be approximated by an additional wall model. The wall model must contain the flow physics present in the inner layer and can be either a quasi-analytical model composed of wall laws or a numerical model like the Thin Boundary Layer (TBL) model described in Balaras (1996) where a simplified one dimensional model is used between the wall and the first LES point in the flow.

Despite their cost, TBL models constitute an interesting framework for the derivation of wall models



(a) Velocity profiles. (b) Temperature profiles. (c) Computational domain.

FIG. 4.1: LES with wall modeling on supersonic plane channel flow compared to Coleman DNS : Mach $= 1.5$ (bottom) and Mach $= 3$ (top).

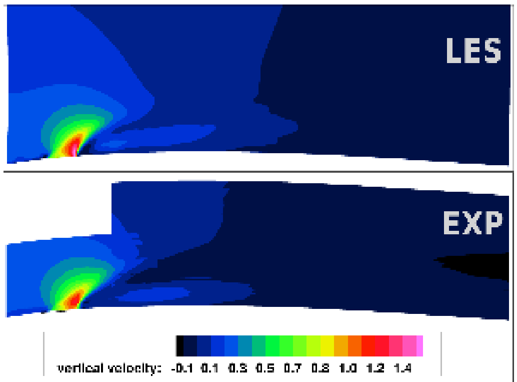
adapted to various physical effects. Thus, a TBL model based on the work of Monfort (2009) and extended to compressible flows has been implemented in the elsA software. This wall model has been validated on a quasi-incompressible channel flow, with friction Reynolds number Re_τ ranging from 1020 to 20000, the latter being representative of the boundary layer at the leading edge of a commercial airplane during cruise. The errors on the friction coefficient C_f and wall heat flux Nu remain below 10% for the range of Reynolds number tested. Then a more discriminatory test case, namely the supersonic channel flow of Coleman (1995), has been used to assess the capability of this approach to handle significant compressibility effects. Figure 4.1 shows the velocity and temperature profiles obtained on a coarse mesh of $(21 \times 21 \times 25)$ points. The excellent agreement obtained on the temperature profile constitutes an encouraging starting point toward LES with wall modeling of compressible flows with convective heat transfer.

Embedded LES
Within the frame of ASTHER project (FRAE funding, AIRBUS-ONERA-CERFACS collaborative work), we have focused on the embedded LES strategy. The idea is to run sequentially a low computational cost RANS simulation in a large domain around the area of interest, so that the influence of boundary conditions can be neglected. Then a LES simulation is performed in a smaller domain centered on the area of interest. The RANS flow is used to define the LES boundary conditions and the initial solution. A schematic view of this method is shown in Fig. 4.2a for a jet in cross flow configuration. Navier-Stokes Characteristic Boundary Condition (NSCBC) are used for the LES domain. As shown in Fig. 4.2b, a good agreement is obtained compared to experimental data [CFD96].

4.1.2 Optimization (M. Montagnac, F. Gallard, M. Mouffe)

Since 2005, CERFACS works in numerical optimization in the context of aircraft preliminary design. The optimization setup of modern aircraft often ends up with several hundreds of design variables and a few constraints. The work is subdivided into three parts that are integrated in the OPTaliA framework of Airbus

(a) Schematic view of the embedded-LES approach.



(b) elsA vertical velocity (top) with the experimental data (bottom) in the symmetry plane.

FIG. 4.2: Jet in cross flow : embedded LES simulation.

France (renamed Worms last year) to perform optimizations.
The first part is dedicated to optimization algorithms, in collaboration with the CERFACS Parallel Algorithms team. Many different metamodels have been tested in a trust-region algorithm [CFD157] and the impact of noisy data on stopping criteria have been studied [CFD139]. After a first study of gradient-based algorithms in the previous years to handle the resolution of optimization problems without constraints or with bound constraints, the introduction of general (non-linear) constraints has been considered [CFD158].
The second part is dedicated to the CFD solver and tools. A high-fidelity solver is required to compute the objective function. The choice of the optimization algorithm is heavily constrained by the computational cost implied by one function evaluation [CFD77]. Thus, gradient-based optimization algorithms are particularly valued for their speed of convergence although they only give a local optimum. Therefore, the gradient of the objective function with respect to the shape variables is computed through the discrete adjoint method that only requires a linear system resolution for each function and constraint. As a consequence, many numerical features have been linearized and integrated in the elsA software to enable optimizations on complex aircraft configurations [CFD157].
The third part (the formulation of the optimization problem) is heading gradually towards MDO (Multidisciplinary Design Optimization). A PhD student (F. Gallard) currently investigates the multipoint optimization and the integration of aeroelastic effects for the design of flexible aircrafts. CERFACS also takes part since 2010 in the OSYCAF project funded by the STAE foundation. The objective is to setup a MDO methodology for an aero-structural optimization process in collaboration with : Onera, ISAE and UPS.

4.1.3 GMRES (M. Montagnac, X. Pinel)

A Jacobian-Free Newton-Krylov framework has been developed in the elsA software and validated on many configurations for both structured and unstructured grids [CFD161]. In this method the Jacobian matrix does not have to be explicitly expressed as in the standard LU-SSOR method for example. Indeed, the former relies only on the matrix-vector product of the Jacobian matrix times a vector that is implemented simply through the computation of the flux balance. As high-order schemes are developed in parallel, this framework will be automatically compatible contrary to the LU-SSOR method that is expected to be changed due to its first-order linearisation scheme. Moreover, this framework may help the convergence in case of highly skewed meshes.

The classical Krylov methods GMRES and FMGRES have been investigated in a matrix-free version. The algorithm is used as a smoother in combination with the multigrid approach. The main issue was to find a good matrix-free preconditioner. Three of them were tested : diagonal preconditioning, scalar LU-SSOR and preconditioned GMRES. The scalar LU-SSOR preconditioner has shown its efficiency on both Euler and Navier-Stokes simulation for structured meshes. The FGMRES method is more efficient with unstructured meshes (A350 Wing-Body configuration).

4.1.4 Non conforming mesh boundary condition (M. Montagnac, B. François)

The meshing process is a crucial point for simulations of complex aircraft and turbomachinery configurations, especially for body-fitted structured solvers. The key point is the type of interface to set between two zones, either structured or unstructured. Particularly, for matching interfaces in the structured approach, local refinements around the geometry tend to spread through the whole configuration domain. This can lead to very large grids and make the meshing process tedious. In addition, matching interfaces cannot be prescribed anymore when facing moving parts (such as high-speed propellers or rotor/stator interactions).

CERFACS developed the efficient technique of conservative non coincident interface boundary condition to address these issues. Two zones must have a common adjacent (2D) interface, contrary to chimera technique, but grid points of both interfaces do not have to be at the same location or coincident, preventing the spreading of mesh points from one block to another. A complex mesh can be created with addition of independent non overlapping zones, which is the base of our approach for hybrid meshes generation composed of structured zones and multi-element unstructured zones.

This functionality has been made compatible for computations in a relative frame with an absolute velocity formulation and CPU performance has been improved, which has benefited to CROR simulations in particular (see Sec. 4.2.1). Recently, this development has been extended to unstructured and hybrid meshes (see Sec. 4.3.1).

4.1.5 Vortex confinement (D. Kolomenskiy, J.-F. Boussuge)

One of the features of aircraft trailing wakes that makes them difficult for numerical simulation is that the vortex cores are very thin compared to the wing span and the length of the vortex system is very large. This is particularly challenging for low-order numerical methods as they require extremely high grid resolution to preserve fine structures. However, in many applications, the velocity distribution in the vortex core is unimportant and only the vortex strength has to be predicted adequately. Vorticity confinement schemes can serve this purpose. The basic idea of vorticity confinement methods [4, 25] is to add anti-diffusive terms to the momentum equations of the fluid. It results in a reduced diffusion of vorticity with little extra computational cost. This approach has been implemented in *elsA* and validated on an academic test case (advection of a two-dimensional vortex in a periodic domain). An industrial configuration (fuselage-wing-pylon-nacelle) is envisaged in a near future.

4.2 Applications for external flows

4.2.1 CROR (B. François, J-F. Boussuge)

With increasing costs of fuel, the development of new aircraft concepts is mainly driven by the fuel burn reduction. In this context, new engine concepts such as Counter Rotating Open-Rotors (CROR) appear to be suitable options for the single aisle segment, currently dominated by the Airbus A320 and Boeing 737.

Counter-Rotating Open-Rotors raise many technical challenges where CFD have an important role to play.

