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. 2006 – Dec. 2007

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Foreword

Welcome to the 2006-2007 issue of the CERFACS Scientific Activity Report.

Before turning to more scientific issues it is worth recalling a main event which took place during the period : on October first, 2006, ONERA, the French Aerospace Lab, became the sixth CERFACS shareholder. This brought new support to CERFACS' research activities such as aerodynamics and code coupling, among others. It is also important to mention that CERFACS celebrated its 20^{th} anniversary on October 12, 2007, which offered the opportunity for a large crowd of CERFACS' alumnis and all-time friends to gather on the premises to listen to stimulating talks and enjoy getting together again.

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

Parallel Algorithms

Highlights of the activity during the period include :
- development of a new flexible variant of the GMRES solver, based on deflation and outperforming the previous flexible schemes, and application to RCS computations in electromagnetics ;
- development of multigrid preconditioned Krylov methods for the scalable solution of very large three-dimensional Helmholtz linear systems on massively parallel computers to simulate wave propagation problems, and application to depth imaging in geophysics ;
- development of hybrid direct/iterative solver on distributed memory computers, and application to electromagnetics or structural mechanics ;
- improvement of the ScaLAPACK software based on packed format for storage, leading to halving the necessary memory space without degrading the speed of computation, and application to gravity field computations in geodesy ;
- use of multigrid trust region methods in bound constrained optimization, and application to calculus of variations ;
- development of new Ritz preconditioned trust region algorithm for data assimilation.

To better disseminate these and other results, the series of "Sparse Days" meetings was continued (CERFACS, June 15-16, 2006, and October 10-12, 2007). On a greater scale the team co-organized with ENSEEIHT the 2007 international conference on "Preconditioning techniques for large sparse matrix problems in scientific and industrial applications (PRECOND-07)" on July 9-12, 2007, with a large European and overseas participation.

Computational Fluid Dynamics

The work is now entirely organized around two simulation codes : on the one hand, AVBP is used for combustion studies by CERFACS and many other laboratories and institutes around Europe and overseas while, on the other hand, elsA, developed together with ONERA, is used for aerodynamics.

Simulation methods for turbulent combustion kept progressing at a very rapid pace. Let us just mention a few highlights in this field :

- development of large-eddy simulations (LES) for reacting flows, with world-premier applications dealing with the simulation of a full combustion chamber in real industrial configurations, including all chamber components (casing, walls, swirlers, exhaust nozzle) and all burners (15) ;
- development of LES for piston engines (with IFP), with world-premiere applications in simulation of multiple successive cycles ;

These achievements made possible thanks, in part, to the very efficient AVBP code, now a ”standard” code for massively parallel machines tested on almost all computers belonging to the Top 10. They led to the success of the Marie-Curie ”ECCOMET” project under FP7, aimed at training experts in two-phase flow combustion and providing grants for 12 PhD students coming from Europe and overseas. They also convinced SNECMA to initiate the C3S project, a first step towards industrialization of the AVBP code.

Highlights of the aerodynamics activity during the period include :

- numerical simulation of the distortion generated by crosswind inlet flows, and application to nacelle design ;
- numerical simulation of casing treatment for turbomachines, with extension of the compressor operability and increase of the pressure ratio ;
- spatial simulation of wave-vortices fusion during take-off and landing ;
- first attempt toward the simulation of a whole gas turbine. Most of these studies take, or will take, advantage of the massively-parallel version of elsA, which is under active development on CERFACS' new IBM Blue Gene computer.

Additional CFD activities have been concerned with new applied simulations of ventilation in aircraft painting halls and within office buildings, and with wind simulation within urban districts or flow simulation in a computer room for the blow-out plenum.

Computational Electromagnetism

Among the main achievements which took place over the period one should mention :

- development of the fast multipole method for scattering problems with an impedance surface, and application to the evaluation of the impact of a wind turbine farm on a VOR antenna ;
- further development of domain-decomposition methods and of the coupling of integral equations with finite-element solution ;
- first application of the linear-sampling method to reconstruct images of dielectric objects ;
- improvement of the Galbrun method to describe the sound propagation inside any prescribed subsonic flow.

Climate Modelling

Using the fingerprint method allowed CERFACS' researchers to estimate that about two-thirds of the 1990's observed warming over France can be attributable to human influence, with the rest explained by natural variability. Further studies at the subregional spatial scale showed that large modifications of the precipitations and of the other components of the hydrological cycle are to be expected over France at the 2050 horizon.

A promising result for seasonal forecasting was obtained through the use of statistical modelling : if the phase and amplitude of the Maden-Julian oscillation (MJO) are used as predictors, the sign of the North-Atlantic oscillation (NAO) 12 days later can be correctly predicted in approximately 70% of the cases.

It is also important to mention the participation in the French contribution in the 5^{th} IPCC report (IPCC AR-5), including the development of a high-resolution coupled ocean-atmosphere model in collaboration with CNRS, IFREMER and Earth Simulator Center in Japan ;

Coupling

Couplers were still actively developed over the period, with :

- OASIS.4 being more and more widely chosen by climate groups, including now the Met Office in the UK and the Bureau of Meteorology of Australia, and being at the core of the new FP'7 METAFOR project to describe in a standard way the climate data as well as the numerical models and their coupling algorithms that produce this data ;
- PALM is successfully used for more and more coupling applications (data assimilation in the ocean for atmospheric chemistry and for neutronics, hydrology, ecosystem modelling, model nesting, fluid-structure coupling, optimization, ...). The newly developed version (2_4_0) accounts for dynamic object size and is available on a number of computing platforms. It can be found in the new Web site, and specific training for all types of users is organized at very short notice.

Data Assimilation

Data assimilation methods have been applied to oceanic, atmospheric-chemistry, and neutronic problems :

- development of an advanced variational ocean data assimilation system called NEMOVAR, in collaboration with ECMWF, the Met Office in the UK, and INRIA. It is based on the earlier OPAVAR system but is redesigned for the new NEMO model, and includes features such as 3D-Var with multivariate covariances, assimilation of in situ profiles, surface temperature, and multi-satellite altimeter data, and can run on distributed memory machines ;
- using the PALM software and the MOCAGE model, data assimilation of atmospheric ozone showed that the various satellite-borne sensors are suffering from different biases, and that a reference analysis of the ozone field has then to be constructed ;
- using mock-ups of the EDF Kaféine and Manara models together with the PALM coupler, the neutronic activity in the core of a nuclear power plant has been optimally reconstructed from all the available measurements, with a new application aiming at determining the efficiency of this reconstruction as a function of the number of measurements.

Oceanography

The MERCATOR group successfully contributed to the study of the seasonal oceanic structure using the eddy-permitting version of the model at $1/4^{th}$ degree resolution, and was instrumental in developing the new eddy-resolving model at $1/12^{th}$ degree resolution.

Aviation and Environment

With the aim of developing a parameterization of air traffic for inclusion within climate models, and using the suite of NTMIX and Meso-NH models, 3D simulations of an aircraft wake have been realized, which include all dynamical, chemical, and microphysical processes. The resulting contrails exhibit very realistic distribution and size of ice particles ; Similar studies are also being developed for ship-plume simulations.

Technology Transfer

The N'S'^{3} solution, for collaborative working for the extended enterprise, benefited from additional new functionalities. It is now organized as a Web application, with secure access, secure data exchange, and data-access management per user.

Computing resources

A new computer (IBM Blue Gene L) was installed in the summer of 2007, with a peak capacity of 5.7 TFlop/s, and with an accompanying increase of the storage capacity.

CERFACS scientific production is still high :
- the number of high-standard publications, i.e. in internationally-refereed journals, is close to 90 for the period, showing an increase as compared to past years when the mean rate of publications was closer to 30 to 35 per year ; CERFACS' researchers have also produced over the period approximately 200 technical reports, book chapters, and papers in conference proceedings ;
- training of new researchers is very intense, with 24 Ph. D. theses being awarded over the period.
- it is also worth mentioning that among the 12 proposals which CERFACS submitted to the 7^{th} Framework Programme of the European Union in response to its 2007 calls, 7 of them were successful, achieving quite a high success rate close to 60% ;
- finally CERFACS researchers and engineers are also very active in applied research, with more than 50 grants per year being held over the period, awarded either by national funding agencies or industrial partners.

During 2006 and 2007, the mean total number of (full-time equivalent) people working at CERFACS has been 94 (see Tables ii to ix), with a global annual budget rising from 6.3 to 7.3 M€.

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

Enjoy your reading.

Jean-Claude ANDRÉ
CERFACS Director

CERFACS Structure

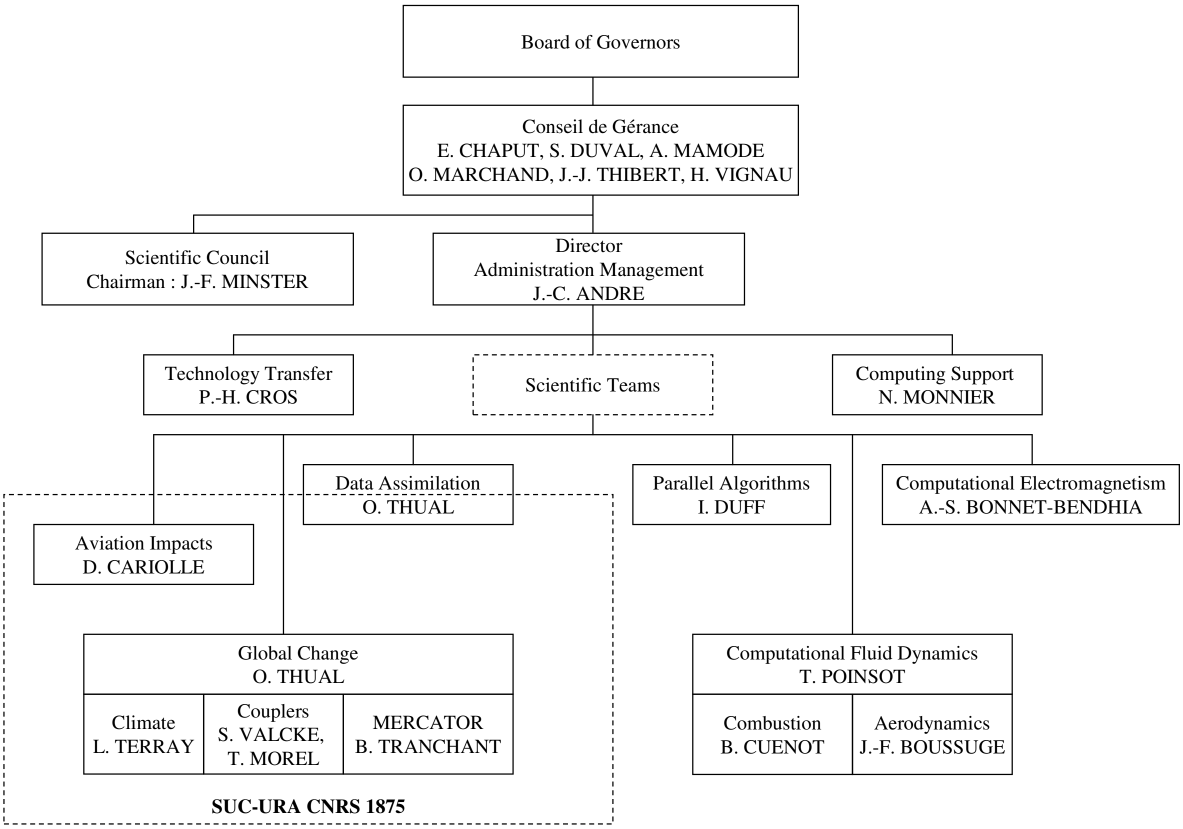
As a ”Société Civile” CERFACS is governed by two bodies.
Firstly, the ”Conseil de Gérance”, composed of only 6 managers (in French, ”Gérants”) nominated by the 6 shareholders (see table i, where the 6th shareholder, ONERA, joined on Oct. 1st, 2006), follows quite closely the CERFACS activities and the financial aspects. It met 9 times during the period (12 April 2006, 18 May 2006, 23 June 2006, 12 September 2006, 20 December 2006, 25 April 2007, 2 July 2007, 10 September 2007 and 20 December 2007).
Secondly the Board of Governors (in French ”Assemblée des Associés”), composed of representatives of CERFACS shareholders and of 3 invited personalities, including the Chairman of the Scientific Council. It met 4 times during the period (18 January 2006, 4 October 2006, 17 January 2007 and 26 September 2007).

CERFACS Scientific Council met for the tenth time, on 9 January 2007, under the chairmanship of Prof. Jean-François MINSTER.

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

CENTRE NATIONAL D’ÉTUDES SPATIALES (CNES)	23.4 %
ÉLECTRICITÉ DE FRANCE (EDF)	23.4 %
MÉTÉO-FRANCE	23.4 %
EUROPEAN AERONAUTIC DEFENCE AND SPACE COMPANY (EADS)	9.9 %
SAFRAN	9.9%
OFFICE NATIONAL D’ÉTUDES ET DE RECHERCHES AÉROSPATIALES (ONERA)	9.9%

Table i : Société Civile Shareholders



CERFACS chart as of Dec. 31, 2007

CERFACS Staff

NAME	POSITION	PERIOD
DUFF	Project Leader	1988/11
CHATELIN	Group leader	1988/09
GRATTON	Senior	2002/07-2007/06
VASSEUR	Senior Post Doc	2007/05 2005/10-2007/04
BABOULIN	Post Doc Ph.D student	2006/04 2003/09-2006/03
BASTIN	Post Doc	2005/01-2006/12
GARCIA ARAUJO	Post Doc	2006/04
TSHIMANGA	Post Doc	2007/11
UCAR	Post Doc	2007/01
AHMADNASAB	Ph.D student	2003/08
BOESS	Ph.D student	2006-05-2007/04
HAIDAR	Ph.D student	2005/03
MOUFFE	Ph.D student	2005/10
PINEL	Ph.D student Student	2006/10 2006/04-2006/09
SLAVOVA	Ph.D student	2005/03
TROELTZCH	Ph.D student Student	2007/05 2006/10-2007/03
AMESTOY	Engineer	2005/12-2006/03
LE BERRE	Engineer	2005/06
FEZZANI	Student	2007/04-2007/09
GAYOU	Student	2007/02-2007/08

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

NAME	POSITION	PERIOD
POINSOT	Project Leader	1992/09
CHEVALIER	Senior	1999/11-2006/01
CUENOT	Senior	1996/10
DENIAU	Senior	2006/11
JOUHAUD	Senior	2001/10
GICQUEL	Senior	2004/02
MONTAGNAC	Senior	2000/11
PAOLI	Senior	2004/07
PUIGT	Senior	2005/12
VERMOREL	Senior Post Doc	2007/11 2005/11-2007/10
BOUSSUGE	Research Engineer	2002/02
SOMMERER	Research Engineer	2002/04-2006/05
BOIN	Post Doc	2004/12-2006/06
BOUDIER	Post Doc Ph.D student	2007/10 2004/10-2007/09
BRACONNIER	Post Doc	2007/01
DUCHAINE	Post Doc Ph.D student	2007/11 2004/10-2007/09
DUFOUR	Post Doc	2007/06
GOURDAIN	Post Doc	2006/02
LAMARQUE	Post Doc Ph.D student	2007/11 2004/10-2007/10
LANDMANN	Post Doc	2006/08
MENDEZ	Post Doc Ph.D student	2007/11 2004/10-2007/09
PORTA	Post Doc Ph.D student	2007/04 2004/04-2007/03
STAFFELBACH	Post Doc Ph.D student	2006/06 2002/10-2006/05
ALBOUZE	Ph.D student	2005/10
AMAYA	Ph.D student Student	2006/10 2006/02-2006/08
AUFFRAY	Ph.D student	2003/10-2006/12
BLANC	Ph.D student Engineer	2006/09 2005/10-2006/08
BODOC	Ph.D student	2007/07
CABRIT	Ph.D student Student	2006/10 2006/02-2006/08
COLIN	Ph.D student	2004/12
DAUPTAIN	Ph.D student	2002/10-2006/03
DEVESA	Ph.D student	2003/10-2006/10
ENAUX	Ph.D student Student	2006/10 2006/02-2006/08
FOSSO	Ph.D student Student	2007/10 2007/04-2007/09