Among them, the prediction of 1P-forces is essential for aircraft manufacturers because it impacts the sizing of major parts of the aircraft (pylon, HTP, VTP). 1P-forces are unsteady transversal efforts on the rotation axis of the propellers which are created when the inflow is inhomogeneous (incidence/sidestream conditions, installation effect).
To evaluate 1P-forces, unsteady simulations of isolated Airbus generic CROR design using full 360 ° meshes were computed. These large meshes are required to capture incidence and installation effects. Advanced grid techniques (chimera or sliding mesh) are used in order to enable communication between the different rotating parts (front and rear rotor) and the fixed parts (far field area) [CFD31]. The unsteady pressure field over the whole CROR enables to calculate the 1P-forces (see figure 4.3).

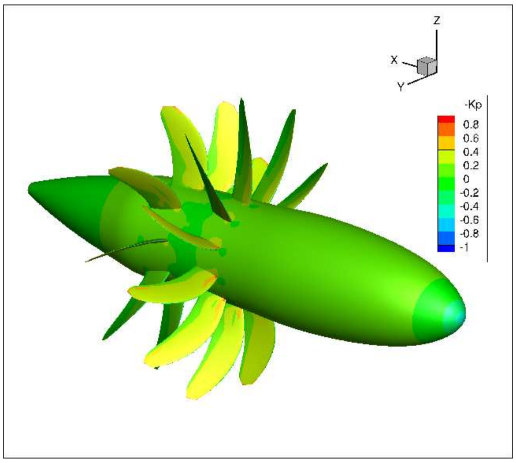


FIG. 4.3: Pressure coefficient field with incidence effect

4.2.2 Air inlet (F. Sicot, G. Dufour, J.-F. Boussuge)

The air inlet of a jet engine plays a key role on engine operability : it channels the flow to the fan in such a way that it should be as smooth and uniform as possible. Therefore the region between the nacelle tip and the fan should be long enough to smooth out any disturbance and non-uniformity of the flow. The current trend is to reduce this length to reduce the weight and drag of the nacelle and increase overall performances. One of the most critical operating point is take-off in the presence of cross-winds which can generate detached flow at the nacelle tip and lead to high distortions on the fan. These distortions must be minimized and CFD can help engineers to estimate flow distortion on the fan and improve the nacelle design. First studies [3] were performed at CERFACS for the nacelle alone. New studies including the fan started in 2011 (Fig. 4.4).

4.2.3 Jet in cross-flow (J-C. Jouhaud, Y. Hallez)

Aerothermal flows involving a jet in cross-flow are very common in aeronautics. A classical example is the nacelle anti-ice system where a hot jet in cross-flow interacts with the wall of a turbo-fan engine nacelle. An accurate description of the thermal boundary conditions is essential in this case : heat fluxes at the wall have a strong influence on the flow/structure interaction. Thus, an accurate thermal boundary condition for the fluid flow is obtained by coupling the fluid solver with a heat transfer solver in the walls [CFD96]. The compressible LES solver AVBP has been used to solve the fluid flow and the heat transfer problem inside the scoop top wall has been addressed with the heat conduction solver AVTP (see Fig. 4.5a). The organization of communications between these two codes is handled with the open source PALM library.

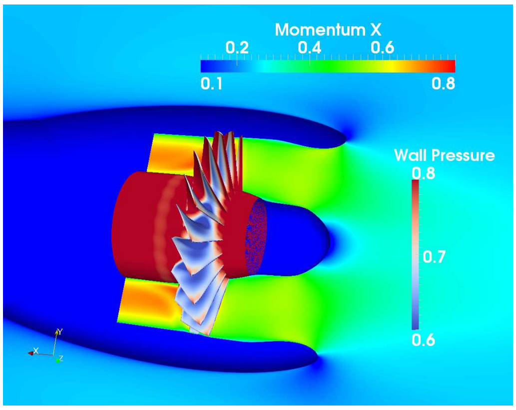
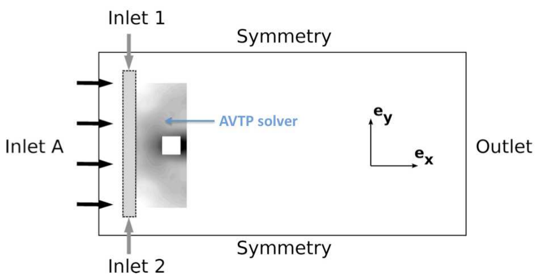
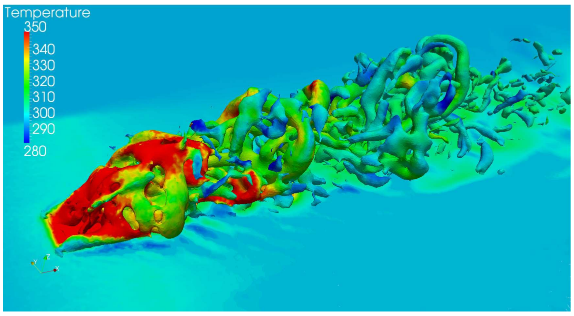


FIG. 4.4: Fan/Nacelle Configuration (axial momentum and blade pressure)



(a) Anti-ice system computational domain



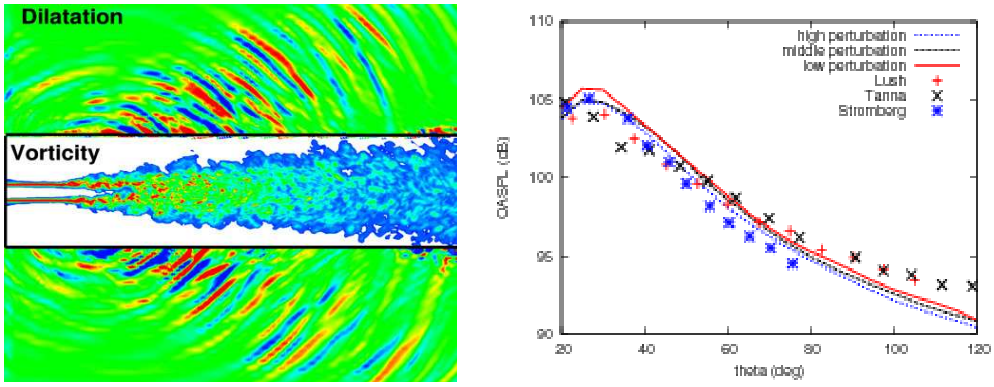
(b) Iso-Q criteria colored by temperature

FIG. 4.5: Coupled simulation between LES (AVBP solver) and the scoop temperature field (AVTP solver).

The compressible LES solver AVBP has been used to solve the fluid flow and the heat transfer problem inside the scoop top wall has been addressed with the heat conduction solver AVTP (see Fig. 4.5a). The organization of communications between these two codes is handled with the open source PALM library.

4.2.4 Jet noise (H. Deniau, A. Fosso-Pouangué, J.-F. Boussuge)

The noise associated to the turbulent mixing of a jet with the ambient fluid is one of the most complicated case to simulate. It requires advanced numerical ingredients (high-order schemes, non reflecting boundary conditions, inlet turbulence generation) to be able to capture very small pressure fluctuations associated to sound sources. During the past years, a lot of efforts have been done to implement such ingredients into the elsA software. The far-field acoustic calculation is performed with KIM (ONERA) using a FW-H method. The method was validated on academical test cases [9] and is now used for aeroacoustics computations. We studied the influence of many numerical parameters on a classical single jet test case ($Mach = 0.9$ and $Re = 4.0\,10^5$). A key point for a jet noise simulation is to accurately reproduce the turbulence activity at the nozzle exhaust which is related to the inlet perturbations. This can be achieved (see Fig. 4.6a)) when perturbations are correctly discretized ; in that case the results are insensitive to the amplitude magnitude (see Fig. 4.6b). In addition to single jet simulations a co-axial configuration has been studied with the PPRIME institute (Poitiers). Currently, aerodynamics results agree very well with experimental data. A new activity on supersonic jet noise also started six months ago where the 6th order compact Lele scheme



(a) Near-field vorticity magnitude and far-field sound (shown using dilatation contours).

(b) Influence of the perturbation intensity imposed at the jet inlet.

FIG. 4.6: Noise computation of a subsonic jet.

was adapted to simulate shocks.

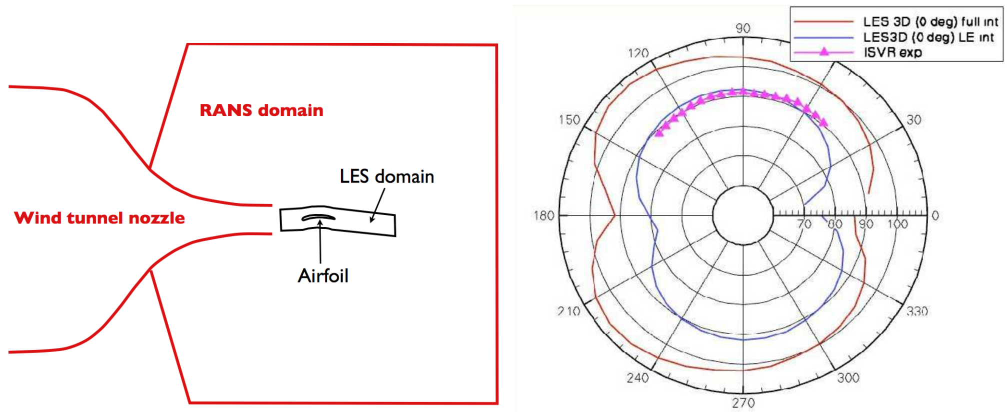
4.2.5 Airfoil noise (H. Deniau, G. Dufour, J.-F. Boussuge)

Broadband noise generation and radiation from rotating blades due to the ingestion of turbulence is a topic of major interest for fan manufacturers. It becomes the main broadband noise source when the ingested turbulence is at least stronger than two or three % of the relative mean flow on the blades. In that context, turbulence-interaction noise due to isotropic turbulence impacting a thick cambered airfoil has been simulated for the first time at high Reynolds number ($Rec = 6.5\ 10^5$) by a compressible Large Eddy Simulation (LES) accounting for the installation effects. The full wind-tunnel has been simulated by a two dimensional Unsteady Reynolds-Averaged Navier-Stokes (URANS) simulation that provides the realistic boundary conditions for the LES on a restricted domain embedded in the potential core of the wind-tunnel jet (Fig. 4.7a). Radiative boundary conditions are applied around the LES domain to prevent reflection or drift of flow parameters. Synthetic turbulence is injected at the inlet of the LES domain. Comparison with experimental data shows excellent agreement for the noise level and directivity if the sources are restricted to the leading edge area (Fig. 4.7b). Yet LES also shows some extra noise sources at the trailing edge caused by a large recirculation bubble close to the leading edge yielding some large vorticity up to the trailing edge, and a late transition on the suction side [CFD27, CFD53].

4.2.6 Landing-gear noise (J-C. Giret, J-C. Jouhaud, J.-F. Boussuge)

Understanding and predicting aerodynamic noise generation is nowadays of a great importance. Particularly, since huge progresses have been made on the noise reduction of turbofan engines through high bypass ratios, the design of new aircraft requires the prediction and if needed the reduction of airframe noise (landing gear and high-lift devices), which is a major source in approach conditions.

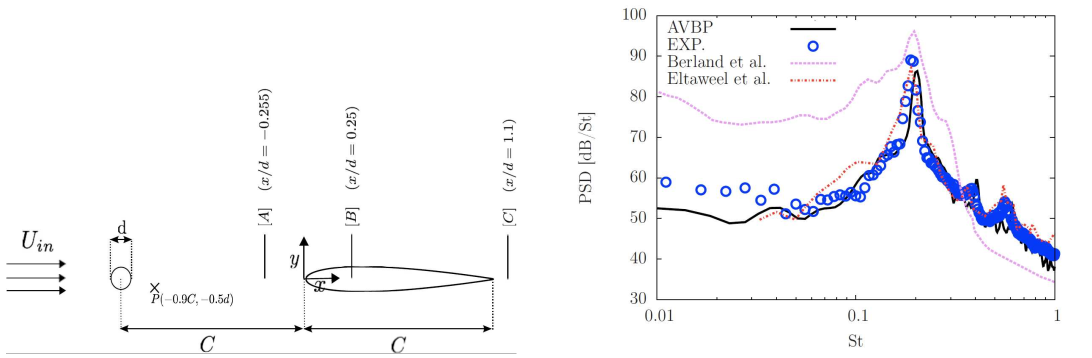
A requirement for such simulations is the ability to handle complex geometries. Most numerical aeroacoustics studies have been performed on structured meshes as it enables the use of high-order schemes. However, meshing a complex geometry with a block-structured mesh can be at least difficult and at worst impossible. In order to overcome such limitations, overset grids or unstructured meshes can be used. This study focuses on the use of unstructured meshes with a special care on accuracy issues.



(a) Domain decomposition for RANS and LES

(b) OASPL directivity (dB)

FIG. 4.7: Airfoil turbulence interaction noise.



(a) Sketch of the rod-airfoil configuration.

(b) Power spectral density of the acoustic pressure at 90 and at 1.85m.

FIG. 4.8: 3D LES simulation of a rod-airfoil interaction. Comparison with experiment.

The rod-airfoil test case performed by Jacob *et al.* at ECL [11] is a good benchmark for airframe noise : it produces a quasi-tonal noise due to the periodic shedding of vortices at the rod and the broadening of the spectra due to the impingement of the developed turbulent wake on the airfoil. This test case has then been used in numerous studies to validate numerical methods for airframe noise (Fig. 4.8a). A simulation of the rod-airfoil configuration has been performed using AVBP. The far-field acoustic propagation has been achieved using a Ffowcs Williams and Hawkings (FW-H) analogy implemented in KIM (Fig. 4.8b).

4.3 Software engineering

4.3.1 Hybrid grid computations (G. Puigt, M. Montagnac, J.-F. Boussuge)

RANS simulations based on structured grids / structured codes have proved their efficiency for a long time and are used routinely in industry. Even with advanced meshing techniques like chimera grids or non abutting block interfaces, a meshing strategy must be adopted, which is strongly linked with mesh expertise and with predefined mesh shapes choices following canonical CADs. Structured grids are suitable to maintain mesh lines aligned with the flow anisotropy, especially in the boundary layer where the variables are mainly varying in the direction normal to the wall. Moreover, structured numerical techniques help to improve the global performance and robustness of the structured approach. The structured mesh generation process must be performed by experts and the solution can be computed very accurately and quickly when the mesh lines are aligned with the flow.

Nowadays, an industrial tendency is to increase the CAD complexity in order to compute flows with a higher accuracy. For planes, one can for instance consider thermal computation between engine and nacelle or flows around landing gears. For turbomachinery, passive wall treatments are added to increase the stability area of the propeller system and cannot be meshed easily. For those examples, the global structured mesh strategy fails at a reasonable human cost and it is clear that complex CAD must be computed with unstructured capabilities. The unstructured mesh generation process is very efficient but the prize to pay lays in the global accuracy of the computation : it is very difficult to impose mesh lines which are aligned with the flow and the accuracy can finally be lower than for structured grids. This point has been highlighted as a conclusion of the 4th Drag Prediction Workshop held in June 2009 : “More scatter from unstructured methods than from structured grid methods. Suspect this is more due to grid than to code.” A way to overcome this drawback is to authorize unstructured grids composed of different element shapes with hexahedra and prisms in the anisotropy flow region, tetrahedra elements where the flow is isotropic and pyramids in the buffer region from four-nodes element faces to three-nodes element faces. This is what is called a *hybrid mesh approach* in the literature but we prefer to call them *mixed-elements grids*. Compared with a structured grid, an unstructured equivalent induces a memory overhead due to connectivity and indirect memory addressing and since the global mesh structure is left away, it is difficult to implement efficient algorithms such as implicit schemes.

An interesting approach seems finally to associate both techniques. Therefore, we consider meshes composed at the same time of structured blocks and unstructured mixed-elements zones : this is what we call a *hybrid approach*. This approach corresponds to the current Airbus needs (and strategy) who would like to benefit from the two worlds at the same time.

In that context and in collaboration with ONERA, CERFACS actively participates to the development of unstructured capabilities in elsA. We are now able to simulate RANS three-dimensional unstructured grids on parallel platforms. Advanced validations on industrial configurations are on-going. The next step consists in handling hybrid grids. CERFACS is involved in the numerical treatment of interfaces between structured zones and unstructured ones. This is a consequence of the impossibility to implement identical numerical schemes for structured and unstructured zones. This activity can be related to coupling algorithms.