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

GARCIA	Ph.D student	2005/10
GIAUQUE	Ph.D student	2003/09-2007/02
GULLAUD	Ph.D student Student	2007/11 2007/04-2007/09
GUTIERREZ	Ph.D student	2006/12
JAEGLE	Ph.D student	2006/09
LACAZE	Ph.D student	2005/11
LAVEDRINE	Ph.D student	2004/10
LEGRAS	Ph.D student	2007/11
LEYKO	Ph.D student	2006/09
MAGLIO	Ph.D student	2007/07
NYBELEN	Ph.D student	2004/11
OZEL	Ph.D student	2007/09
PASCAUD	Ph.D student	2002/10-2006/01
RIBER	Ph.D student	2003/10-2007/03
ROUX Seb	Ph.D student Ph.D student	2003/10-2006/12 2001/10-2004/12
ROUX A	Ph.D student	2005/10
SAN JOSE	Ph.D student Student	2006/10 2006/02-2006/08
SCHMITT	Ph.D student	2005/10
SENGISSEN	Ph.D student	2002/10-2006/02
SENONER	Ph.D student	2007/01
SENSIAU	Ph.D student	2005/03
SICOT	Ph.D student Engineer Student	2006/09 2006/04-2006-07 2005/09-2006/02
SILVA GARZON	Ph.D student Student	2007/08 2007/04-2007/07
WAGNER	Ph.D student	2006/10
WIECZOREK	Ph.D student	2007/06
WOLF	Ph.D student	2007/10
WUNSCH	Ph.D student	2006/12
ZEREN	Ph.D student	2006/12
ZUZIO	Ph.D student	2007/08
BOILEAU	Engineer Ph.D student	2007/05 2003/10-2007/02
BENOIT	Engineer	2006/05-2007/11
CHANAUD	Engineer	2007/09-2007/10
JOUBERT	Engineer	2007/06
ROUMEAS	Engineer	2007/06
TOURNIER	Engineer	2005/04-2006/09

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

AYACHE	Student	2007/06-2007/08
BEN AHMED	Student	2007/04-2007/09
COMBE	Student	2007/09
DASSE	Student	2007/02-2007/08
	Student	2006/06-2006/09
ETIENNE	Student	2006/06-2006/09
EYSSARTIER	Student	2007/06-2007/08
GERMAINE	Student	2007/04-2007/09
GRAU	Student	2007/07-2007/09
GUEZENNEC	Student	2006/03-2006/08
MARGER	Student	2006/03-2006/08
MYRCZIK	Student	2006/03-2006/08
PEDOT	Student	2007/02-2007/03
ROUX Ste	Student	2006/06-2006/09
STOLL	Student	2007/06-2007/11
VAN LEEUWEN	Student	2006/09-2007/02
VICQUELIN	Student	2006/04-2006/10
BOLLWEG	Visitor/Ph.D student	2006/10-2007/01
BREAR	Visitor	2005/09-2006/01
HERNANDEZ	Visitor/Ph.D student	2007/09-2007/12
KAESS	Visitor/Ph.D student	2006/09-2006/11
MULLER	Visitor	1997/11/
NICOUD	Visitor	2001/10
RICHARDSON	Visitor/Ph.D student	2007/02-2007/05
RIZZI	Visitor	1987/10
SAGAUT	Visitor	2003/12
SCHONFELD	Visitor	2001/01

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

NAME	POSITION	PERIOD
THUAL	Project Leader	1991/09
ROGEL	Senior	1998/10
TERRAY	Senior	1992/10
WEAVER	Senior	1999/11
MASSART	Senior	2004/12
BOURIQUET	Research Engineer Engineer	2006/08 2005/11-2006/07
MAISONNAVE	Research Engineer	2000/12
MOREL	Research Engineer	2000/03
VALCKE	Research Engineer	1997/02
DAMASIO DA COSTA	Post Doc	2006/10
MUNOZ	Post Doc	2007/10
RICCI	Post Doc CNRS	2007/11 2006/10-2007/10
SANCHEZ	Post Doc	2005/05-2007/04
DAGET	Ph.D student	2005/05
MINVIELLE	Ph.D student	2005/09
MIROUZE	Ph.D Student	2007/10
NAJAC	Ph.D student	2005/10
BOE	Engineer Ph.D student	2007/12 2004/10-2007/11
CAMINADE EPITALON	Engineer Ph.D Student Engineer Engineer	2007/09-2007/12 2003/10-2007/08 2007/01-2007/12 2005/09-2006/08
GHATTAS	Engineer	2005/02-2006/07
MOINE	Engineer	2007/03-2007/12
RODRIGUEZ	Engineer	2005/09-2006/05
THEVENIN	Engineer	2007/12
AUGER	Student	2007/02-2007/06
BABQIQI	Student	2006/02-2006/06
CHARLES	Student	2006/06-2006/09
DUFOUR	Student	2007/02-2007/09
GUILLERM	Student	2007/01-2007/06
LABI	Student	2006/06-2006/07
PAJOT	Student	2006/01-2006/01
PEINGS	Student	2006/05-2006/06
PERE	Student	2006/05-2006/06
TRIVINO	Student	2007/02-2007/08
YANG	Student	2006/06-2006/09
ARGAUD	Visitor	2006/07
BUIS	Visitor	2006/01-2006/06
GACON	Visitor	2003/04 -2006/04
PIACENTINI	Visitor	2007/06
CASSOU	CNRS	2002/11
LORANT	CNRS	2004/09-2006/08
COQUART	CNRS Engineer	2006/12 2006/09-2006/11

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

NAME	POSITION	PERIOD
DREVILLON	Senior Post Doc	2006/06 2004/06-2006/05
TRANCHANT	Senior	2001/07
GARRIC	Senior	2005/03-2006/12
LELLOUCHE	Senior	2002/10
REMY	Senior	2003/12
BOURDALLE-BADIE	Research Engineer	2001/01
DERVAL	Research Engineer	2003/07
DRILLET	Research Engineer	1999/03
REFFRAY	Post Doc	2006/12-2007/11
CHANUT	Post Doc	2006/01-2007/12
DHOMPS	Engineer	2006/09-2006/11
LABORIE	Engineer	2005/08-2006/02
LEGALLOUDEC	Engineer	2006/03-2007/09

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

NAME	POSITION	PERIOD
BENDALI	Project Leader	1996/01
FARES	Senior	1992/06
MILLOT	Senior	1995/11
PERNET	Senior Post Doc	2007/03 2005/03-2007/02
ZERBIB	Ph.D.student	2002/10-2006/03
LE BRIS	Student	2007/07-2007/09
COLLINO	Visitor	1994/04

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

NAME	POSITION	PERIOD
CARIOLLE	Project Leader	2003/08
PAOLI	Senior	2004/07
CHOSSON	Post Doc	2006/05
LE BERRE	Engineer	2007/01
HEUFEU-TONKEU	Student	2007/03-2007/08
LAVEAU	Student	2006/01-2006/06
PEBERNET	Student	2007/02-2007/08
SOURICE	Student	2006/06-2006/09
VIZCAINO	Student	2007/03-2007/09
PAUGAM	Ph.D Student	2005/01
PIACENTINI	Visitor Engineer	2007/10 2005/11-2006/04

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

NAME	POSITION	PERIOD
CROS	Project leader	1997/04
JONVILLE	Engineer	2000/10
MAGLARAS	Engineer	2007/05-2007/09
MILHAC	Engineer	2004/01
OLIVEIRA	Technician	2007/06

TAB. viii – List of members of the ENScube group.

NAME	POSITION	PERIOD
MONNIER	Project Leader	1996/12
D'AST	Engineer	1996/10
LAPORTE	Engineer	1988/04
DEJEAN	Technician	1990/11
FLEURY	Technician	1999/10
CHANAUD	Student	2007/02-2007/08
DURAND	Student	2006/04-2006/06
JONQUET	Student	2007/04-2007/06
POMES	Student	2006/04-2006/06

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

CERFACS Wide-Interest Seminars

Anne-Sophie Bonnet (ENSTA, POEMS) : *Simulation du rayonnement acoustique dans un écoulement cisaillé.* (Jan. 10th, 2006)

Marzio Sala (ETHZ Computational Laboratory) : *Object-oriented programming techniques for sparse linear system solvers.* (Jan. 12th, 2006)

Alison Ramage (Univ. Strathclyde, Dpt. Math.) : *Multigrid solution of discrete convection-diffusion equations.* (March 24th, 2006)

Georges Duffa (CEA/CESTA) : *Protections thermiques ablatables pour la rentrée hypersonique. Le point de vue "calcul scientifique".* (April 4th, 2006)

Carlos Roberto Mechoso (Univ. California) : *What can be learned from 'sensitivity studies' with General Ciculation Models ?* (Nov. 6th, 2006)

Thilo Schönfeld (Aerospace Valley, Toulouse) : *Introduction to the 7th European Research Framework Program and the first call in the aeroautics area.* (Feb. 14, 2007)

David Keyes (Columbia Univ.) : *Scalable solver infrastructure for computational science and engineering.* (March 15, 2007)

Didier Swingedouw (CERFACS) : *Influence of ocean - ice sheets interaction on global warming projections.* (April 9th, 2007)

Andrew M. Moore (Univ. California, Santa Cruz) : *A nonnormal view of ocean variability stochastically forced by the North Atlantic Oscillation.* (June 11th, 2007)

Julian Hunt (Univ. College London) : *Using models of mesoscale flows over orography and urban areas to examine effects of climatic and environmental trends.* (Oct. 8th, 2007)

Jean-Philippe Argaud (EDF R&D and CERFACS) : *On mathematics for finance.* (Nov. 27th, 2007)

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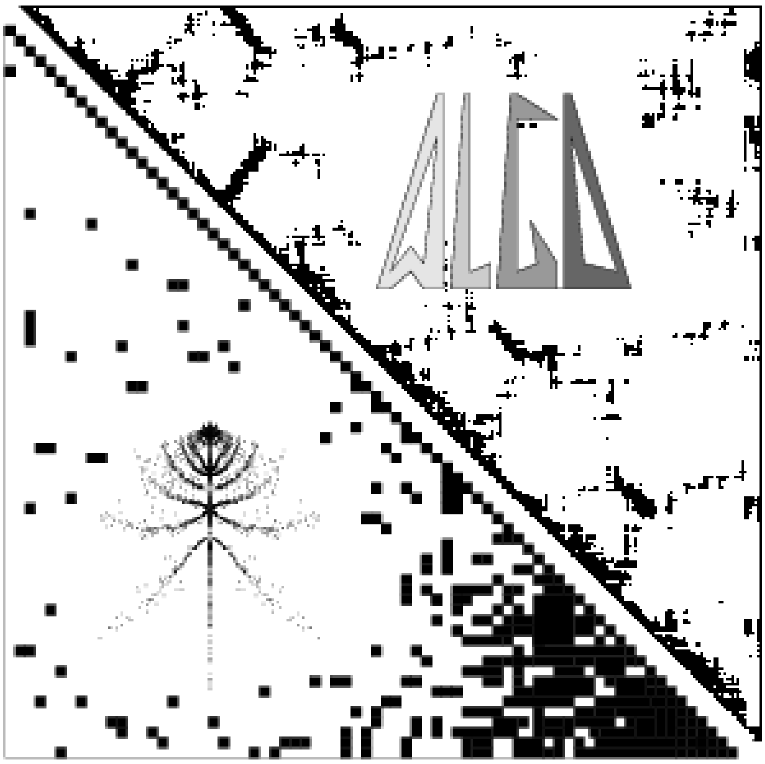
Parallel Algorithms Project



1 Introduction

1.1 Introduction

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

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

Members of the Team very much play their full part in the wider academic and research community. They are involved in Programme Committees for major conferences, are editors and referees for frontline journals, and are involved in research and evaluation committees. These activities both help CERFACS to contribute to the scientific life of France, Europe and the world while at the same time maintaining the visibility of CERFACS within these communities. Some measure of the visibility of the Parallel Algorithms Project can be found from the statistics of accesses to the CERFACS Web pages where a major part of all the hits for CERFACS projects are on the Algo web pages.

Our main approach in the direct solution of sparse equations continues to be the multifrontal technique originally pioneered at Harwell in the early 1980s. During this last period we have further developed the MUMPS package in conjunction with our colleagues at ENSEEIHT, INRIA-Lyon, and INRIA-Bordeaux. The release currently being distributed is Version 4.7.3. Some research work that will most likely have an impact on future releases is discussed in the following sections, in particular in Section 3.3. The code continues to be downloaded on a daily basis by researchers throughout the world. The complex version has been accessed extensively and used in many applications, particularly in electromagnetics. Along with our colleagues from ENSEEIHT, Lyon, and Bordeaux, we were awarded 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. Much of the work described in Sections 3 and 4 is supported by this ANR programme. We were also awarded a Franco-Berkeley Fund grant in 2007 for working in related areas although we do not plan to start work on this until March 2008.

Most of the work discussed in Section 3 is concerned with the direct factorization of symmetric indefinite and general sparse matrices. Considerable work has been done to understand and develop robust approaches to the case of symmetric indefinite matrices. Research on examining the out-of-core parallel solution for one or many right-hand sides is progressing well and will hopefully also result in future improvements to MUMPS. The current *A*chilles Heel of parallel direct methods is in the preliminary analysis stages involving mainly symbolic and combinatorial aspects. This is being addressed by some tasks from SOLSTICE and we discuss some of this work in Section 3 (e.g. Sections 3.1, 3.3, 3.9). We discuss the more downstream aspects of direct solvers including the use of MUMPS in a major code of our partners and the accurate detection of rank and null space bases that can be important both in its own right and in the development of preconditioners.

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

The main area of interest for the Qualitative Computing Group 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 by the Qualitative Computing Group.

A major focus of our work on nonlinear systems and optimization has been in joint work with the PALM Project and the Climate Modelling Group on data assimilation. This area is becoming one of the main interdisciplinary focus points at CERFACS. We are particularly involved in a study of solution techniques for linear least-squares computations that lie at the heart of data assimilation algorithms, and we have investigated several aspects of this including further studies on Gauss-Newton methods and model reduction techniques. Some of this work has been done in collaboration with scientists from the UK through a grant from the Alliance programme. We are also continuing the development of software for solving large dense linear least-squares in a parallel environment and have studied component conditioning and parallel tools for cases when the least-squares problem has constraints added in an incremental manner. Other work has involved the use of neural networks particularly as a preconditioning technique for more general optimization. Much of our optimization work involves trust region methods including the innovative combination of multilevel schemes with trust region methods for optimization problems including those arising in the solution of partial differential equations. We are greatly aided in our optimization work by Philippe Toint who is now a consultant to CERFACS in this area.

The Parallel Algorithms Project is heavily involved in the Advanced Training aspects of CERFACS' mission. We ran internal training courses for new recruits to all Projects at CERFACS to give them a basic understanding of high performance computing and numerical libraries. This course was open to the shareholders of CERFACS. 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 four stagiaires : Anke Tröltzsch from Germany, Xavier Pinel from UPS, Riadh Fezzani from UPS, and Antoine Gayou from Pau. It is good to record that the first two stagiaires are now PhD students working at CERFACS hopefully the right career choice for both the stagiaire and CERFACS. Members of the Team have assisted in many lecture courses at other centres, including ENSICA, INPT, Toulouse 1 and INSA. Marc Baboulin completed his PhD thesis on “Solving large dense linear least squares problems on parallel distributed computers. Application to the Earth’s gravity field computation” in March, 2006. I am delighted to record that the thesis was of such a high standard that Marc was awarded a Prix Léopold Escande by INPT. This maintains our impressive record and is the third Algo thesis to receive this accolade. Morad Ahmadnasab completed his PhD thesis, submitted to Université Toulouse 1, on “Homotopic deviation theory : a qualitative study” in October 2007 and was awarded it with a mention “summa cum laude”.

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.

As always, it was a pleasure to welcome on two occasions Gene Golub from Stanford who is a great source of inspiration especially to our younger students. It was with very great sorrow that we received news in November of the sudden death of Gene only a month after he had presented a plenary talk at the CERFACS Anniversary meeting. We are planning to join the world community in commemorating Gene in the celebrations planned for 29th February 2008 on the day that would have been Gene’s 19th birthday.

We continue to have a “Sparse Days at CERFACS” meeting each year. On 15-16 June 2006, our theme was on optimization and we attracted an attendance of 51 from 16 countries with 21 talks and posters. In 2007, we had in effect two sets of Sparse Days. For the first we collaborated with ENSEEIHT to host the Preconditioning 2007 meeting (a series held every two years since 1999, previously only in the US) at the main Météo Conference Centre from 9-12 July. There were 62 presentations and the meeting attracted 107 people from 24 countries. Then we combined a Sparse Days with the meeting organized at CERFACS on October 11 and 12 to commemorate the 20th Anniversary of the start of CERFACS. One special feature of this Sparse Days was that the Friday was devoted to talks by CERFACS old boys who gave very interesting talks on their current work and related it to their CERFACS experience. This meeting attracted over 60 people from 14 countries (illustrating the strength of the Algo diaspora) and was concluded by a very memorable dinner on the Friday evening. A number of distinguished scientists who came to this meeting also visited CERFACS and met members of the Team.

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 a project with EADS on preconditioning techniques in electromagnetics. We have continued our joint effort with the CERFACS electromagnetics project on the solution of discretized Maxwell equations using the boundary element method in the framework of a DGA/Dassault contract. This has been an occasion for us to use techniques developed for perfect conductors in the more general context of impedance, and to modify the GMRES-DR algorithm so that it can cope with flexible preconditioners.