4.3.2 High Performance Computing (M. Montagnac)

The emergence of large-scale HPC computing platforms based on multicore and manycore technologies, processor-based CPU and hybrid CPU / GPU, involves the modification of the legacy software to ensure optimal use of these capabilities in the future. CERFACS is involved in these two aspects. The first point is on hardware accelerators and especially GPU. elsA has been ported on GPU platforms after rewriting some parts of the code in CUDA-C. Results show an acceleration factor of about ten between one GPU card and one core of an Intel Westmere processor. Many GPU cards can be addressed for parallelism but more validations are required to make conclusions.

The second point focuses on multicore hardware architecture. A simplified model of elsA has been developed in order to assess many different techniques that aim to maximize both the individual CPU performance and the shared-memory multicore performance. This effort will continue in the project SONATE+.

4.3.3 Flow Simulation Data Manager (M. Montagnac)

In an industrial context, experts in numerical calculations deliver computational frameworks to their end-users to design products. Obviously, these multidisciplinary frameworks include many third-party tools and legacy codes, which exchange data. Airbus France has developed a proprietary software architecture to enable code coupling and multi-physics simulations. Since these simulations often include an aerodynamics solver, elsA has been introduced as a python module in this framework. The purpose of the main module, called the Data Manager, is to contain all information about the simulation. 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 CERFACS 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 contains 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).

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5 Publications

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7

Aviation and Environment

1 Introduction

The aircraft emissions have an impact on atmospheric chemistry and on the radiative balance of the atmosphere. For example, contrails formed by condensation of water vapor onto exhaust aerosols and soot particles trigger the formation of cirrus clouds. Emissions of nitrogen oxides perturb the natural chemical cycles and lead to ozone production or destruction depending on local air mass composition and insolation. These ozone perturbations along with the emissions of CO_2, water vapour and ice particles formation, soot particles, sulphuric aerosols from the burning kerosene give an additional contribution to the green house forcing.
The most recent evaluations of those effects show the existence of an amplification factor of about 2 to 3 for green house potential factor from aircraft emission : a molecule of CO_2 emitted from a jet airplane is a factor of 2/3 more efficient for green house forcing than a similar molecule emitted at ground level.
Given the exponential increase of the air traffic it is anticipated that the aircraft emissions will double by year 2020 compared to present. The air traffic would then be a major player of the climate change. There is no doubt that in future negotiation processes for the limitation of green house gas emissions aviation sources will be a central issue. It is therefore important that the regulations that could be imposed on aviation be based on well-sound scientific studies.

The main objective of the scientific investigations conducted within the Aviation Environment team is to better quantify the chemical and radiative atmospheric impacts of aviation at the various scales from the aircraft near field to the global atmosphere. An integrated evaluation of the different steps that involves the emission transformations must be performed, from the gaseous and particulate species generation in the combustion chambers, their chemical and microphysical transformations in the aircraft near field, their vertical and horizontal dilution in the far wake along the contrail path, up to the formation of corridors by the fleets and their transport by the general circulation of the atmosphere. At each of those steps the chemical and radiative atmospheric perturbations must be assessed.

During this last 2 years we have made significant model developments and we have now all the ingredients needed to evaluate the chemical and radiative impact of aircraft exhausts. At small and mesoscale the numerical models NTMIX and Méso-NH are used. They both include the microphysic needed to describe the ice particle formation and evolution several hours after injection in the atmosphere. The NTMIX model also includes the gas-phase and heterogeneous chemical schemes to compute the evolution of the nitrogen species and their partitioning. During the period covered by this report, emphasis was placed on the evaluation of the role of atmospheric turbulence on the development of contrails and on the importance of the aircraft type (number of engines) in the contrail properties.

For the larger scale, a study on the climate impact of transportation modes has been conducted with the CNRM. Despite a rather simplified parameterization of the radiative impact of contrails, it is found that the non-CO_2 effects are essential when attempt is made to quantify the influence of aviation on climate. At the time horizon of the end of the century, the forcing by contrails and contrail-currus and the ozone formation by aviation NOx release encompass the greenhouse effects due to the CO_2 release by aviation. Those results have been published in the Atmospheric Chemistry and Physic Discussion journal. In addition, within the SWAFEA project, we have evaluated the possible atmospheric impact of the use of agrofuels instead of regular kerosene. The agrofuels are expected to release less soot particles and NOx emissions. If those assumptions are right the aircraft using agrofuel should have slightly less atmospheric impact, but uncertainties are large due to very limited data existing on emissions by engines using agrofuels.

In addition, a new project has been initiated to evaluate the atmospheric impact of the solid propellants used by the Ariane V and VEGA rockets, and by the SOYOUZ rocket that uses kerosene as a propellant. In the case of rockets using solid propergol a significant fraction of the chlorine from the propellant is released in form of chlorine radicals and gases, Cl, ClO, Cl_2, that can locally destroy the atmospheric ozone. Evaluations of these effects have been performed with a simple chemistry-diffusion model. The results obtained show a significant ozone destruction regionally above the launch site and are consistent with observations reported for the US shuttle launches. In the case of Soyouz, preliminary calculations show that a moderate ozone destruction can be found in the upper stratosphere due to the water vapour emissions whereas negligible effects are expected in the lower stratosphere. The impact of soot emissions and the possible formation of ice in the stratosphere remains to be evaluated.

We have developed numerous cooperations within the present research activities. With the CNRM for the use of Méso-NH and ARPEGE/Climat and MOCAGE models, with the LSCE for implementation of our plume parameterization, with the ONERA for the near aircraft field simulations, and at the european level within the SWAFEA project coordinated by ONERA to study the impact of alternate fuel to the kerosene. Further, the “RTRA Sciences et Technologie pour l’Aéronautique et l’Espace” is supporting the ITAAC project that is coordinated by CERFACS and IMFT, and includes research teams from the CNRM, the IMFT, the ISAE, the LAPLACE laboratory and the SAFIRE unit.
The study of the possible impact of rocket launches on the atmospheric ozone content has been supported by the CNES.

The next sections detail the results obtained within the period covered by this report.

2 Simulations of aircraft wakes and rocket launch emissions

2.1 Wake simulation in the vortex regime (R. Paoli, J. Picot, O. Thouron, D. Kolomenskiy)

2.1.1 Interactions between jets and wing vortices (D. Kolomenskiy, R. Paoli)

Wing-tip vortices have a major influence on the dynamics of condensation trails. Numerical simulation of their initial development requires an adequate approximation to boundary layers on the wing surfaces. On the other hand, important hydrodynamic instabilities occur in the wake on a much larger scale. Therefore, it seems reasonable to decompose the simulation in an upstream domain comprising the solid boundaries, and a downstream domain that only contains the vortex wake. In the upstream domain, a RANS computation is performed. Its outputs are then used as inflow conditions for an LES computation in the downstream domain.

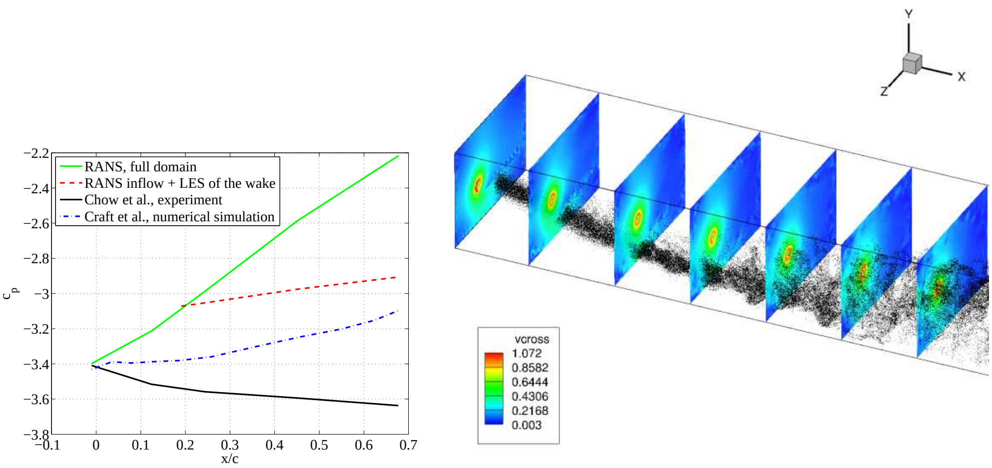

FIG. 2.1: Left : minimum static pressure coefficient along the vortex centreline. Right : instantaneous crossflow velocity field (colour) and particles location (dots).