We are represented in the CCT of CNES on orbitography and have developed a strong collaboration with them in the parallel distributed generation of normal equations and their subsequent Choleski factorization

for applications in geodesy and computational electromagnetics. We also took part in the organisation of a workshop on code optimization for navigation and space communication, in collaboration with the CCT of CNES on ”Positionnement et Datation par Satellites” (PDS).
We have had detailed discussions with EDF on both parallel sparse direct methods and domain decomposition methods for the solution of industrial problems in structural mechanics in the framework of Code_Aster. We have also had discussions on embedded iterations when solving generalized eigenproblems in neutronics. More recent collaboration with EDF has concerned the work on null space bases in the context of the ANR Solstice Project.
Our work on the optimization and linear algebraic aspects of data assimilation has been of great interest to and the subject of some discussions with the Climate Modelling and Global Change Group and Météo France. We now have a strong and growing collaboration with the Climate Modelling Team on aspects of data assimilation, and continue to co-host Jean Tshimanga, a researcher from Belgium who is doing a PhD at Namur with Annick Sartenaer. Jean has since joined us as a postdoc to continue his work in this area. In the context of this work, we have also hosted visits from Amos Lawless from the UK MET Office, from Nancy Nichols of the University of Reading who works partly in numerical analysis and partly with the meteorology department, and from Reading University students supported by our Alliance Programme Grant.
One of our new PhD students, Anke Tröltzsch, is doing a PhD in collaboration with Airbus on shape optimization for drag minimization under lift constraints. 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.
We have been working closely with TOTAL on the development of efficient parallel solvers for Helmholtz problems arising in their geophysical applications and have been awarded a grant by them for a PhD to help with this work.
We help 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 on advice on the accuracy of their computations in a parallel environment, and many aspects of numerical algorithms with Global Change. We are involved in close collaborations over linear solvers in electromagnetic codes with the EMC team. We have also interacted with the CSG group on issues concerning new computer chips and technologies.

As a postscript, I should record my thanks to my two seniors, Serge Gratton and Xavier Vasseur, for doing all the hard work to ensure the smooth running of the Team. Sadly Serge’s sabbatical from CNES came to an end in the summer of 2007 but I am delighted to report that his employers have seen the wisdom of allowing him to devote a substantial amount of time to continue with the research programme of the Team and to continue his supervision or joint-supervision of 3 students. It is now Xavier who has to bear the many responsibilities of the day-to-day management. I am very pleased to say that he does so in an excellent fashion and is well supported in his efforts by our enthusiastic and talented postdocs and our students who all contribute hugely to the ambience and atmosphere that many visitors remark on with great appreciation and fondness.
I should also pay tribute to the support we receive from our ex-team members who are now working at ENSEEIHT. Patrick Amestoy jointly supervises one student and interacts greatly with another and collaborates in our programmes on direct and hybrid solvers. Luc continues to supervise a student and is always on hand for good advice on our programme and interaction with partners and other teams. Daniel Ruiz is collaborating with us on aspects of the SOLSTICE project and Michel Daydé interacts closely with us on networking, computing, and GRID topics. It is our local diaspora in action !

Iain S. Duff.

Visitors to Parallel Algorithm Project in 2006-2007

In alphabetical order, our visitors in the years 2006-2007 included :
LINA ABDALLAH (INRETS, France),
MORAD AHMADNASAB (University Toulouse I, France),
PATRICK AMESTOY (ENSEEIHT-IRIT, France),
MARIO ARIOLI (RAL, U.K.),
ANGELA BERNARDINI (University of Pau, France),
AKE BJÖRCK (Linköping University, Sweden),
CAROLINE BOESS (Bremen University, Germany),
LUIZ MARIANO CARVALHO (Universidade do Estado do Rio de Janeiro, Brazil),
TIM DAVIS (University of Florida Gainesville, U.S.A),
MICHEL DAYDÉ (ENSEEIHT-IRIT, France),
JACK DONGARRA (The University of Tennessee, U.S.A.),
TONY DRUMMOND (Lawrence Berkeley National Laboratory, Berkeley, U.S.A.),
ALAN EDELMAN (Massachusetts Institute of Technology, U.S.A.),
LUC GIRAUD (ENSEEIHT-IRIT, France),
GENE GOLUB (Stanford University, U.S.A.),
NICK GOULD (University of Oxford, U.K.),
JULIAN HALL (University of Edinburgh, U.K.),
NICK HIGHAM (University of Manchester, U.K.),
DAVID KEYES (Columbia University, New-York, U.S.A),
PHILIP KNIGHT (University of Strathclyde, U.K.),
JULIEN LANGOU (The University of Colorado at Denver, U.S.A.),
AMOS LAWLESS (University of Reading, U.K.),
JEAN-YVES L'EXCELLENT (INRIA-ENS, Lyon, France),
OSNI MARQUES (Lawrence Berkeley National Laboratory, Berkeley, U.S.A.),
GÉRARD MEURANT (CEA, Bruyères-le-Châtel, France),
SERGEY NAZIN (Institute of Control Sciences, Moscow, Russia),
NANCY NICHOLS (University of Reading, U.K.),
ADELA PAGES (Universitat Politecnica de Catalunya, Spain),
ALEX POTHEN (Old Dominion University, Norfolk VA, U.S.A.),
STÉPHANE PRALET (SAMTECH, Belgium),
ALISON RAMAGE (University of Strathclyde, U.K.),
MARIELBA ROJAS (Technical University of Denmark, Denmark),
JEAN ROMAN (INRIA Futurs, LaBRI, Talence, France),
DANIEL RUIZ (ENSEEIHT-IRIT, France),
MARZIO SALA (ETH Zürich, Switzerland),
ANNICK SARTENAER (The University of Namur, Belgium),
MICHAEL SAUNDERS (Stanford University, U.S.A.),
JENNIFER SCOTT (Rutherford Appleton Laboratory, U.K.),
MASHA SOSONKINA (University of Minnesota Duluth, U.S.A.),
PHILIPPE TOINT (The University of Namur, Belgium),
JEAN TSHIMANGA (The University of Namur, Belgium),
MARTIN VAN GIJZEN (Delft University of Technology, The Netherlands),
CHRISTOPH VÖMEL (ETH Zürich, Switzerland),
FRED WUBS (University of Groningen, The Netherlands),
GAETANO ZANGHIRATI (University of Ferrara, Italy).

2 List of Members of the Algo Team

IAIN DUFF - Project Leader
FRANÇOISE CHAITIN-CHATELIN - Qualitative Computing Group Scientific Advisor
SERGE GRATTON - Senior Researcher
XAVIER VASSEUR - Senior Researcher
MARC BABOULIN - Post. Doc.
FABIAN BASTIN - Post. Doc., until December 2006
MILAGROS GARCIA - Post. Doc.
JEAN TSHIMANGA - Post. Doc., from October 2007
BORA UCAR - Post. Doc., from January 2007
CAROLINE BOESS - Ph.D. Student, from May 2006 until May 2007
AZZAM HAIDAR - Ph.D. Student
MÉLODIE MOUFFE - Ph.D. Student
XAVIER PINEL - Ph.D. Student
TZVETOMILA SLAVOVA - Ph.D. Student
ANKE TRÖLTZSCH - Ph.D. Student
MORAD AHMADNASAB - Visitor, University Toulouse I, France
PATRICK AMESTOY - Senior Visitor, ENSEEIHT-IRIT, France
LUC GIRAUD - Senior Visitor, ENSEEIHT-IRIT, France
RIADH FEZZANI - Trainee
ANTOINE GAYOU - Trainee
NICOLE BOUTET - Administration, from end of January 2006
BRIGITTE YZEL - Administration

3 Dense and Sparse Matrix Computations

3.1 Analysis of the Solution Phase of a Parallel Multifrontal Approach

P. R. Amestoy : ENSEEIHT-IRIT, *France* ; **I. S. Duff** : CERFACS, *France and* RUTHERFORD APPLETON LABORATORY, *England* ; **A. Guermouche** : LABRI, UNIV. BORDEAUX 1 / INRIA FUTURS, *France* ; **Tz. Slavova** : CERFACS, *France*

In [ALG31] 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).

3.2 Towards Stable Mixed Pivoting Strategies for the Sequential and Parallel Solution of Sparse Symmetric Indefinite Systems

I. S. Duff : CERFACS, *France and* RUTHERFORD APPLETON LABORATORY, *England* ; **S. Pralet** : ENSEEIHT-IRIT, *France*

In [ALG11] we consider the direct solution of sparse symmetric indefinite matrices. We develop new pivoting strategies that combine numerical pivoting and perturbation techniques. Then an iterative refinement process uses our approximate factorization to compute a solution. We show that our pivoting strategies are numerically robust, that few steps of iterative refinement are required, and that the factorization is significantly faster than with previous methods. Furthermore, we propose original approaches that are designed for parallel distributed factorization. A key point of our parallel implementation is the cheap and reliable estimation of the growth factor. This estimation is based on an approximation of the off-diagonal entries and does not require any supplementary messages.

3.3 A parallel matrix scaling algorithm

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

Based on [3], we worked on an iterative procedure which asymptotically scales the infinity norm of both rows and columns of a given matrix to 1. In [2], we propose a parallelization of the scaling procedure. We argue that the parallelization requires a careful partitioning of two diagonal matrices in addition to a standard sparse matrix partitioning for parallel matrix-vector multiply operations. We propose a method based on an all-reduce operation to partition the diagonal matrices. We present performance results on a PC cluster where good speedups are obtained for matrices having a reasonably large number of nonzeros. We plan to perform more experiments on a larger set of matrices and investigate the merits of the proposed parallelization approach. The parallel algorithms are implemented in Fortran, and the resulting codes are integrated into the MUMPS [1] solver.

[1] P. R. Amestoy, I. S. Duff, and J.-Y. L'Excellent, (1998), MUMPS MUltifrontal Massively Parallel Solver Version 2.0, Technical Report TR/PA/98/02.

[2] P. R. Amestoy, I. S. Duff, D. Ruiz, and B. Uçar, (2008), A parallel matrix scaling algorithm, In *Proceedings of VECPAR'08-International Meeting-High Performance Computing for Computational Science* (to appear).

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

3.4 Computing a class of matchings in parallel

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

One of the most powerful preprocessing methods for direct solvers is known as the maximum product matching ordering. Given an $n \times n$ matrix A, the objective is to find a permutation M such that the diagonal product of the permuted matrix, $\prod \mathrm{diag}(AM)$, is maximum (in magnitude) among all permutations. It is well known that the standard algorithms (see [4]) for this problem are not amenable to parallelization. We follow a different path. We start from the property that an optimal diagonal is invariant under matrix scaling. Based on this, we have designed the following algorithm :

(1) Scale the matrix in parallel such that each row and column contains one entry of magnitude 1.0 ;

(2) find a maximum cardinality matching using only the entries of magnitude 1.0 ;

(3) if the matching is perfect, we are done.

(4) If not, select a particular entry and update the scaling factors as well as the matching.

This process is repeated until a perfect matching is found. We have observed that on many matrices, applying the first three steps above is sufficient to obtain the optimal matching where the algorithm happens to boil down to selecting a maximum entry in each row or column. For the others we have envisaged an approximate approach, where the resulting matching is not guaranteed to be of maximum product, but empirically observed to have an almost equal impact on the factorization as a maximum product one. The results obtained so far will be discussed in SIAM conference in March, 2008 [5].

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

[5] I. S. Duff, D. Ruiz, and B. Uçar, Computing a class of bipartite matchings in parallel. Abstract has been accepted to be presented at *SIAM Conference on Parallel Processing for Scientific Computing (*PP08), to be held in Atlanta, USA. 12–14 March, 2008.

3.5 On block triangular form of symmetric matrices

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

We report observations on the block triangular form of symmetric, structurally rank deficient, square, sparse matrices. As the matrix is square and structurally rank deficient, it has at least one underdetermined and one overdetermined block. We prove that these blocks are transposes of each other. Furthermore, we show that the fine decomposition of the square block consists of matrices whose row set is equal to its column set or whose row set and column set are disjoint. The properties shown help us recover symmetry around the anti-diagonal in the block triangular matrix. The main results are carried over to full rank symmetric matrices as well. At the time of writing a paper [6] was under preparation.

[6] I. Duff and B. Uçar, (2008), On block triangular form of symmetric matrices. Manuscript in preparation.

3.6 Heuristics for a matrix symmetrization problem

B. Uçar : CERFACS, *France*

We consider the following variant of the matrix symmetrization problem. Given a square, unsymmetric sparse matrix, find a permutation of the columns of the matrix to yield a zero-free diagonal and to maximize the structural symmetry. The problem is known to be NP-hard. We had proposed a fairly fast heuristic and performed extensive tests empirically demonstrating results around 75% of the optimum [ALG61]. A solution to the matrix symmetrization problem can be used in different contexts. First, the method can be used as a preprocessing tool for some algorithms which are originally designed for structurally symmetric matrices. We have obtained promising results with the algorithms that are used for reducing bandwidth, and also with those that are used for obtaining doubly bordered block diagonal forms. Second, direct solvers for unsymmetric systems can take advantage of structural symmetry. We plan to modify the proposed heuristic to plug it into a direct solver.

3.7 Adapting iterative-improvement heuristics for scheduling file-sharing tasks on heterogeneous platforms

K. Kaya : BILKENT UNIVERSITY, *Turkey*; **B. Uçar** : CERFACS, *France*; **C. Aykanat** : BILKENT UNIVERSITY, *Turkey*

We consider the problem of scheduling an application on a computing system consisting of heterogeneous processors and one or more file repositories. The application consists of a large number of file-sharing, otherwise independent tasks. The files initially reside on the repositories. The interconnection network is heterogeneous. We focus on two disjoint problem cases. In the first case, there is only one file repository which is called as the master processor. In the second case, there are two or more repositories, each holding a distinct set of files. The problem is to assign the tasks to the processors, to schedule the file transfers from the repositories, and to order the executions of tasks on each processor in such a way that the turnaround time is minimized. In [7], we surveys several solution techniques and discuss how iterative-improve-based heuristics can be made to be efficient and effective in similar scheduling problems.

[7] K. Kaya, B. Uçar, and C. Aykanat, (2008), Adapting iterative-improvement heuristics for scheduling file-sharing tasks on heterogeneous platforms, In *Metaheuristics for Scheduling*, F. Xhafa and A. Abraham, eds., vol. II : in distributed computing environments of Studies in Computational Intelligence, Springer.

3.8 Performance analysis of the direct sparse linear solver MUMPS into CODE_ASTER

O. Boiteau : EDF DIVISION R&D, *France* ; **F. Hülsemann** : EDF DIVISION R&D, *France* ; **X. Vasseur** : CERFACS, *France*

The goal of this collaboration is the integration of the parallel, direct sparse linear solver MUMPS into CODE_ASTER, a structural mechanics code developed at EDF. A comparison of the linear solver MUMPS with the inbuilt serial multifrontal out-of-core solver of CODE_ASTER has been performed on a serial platform [ALG37]. We have compared the in-core linear algebraic solver MUMPS to the multifrontal solver of CODE_ASTER in terms of run time performance and stability with help of backward error estimate. The test cases are linear elasticity problems in two and three space dimensions proposed by EDF. It has been found that MUMPS is an attractive alternative to the current multifrontal solver in CODE_ASTER as its run time behaviour is more predictable and as it offers error diagnostic and iterative refinement features that are currently not available in the inbuilt solver. With iterative refinement, it has been checked that MUMPS reduces the error to the level of the machine accuracy. Following this comparison on serial platforms, it has been decided to consider MUMPS as a direct solver within the framework of CODE_ASTER also for parallel computations.

3.9 Null space detection for large rank-deficient sparse matrices

P. R. Amestoy : ENSEEIHT-IRIT, *France* ; **S. Gratton** : CNES AND CERFACS, *France* ; **J.Y. l'Excellent** : ENS-LYON, LIP, INRIA RHÔNE-ALPES, *France* ; **X. Vasseur** : CERFACS, *France*

The analysis of rank deficiency of possibly large matrices is an open problem occuring in various algorithms (constrained optimization, solution of indefinite eigenvalue problems, solution of linear systems by algebraic multigrid methods or non-overlapping domain decomposition methods). Whereas various rank-revealing procedures have been proposed for dense matrices, this question is rarely addressed for possibly large sparse matrices.

The goal of this collaboration is to obtain a reliable and robust algorithm based on a multifrontal Gaussian elimination to detect the deficiency of a sparse matrix and to compute accurately a null space basis. The proposed algorithm implemented within MUMPS combines an on the fly detection of null pivots during the sparse multifrontal Gaussian factorisation, a postponing of (pseudo)singularities to the root of the tree and the use of a dense rank-revealing factorisation of the root matrix (QR factorization with column pivoting). Combination of both the on the fly and root informations allows to compute a null space basis of the sparse matrix.

This algorithm has been evaluated when computing null space informations of large sparse matrices coming from structural mechanics (collaboration with O. Boiteau EDF R&D within the ANR Solstice project) and electromagnetism. On this set of semidefinite symmetric positive matrices it has been found that the proposed algorithm did obtain reliably both the deficiency and an accurate null space basis. Further investigations are ongoing for addressing the general case of rank-deficient matrices.