A wind-tunnel experiment with a NACA 0012 wing (Chow et al., 1997) has been used to test these techniques. It was found, in agreement with previous studies (Craft et al., 2006), that RANS computations may overestimate the rate of decay of the trailing vortex. The choice of turbulence model is crucial. Satisfactory results have been obtained with a differential Reynolds stress model in the very near field. Downstream, an LES computation supplied with the required inflow condition can provide an accurate prediction of the vortex wake properties. This is shown in figure 2.1(left), which shows the minimum static pressure coefficient in the vortex core as a function of the non-dimensional distance from the trailing edge.

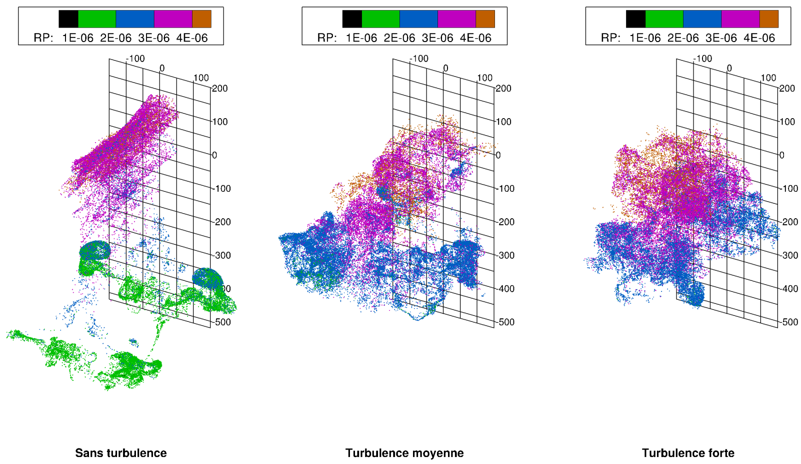

FIG. 2.2: Spatial distribution of ice crystals for different atmospheric situations : from left to right : no turbulence, mild turbulence and strong turbulence.

Figure 2.1(right) displays a snapshot of the crossflow velocity field obtained in the LES computation and the location of passive tracer particles that were injected at the inflow plane to simulate the engine exhaust emissions. Similar approach will be used to compute the condensation trails behind an airliner.

– J. S. Chow and G. Zilliac and P. Bradshaw. Turbulence measurements in the near field of a wingtip vortex. NASA Technical Memorandum 110418, 1997.
– T. J. Craft and A. V. Gerasimov and B. E. Launder and C. M. E. Robinson. A computational study of the near-field generation and decay of wingtip vortices. Int. J. of Heat and Fluid Flow.27, 684-695, 2006.

2.1.2 Influence of turbulence on the vortex evolution (J. Picot, R. Paoli, O. Thouron)

The objective of this study was to understand the effects of atmospheric turbulence on the evolution of a contrail in the far-field wake up to 5 minutes after emissions (vortex regime). In order to get statistically steady conditions and avoid the decay of kinetic energy over time, turbulence was sustained by means of a stochastic low wavenumber forcing scheme by Paoli and Shariff (2009), which allows the nonlinear cascade to determine fluctuations at smaller scales. Large-eddy simulations were performed using NTMIX with ice crystals tracked using a Lagrangian approach and the initial conditions obtained from a pre-simulation covering the first 10 seconds after emission (jet regime). Figure 2.2 shows the spatial distributions of particles colored with ice crystals radius at the end of the simulation for three atmospherics situations : no turbulence, mild and strong turbulence, respectively. The figure indicates that turbulence strongly affects the structure of the contrail by increasing mixing with ambient air. This leads to a homogenization of ice crystals with a strong reduction of the gap between the primary and secondary wakes (which are almost indistinguishable in the strong turbulence case). In addition, mixing with supersaturated air enhances the process of condensation of water vapor with the formation of larger ice crystals especially in the upper secondary wake.
A follow-up of this study will be to analyze the dissipation of the contrail up to a wake age of a few hours (diffusion regime) using these data to initialize the MesoNH atmospheric code.

– R. Paoli and K. Shariff. Turbulent Condensation of Droplets : Direct Simulation and a Stochastic Model Journal of the Atmospheric Sciences, Vol. 66, pp. 723-740, 2009.

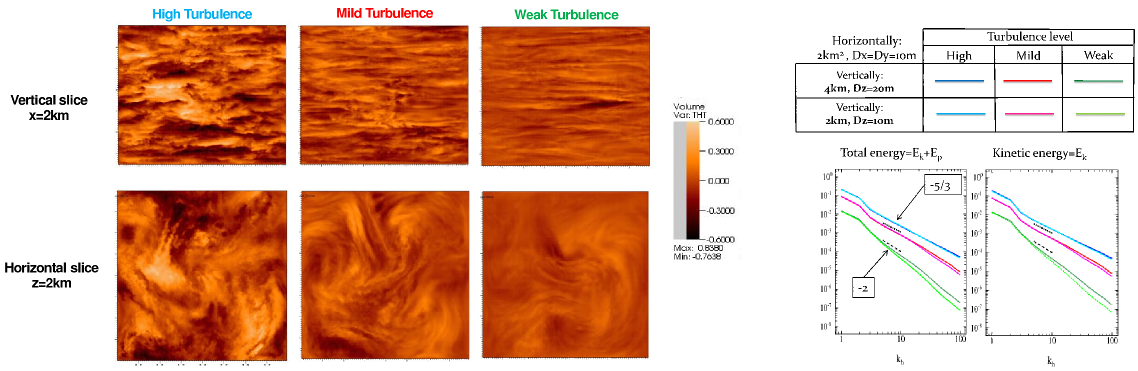

FIG. 2.3: Large-eddy simulations of atmospheric turbulence at Kilometer scale : Snapshots of potential temperature fluctuations (left) and spectra of turbulent kinetic energy (right)

2.2 Wake simulation in the diffusion regime (O. Thouron, R. Paoli, D. Cariolle)

2.2.1 Direct simulation of the atmospheric turbulence (O. Thouron, R. Paoli)

The objective of this study was to understand the properties of atmospheric turbulence in the upper troposphere lower stratosphere (UTLS) at scale of $\mathcal{O}(1$ Km), which are of interest for the dispersion of contrails in the diffusion regime. Large-eddy simulations of stratified turbulence have been carried out in cubic computational domains that are representative of portions of the UTLS. The forcing scheme by Paoli and Shariff (2009) used to sustain turbulence was implemented in MesoNH, the mesoscale model of the atmospheric research community jointly developed by CNRM and Laboratoire d'Aérologie.
Preliminary studies have been carried out to determine the optimal resolution required by the physics of the problem : (i) for typical atmospheric density gradient, small-scale turbulence simulations with 1 cm resolution showed that isotropic turbulence can be achieved up to scales of about 10 m ; (ii) using LES in 100 m^3, 200 m^3 and 400 m^3 cubic domains it was shown that resolution of $\mathcal{O}(1$ m) is necessary to insure the turbulence model represents correctly sub-grid scale fluctuations.
Based on these tests, simulation of 2 km and 4 km cubic domain with uniform 10 m, 20 m and 40 m resolution have been performed. Three large-scale turbulence levels have been considered, which are representative of 'strong', 'mild' and 'weak' turbulence as retrieved from available measurements in the UTLS (Wroblewski et al., 2010), see Fig. 2.3(left).
This work allowed the establishment of optimal numerical configuration to study stratified turbulence in the UTLS. As suggested by Waite (2011) the resolution has to be higher than buoyancy scale (which depends on turbulence intensity) to correctly represent the turbulence. In addition, it was shown that for typical UTLS turbulence the minimum vertical domain size must be at least 4 Km to ensure that turbulent eddies are not confined. The outcome from these simulations gave a first contribution to the understanding of stratified turbulence in the UTLS at the scales of interest to aviation. The analysis showed that at scales of 10 to 100 km the slopes of kinetic and potential energy spectra get closer to -5/3 as turbulence intensity increases, and that lowering the turbulence intensity leads to steeper slopes and smaller vertical extensions of turbulent eddies (see Fig. 2.3(right)). Finally, this study allowed setting up MesoNH and preparing the computational framework for large-scale simulations of atmospheric turbulence (4 Km computational domains with 2 m resolution, grid size of 8 billions points) that will be carried out in 2012 on massively parallel computers of PRACE and INCITE infrastructures.

– Waite, M. L. Stratified turbulence at the buoyancy scale, 23, 066602, 2011

– Wroblewski, D. E., Coté, O. R., Hacker, J. M., and Dobosy, R. J. Velocity and Temperature Structure Functions in the Upper Troposphere and Lower Stratosphere from High-Resolution Aircraft Measurements J. Atmos. Sci., 67, 1157-1170, 2010.

2.3 Impact of rocket launches on atmospheric O_3 (D. Cariolle, A. Poubeau, R. Paoli, O. Thouron)

2.3.1 Simulation of a rocket jet (A. Poubeau, R. Paoli)

The first objective of this study is to obtain large-eddy simulations using the AVBP code of the jet generated by a rocket booster. The results of these simulations (at various altitudes) will then be used as an input to the Meso-NH code to determine the influence of rocket emissions on the atmosphere at large scale.

Some two-dimensional simulations were run in order to set up all the parameters (boundary conditions, artificial viscosities...) and have a first idea of the structure that should be observed at the exit of the nozzle. The computational domain is composed of the nozzle, whose exit was connected to a box representing the atmosphere. A tentative approach was to inject high pressure air at the entrance of the nozzle at a high pressure. This configuration rapidly showed its limits, as a shock was formed right at the entrance of the nozzle due to the high pressure imposed as a boundary condition. A solution to this problem was to add a large tank that would discharge gas through the nozzle to the atmosphere. The following step was to run a simulation that would correspond to the case of the rocket flying at an altitude of 20 km (where the ozone concentration is maximum). The fact that the nozzle verifies the one-dimensional isentropic relations made it possible to set the boundary conditions using the available data. The result presents all the characteristics of an under-expanded jet. However, the turbulence in the mixing layer could not be observed in this 2D configuration.

Following these results, some three-dimensional simulations were performed using the same parameters (figure 2.4, left). To be closer to the actual case, the air injected in the nozzle was replaced by a gas thermodynamically equivalent to the real gas (with the same C_p, γ and R). Again, the results show a highly supersonic, under-expanded jet, as it can be seen on figure 2.4 (right).

The next objective is to validate these simulations by the study of the spreading and the centerline property decay rates of jets for which experimental data exist in the literature. Then the chemistry will be added to represent fully the exhaust plume.

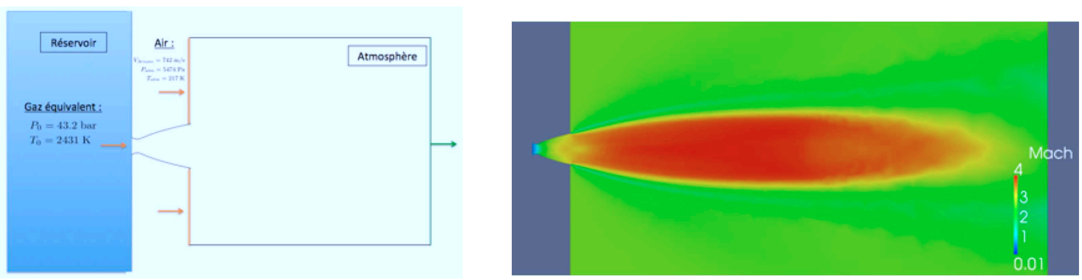

FIG. 2.4: Computational domain (left) and Mach number in a longitudinal cut (right)

2.3.2 Simulations of the plume dilution and its impact on the atmosphere (D. Cariolle, O. Thouron, R. Paoli)

The space industry now provides an important component of the societys infrastructure and economy. It plays a key role in several sectors such as telecommunications, broadcasting, or earth observation. Rockets are the vectors of space activities with the rocket launch being the most visible manifestation of a space mission. During a launch, the burning of massive amounts of propellants within minutes leads to vast emissions of chemically and/or climate-forcing (i.e. radiatively active) gases and particles into the atmosphere, resulting in perturbations of atmospheric chemical composition and radiative balance. Gases and particles are emitted either directly from engines or produced as secondary products of processes occurring in rocket plumes. The principal compounds emitted by the european launcher Ariane 5, Vega, Soyuz are carbon dioxide (CO_2) and water vapour (H_2O), chlorine compounds (HCl, chlorine radicals) for Ariane and Vega, nitrogen oxides (NO and NO_2, jointly referred to as NOx), carbon monoxide (CO), aluminium oxide (Al_2O_3) particles for Ariane and Vega and soot particles for Soyuz.
CO_2 and H_2O are powerful greenhouse gases. The other exhaust products are not climate forcers but they play an influential role in atmospheric chemistry, especially chlorine and nitrogen oxides who are involved in the production and destruction of ozone, an important climate forcer.
In a 'clean' atmosphere without anthropogenic emissions, ozone is mainly produced by photodissociation of molecular oxygen and the main reactions that control its concentration are the following :

$$\begin{array}{lllll} O_2 & + \ h\nu & \rightarrow \ O(^3P) & + \ O(^3P) & \qquad (\lambda < 242nm) \\ O(^3P) & + \ O_2 & \rightarrow \ O_3 & & \\ O(^3P) & + \ O_3 & \rightarrow \ O_2 & + \ O_2 & \end{array}$$

When reactive emissions are introduced, like the chlorine species from propergol combustion, the ozone content is reduced by the following catalytic cycle :

$$\begin{array}{llllll} & Cl & + \ O_3 & \rightarrow \ ClO & + \ O_2 \\ & ClO & + \ O & \rightarrow \ Cl & + \ O_2 \\ \hline Bilan: & O_3 & + \ O & \rightarrow \ 2O_2 & \end{array}$$

In that context we have studied the impact on stratospheric ozone of a launch of a rocket using propergol, like Ariane, Vega or the U.S. Titan. Emphasis has been placed on the regional impact above the launch site and on the ozone destruction within a few hours after the launch. This period is critical since the rocket exhausts are still very large and their impact on ozone is maximum. To this end we have developed a transport-chemistry model which computes the chemical composition of the plumes during their dispersion phase. The transport is introduced with a diffusion model in cylindric geometry. The chemical scheme is composed of 29 species and about 80 reactions which account for the main reactions of the Ox, NOx, Clx and HOx species. The models solves the system :

$$dC_i/dt = ... - div(K.grad(C_i)) - KC_jC_i + ... \qquad (2.1)$$

where C_i are the concentrations and K the diffusion coefficient. The resulting set of equations is integrated using the chemical solver described in section 3.1. Fig. 2.5 shows the ozone evolution after Titan 4 launch at midnight at 15 et 40 km. At sunrise, at 6 am, the ozone is rapidly destroyed within the launcher plume. The ozone destruction reaches about 70$\%$ at 15 km and almost all the ozone is removed within the plume at 40 km. Those pictures are in good agreement with in-situ measurements in the lower stratosphere obtained by aircraft in the plume after a Titan 4 launch. The local ozone destruction persists over a day before it is completely mixed with the surrounding atmosphere.

This work is still in development, next steps will focus on the initialisation of the radical concentration using outputs from the AVBP code (see section 2.3.1), on the atmospheric impact of rockets that use kerosene and on the improvement of the representation of transport processes by atmospheric turbulence.

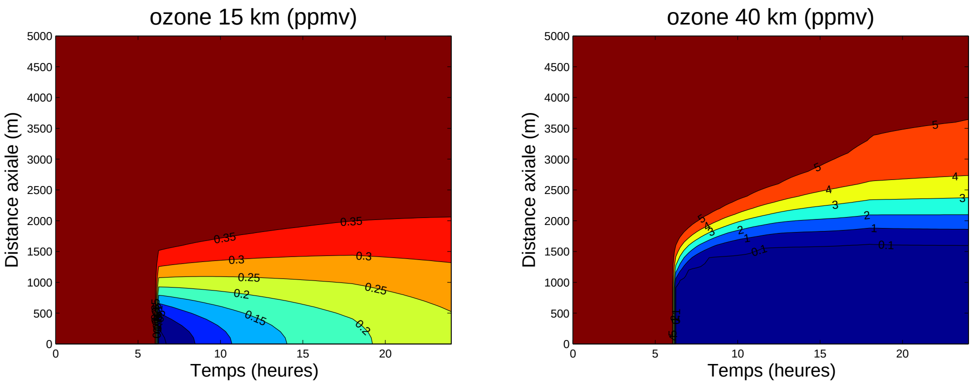

FIG. 2.5: Time evolution of the ozone content after an Titan 4 launch at 15 et 40 km.