4 Iterative Methods and Preconditioning

4.1 Parallel distributed numerical simulations in aeronautic applications

G. Alléon : EADS-CRC, *France* ; **S. Champagneux** : CERFACS, *France* ; **G. Chevalier** : CERFACS, *France* ; **L. Giraud** : ENSEEIHT-IRIT, *France* ; **G. Sylvand** : EADS-CRC, *France*

The numerical simulation plays a key role in industrial design because it enables to reduce the time and the cost to develop new products. Because of the international competition, it is important to have a complete chain of simulation tools to perform efficiently some virtual prototyping. In this paper [ALG1], we describe two components of large aeronautic numerical simulation chains that are extremely consuming of computer resource. The first is involved in computational fluid dynamics for aerodynamic studies. The second is used to study the wave propagation phenomena and is involved in acoustics. Because those softwares are used to analyze large and complex case studies in a limited amount of time, they are implemented on parallel distributed computers. We describe the physical problems addressed by these codes, the main characteristics of their implementation. For the sake of re-usability and interoperability, these softwares are developed using object-oriented technologies. We illustrate their parallel performance on clusters of symmetric multi-processors. Finally, we discuss some challenges for the future generations of parallel distributed numerical software that will have to enable the simulation of multi-physic phenomena in the context of virtual organizations also known as the extended enterprise.

4.2 A Note on GMRES Preconditioned by a Perturbed LDL^T Decomposition with Static Pivoting

M. Arioli : RUTHERFORD APPLETON LABORATORY, *England* ; **I. S. Duff** : CERFACS, *France and* RUTHERFORD APPLETON LABORATORY, *England* ; **S. Gratton** : CNES AND CERFACS, *France* ; **S. Pralet** : ENSEEIHT-IRIT, *France*

A strict adherence to threshold pivoting in the direct solution of symmetric indefinite problems can result in substantially more work and storage than forecast by a sparse analysis of the symmetric problem. One way of avoiding this is to use static pivoting where the data structures and pivoting sequence generated by the analysis are respected and pivots that would otherwise be very small are replaced by a user defined quantity. This can give a stable factorization but of a perturbed matrix. The conventional way of solving the sparse linear system is then to use iterative refinement, but there are cases where this fails to converge. In this paper [ALG3], we discuss the use of more robust iterative methods, namely GMRES and flexible GMRES (FGMRES). We show both theoretically and experimentally that both approaches are more robust than iterative refinement and furthermore that FGMRES is far more robust than GMRES and that, under reasonable hypotheses, FGMRES is backward stable. We also show how restarted variants can be beneficial, although again the GMRES variant is not as robust as FGMRES.

4.3 Partitioning sparse matrices for parallel preconditioned iterative methods

B. Uçar : CERFACS, *France* ; **C. Aykanat** : BILKENT UNIVERSITY, *Turkey*

We address the parallelization of the preconditioned iterative methods that use explicit preconditioners such as approximate inverses in [ALG60]. Parallelizing a full step of these methods requires the coefficient and preconditioner matrices to be well partitioned. We first show that different methods impose different partitioning requirements for the matrices. Then, we develop hypergraph models to meet those requirements. In particular, we develop models that enable us to obtain partitionings on the coefficient and preconditioner matrices simultaneously. Experiments on a set of unsymmetric sparse matrices show that the proposed models yield effective partitioning results. A parallel implementation of the right preconditioned BiCGStab method on a PC cluster verifies that the theoretical gains obtained by the models hold in practice.

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

C. Aykanat : BILKENT UNIVERSITY, *Turkey* ; **B. B. Cambazoglu** : OHIO STATE UNIVERSITY, *USA* ; **B. Uçar** : CERFACS, *France*

K-way hypergraph partitioning has an ever-growing use in parallelization of scientific computing applications. In [8], we claim that hypergraph partitioning with multiple constraints and fixed vertices should be implemented using direct K-way refinement, instead of the widely adopted recursive bisection paradigm. Our arguments are based on the fact that recursive-bisection-based partitioning algorithms perform considerably worse when used in the multiple constraint and fixed vertex formulations. We discuss possible reasons for this performance degradation. We describe a careful implementation of a multi-level direct K-way hypergraph partitioning algorithm, which performs better than a well-known recursive-bisection-based partitioning algorithm in hypergraph partitioning with multiple constraints and fixed vertices. We also experimentally show that the proposed algorithm is effective in standard hypergraph partitioning.

[8] C. Aykanat, B. B. Cambazoglu, and B. Uçar, (2007), Multi-level direct K-way hypergraph partitioning with multiple constraints and fixed vertices, *Journal of Parallel and Distributed Computing*, **(accepted for publication)**.

4.5 Parallel multigrid preconditioned Krylov subspace methods for the solution of three-dimensional wave propagation problems

H. Calandra : TOTAL, *France* ; **S. Gratton** : CNES AND CERFACS, *France* ; **X. Pinel** : CERFACS, *France* ; **X. Vasseur** : CERFACS, *France*

We have developed preconditioning strategies for the iterative solution of the three-dimensional Helmholtz problem arising in geophysics. Finite difference discretization of this problem leads to a linear system with a large complex sparse matrix that is generally ill-conditioned and indefinite. Krylov subspace methods are the method of choice for solving these very large problems (up to one billion of unknowns for high frequency problems). We have developed and implemented parallel geometric multigrid based preconditioners for flexible Krylov subspace methods where the coarse grid is fine enough to capture the characteristics of the physical problem. We have studied the robustness of the numerical method with respect to the wavenumber and the scalability issue on massively parallel computers (Blue Gene L computer up to

2048 processors) on both homogeneous and heterogeneous problems. At the time of writing a paper is under preparation.

4.6 Additive and Multiplicative Two-Level Spectral Preconditioning for General Linear Systems

B. Carpentieri : CERFACS, *France* ; **L. Giraud** : ENSEEIHT-IRIT, *France* ; **S. Gratton** : CNES AND CERFACS, *France*

In this paper [ALG8] we introduce new preconditioning techniques for the solution of general symmetric and unsymmetric linear systems $Ax = b$. These approaches borrow some ideas of the multigrid philosophy designed for the solution of linear systems arising from the discretization of elliptic partial differential equations. We attempt to improve the convergence rate of a prescribed preconditioner M_1. In a two-grid framework, this preconditioner is viewed as a smoother and the coarse space is spanned by the eigenvectors associated with the smallest eigenvalues of M_1A. We derive both additive and multiplicative variants of the resulting iterated two-level preconditioners for unsymmetric linear systems that can also be adapted for Hermitian positive definite problems. We show that these two-level preconditioners shift the smallest eigenvalues to one and tend to better cluster around one those eigenvalues that M_1 already succeeded in moving into the neighborhood of one. We illustrate the behavior of our method through extensive numerical experiments on a set of general linear systems. Finally, we show the effectiveness of these approaches on two challenging real applications ; the first comes from a nonoverlapping domain decomposition method in semiconductor device modeling, the second from industrial electromagnetism applications.

4.7 Multigrid based preconditioners for the numerical solution of two-dimensional heterogeneous problems in geophysics

I. S. Duff : CERFACS, *France and* RUTHERFORD APPLETON LABORATORY, *England* ; **S. Gratton** : CNES AND CERFACS, *France* ; **X. Pinel** : CERFACS, *France* ; **X. Vasseur** : CERFACS, *France*

We have studied numerical methods for the solution of the Helmholtz equation for two-dimensional applications in geophysics [ALG12]. The common framework of the iterative methods in this study is a combination of an inner iteration with a geometric multigrid method used as a preconditioner and an outer iteration with a Krylov subspace method. The preconditioning system is based on either a pure or shifted Helmholtz operator. A multigrid iteration is used to approximate the inverse of this operator. The proposed solution methods are evaluated on a complex benchmark in geophysics involving highly variable coefficients and high wavenumbers (Marmousi problem). We have compared this preconditioned iterative method with a direct method (MUMPS) and a hybrid method that combines our iterative approach with a direct method on a reduced problem. The conclusion of these sequential numerical experiments is that the hybrid method outperforms both a direct approach and an iterative one based on a shifted Helmholtz operator.

4.8 On the Sensitivity of Some Spectral Preconditioners

L. Giraud : ENSEEIHT-IRIT, *France* ; **S. Gratton** : CNES AND CERFACS, *France*

It is well known that the convergence of the conjugate gradient method for solving symmetric positive definite linear systems depends to a large extent on the eigenvalue distribution. In many cases, it is observed that ”removing” the extreme eigenvalues can greatly improve the convergence. Several preconditioning techniques based on approximate eigenelements have been proposed in the past few years that attempt to tackle this problem. The proposed approaches can be split into two main families, depending on whether the extreme eigenvalues are moved exactly to one or are shifted to close to one. The first technique is often referred to as the deflation approach, while the latter is referred to as a coarse grid preconditioner by analogy to techniques first used in domain decomposition methods. Many variants exist in the two families that reduce to the same preconditioners if the exact eigenelements are used. In this paper [ALG14] we investigate the behavior of some of these techniques when the eigenelements are known only approximately. We use the first-order perturbation theory for eigenvalues and eigenvectors to investigate the behavior of the spectrum of the preconditioned systems using first-order approximation. We illustrate the sharpness of the first-order approximation and show the effect of the inexactness of the eigenelements on the behavior of the resulting preconditioner when applied to accelerating the conjugate gradient method.

4.9 Convergence in Backward Error of Relaxed GMRES

L. Giraud : ENSEEIHT-IRIT, *France* ; **S. Gratton** : CNES AND CERFACS, *France* ; **J. Langou** : THE UNIVERSITY OF TENNESSEE, DEPARTMENT OF COMPUTER SCIENCE, *France*

This work [ALG15] is the follow-up of the experimental study presented in [A. Bouras and V. Frayssé, SIAM J. Matrix Anal. Appl., 26 (2005), pp. 660-678]. It is based on and extends some theoretical results in [V. Simoncini and D. B. Szyld, SIAM J. Sci. Comput., 25 (2003), pp. 454-477 ; J. van den Eshof and G. L. G. Sleijpen, SIAM J. Matrix Anal. Appl., 26 (2004), pp. 125-153]. In a backward error framework we study the convergence of GMRES when the matrix-vector products are performed inaccurately. This inaccuracy is modeled by a perturbation of the original matrix. We prove the convergence of GMRES when the perturbation size is proportional to the inverse of the computed residual norm ; this implies that the accuracy can be relaxed as the method proceeds which gives rise to the terminology relaxed GMRES. As for the exact GMRES we show under proper assumptions that only happy breakdowns can occur. Furthermore, the convergence can be detected using a byproduct of the algorithm. We explore the links between relaxed right-preconditioned GMRES and flexible GMRES (FGMRES). In particular, this enables us to derive a proof of convergence of FGMRES. Finally, we report results of numerical experiments to illustrate the behavior of the relaxed GMRES monitored by the proposed relaxation strategies.

4.10 Incremental spectral preconditioners for sequences of linear systems

L. Giraud : ENSEEIHT-IRIT, *France* ; **S. Gratton** : CNES AND CERFACS, *France* ; **E. Martin** : CERFACS, *France*

A technique suited for the solution of sequences of linear systems is described in [ALG16]. This technique is a combination of a low rank update spectral preconditioner and a Krylov solver that computes on the fly approximations of the eigenvectors associated with the smallest eigenvalues. A set of Matlab examples illustrates the behaviour of this technique on academic sparse linear systems and its clear interest is showed in large parallel calculations for electromagnetic simulations. In this latter context, the solution technique enables the reduction of the simulation times by a factor of up to eight ; these simulation times previously exceeded several hours of computation on a modern high performance computer.

4.11 Parallel scalability study of hybrid preconditioners in three dimensions

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In this work, we study the parallel scalability of variants of additive Schwarz preconditioners [9] for three dimensional non-overlapping domain decomposition methods. To alleviate the computational cost, both in terms of memory and floating-point complexity, we investigate variants based on a sparse approximation or on mixed 32- and 64-bit calculation. This latter strategy is mainly motivated by the observation that many recent processor architectures exhibit 32-bit computational power that is significantly higher than that for 64-bit [10]. The robustness of the preconditioners is illustrated on a set of linear systems arising from the finite element discretization of elliptic and non-elliptic PDEs through extensive parallel experiments on more than a thousand processors. Their efficiency from a numerical and parallel performance view point are studied. A set of experiments are performed on two class of matrices (symmetric and unsymmetric), and for various problems difficulty (heterogeneous, anisotropic, comvection-dominant). Although many runs have been performed on various parallel platforms, we mainly report on experiments conducted on the IBM Blue Gene/L computing facility at CERFACS and the System X supercomputer installed at Virginia Tech (USA). On those plateforms, 3D problems with a few tens of millions of unknowns have been solved.

Some results of this study are presented in [11].

[9] L. M. Carvalho, L. Giraud, and G. Meurant, (2001), Local preconditioners for two-level non-overlapping domain decomposition methods, *Numerical Linear Algebra with Applications*, **8**, 207–227.

[10] L. Giraud, A. Haidar, and L. T. Watson, (2008), Mixed-precision preconditioners in parallel domain decomposition solvers, *Springer*, 357–364.

[11] L. Giraud, A. Haidar, and L. T. Watson, (2008), Parallel scalability study of hybrid preconditioners in three dimensions, *Parallel Computing*, **to appear**.

4.12 On the parallel solution of large industrial wave propagation problems

L. Giraud : ENSEEIHT-IRIT, *France* ; **J. Langou** : THE UNIVERSITY OF TENNESSEE, DEPARTMENT OF COMPUTER SCIENCE, *USA* ; **G. Sylvand** : EADS-CRC, *France*

In [ALG17] the use of Fast Multipole Methods (FMM) combined with embedded Krylov solvers preconditioned by a sparse approximate inverse is investigated for the solution of large linear systems arising in industrial acoustic and electromagnetic simulations. We use a boundary elements integral equation method to solve the Helmholtz and the Maxwell equations in the frequency domain. The resulting linear systems are solved by iterative solvers using FMM to accelerate the matrix-vector products. The simulation code is developed in a distributed memory environment using message passing and it has out-of-core capabilities to handle very large calculations. When the calculation involves one incident wave, one linear system has to be solved. In this situation, embedded solvers can be combined with approximate inverse preconditioner to design extremely robust algorithms. For radar cross section calculations, several linear systems have to be solved. They involve the same coefficient matrix but dif- ferent right-hand sides. In this case, we propose a block variant of the single right-hand side scheme. The efficiency, robustness and parallel scalability of our approach are illustrated on a set of large academic and industrial test problems.

4.13 A Comparative Study of Iterative Solvers Exploiting Spectral Information for SPD Systems

L. Giraud : ENSEEIHT-IRIT, *France* ; **D. Ruiz** : ENSEEIHT-IRIT, *France* ; **A. Touhami** : ENSEEIHT-IRIT, *France*

When solving the symmetric positive definite (SPD) linear system $\mathbf{A}\mathbf{x}^\star = \mathbf{b}$ with the conjugate gradient method, the smallest eigenvalues in the matrix $\mathbf{A}$ often slow down the convergence. Consequently if the smallest eigenvalues in $\mathbf{A}$ could somehow be "removed," the convergence may be improved. This observation is of importance even when a preconditioner is used, and some extra techniques might be investigated to further improve the convergence rate of the conjugate gradient on the given preconditioned system. Several techniques have been proposed in the literature that consist of either updating the preconditioner or enforcing conjugate gradient to work in the orthogonal complement of an invariant subspace associated with the smallest eigenvalues. The goal of this work [ALG18] is to compare several of these techniques in terms of numerical efficiency. Among various possibilities, we exploit the Partial Spectral Factorization algorithm presented in [M. Arioli and D. Ruiz, Technical Report RAL-TR-2002-021, Rutherford Appleton Laboratory, Atlas Center, Didcot, Oxfordshire, England, 2002] to compute an orthonormal basis of a near-invariant subspace of $\mathbf{A}$ associated with the smallest eigenvalues. This eigeninformation is used in combination with different solution techniques. In particular we consider the deflated version of conjugategradient. As representative of techniques exploiting the spectral information to update the preconditioner we consider also the approaches that attempt to shift the smallest eigenvalues close to one where most of the eigenvalues of the preconditioned matrix should be located. Finally, we consider an algebraic two-grid scheme inspired by ideas from the multigrid philosophy. In this paper, we describe these various variants and we compare their numerical behavior on a set of model problems from Matrix Market or arising from the discretization via the finite element technique of some two-dimensional (2D) heterogeneous diffusion PDE problems. We discuss their numerical efficiency, computational complexity, and sensitivity to the accuracy of the eigencalculation.

4.14 Bounds on the eigenvalue range and on the field of values of non-Hermitian and indefinite finite element matrices

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In the early seventies, Fried formulated bounds on the spectrum of assembled Hermitian positive (semi-) definite finite element matrices using the extreme eigenvalues of the element matrices. In this paper [ALG22] we will generalise these results by presenting bounds on the field of values, the numerical radius and on the spectrum of general, possibly complex matrices, for both the standard and the generalised problem. The bounds are cheap to compute, involving operations with element matrices only. We illustrate our results with an example from acoustics involving a complex, non-Hermitian matrix. As an application, we show how our estimates can be used to derive an upper bound on the number of iterations needed to achieve a given residual reduction in the GMRES-algorithm for solving linear systems.