3 Large scale atmospheric composition

3.1 Introduction of chemistry into large-scale atmospheric models (D. Cariolle, R. Paoli)

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All the models that include atmospheric chemistry need to adopt a numerical solver to integrate the transport-chemical continuity equations. This is usually done by the integration of successive operators working on the integration of the transport equation followed by the calculation of the evolution of the chemical species. For instance, with the MOCAGE CTM from Météo-France, the model first solves the evolution of the species due to advection with a semi-lagrangien scheme, followed by the chemical evolution of species solved using a semi-implicit solver. Both of those schemes do not assure mass conservation and hence may introduce drifts in the numerical integration which could become large for long term multi-year simulations. To study the properties of some advection and chemical solvers we have developed within the SOLSTICE project a reduced 2D model that mimic the evolution of the atmospheric composition on a latitude-longitude plane from pole to pole. On that geometry the model solves the coupled set of continuity equations :

$$dC_i/dt = ... - div(V.C_i) - K_{ij}C_jC_i + ... \tag{3.1}$$

Where C_i are the species concentrations and V the velocity. To integrate the transport part of the above equation, the divergence of the fluxes, we have used the so called 'slope scheme' which adopts a volume finite formulation, is characterised by its mass conservation, and assures the positivity of the solution if a slope limiter is used. For the integration of the chemistry par of the equation we have developed a semi-implicit scheme which is mass conserving and is preconditioned to insure positivity in most cases. The discretisation writes as follow :

$$(C_i^{t+1} - C_i^t)/dt = -\delta K_{ij}C_j^tC_i^{t+1} - (1-\delta)K_{ij}C_j^{t+1}C_i^t \tag{3.2}$$

The C^{t+1} concentrations are obtained by inversion of the matrix obtained from the above equation. The matrix is of the order on the number of species. On scalar computers we use the direct DGES software from the Scalapack library to invert the system. In a preliminary version the value of δ was fixed according to the user's knowledge of the stiffness of the system, but il was found that a much stable solution was obtained by evaluating its value using the species concentrations at time t. Best results were obtained with the formulation : $\delta = C_j^t/(C_j^t + C_i^t)$, coupled to the determination of the time step dt function of the curvature of the solution.

We have first tested the above choices in the framework of the reduced model. The chemical system is composed of 30 species representative of the Ox, HOx, NOx and Clx chemistry in the stratosphere. The model performed very well, Fig. 3.1 shows for instance the concentration of the $HOCl$ radical after more than 1000 iterations of the system. As can be seen the solution exhibits filamentations of the field, which are a result of the combination of advection and chemistry. In the atmosphere this sort of situation is encountered for air masses at the boundary of the ozone hole in the stratosphere. The chemical solver was then introduced in the CNRM general circulation model. Preliminary results show a satisfying behaviour, although with a numerical cost which will be only affordable if the model is integrated in parallel mode on a scalar computer. The solver was also tested with success in the LATMOS chemical transport model applied to the atmosphere of Mars.

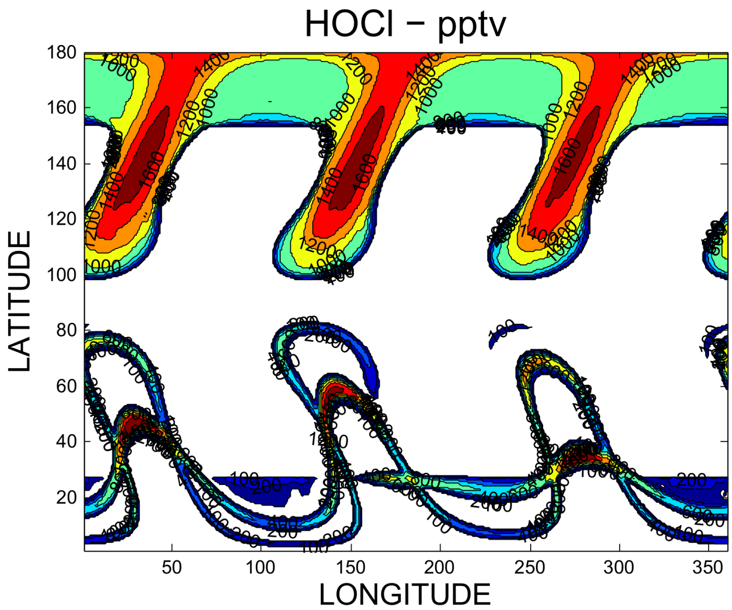

FIG. 3.1: Distribution of the concentration of $HOCl$ computed by the reduced model

3.2 A finite volume model for the advection of tracers on a sphere (D. Cariolle, A. Praga, L. Giraud).

In the context of three-dimensionnal tracer advection on the sphere, as discussed in the previous section, we are studying finite-volume schemes on an area-preserving grid. The objective is to develop an efficient mass conservative scheme with a good scalability on HPC that will be coupled to the chemical solver described in section 3.1. In order to avoid the problem of convergence of the longitudes at the poles, the adopted grid conserves an equally spacing of the latitudes but, from equator to pole, reduces progressively the number of points on each latitudinal circle. The number of point on each latitude is chosen to obtain model cells that have approximatively the same surface, so that for a given velocity vector the maximum possible time step is uniform all over the globe. Grid properties are set by specifying a reference cell at the equator. In our preliminary tests , a cell of 1° by 1° was used.

On that grid the bidimensionnal advection is done by successive transports in each direction. For each one-dimensionnal case, we use a finite volume scheme, a standard scheme in the climate modelling community. We chose a Van Leer's second-order scheme, which is accurate and conservative by construction. Comparison with others schemes such as Prather's or Godunov's makes it interesting in terms of the accuracy/storage ratio. With slope limitations, we also ensure positivity of the solution, a property that is required for subsequent coupling with the chemical solver.

A first implementation was done as a sequential version in Matlab. The scheme was integrated on a standard test suite where winds and concentrations have analytical solutions. This allows us to check the performance

of the scheme in terms of accuracy and shape preservation, which are important properties for the modelling of atmospheric flows.
For example, Fig. 3.2 shows the result of a 2D advection for a Gaussian shape concentration distribution. Winds were set as to create a vortex centered on the Equator. Each grid cell is represented as a single point and colorised according to its concentration. We can see that the scheme preserve the filament shape, even after several rotations.

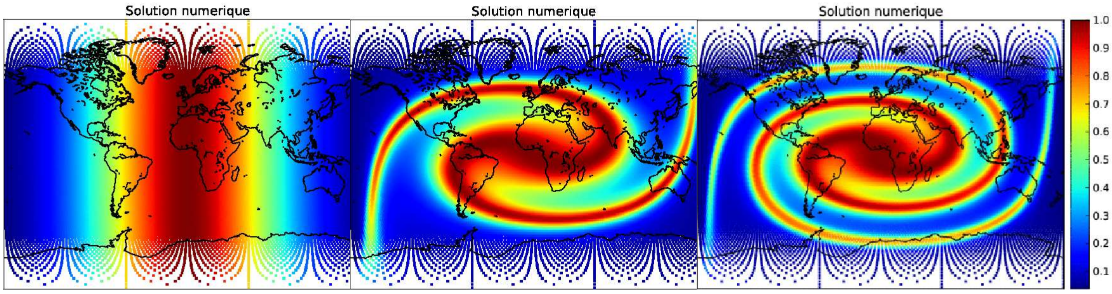

FIG. 3.2: Evolution of a Gaussian concentration advected by vortex centred at the equator. Left : initial state, middle : after 600 iterations, right : after 1000 iterations.

In this reduced grid, the address of neighbour cells are obtained by analytical formulas. This property will be used for building a massively parallel code in Fortran 90 based on domain decomposition. For that purpose, the grid will be partitioned at two levels. First, a three sectors division arises naturally when building the grid. Then the remaining partitioning will be done according to the number of processors. The next steps will be the introduction of a chemical scheme similar to the one used in chemical transport models in order to study the scalability of the code for representative atmospheric situations.