4.15 Adaptive preconditioners for nonlinear systems of equations

D. Loghin : CERFACS, *France* ; **D. Ruiz** : ENSEEIHT-IRIT, *France* ; **A. Touhami** : ENSEEIHT-IRIT, *France*

The use of preconditioned Krylov methods is in many applications mandatory for computing efficiently the solution of large sparse nonlinear systems of equations. However, the available preconditioners are often sub-optimal, due to the changing nature of the linearized operator. In this work [ALG21] we introduce and analyse an adaptive preconditioning technique based on the Krylov subspace information generated at previous steps in the nonlinear iteration. In particular, we use an adaptive technique suggested in [J. Baglama, D. Calvetti, G.H. Golub, L. Reichel, Adaptively preconditioned GMRES algorithms, SIAM J. Sci. Comput. 20(1) (1998) 243-269] for restarted GMRES to enhance existing preconditioners with information available from previous stages in the nonlinear iteration. Numerical experiments drawn from domain decomposition techniques and fluid flow applications are used to validate the increased efficiency of our approach.

4.16 A numerical study on Neumann-Neumann methods for hp approximations on geometrically refined boundary layer meshes II. Three-dimensional problems

A. Toselli : ETH ZÜRICH, *Switzerland.* ; **X. Vasseur** : CERFACS, *France*

We present extensive numerical tests showing the performance and robustness of a Balancing Neumann-Neumann method for the solution of algebraic linear systems arising from hp finite element approximations of scalar elliptic problems on geometrically refined boundary layer meshes in three dimensions [ALG24]. The numerical results are in good agreement with the theoretical bound for the condition number of the preconditioned operator derived in [Toselli and Vasseur, IMA J. Numer. Anal. 24 (2004) 123-156]. They confirm that the condition numbers are independent of the aspect ratio of the mesh and of potentially large jumps of the coefficients. Good results are also obtained for certain singularly perturbed problems. The condition numbers only grow polylogarithmically with the polynomial degree, as in the case of p approximations on shape-regular meshes.

4.17 Convergence and round-off errors in a two-dimensional eigenvalue problem using spectral methods and Arnoldi-Chebyshev algorithm

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An efficient way of solving 2D stability problems in fluid mechanics is to use, after discretization of the equations that cast the problem in the form of a generalized eigenvalue problem, the incomplete Arnoldi-Chebyshev method. This method preserves the banded structure sparsity of matrices of the algebraic eigenvalue problem and thus decreases memory use and CPU time consumption. The errors that affect computed eigenvalues and eigenvectors are due to the truncation in the discretization and to finite precision in the computation of the discretized problem. In this paper [ALG27] we analyze those two errors and the interplay between them. We use as a test case the 2D eigenvalue problem yielded by the computation of inertial modes in a spherical shell. This problem contains many difficulties that make it a very good test case.

It turns out that single modes (especially most-damped modes i.e. with high spatial frequency) can be very sensitive to roundoff errors, even when apparently good spectral convergence is achieved. The influence of roundoff errors is analyzed using the spectral portrait technique and by comparison of double precision and extended precision computations. Through the analysis we give practical recipes to control the truncation and roundoff errors on eigenvalues and eigenvectors.

5 Qualitative Computing

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

The work of Qualitative Computing (QC) Group deals with stability and reliability issues in Numerical Simulation which are too difficult to be resolved at the software engineering level only. Such difficulties come from the increased mathematical complexity of the models used in industry. Therefore a sound mathematical understanding of the underlying phenomena is required before one can turn reliably to software solutions.
In the last four decades, the increasing complexity of methods has been a serious challenge for applied mathematicians summarized by the two words : nonlinearity and coupling. A lot has been already accomplished by the scientific community. Some 40 years ago, the pessimistic view prevailed that one could not reliably compute in the chaotic regime. However, thanks to the invention of more refined notions of stability and backward errors, a reliability path was gradually opened in the jungle of seemingly random results.

The very success of Scientific Computing in meeting their needs has led high tech industries to shift from laboratory experiments (wind tunnels in Aeronautics, for example) to Computer Simulation only. This novel situation forces us to face the new frontier in Scientific Computing, which can be summarized as follows :

Assess the validity of computer simulations for highly unstable physical phenomena.

High instability, such as turbulence and chaos, is inherently present in CFD. This represents a formidable challenge.

Contributing to the exploration of this new frontier has been the goal of the QC Group during its 20 years at Cerfacs. QC looks at the autonomous evolution of numerical methods / algorithms in the neighborhood of the *singularities* of the model. A prerequisite is that the approximation methods (resp. algorithms) are demonstrated numerically stable with respect to perturbations in the model (resp. round off, that is finite precision of the computer arithmetic). Such robustness to perturbations can be established at all *regular* points where the model does not display any singular behaviour. This task is an important component of the classical activity of numerical software assessment : prove that the software works well *away* from singularities.
The neighbourhood of singularities, is where Qualitative Computing operates, a domain where results are declared unreliable by the classical measures developed after Wilkinson by the Numerical Linear Algebra community. The underlying reason is that these tools are intrinsically based on a *linear* view of things. They quantify first order effects, hence they cannot handle serious nonlinearity. They are local and do not provide the global understanding of computation required by complex models.
This explains why the classical books of Numerical Analysis (such as the popular text books by Golub - Van Loan, or Higham ...) cannot suggest any valuable research direction : all problems set in the neighborhood of singularities are declared ill-conditioned, without discrimination. Such an answer is very unsatisfactory.

How can we go *beyond* the too limited linear viewpoint of the numerical software developers ? The approach of QC has been to create a theory of Nonlinear Computation which extends radically the backward analysis of Wilkinson by providing a *global* understanding of the computational dynamics. This new theory has the two following components i) Homotopic Deviation theory, and ii) Dickson algebras.
We review below the work accomplished in the years 2006 and 2007 with respect to each component of the Qualitative Computing theory.

5.1 Homotopic Deviation in Linear Algebra

In the first component, we address nonlinearity by maintaining the linearity of the framework for Computation (*linear* vector spaces) while focusing on the nonlinearity of Computation itself resulting from the spectral analysis of a coupling. This is the basis for the new theory of Homotopic Deviation (HD). One considers the linear coupling $A(t) = A + tE$ between 2 square matrices A and E of order n by the complex parameter $t \in \hat{\mathbb{C}} = \mathbb{C} \cup \{\infty\}$. The nonlinearity is expressed by the spectral field $t \in \hat{\mathbb{C}} \mapsto \sigma(A(t)) \in \mathbb{C}^n$. The coupling $A(t)$ is linear, but the spectral analysis of $A(t)$ is based on the formal *multiplicative* representation of the resolvent matrix

$$(A(t) - zI)^{-1} = (A - zI)^{-1}[I + tE(A - zI)]^{-1},$$

and uses the SVD of E. The spectral analysis of $A(t)$ is equivalent to a *transcendental* (not algebraic) coupling between the two parameters t and z in $\hat{\mathbb{C}} \times \mathbb{C}$. The coupling is closed in t but open in z. t is the intensity of the coupling, and z is the observation point. The point at ∞ ($|t| = \infty$) is a singularity which plays an essential role reflected computationally at finite distance for z. When E is singular, there exist complex observation points (attracting and repelling) which organize the flow of the spectral field $\sigma(A(t))$ as $|t|$ increases and $\to \infty$. The localization of these points is essential to understand the global evolution of the complex coupling of two phenomena realized by spectral analysis [ALG28, 14, 19].

This complex coupling is one of the mechanisms by which new laws of computation can emerge. The algebraic singularities of $A(t)$ can be analyzed dynamically at a transcendent level only. The dynamics of computation is organized at a metalevel which is *not* algebraic. This explains why the effects cannot be purely local, as experience tells us [ALG28, 14].

Linearization of quadratic eigenproblems often leads to a situation where $0 \in \sigma(E)$ is semi-simple. The paper [ALG9] treats an example from computational Acoustics, where t represents the complex admittance (joint work with M. Van Gijzen). It consists of a practical application where the homotopy parameter is $complex$. The points z where the matrix pencils $(A - zI) + tE$ have no finite eigenvalues are given a physical interpretation : they are points where $no\ \ resonance$ can occur.

An application to the incomplete Arnoldi method (E singular defective of rank 1) has been made. Numerical experiments are described in [ALG28]. An application of HD to matrix pencils has been presented at ICIAM07 by M. Ahmadnasab [12, 13]. The PhD thesis of M. Ahmadnasab was successfully defended on October 24, 2007 (Université Toulouse 1 and Cerfacs). The jury awarded it with mention “summa cum laude” (félicitations du jury).

[12] M. Ahmadnasab, Parameter analysis of the structure of regular matrix pencils by Homotopic Deviation theory. presented during the 6th International Congress on Industrial and Applied Mathematics, Zurich, Switzerland, 16-20 July 2007.

[13] M. Ahmadnasab and F. Chaitin-Chatelin, Matrix pencils under Homotopic Deviation theory. to be presented at NAA 2008, Rousse, Bulgaria.

[14] F. Chaitin-Chatelin, The dynamics of spectral analysis by Homotopic Deviation. Part I : The spectral field, Cerfacs TR/PA/07/118, Part II : The evolution field, Cerfacs TR/PA/08/03.

[15] F. Chatelin, (2008), *Qualitative Computing*, World Scientific, Singapore, (to appear).

5.2 Dickson Algebras for Nonlinear Computation

The second component in our analysis of nonlinearity drops the linearity assumption for the algebraic framework. This is the most daring step. Albeit quite natural from the point of view of nonlinear computation, this step has not been seriously considered by applied mathematicians so-far. The novel idea consists in considering the framework of computation, the algebraic structure, as inherently *nonlinear*. This requires to define the *multiplication* of vectors, and this restricts the dimension n for vectors to be 2^k,

$k \geq 0$. Starting from the basis field $\mathbb{R}$ ($k = 0$) one gets $\mathbb{C}$ ($k = 1$) and the quaternions ($k = 2$). At $k = 3$ occurs a bifurcation point. One can either define Clifford algebras which maintain associativity (at the expense of computing potential), or consider Dickson algebras which maintain the evolution of the computing capabilities by recursive complexification (at the expense of associativity).

The mathematicians and physicists of the 20th Century favoured associativity and Clifford algebras. However there are clues from Nature that Computation favours non associative algebras for its autonomous evolution by successive complexification. Hypercomputation in nonassociative Dickson algebras of dimension 16 (and up) creates new computing opportunities, some of which shed new light on *chaotic* computations [ALG39, ALG63].

Associativity puts an arbitrary limit to the type of nonlinearities which can be considered : they cannot be chaotic. The possibility to go beyond this limit is numerically very important to assess the validity of computer simulations in the chaotic regime. This ambitious goal implies to go even beyond division algebras, into the framework of Dickson algebras A_k of dimension 2^k, $k \geq 4$, where multiplication is neither associative nor isometric, but remains quadratic and flexible. A body of theory is developing [ALG39, ALG63, ALG38, 18], which connects various aspects of Computation (Analysis, Algebra, Geometry and Arithmetics) in new $algorithmic$ ways. It was presented in [17].

SVD computations are sensitive to logical paradoxes in the presence of zerodivisions. This emerging phenomenon is related to the inductive process of complexification for Dickson algebras of dimension ≥ 16. This algorithmic complexification drives the dynamics of Computation in a way described in [ALG38]. A key point for understanding the chaotic regime is the analysis of the evolution of anisometry in A_k as $k \to \infty$ [ALG39].

A complete account of Qualitative Computing will be published in 2008 [19]. The theoretical foundations have been laid to serve as a basis for the assessment of the quality of software for highly unstable phenomena which are now encountered in high-tech. industries.

[16] F. Chaitin-Chatelin, *Computing beyond classical logic* : SVD *computation in nonassociative* $Dickson\ algebras$. in Randomness and Complexity (C. Calude ed.) pp. 13-23, World Scientific, Singapore, 2007.

[17] F. Chaitin-Chatelin, Scientific Computation in nonassociative Dickson algebras. Invited talk, Symposium in honour of Prof. J. Fleckinger, 1 July, 2006.

[18] F. Chaitin-Chatelin and E. Traviésas-Cassan, (Chapter 5 in B. Einarsson (ed.), *Accuracy and Reliability in Scientific Computing,* SIAM, Philadelphia, 2005, pp. 77-92), Qualitative Computing.

[19] F. Chatelin, (2008), *Qualitative Computing*, World Scientific, Singapore, (to appear).

6 Nonlinear Systems and Optimization

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

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We address the accuracy of the results for the overdetermined full rank linear least squares problem. We recall theoretical results obtained in [ALG2] on conditioning of the least squares solution and the components of the solution when the matrix perturbations are measured in Frobenius or spectral norms. Then we define computable estimates for these condition numbers and we interpret them in terms of statistical quantities. In particular, we show that, in the classical linear statistical model, the ratio of the variance of one component of the solution by the variance of the right-hand side is exactly the condition number of this solution component when perturbations on the right-hand side are considered. We also provide, similarly to [22], fragment codes using LAPACK [20] and ScaLAPACK [21] routines to compute the variance-covariance matrix and the least squares conditioning and we give the corresponding computational cost. Finally we present a small historical numerical example that was used by Laplace for computing the mass of Jupiter and experiments from the space industry with real physical data.

[20] E. Anderson, Z. Bai, C. Bischof, S. Blackford, J. Demmel, J. Dongarra, J. D. Croz, A. Greenbaum, S. Hammarling, A. McKenney, and D. Sorensen, (1999), *LAPACK Users' Guide*, Society for Industrial and Applied Mathematics, 3 ed.

[21] L. S. Blackford, J. Choi, A. Cleary, E. D'Azevedo, J. Demmel, I. Dhillon, J. Dongarra, S. Hammarling, G. Henry, A. Petitet, K. Stanley, D. Walker, and R. C. Whaley, (1997), *ScaLAPACK Users' Guide*, Society for Industrial and Applied Mathematics.

[22] T. N. A. Group", (2006), *NAG Library Manual, Mark 21*, NAG.

6.2 Parallel tools for solving incremental dense least squares problems. Application to space geodesy

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We implemented a parallel distributed solver that enables us to solve incremental dense least squares arising in some parameter estimation problems. This solver is based on ScaLAPACK [23] and PBLAS [24] kernel routines. In the incremental process, the observations are collected periodically and the solver updates the solution with new observations using a QR factorization algorithm. It uses a recently defined distributed packed format [ALG4] that handles symmetric or triangular matrices in ScaLAPACK-based implementations. We provide performance analysis on IBM pSeries 690. We also present an example of application in the area of space geodesy for gravity field computations with some experimental results.

[23] L. S. Blackford, J. Choi, A. Cleary, E. D'Azevedo, J. Demmel, I. Dhillon, J. Dongarra, S. Hammarling, G. Henry, A. Petitet, K. Stanley, D. Walker, and R. C. Whaley, (1997), *ScaLAPACK Users' Guide*, Society for Industrial and Applied Mathematics.

[24] J. Choi, J. Dongarra, L. Ostrouchov, A. Petitet, D. Walker, and R. Whaley, (1995), A Proposal for a Set of Parallel Basic Linear Algebra Subprograms, tech. rep. LAPACK Working Note 100.

6.3 A retrospective trust-region method for unconstrained optimization

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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 retro- spectively 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. For more details about this work, please refer to [ALG36].

6.4 Trust-region methods with dynamic accuracy and nonlinear least-squares

F. Bastin : CERFACS, *France* ; **S. Gratton** : CNES AND CERFACS, *France*

We consider trust-region techniques with adaptive strategies for stochastic programming. We have constructed a convergent method designed for stochastic programs based on expected values [25, ALG7], and have applied it for mixed logit models, a class of problems encountered in discrete choice theory. We have however identified problems arising when using some popular classes of Hessian approximations, especially the BHHH one [ALG6]. Such difficulties are similar to those that can be encountered with nonlinear least-square problems for the Gauss-Newton method. These similarities are at the origin of a project where we consider these problems inside an unified framework. We have identified the origins of the poor numerical performance and we consider hybrid strategies such as that developed by Dennis et al. [26], which can be shown to be convergent. Preliminary numerical experimentations have been performed and presented at the SMAI (Société de Mathémathiques Appliquées et Industrielles) conference in 2006, confirming the potential of the approach.

[25] F. Bastin, (2005), An adaptive trust-region approach for nonlinear stochastic optimisation with an application in discrete choice theory, In *Algorithms for Optimization with Incomplete Information*, S. Albers, R. H. Möhring, G. C. Pflug, and R. Schultz, eds., no. 05031 in Dagstuhl Seminar Proceedings, Internationales Begegnungs- und Forschungszentrum (IBFI), Schloss Dagstuhl, Germany.

[26] J. E. Dennis Jr, D. Gay, and R. E. Welsch, (1981), An adaptive nonlinear least-squares algorithm, *ACM Transactions on Mathematical Software*, **7**, 348–368.

6.5 Trust-Region algorithms applied to discrete choice modelling

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In this research, we have considered the application of trust-region methods to discrete choice models involving random parameters, so that the problem can be viewed as a stochastic program [27, ALG5]. We have more specically studied a model of activity and trip scheduling that combines three elements that have previously been investigated in isolation : the duration of activities, the time-of-day preference for activity participation and the effect of schedule delays on the valuation of activities. The model was tested using a 2001 data set from the Netherlands and results are presented in [ALG13]. The method is convergent, and error components included in the model suggest that there is considerable unobserved heterogeneity with respect to mode preferences and schedule delay.

[27] F. Bastin, (2005), An adaptive trust-region approach for nonlinear stochastic optimisation with an application in discrete choice theory, In *Algorithms for Optimization with Incomplete Information*, S. Albers, R. H. Möhring, G. C. Pflug, and R. Schultz, eds., no. 05031 in Dagstuhl Seminar Proceedings, Internationales Begegnungs- und Forschungszentrum (IBFI), Schloss Dagstuhl, Germany.

6.6 Formulation and solution strategies for nonparametric nonlinear stochastic programs

F. Bastin : CERFACS, *France*; **C. Cirillo** : FUNDP - UNIVERSITY OF NAMUR, *Belgium*; **Ph. L. Toint** : FUNDP - UNIVERSITY OF NAMUR, *Belgium*

We consider a class of stochastic programming models where the uncertainty is classically represented using parametric distributions families. The parameters are then usually estimated together with the optimal value of the problem. However, misspecification of the underlying random variables often leads to irrealistic results when little is known about their true distributions. We propose to overcome this difficulty by introducing a nonparametric approach where we replace the estimation of the distribution parameters by that of cumulative distribution functions (CDF). We have designed a practical algorithm which achieves this goal by using a monotonic spline representation of the inverse marginal CDF's and a projection-based trust-region globalization. The method has been assessed on discrete models in the transportation field [ALG62].

6.7 Using model reduction techniques within variational data assimilation

C. Boess : CERFACS, *France*; **A.S. Lawless** : UNIVERSITY OF READING, *UK*; **N.K. Nichols** : UNIVERSITY OF READING, *UK*; **A. Bunse-Gerstner** : UNIVERSITY OF BREMEN, *Germany*

Incremental four-dimensional variational data assimilation is the method of choice in many operational atmosphere and ocean data assimilation systems. It allows the four dimensional variational technique (4D-Var) to be implemented in a computationally efficient way by using approximate Gauss-Newton methods where the minimization of the full nonlinear 4D-Var cost function is replaced by the minimization of a series of simplified cost functions. In practice these simplified functions are usually derived from a spatial or spectral truncation of the full system being approximated. We propose a new method for deriving the simplified problems in incremental 4D-Var, based on model reduction techniques developed in the field of control theory. We show how these techniques can be combined with incremental 4D-Var to give an assimilation method that retains more of the dynamical information of the full system. Numerical experiments using a shallow-water model illustrate the superior performance of model reduction to standard truncation techniques [28, 29].

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

[29] A. Lawless, N. Nichols, C. Boess, and A. Bunse-Gerstner, (2008), Using model reduction methods within incremental four-dimensional variational data assimilation, *Accepted for publication in Monthly Weather Review*.

6.8 Benchmarking of bound-constrained optimization software

S. Gratton : CNES AND CERFACS, *France* ; **Ph. L. Toint** : UNIVERSITY OF NAMUR, *Belgium* ; **A. Tröltzsch** : CERFACS, *France*

In this work, we compare different algorithms solving nonlinear optimization problems with simple bounds on the variables. Moreover, we would like to come out with an assessment of the optimization library DOT (Design Optimization Tools) used at Airbus to optimize aerodynamic design problems. DOT is mainly based on line search techniques and the purpose of this study is to compare it with more recent line search solvers and with other solvers based on different approaches such as trust region and interior point method. We focus on the case where function and gradient evaluations are possible, but where the Hessian of the problem, when needed, has to be approximated using e.g. quasi-Newton updates. DOT is compared with a set of well-known optimization codes which are freely available for academic use as there are TN-BC, L-BFGS-B, Lancelot B and IPOPT. The numerical experiments in the testing environment CUTEr show that the trust region based solver Lancelot B performs best of the considered solvers both for CPU time and number of function and gradient evaluations. For more details of this study we refer to [ALG59].

6.9 Neural Networks : low-memory training regularization techniques

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With the intention of using easy-to-compute and differentiable surrogate mod- els for the optimization of computationally expensive objective functions [32], we have studied the artificial neural network methodology [31]. We describe a low-memory Levenberg-Marquardt algorithm for the supervised training of artificial neural networks. It is based on the use of the forward and reverse modes of the algorithmic differentiation [30]. We also have combined three different strategies of regularization to build neural networks that generalize well.

[30] A. Griewank, (2000), *Evaluating derivatives*, Society for Industrial and Applied Mathematics (SIAM), Philadelphia.

[31] K. Hornik, M. Stinchcombe, and H. White, (1989), Multilayer feedforward networks are universal approximators, *Neural Networks*, **2**, 359–366.

[32] R. Jin, W. Chen, and T. Simpson, (2001), Comparative studies of metamodeling techniques under multiple modeling criteria, *Structural and Multidisciplinary Optimization*, **1**, 1–13.

6.10 Neural networks based trust region methods for bound constrained optimization problems

M. Garcia : CERFACS, *France* ; **S. Gratton** : CNES AND CERFACS, *France* ; **Ph. L. Toint** : FUNDP, *Belgium*

We explore how neural network techniques [33] can be combined with trust-region methods in the framework of bound-constrained optimization. The resulting algorithms converge to first order critical point for any starting point and often enjoy interesting properties when applied to highly oscillatory problems. In these cases a local optimiser might be stalled, whereas a coarse model seems to be much easier to solve. Bearing this example in mind we propose to use a model of f that is such that the iterates obtained with a minimiser get close to the global minimum [ALG54]. We propose to implement our model in a trust region approach because trust region methods have strong convergence properties, they converge to critical points from any starting point. We also suppose that we have access to the gradient, so a linear term can be add such that f and the model m have the same gradient.

[33] M. V. Grieken, (2004), *Optimisation pour l'apprentissage et apprentissage pour l'optimisation*, PhD thesis, Paul Sabatier University, Toulouse, France.

6.11 Activation functions in neural netwoks approximation functions

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In many cases neural networks have given good results in function approximations, even if there exist many problems that could not been solved. The selection of the activation functions used in neural network approximations depends on the problem and also on the criterion of the researcher, sometimes this selection is done by test. Commonly, the function of activation logistic has been more frequently used given good results. In the literature a standard criterion does not exist for the selection of these activation functions in neural networks, an exhaustive research neither does exist in this topic. The choice of transfer functions may strongly influence complexity and performance of neural networks used in function approximations [34]. It is for this reason that the principal aim of this work is to obtain a criterion of selection of activation functions in a feedforward neural network with only one hidden layer, comparing their performances. A new activation function based in logistic activation function is proposed. Several test functions with varying problem dimensions and degrees of nonlinearity are used to compare the accuracies of the neural networks using different activation functions. We consider several performance criteria such as neural network accuracy, effect of problem dimension and computational complexity.

[34] F. Piekniewski. and L. Rybicki, (2004), Visual comparison of performance for different activation functions in MLP networks, In *IEEE International Joint Conference on Neural Networks*, 2947–2952.

6.12 Convergence properties of trust-region methods with application to multigrid optimization

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A multilevel algorithm is proposed to solve unconstrained optimization problems, that puts together ingredients taken both from the multigrid and trust-region based optimization domains. The resulting algorithm, presented in [ALG54] is globally convergent and performs very well in practice. Indeed, it is shown in [ALG53], that it behaves similarly as linear multigrid solvers on convex-quadratic problem, and exhibits interesting performance even for non quadratic test-cases, such as the solid ignition optimal control problem and the minimum surface problem. In this method, the smoothing step consists in the approximate solution of the trust-region local subproblem, using the sequential coordinate minimisation ; this procedure generalizes the Gauss-Seidel smoother in the local trust-region. Since the algorithm only explores directions aligned with the prolongated coordinate axis, information on negative curvature directions at a given iteration may either be incom- plete or simply missing, causing the assumption required for second-order convergence to fail. However we showed in [ALG20] that a weaker form of the second-order convergence can still be obtained under some additional but algorithmically realistic conditions.

The method is currently being extended to the case of the minimization of problems with simple bound contraints [ALG52]. For compatibility with the bounds, the trust-region is defined using the infinity norm and the coarse grid bounds are chosen so that the prolongation of a step always remains feasible for the bounds, whereas a bounded violation of the trust-region is allowed. Preliminary results show the good performance of the algorithm for academic test problems.

6.13 Preconditioners for Data Assimilation

S. Gratton : CNES AND CERFACS, *France* ; **A. Sartenaer** : FUNDP UNIVERSITY OF NAMUR, *Belgium* ; **J. Tshimanga** : CERFACS AND FUNDP UNIVERSITY OF NAMUR, *Belgium* ; **A. Weaver** : CERFACS, *France*

Incremental four-dimensional variational assimilation (4D-Var) is an algorithm that approximately solves a nonlinear minimization problem by solving a sequence of linearized (quadratic) minimization problems. In [36] we designed a family of limited-memory preconditioners (LMPs) for accelerating the convergence of conjugate gradient (CG) methods used to solve quadratic minimization problems such as those encountered in incremental 4D-Var. The family is constructed from a set of vectors $\mathbf{s}_i$, $i = 1, \ldots, l$, where each $\mathbf{s}_i$ is assumed to be conjugate with respect to the (Hessian) matrix $\mathbf{A}$. In incremental 4D-Var, approximate LMPs from this family can be built using conjugate vectors generated during the CG minimization on previous outer iterations. The spectral and quasi-Newton LMPs employed in many operational 4D-Var systems are shown to be special cases of the family of LMPs proposed here. In addition, a new LMP based on Ritz vectors (approximate eigenvectors) is derived. The Ritz LMP is shown to be more effective than, or at least as effective as, the spectral and quasi-Newton LMPs in our 4D-Var experiments. Our experiments also illustrate for this particular application the importance of limiting the number of CG (inner) iterations on certain outer iterations to avoid divergence of the cost function on the outer loop. This phenomenon is well-known, and has been intensively described in [35].

[35] A. R. Conn, N. I. M. Gould, and P. L. Toint, (2000), *Trust-region methods*, Society for Industrial and Applied Mathematics, Philadelphia, PA, USA.

[36] J. Tshimanga, S. Gratton, A. Weaver, and A. Sartenaer, (2008), Limited-memory preconditioners with application to incremental 4D-Var, Technical Report, CERFACS, Toulouse, France. In preparation, also submitted to QJRMS.

6.14 Approximate Gauss-Newton methods for nonlinear least squares problems

A. Lawless : UNIVERSITY OF READING, *UK* ; **S. Gratton** : CNES AND CERFACS, *France* ; **N. K. Nichols** : UNIVERSITY OF READING, *UK*

The Gauss-Newton algorithm is an iterative method regularly used for solving nonlinear least squares problems. It is particularly well suited to the treatment of very large scale variational data assimilation problems that arise in atmosphere and ocean forecasting. In practice the exact Gauss-Newton method is too expensive to apply operationally in meteorological forecasting, and various approximations are made in order to reduce computational costs and to solve the problems in real time. In [ALG19] we investigate the effects on the convergence of the Gauss-Newton method of two types of approximation used commonly in data assimilation. First, we examine truncated Gauss-Newton methods where the inner linear least squares problem is not solved exactly, and second, we examine perturbed Gauss-Newton methods where the true linearized inner problem is approximated by a simplified, or perturbed, linear least squares problem. We give conditions ensuring that the truncated and perturbed Gauss-Newton methods converge and also derive rates of convergence for the iterations. The results are illustrated by a simple numerical example. A practical application to the problem of data assimilation in a typical meteorological system is presented.

7 Conferences and Seminars

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

February

Stanford University, California, USA. 20 February 2006. I.S. DUFF, visitor.

Lawrence Berkeley National Laboratory, California, USA. 20-21 February 2006. I.S. DUFF, visitor.

SIAM Parallel Processing Meeting, San Franciso, California, USA. 21-24 February 2006. I.S. DUFF, attendee and secretary of SIAM SIAG.

SIAM Parallel Processing Meeting, San Franciso, California, USA. 21-24 February 2006. M. BABOULIN, *A distributed packed storage for large parallel calculations*, joint work with L. Giraud and S. Gratton, Contributed talk.

March

13th Han-sur-Lesse Conference on Mathematical Programming. Han-sur-Lesse, Belgium. 16-17 March 2006. M. MOUFFE, *Use of multi-level trust-region techniques for nonlinear bound constrained optimization problems*, joint work with S. Gratton, A. Sartenaer and Ph. L. Toint, Seminar.

April

Copper Mountain Conference on Iterative Methods, Copper, Colorado, USA. 2-7 April 2006. M.ARIOLI, I.S. DUFF[†], S. GRATTON, AND S. PRALET, *A note on GMRES preconditioned by a perturbed* LDL^T *decomposition with static pivoting*, Talk, Workshop Chair, Organizing Committee.

CIMOD06 2006, International Conference on Mathematics of Optimization and Decision Making, Pointe–Pitre, France, April 18-21 M. VAN GRIEKEN. *Neural networks : a model for solving nonlinear optimization problems*, joint work with S. Jan and M. Masmoudi, contributed talk.

CIMOD06 2006, International Conference on Mathematics of Optimization and Decision Making, Pointe–Pitre, France, April 18-21 F. BASTIN, *On second-order approximations for nonlinear least-squares and nonlinear stochastic programming in discrete choice theory*, joint work with S. Gratton.

May

Shanghai Forum on Industrial and Applied Mathematics, Shanghai, China. 25-26 May 2006. I.S. DUFF, *Sparse system solution and the HSL Library,* Invited talk.

June

Workshop on State-of-the-Art in Scientific and Parallel Computing, Umea, Sweden, June 18-21, 2006 M. BABOULIN, *HPC tools for solving accurately the large dense linear least squares problems arising in gravity field calculations,* Contributed talk.

July

Symposium in honour of Prof. J. Fleckinger, Université Toulouse I, 1 July, 2006. F. CHAITIN-CHATELIN, *Scientific Computation in nonassociative Dickson algebras*, Invited talk.

21^{st} European Conference on Operational Research, Reykjavik, Iceland. July 2-5, 2006. PH.L. TOINT, *A non-parametric sampling approach for nonlinear stochastic programming*, joint work with Fabian Bastin (Organizer of the session *Adaptive and innovative samplings techniques*, and *Stochastic Programming*) and Cinzia Cirillo.

17th International Conference on Domain Decomposition Methods in St. Wolfgang/Strobl, Austria. July 3-7, 2006. A. HAIDAR, attendee.

SIAM Annual Meeting, Boston, USA. 8-16 July 2006. I.S. DUFF, Attendee and Chairman of the SIAM Board.

ICCG, BICGSTAB, and Jacobi-Davidson. A meeting in honour of Henk van der Vorst. Utrecht, Netherlands. 22 July 2006. I.S. DUFF, *The perfect preconditioner,* Invited talk.

JCCC'07, Journée jeunes chercheurs organisée par le Comité des Chercheurs Calculant au CINES, Juillet 24-27. A. HAIDAR, *Parallel hybrid direct/iterative linear solvers for 2D/3D elliptic problems.*, joint work with L. Giraud and L. T. Watson, contributed talk.

SIAM-GAMM Conference on Applied and Linear Algebra, University of Düsseldorf, Germany, July 24 - 27 X. VASSEUR, *On the computation of the null space of a sparse matrix*, joint work with Serge Gratton, talk.

September

SPEEDUP Workshop on High-Performance Computing, ETH Zürich, Switzerland, September 4-5, 2006. X. VASSEUR, attendee.

PMAA 2006, Fourth International Workshop on Parallel Matrix Algorithms and Applications, IRISA, Rennes, France, September 7-9. TZ. SLAVOVA, *A Preliminary Analysis of the OutofCore Solution Phase of a parallel Multifrontal Approach (presentation),* joint work with P. Amestoy, I. Duff and A. Guermouche, contributed talk.

PMAA 2006, Fourth International Workshop on Parallel Matrix Algorithms and Applications, IRISA, Rennes, France, September 7-9. A. HAIDAR, *Numerical experiments with additive Schwarz preconditioner for nonoverlapping domain decomposition in 3D*, joint work with L. Giraud and S. Mulligan, contributed talk.

Bath-RAL Numerical Analysis Day, University of Bath, England. 18 September, 2006. I. DUFF, *Direct solution of sparse skew symmetric linear systems,* Invited speaker.

October

MUMPS User Day 2006, LIP- ENS Lyon, Lyon, France, October 24. TZ. SLAVOVA, *Out-Of-Core parallel solution*, joint work with P. Amestoy, I. Duff and A. Guermouche, contributed talk.

First International Conference on Numerical Algebra and Scientific Computing (NASC06). Beijing, China, 22-26 October 2006. I. DUFF, *Design and use of a sparse direct solver for skew-symmetric systems,* Invited talk.