3.3 Atmospheric impact of alternate fuel for aviation : the SWAFEA project (D. Cariolle, R. Paoli)

Tropospheric ozone is a gas with a significant contribution to the greenhouse forcing, and is an oxidant that can hump living species and human health at high concentrations. Ozone is formed in the troposphere via several chemical cycles involving methane, NMH and VOC species and the nitrogen oxides. Consequently, emissions of nitrogen oxides tend to increase the ozone formation. As such the aircraft NOx, CO and NMH emissions contribute to the ozone production, especially at cruise altitude near the tropopause in the northern hemisphere. Current evaluations report that about 7% of the ozone at the tropopause in the North Atlantic corridor is due to the NOx injection by the current commercial fleet.
In the SWAFEA project CERFACS has investigated the possible impact of the use of alternate fuels on the ozone formation. This has been done using the MOBIDIC 2D photochemical model using emissions scenarios at the horizon 2026 constructed by AIRBUS based on gas emissions compiled by SAFRAN for current and alternate jet fuels. The scenarios are based on traffic forecasts and evolution of the fleet, and are constructed using the ELISA tool that combines air traffic data, fleet composition, distribution of routes, and calculation of emissions along each mission.
The MOBIDIC model solves the transport-chemistry continuity equations as a function of latitude and height. The chemistry scheme used in MOBIDIC includes the main gas-phase reactions driving the NOx, HOx, $ClOx$, $BrOx$ catalytic cycles, with 32 transported long-lived species, and 32 short-lived species computed using steady-state assumptions. The gas-phase chemical rates have been upgraded according to the recommendations of the JPL-2003-25 report. For the present study the chemical scheme of MOBIDIC

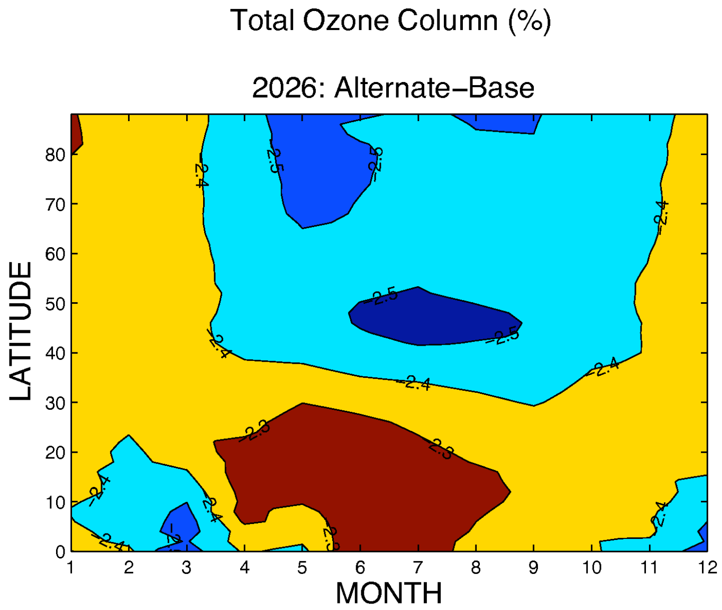

FIG. 3.3: Reduction in the ozone formation due to the use of alternate fuels at the 2026 horizon

has been extended to include ethane, PAN and CH_3CO_3. The NMH emitted by aircraft are assumed to follow an oxidation cycle with rates identical to ethane, which is a fair approximation given the rather short lifetime of NMH in the upper troposphere. The MOBIDIC model uses a dynamical forcing (wind components and temperature) from a transient climate scenario of the ARPEGE-Climat model which takes into account the evolution of trace gases having an impact on radiation and chemistry.

The impact of using alternate fuels is first seen on the NOx atmospheric content. At the 2026 horizon the NOx content would decrease by about 2% at cruise altitude in the NH (about 3 pptv). Consequently less ozone would be produced by the NOx aircraft emissions, an ozone decrease of 200 ppt is calculated at the tropopause level at mid-latitudes. In relative terms the ozone production would decrease by about 2.4% , with little seasonal and latitudinal variations (see Fig. 3.3).

We can conclude that the used of alternate fuel (50% blend of agro-fuel and Jet A-1 kerosene) should have a very modest impact on the ozone atmospheric content. According to our model calculation, the ozone production at the 2026 time horizon would decrease by about 2.4 % when alternate fuel is used. This is a very small number that is at least one order of magnitude lower that variations due to natural variability or changes that are expected to follow the decrease in the stratospheric chlorine loading. In addition, this results is quite uncertain because the NOx index of emission for alternate fuel appears to be very variable from one engine type to another, and also according to the power regime used. Thus, the NOx emission reduction is a result of a delicate balance directly related to the details of the fleet scenario. Most of the NOx decrease seems however to be related to the lowest fuel consumption in the alternate scenario compared to the reference one.

4 Publications

4.1 Journal Publications

[PAE1] M. Claeyman, J.-L. Attié, L. E. Amraoui, D. Cariolle, V.-H. Peuch, H. Teyssèdre, B. Josse, P. Ricaud, S. Massart, A. Piacentini, J.-P. Cammas, N. L. Livesey, H. C. Pumphrey, and D. P. Edwards., (2010), A linear CO chemistry parameterization in a chemistry-transport model : evaluation and application to data assimilation., *Atmos. Chem. Phys.*, **10**, 6097–6115.

[PAE2] M. Claeyman, J.-L. Attié, V.-H. Peuch, L. E. Amraoui, W. A. Lahoz, B. Joss, M. Joly, J. Barré, P. Ricaud, S. Massart, A. Piacentini, T. von Clarmann, M. Höpfner, J. Orphal, J.-M. Flaud, and D. P. Edwards, (2011), A thermal infrared instrument onboard a geostationary platform for CO and O3 measurements in the lowermost troposphere : observing system simulation experiments., *Atmos. Measur. Tech.*, **4**, 1637–1661.

[PAE3] L. El Amraoui, J.-L. Atté, N. Semane, M. Claeyman, V.-H. Peuch, J. Warner, P. Ricaud, J.-P. Cammas, A. Piacentini, B. Josse, D. Cariolle, S. Massart, and H. Bencherif., (2010), Midlatitude stratosphere-troposphere exchange as diagnosed by MLS O_3 and MOPITT CO assimilated fields., *Atmos. Chem. Phys.*, **10**, 2175–2194.

[PAE4] J. Flemming, A. Inness, L. Jones, H. J. Eskes, V. Huijnen, M. G. Schultz, O. Stein, D. Cariolle, D. Kinnison, and G. Brasseur., (2011), Forecasts and assimilation experiments of the Antarctic ozone hole 2008., *Atmos. Chem. Phys.*, **11**, 1961–1977.

[PAE5] P. Huszar, D. Cariolle, R. Paoli, T. Halenka, M. Belda, H. Schlager, J. Miksovsky, and P. Pisoft., (2010), Modeling the regional impact of ship emissions on NOx and ozone levels over the Eastern Atlantic and Western Europe., *Atmos. Chem. Phys.*, **10**, 6645–6660.

[PAE6] S. Massart, B. Pajot, A. Piacentini, and O. Pannekoucke., (2010), On the merits of using a 3D-FGAT assimilation scheme with an outer loop for atmospheric situations governed by transport., *Month. Weather Rev.*, **138**, 4509–4522.

[PAE7] S. Massart, A. Piacentini, and O. Pannekoucke., (2011), Importance of using ensemble estimated background error covariances for the quality of atmospheric ozone analyses., *Quarter. J. Roy. Met. Soc.*, early view.

[PAE8] B. M. Monge-Sanz, M. P. Chipperfield, D. Cariolle, , and W. Feng., (2011), Results from a new linear O3 scheme with embedded heterogeneous chemistry compared with the parent full-chemistry 3-D CTM., *Atmos. Chem. Phys.*, **11**, 1227–1242.

[PAE9] D. Olivié, D. Cariolle, H. Teyssèdre, D. Salas, A. Voldoire, H. Clark, D. Saint-Martin, M. Michou, F. Karcher, Y. Balkanski, M. Gauss, O. Dessens, B. Koffi, and R. Sausen., (2011), Modeling the climate impact of road transport, maritime shipping and aviation over the period 18602100 with an AOGCM., *Atmos. Chem. Phys. Discuss.*, **11**, 19769–19850.

[PAE10] P. Pajot, S. Massart, D. Cariolle, A. Piacentini, O. Pannekoucke, W. A. Lahoz, C. Clerbaux, P. F. Coheur, and D. Hurtmans., (2011), High resolution assimilation of IASI ozone data with a global CTM., *Atmos. Chem. Phys. Discuss.*, **11**, 29357–29406.

[PAE11] R. Paoli, D. Cariolle, and R. Sausen., (2011), Review of effective emissions modeling and computation., *Geosci. Mod. Dev.*, **4**, 643–667.

[PAE12] R. Paugam, R. Paoli, and D. Cariolle., (2010), Influence of vortex dynamics and atmospheric turbulence on the early evolution of a contrail., *Atmos. Chem. Phys.*, **10**, 3933–3952.

[PAE13] O. Thouron, J.-L. Brenguier, and F. Burnet, (2011), Supersaturation calculation in large eddy simulation models for prediction of the droplet number concentration., *Geosci. Mod. Dev. Discuss.*, **4**, 3313–3337.

4.2 Technical Reports

[PAE14] S. Massart and A. Piacentini., (2011), How important is to use ensemble estimated background error covariances for the atmospheric ozone analysis ?, Technical Report TR/AE/11/16, CERFACS.