Meeting in Shanghai, 28 October 2006. I. DUFF, *Design and use of a sparse direct solver for skew-symmetric systems,* Invited talk.

November

University of Newcastle, NSW, Australia. 6-28 November 2006. Visiting senior researcher.

University of Newcastle, NSW, Australia. 20 November 2006. I. DUFF, *Sparse system solution and the HSL library,* Seminar.

January

Séminaire INRIA Rocquencourt, Paris, 11 Janvier 2007. F. CHAITIN-CHATELIN, *Déviation homotopique : l'application* $(t,z) \in \mathbb{C}^2 \mapsto (A + tE - zI)^{-1}$, Invited talk.

ORBEL 2007, 21st annual conference of the Belgian Operational Research, Luxembourg, January 18-19 M. GARCIA *Neural networks based trust-region methods for bound-constrained nonlinear optimization* , joint work with S. Gratton and Ph. Toint, contributed talk.

February

Scientific and Celebratory Conference. In honour of Paul Durham, CCLC Daresbury Laboratory, UK. 5 February 2007. I.S. DUFF, *Combining direct and iterative methods for the solution of large systems in different application areas,* Invited talk.

Dagstuhl Seminar on Web Information Retrieval and Linear Algebra Algorithms, Schloss Dagstuhl, Germany, February 11–16, 2007. B. UCAR, attendee.

SIAM Workshop on Combinatorial Scientific Computing (CSC07), Cost Mesa, California, USA. 17-19 February, 2007. I.S. DUFF, *Recent developments in multifrontal codes,* Invited talk.

March

IMM, DTU, Lyngby. March-April 2007. I.S. DUFF, *Six double lectures on a Course in Advanced Topics in Optimization*, visiting Professor.

SIAM Conference on Mathematical and Computational Issues in the Geosciences (GS07) March 19-22 Santa Fe, USA. X. PINEL, *Flexible GMRES with deflated restarting with the application for the solution of the Helmholtz equation,* joint work with L. Giraud, S. Gratton, X. Vasseur, contributed talk.

Seminar in Informatik og Matematisk Modellering series at DTU, Lyngby. 21 March 2007. I.S. DUFF, *Combining direct and iterative methods for the solution of large systems in different application areas,* seminar.

Seminar to Numerical Analysis Group at DTU, Lyngby. 23 March 2007. I.S. DUFF, *Recent developments in multifrontal codes,* seminar.

Berkeley Lab Scientific Computing Workshop, LBNL, 28 March 2007. I.S. DUFF, *Recent developments in multifrontal codes,* invited talk.

Stanford 50 : State of the Art and Future Durections of Computational Mathematics and Numerical Computing. 29-31 March 2007. I.S. DUFF, *Combining direct and iterative methods for the solution of large systems in different application areas,* Invited talk.

April

EUCCO 2007, Second European Conference on Computational Optimization, Montpellier, France, April 2-4 M. GARCIA *Neural networks based trust-region methods for bound-constrained nonlinear optimization* , joint work with S. Gratton and Ph. Toint, contributed talk.

May

Gene Golub Day, University of Leicester. 23 May 2007. I.S. DUFF, *Direct codes for rank detection and the solution of skew symmetric systems.*

June

Argonne National Laboratory, Illinois, USA. 14 June 2007. I.S. DUFF, *Recent developments in rank detection and skew solvers,* seminar.

Seminar für Analysis und Numerik, University of Basel, Switzerland, June 22 X. VASSEUR *Multigrid preconditioned Krylov subspace methods for the numerical solution of Helmholtz equation in geophysics*, joint work with S. Gratton and X. Pinel, invited seminar.

July

EUROPT-OMS Meeting 2007. Prague, Czech Republic. 4-7 July 2007. M. MOUFFE, *Active constraints identification in the context of multilevel trust-region methods for nonlinear bound constrained optimization problems,* joint work with S. Gratton and Ph. L. Toint, Talk.

International Conference On Preconditioning Techniques For Large Sparse Matrix Problems In Scientific And Industrial Applications July 9-12th, 2007, Toulouse, France. X. PINEL, *Multigrid preconditioned Krylov subspace methods for the numerical solution of three-dimensional Helmholtz problems in geophysics*, joint work with H. Calandra, I.S. Duff, S. Gratton, X. Vasseur, contributed talk.

International Conference On Preconditioning Techniques For Large Sparse Matrix Problems In Scientific And Industrial Applications July 9-12th, 2007, Toulouse, France. A. HAIDAR, *A parallel additive Schwarz preconditioner and its variants for 3D elliptic non-overlapping domain decomposition*, joint work with L. Giraud and L. T. Watson, contributed talk.

ICIAM 2007, Zurich, Switzerland. 15-20 July, 2007. I. DUFF, *Developments in matching and scaling algorithms,* Minisymposium IC/MP/012/E/221 Organizer Alex Pothen Invited minisymposium speaker.

ICIAM 2007, Zurich, Switzerland. 15-20 July, 2007. I. DUFF, *The use of hybrid techniques at CERFACS for the solution of large problems on parallel machines,* Minisymposium IC/MP/010/U/285 Organizers : Sherry Li and Osni Marques. Invited minisymposium speaker.

ICIAM 2007, Zurich, Switzerland, 15-20 July 2007. M. AHMADNASAB, *Parameter analysis of the structure of regular matrix pencils by Homotopic Deviation theory*, joint work with F. Chaitin-Chatelin, contributed talk.

ICIAM 2007, Zurich, Switzerland, 15-20 July 2007. X. PINEL, *Flexible GMRES with deflated restarting*, joint work with L. Giraud, S. Gratton, X. Vasseur, contributed talk.

SciDAC workshop on libraries and algorithms, Snowbird (Utah), USA, July 30- August 2, 2007 M. BABOULIN, *Very large least-squares for parameter estimation : Algorithm and application*, contributed talk.

August

Second Mathematical Programming Society International Conference on Optimization : ICCOPT II and MOPTA 2007. Hamilton, Canada. 13-16 August 2007. M. MOUFFE, *Multilevel infinity-norm trust-region method for bound-constrained optimization*, joint work with S. Gratton, Ph. L. Toint and M. Weber Mendonça, Talk.

International Conference on Applied Mathematics and Interdisciplinary Research, Lijiang, Yunnan Province, China. August 13-18, 2007. I.S. DUFF, *Hybrid techniques for the solution of large scale problems,* Invited plenary talk.

Department of Mathematics, Jiaotong University, Xi'an, China. August 23 , 2007. I.S. DUFF, *Recent developments in multifrontal codes,* Seminar.

September

PPAM 2007, Seventh International Conference on Parallel Processing and Applied Mathematics, Gdansk, Poland, September 9–12, 2007. B. UCAR, *Heuristics for a matrix symmetrization problem*, contributed talk.

Sixth International Conference on Computer Science and Information Technologies (CSIT'2007). Yerevan, Armenia, September 24-28, 2007. I.S. DUFF, *The use of hybrid techniques for the solution of large scale problems,* keynote talk.

October

University of Manchester, October 3, 2007. I.S. DUFF, *The use of hybrid techniques for the solution of large scale problems,* Seminar.

Matrix Analysis and Applications. CIRM Luminy, Marseille, France, October 15-19, 2007. I.S. DUFF, *The use of hybrid techniques at CERFACS for the solution of large scale problems on parallel machines,* Invited talk.

7.2 Conferences and seminars organized by the Parallel Algorithms Project

June

Sparse Days Meeting at CERFACS June 15–16th, 2006 at CERFACS, Toulouse, France.

July

2007 International Conference On Preconditioning Techniques For Large Sparse Matrix Problems In Scientific And Industrial Applications July 9–12th, 2007 at CERFACS, Toulouse, France.

Invited speakers :

MARIO BEBENDORF, (Leipzig University, Germany),
JACEK GONDZIO, (University of Edinburgh, UK),
YVAN NOTAY, (Université Libre de Bruxelles, Belgium),
PADMA RAGHAVAN, (The Pennsylvania State University, USA) ,
STEFAN REITZINGER, (Computer Simulation Technology GmbH (CST), Germany),
SIVAN TOLEDO, (Tel-Aviv University, Israel),
LUDMIL ZIKATONOV, (Pennsylvania State University, USA).

October

Sparse Days Meeting at CERFACS June 10–12th, 2007 at CERFACS, Toulouse, France.

7.3 Internal seminars organized within the Parallel Algorithms Project

January

Object-Oriented Programming Techniques for Sparse Linear System Solvers., January 12, 2006. M. SALA.

March

Solving large dense linear least squares problems on parallel distributed computers. Application to the Earth's gravity field computation., March 21, 2006. Ph.D. thesis defence. M. BABOULIN.
Multigrid Solution of Discrete Convection-Diffusion Equations., March 24, 2006. A. RAMAGE.

April

On some preconditioning techniques for systems with multiple right-hand sides., April 13, 2006. J. TSHIMANGA

May

Mulitilevel ILU preconditioners., May 3, 2006. F. WUBS.
Fast solution of large linear systems in the ocean model THCM., May 10, 2006. F. WUBS.
The Sinkhorn-Knopp Algorithm : Convergence and Applications., May 17, 2006. P. A. KNIGHT.
Use of multi-level trust-region techniques for nonlinear bound constrained optimization problems. , May 31, 2006. M. MOUFFE.

June

On the computation of the null space of a sparse matrix., June 13, 2006. X. VASSEUR.

August

Minimisation des bruits d'avions commerciaux sous contraintes. Recherche de solutions optimales. August 25, 2006. L. ABDALLAH.

September

Numerical experiments with additive Schwarz preconditioner for non-overlapping domain decomposition in 3D., September 5, 2006. A. HAIDAR.

November

Flexible GMRES with Deflated Restarting (FGMRES-DR), application to two-dimensional Helmholtz equations proceeding from geophysics. , November 2nd, 2006. X. PINEL.

December

Parallel approaches to some large-scale optimization problems., December 13, 2006. G. ZANGHIRATI.

January

Spectral analysis of the discrete Helmholtz operator preconditioned with a shifted Laplacian., January 11, 2007. M. VAN GIJZEN.

February

Ellipsoidal and Interval Techniques for State Estimation in Linear Dynamical Systems under Model Uncertainty., February 1, 2007 S. NAZIN.
Using model reduction techniques within Incremental 4-Dimensional Variational Data Assimilation. , February 8, 2007. C. BOESS.

March

Benchmarking of Bound-constrained Optimisation Tools., March 20, 2007. A. TRÖLTZSCH.

October

Homotopic deviation theory : a qualitative study., October 24, 2007. Ph.D. thesis defence. M. AHMADNASAB.

December

Medium-term power planning problem : model and solutions approach., December 11, 2007. A. PAGES.

8 Publications

8.1 Journal Publications

[ALG1] G. Alléon, S. Champagneux, G. Chevalier, L. Giraud, and G. Sylvand, (2006), Parallel Distributed Numerical Simulations in Aeronautic Applications, *J. Applied Mathematical Modelling*, **30**, 714–730.

[ALG2] M. Arioli, M. Baboulin, and S. Gratton, (2007), A partial condition number for linear least-squares problems, *SIAM Journal on Matrix Analysis and Applications*, **29**, 413–433.

[ALG3] M. Arioli, I. S. Duff, S. Gratton, and S. Pralet, (2007), A Note on GMRES Preconditioned by a Perturbed LDL^T Decomposition with Static Pivoting, *SIAM Journal on Scientific Computing*, **29**, 2024–2044.

[ALG4] M. Baboulin, L. Giraud, S. Gratton, and J. Langou, (2007), A distributed packed storage for large dense parallel in-core calculations, *Concurrency and Computation : Practice and Experience*, **19**, 483–502.

[ALG5] F. Bastin, C. Cirillo, and Ph. L. Toint, (2006), An adaptive Monte Carlo algorithm for computing mixed logit estimators, *Computational Management Science*, **3**, 55–79.

[ALG6] F. Bastin, C. Cirillo, and Ph. L. Toint, (2006), Application of an adaptive Monte Carlo algorithm to Mixed Logit estimation, *Transportation Research Part B*, **40**, 577–593.

[ALG7] F. Bastin, C. Cirillo, and Ph. L. Toint, (2006), Convergence theory for nonconvex stochastic programming with an application to mixed logit, *Mathematical Programming*, **108**, 207–234.

[ALG8] B. Carpentieri, L. Giraud, and S. Gratton, (2007), Additive and Multiplicative Two-Level Spectral Preconditioning for General Linear Systems, *SIAM Journal on Scientific Computing*, **29**, 1593–1612.

[ALG9] F. Chaitin-Chatelin and M. B. van Gijzen, (2006), Analysis of parameterized Quadratic Eigenvalue problems in Computational Acoustics with Homotopic Deviation theory, *Numerical Linear Algebra with Applications*, **13**, 487–512.

[ALG10] I. S. Duff and S. Gratton, (2006), The Parallel Algorithms Team at CERFACS, *SIAM News*, **39**, 10–11.

[ALG11] I. S. Duff and S. Pralet, (2007), Towards Stable Mixed Pivoting Strategies for the Sequential and Parallel Solution of Sparse Symmetric Indefinite Systems, *SIAM Journal on Matrix Analysis and Applications*, **29**, 1007–1024.

[ALG12] I. S. Duff, S. Gratton, X. Pinel, and X. Vasseur, (2007), Multigrid based preconditioners for the numerical solution of two-dimensional heterogeneous problems in geophysics, *International Journal of Computer Mathematics*, **84-88**, 1167–1181.

[ALG13] D. Ettema, F. Bastin, J. Polak, and O. Ashiru, (2007), An error-components framework for joint choice models of activity timing and duration, *Transportation Research Part A*, **41**, 827–849.

[ALG14] L. Giraud and S. Gratton, (2006), On the Sensitivity of Some Spectral Preconditioners, *SIAM Journal on Matrix Analysis and Applications*, **27**, 1089–1105.

[ALG15] L. Giraud, S. Gratton, and J. Langou, (2007), Convergence in Backward Error of Relaxed GMRES, *SIAM Journal on Scientific Computing*, **29**, 710–728.

[ALG16] L. Giraud, S. Gratton, and E. Martin, (2007), Incremental spectral preconditioners for sequences of linear systems, *Appl. Numer. Math.*, **57**, 1164–1180.

[ALG17] L. Giraud, J. Langou, and G. Sylvand, (2006), On the parallel solution of large industrial wave propagation problems, *J. Computational Acoustics*, **14**, 83–111.

[ALG18] L. Giraud, D. Ruiz, and A. Touhami, (2006), A Comparative Study of Iterative Solvers Exploiting Spectral Information for SPD Systems, *SIAM Journal on Scientific Computing*, **27**, 1760–1786.

[ALG19] S. Gratton, A. Lawless, and N. Nichols, (2007), Approximate Gauss-Newton methods for nonlinear least squares problems, *SIAM J. on Optimization*, **18**, 106–132.

[ALG20] S. Gratton, A. Sartenaer, and P. Toint, (2006), Second-order convergence properties of trust-region methods using incomplete curvature information, with an application to multigrid, *Journal of Computational Mathematics*, **24**, 676–692. see also TR/PA/06/34.

[ALG21] D. Loghin, D. Ruiz, and A. Touhami, (2006), Adaptive preconditioners for nonlinear systems of equations, *J. Comput. Appl. Math.*, **189**, 362–374.

[ALG22] D. Loghin, M. van Gijzen, and E. Jonkers, (2006), Bounds on the eigenvalue range and on the field of values of non-Hermitian and indefinite finite element matrices, *J. Comput. Appl. Math.*, **189**, 304–323.

[ALG23] D. Mariano-Goulart, P. Maréchal, S. Gratton, and L. Giraud, (2007), A priori selection of the regularization parameters in emission tomography by Fourier synthesis, *Computerized Medical Imaging and Graphics*, **31**, 502–509.

[ALG24] A. Toselli and X. Vasseur, (2006), A numerical study on Neumann-Neumann methods for hp approximations on geometrically refined boundary layer meshes II. Three-dimensional problems, *Mathematical Modelling and Numerical Analysis*, **40**, 99–122.

[ALG25] B. Uçar and C. Aykanat, (2007), Partitioning Sparse Matrices for Parallel Preconditioned Iterative Methods, *SIAM Journal on Scientific Computing*, **29**, 1683–1709.

[ALG26] B. Uçar and C. Aykanat, (2007), Revisiting Hypergraph Models for Sparse Matrix Partitioning, *SIAM Review*, **49**, 595–603.

[ALG27] L. Valdettaro, M. Rieutord, T. Braconnier, and V. Fraysse, (2007), Convergence and round-off errors in a two-dimensional eigenvalue problem using spectral methods and Arnoldi-Chebyshev algorithm, *J. Comput. Appl. Math.*, **205**, 382–393.

8.2 Theses

[ALG28] M. Ahmadnasab, (2007), *Homotopic deviation theory : a qualitative study*, Ph.D. dissertation, University Toulouse I. TH/PA/07/120.

[ALG29] M. Baboulin, (2006), *Solving large dense linear least squares problems on parallel distributed computers. Application to the Earth's gravity field computation.*, Ph.D. dissertation, INPT. TH/PA/06/22.

8.3 Technical Reports

[ALG30] M. Ahmadnasab and F. Chaitin-Chatelin, (2007), Matrix pencils under Homotopic Deviation theory, Technical Report TR/PA/07/108, CERFACS.

[ALG31] P. Amestoy, I. S. Duff, A. Guermouche, and T. Slavova, (2007), Analysis of the out-of-core solution phase of a parallel multifrontal approach, Technical Report TR/PA/07/48, CERFACS.

[ALG32] M. Baboulin, J. Dongarra, S. Gratton, and J. Langou, (2007), Computing the conditioning of the components of a linear least squares solution, Technical Report TR/PA/07/101, CERFACS. Also appeared as LAPACK Working Note 193.

[ALG33] M. Baboulin, L. Giraud, and S. Gratton, (2006), Solution of an inverse problem for the GOCE satellite mission, Contract Report CR/PA/06/78, CERFACS.

[ALG34] M. Baboulin, L. Giraud, S. Gratton, and J. Langou, (2006), Parallel tools for solving incremental dense least squares problems. Application to space geodesy., Technical Report TR/PA/06/63, CERFACS. Also available as LAPACK Working Note 179.

[ALG35] F. Bastin, C. Cirillo, and P. L. Toint, (2006), Estimating mixed logit with non-parametric random variables, Technical Report TR/PA/06/87, CERFACS.

[ALG36] F. Bastin, V. Malmedy, M. Mouffe, P. L. Toint, and D. Tomanos, (2007), A Retrospective Trust-Region Method for Unconstrained Optiomization, Technical Report TR/PA/07/136, CERFACS.

[ALG37] O. Boiteau, F. Huelsemann, and X. Vasseur, (2006), Comparison of the linear algebraic solvers Mumps and the multifrontal solver of Code ASTER, Contract Report CR/PA/06/11, CERFACS.

[ALG38] F. Chaitin-Chatelin, (2006), Calcul Algébrique non linéaire dans les algèbres de Dickson, Technical Report TR/PA/06/07, CERFACS.

[ALG39] F. Chaitin-Chatelin, (2007), About an organic logic ruling the continuous evolution of SVD measurement with Dickson hypercomplex numbers., Technical Report TR/PA/07/55, CERFACS.

[ALG40] F. Chaitin-Chatelin, (2007), Computing beyond classical logic : SVD computation in nonassociative Dickson algebras, Technical Report TR/PA/07/54, CERFACS.

[ALG41] F. Chaitin-Chatelin, (2007), The dynamics of spectral analysis by Homotopic Deviation. Part I : The spectral field., Technical Report TR/PA/07/118, CERFACS.

[ALG42] I. S. Duff, S. Gratton, X. Pinel, and X. Vasseur, (2007), Multigrid based preconditioners for the numerical solution of two-dimensional heterogeneous problems in geophysics, Technical Report TR/PA/07/03, CERFACS. Preliminary version of an article published in International Journal of Computer Mathematics, vol. 84-8, pp 1167-1181.

[ALG43] I. S. Duff, (2007), The design and use of a sparse direct solver for skew symetric matrices, Technical Report TR/PA/07/04, CERFACS.

[ALG44] D. Ettema, F. Bastin, J. Polak, and O. Ashiru, (2006), An Error-Components Framework for Joint Choice Models of Activity Timing and Duration, Technical Report TR/PA/06/02, CERFACS.

[ALG45] V. Frayssé, L. Giraud, and S. Gratton, (2006), A Set of Flexible GMRES Routines for Real and Complex Arithmetics on High Performance Computers, Technical Report TR/PA/06/09, CERFACS. This report supersedes TR/PA/98/07.

[ALG46] M. Garcia, S. Jan, and M. Masmoudi, (2007), Neural networks : low-memory training and regularizatio techniques, Technical Report TR/PA/07/25, CERFACS.

[ALG47] A. E. Ghazi, S. E. Hajji, L. Giraud, and S. Gratton, (2006), A short note on backward errors for the common eigenvector problem, Technical Report TR/PA/06/13, CERFACS.

[ALG48] L. Giraud, S. Gratton, and J. Langou, (2006), Convergence in backward error of relaxed GMRES, Technical Report TR/PA/06/08, CERFACS. This report supersedes TR/PA/04/132.

[ALG49] L. Giraud, S. Gratton, and X. Pinel, (2007), Classical and flexible Krylov subspace methods with deflated restarting for the solution of electromagnetics problems with impedance boundary conditions, Contract Report CR/PA/07/53, CERFACS. Also appeared as ENSEEIHT-IRIT Technical report RT/APO/07/09.

[ALG50] L. Giraud, A. Haidar, and L. T. Watson, (2006), Mixed-precision preconditioners in parallel domain decomposition solvers, Technical Report TR/PA/06/84, CERFACS. Also appeared as IRIT Technical report ENSEEIHT-IRIT RT/APO/06/08.

[ALG51] L. Giraud, A. Haidar, and L. T. Watson, (2007), Parallel scalability study of three dimensional additive Schwarz preconditioners in non-overlapping domain decomposition, Technical Report TR/PA/07/05, CERFACS. Also appeared as ENSEEIHT-IRIT Technical report RT/APO/07/01.

[ALG52] S. Gratton, M. Mouffe, P. L. Toint, and M. Weber-Mendonça, (2007), Global convergence of a recursive trust-region method in infinite norm for bound-constrained optimization, Technical Report TR/PA/07/42, CERFACS.

[ALG53] S. Gratton, A. Sartenaer, and P. L. Toint, (2006), Numerical Experience with a Recursive Trust-Region Method for Multilevel Nonlinear Optimization, Technical Report TR/PA/06/33, CERFACS.

[ALG54] S. Gratton, A. Sartenaer, and P. L. Toint, (2006), Recursive Trust-Region Methods for Multiscale Nonlinear Optimization, Technical Report TR/PA/06/32, CERFACS.

[ALG55] S. Gratton, A. Sartenaer, and P. L. Toint, (2006), Second-order convergence properties of trust-region methods using incomplete curvature information, with an application to multigrid, Technical Report TR/PA/06/34, CERFACS.

[ALG56] P. A. Knight, (2006), The Sinkhorn-Knopp Algorithm : Convergence and Applications, Technical Report TR/PA/06/42, CERFACS.

[ALG57] A. S. Lawless, S. Gratton, and N. K. Nichols, (2006), An investigation of incremental 4D-Var using non-tangent linear models, Technical Report TR/PA/06/10, CERFACS.

[ALG58] T. P. A. Project, (2006), Scientific Report for 2006, Technical Report TR/PA/06/107, CERFACS.

[ALG59] A. Tröltzsch, S. Gratton, and P. L. Toint, (2007), Benchmarking of bound-constrained optimization software, Working Notes WN/PA/07/143, CERFACS.

[ALG60] B. Ucar and C. Aykanat, (2007), Partitioning sparse matrices for parallel preconditioned iterative methods, Technical Report TR/PA/07/23, CERFACS. Preliminary version of an article published in SIAM Journal on Scientific Computing, vol. 29, nber 4, pp 1683-1709.

[ALG61] B. Ucar, (2007), Heuristics for a matrix symmetrization problem, Technical Report TR/PA/07/91, CERFACS.

8.4 Conference Proceedings

[ALG62] F. Bastin, C. Cirillo, and P. L. Toint, (2006), Estimating mixed logit with non-parametric random variables, In *Proceedings of European Transport Conference (CD-ROM)*, Strasbourg, France, PTRC.

[ALG63] F. Chaitin-Chateli, (2007), *Computing beyond classical logic* : SVD *computation in nonassociative* $Dickson\ algebras$, In *Randomness and Complexity*, C. C. ed., ed., World Scientific, Singapore, 13–23.

[ALG64] I. S. Duff, (2007), Combining direct and iterative methods for the solution of large systems in different application areas, In *Modern Mathematical Models, Methods and Algorithms for Real World Systems*, A. Siddiqi, I. Duff, and O. Christensen, eds., Anamaya Publishers, New Delhi, India, 402–419.

[ALG65] I. S. Duff, (2007), Sparse system solution and the HSL Library, In *Some Topics in Industrial and Applied Mathematics*, R. Jeltsch, T.-T. Li, and I. H. Sloan, eds., Series in Contemporary Applied Mathematics CAM 8, World Scientific, Singapore, 78–94.

[ALG66] B. Uçar, (2007), Heuristics for a matrix symmetrization problem, In *Proceedings of 7th International conference on parallel processing and applied mathematics (PPAM'07)* (to appear), Gdansk, Poland.

2

Data Assimilation

1 Introduction

Data assimilation is used to combined observations of a physical system with the models that describe it or predict its evolution.

Data assimilation is now recognized as a major component of modelling along with the parametrisation of physical processes, numerical simulation or coupling. Data assimilation requires a good physical knowledge of the modelled system, of its statistical properties and efficient optimisation algorithms.

Crucial for weather prediction for which it has been strongly developed, data assimilation is now spreading to all the fields where models and observations are mature enough. In some domains, it is referred as “data reconciliation” or “parameter calibration”.

CERFACS is presently active in data assimilation developments in four modelling domains :
– Data assimilation for oceanography
– Data assimilation for atmospheric chemistry
– Data assimilation for nuclear plants
– Data assimilation for hydrology

Only the three first items are described in this scientific report since the last one started in September 2007. Strong collaborations with the experts of the respective modelling fields, such as METEO-FRANCE for atmospheric chemistry or EDF for nuclear plants, are the key for this research activity success. Most of these projects are using the PALM software to develop their data assimilation algorithms.

2 Data assimilation for oceanography

2.1 A three-dimensional ensemble variational data assimilation system for the global ocean (N. Daget, A. Weaver)

Further developments have been made to the global-ocean variational data assimilation system, OPAVAR, for the OPA ocean general circulation model. The global system is based on an earlier system developed for the tropical Pacific ([4], [3], [2]), but has been extended to incorporate new features including fully multivariate background-error covariances [DA12] and the capacity to produce ensembles of ocean analyses for climate studies and forecast initialization [1]. The ensembles are created by perturbing the surface forcing fields (wind-stress, fresh-water flux and heat flux) and the observations (temperature and salinity profiles) used in the assimilation process. A 3D-Var (FGAT) version of the ensemble OPAVAR system has been applied in the ENSEMBLES (FP6) project to produce multiple historical reanalyses over the period 1960-2006.

Cycled 3D-Var experiments over the period 1993-2000 have also been performed to test the sensitivity of the analyses to two flow-dependent formulations of the background error standard deviations (σ^b) for temperature and salinity [1]. The first formulation is based on an empirical parameterization of σ^b in terms of the vertical gradients of the background temperature and salinity fields, while the second formulation involves a more sophisticated approach that derives σ^b from the spread of an ensemble of analyses. The ensemble system is illustrated schematically in Fig. 2.1. In both experiments, the observation error standard deviations (σ^o) are geographically dependent and have been estimated from a model-data comparison prior to assimilation. An additional 3D-Var experiment that employs the parameterized σ^b but a simpler σ^o formulation, and a control experiment involving no data assimilation have also been conducted and used for comparison.

All 3D-Var experiments produce a significant reduction in the mean and standard deviation of the temperature and salinity innovations compared to those of the control experiment. Comparing innovation statistics from the two σ^b formulations shows that, on the global average, both formulations give similar results below 150 m but the parameterized σ^b give slightly better results above 150 m where statistical consistency checks suggest that the ensemble σ^b are underestimated. The temperature and salinity error growth between cycles, however, is shown to be much reduced with the ensemble σ^b, suggesting that the analyses produced with the ensemble σ^b are in better balance than those produced with the parameterized σ^b. Sea surface height (SSH) anomalies in the northwest Atlantic and zonal velocities in the equatorial Pacific, which are fields not directly constrained by the observations, are clearly improved with the ensemble σ^b than with the parameterized σ^b when compared to independent data (Fig. 2.2). Comparisons with the control are less conclusive, and indicate that, while some aspects of those variables are improved (currents in the central and eastern Pacific), other aspects are degraded (SSH anomalies in the northwest Atlantic, currents in the western Pacific). There are several areas for improving the ensemble method and for making better use of the ensemble information which are currently being explored.

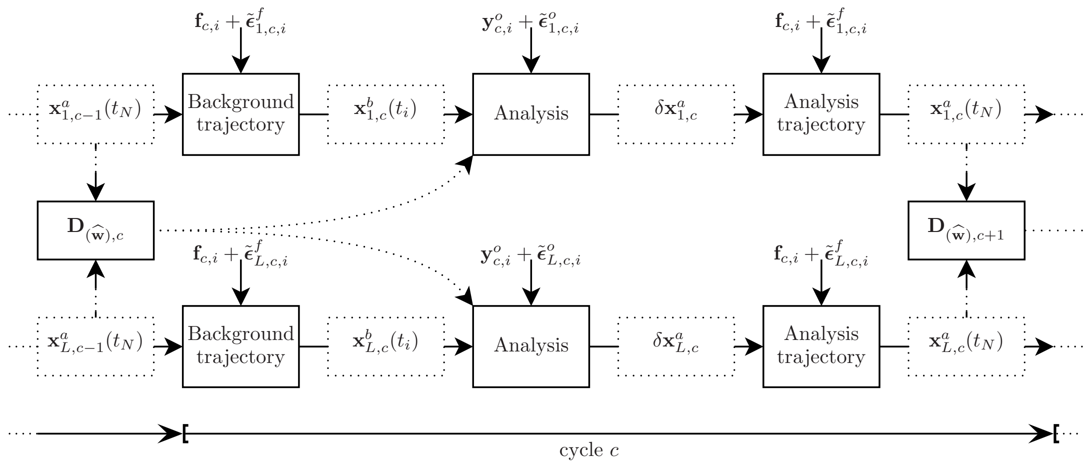
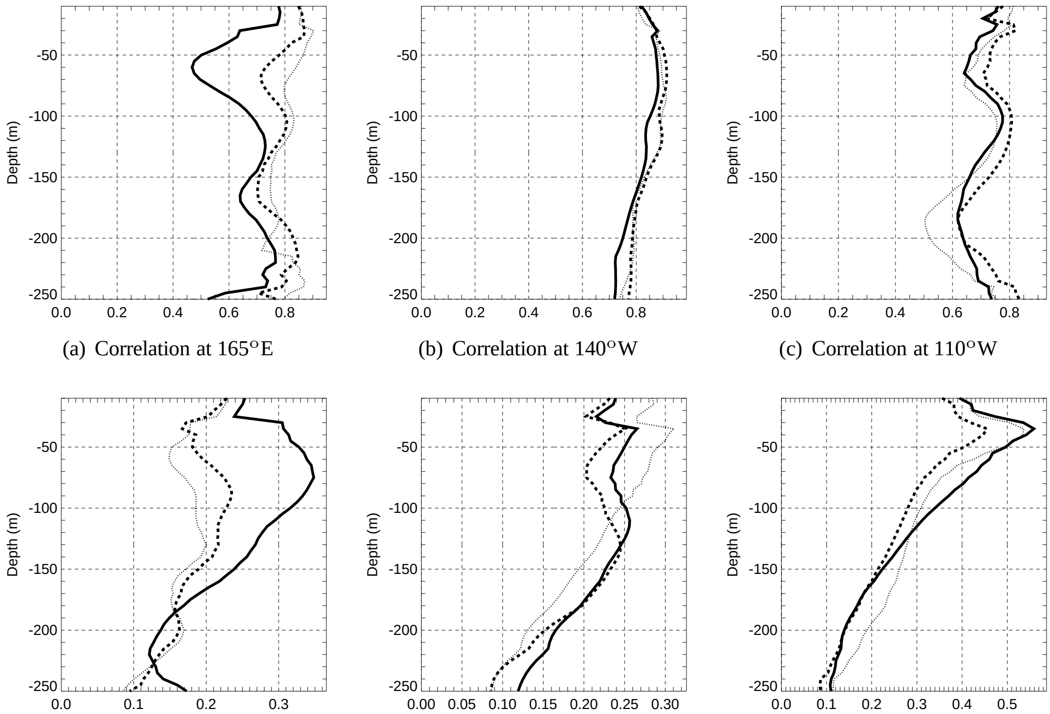


FIG. 2.1 – Schematic illustration of the ensemble 3D-Var system. The ensemble of analysis states $\mathbf{x}^a_{l,c-1}(t_N)$, $l = 1, \ldots L$, at the end of cycle $c-1$ are used to initialize the background trajectories of each ensemble member on the next cycle c. The background trajectory of each member l is produced by integrating the model with a perturbed set of forcing fields (wind-stress, fresh-water flux, heat flux), $\mathbf{f}_{c,i} + \tilde{\epsilon}^f_{l,c,i}$, from the initial condition $\mathbf{x}^b_{l,c}(t_0) = \mathbf{x}^a_{l,c-1}(t_N)$. Each background trajectory is compared with a set of perturbed observations $\mathbf{y}^o_{c,i} + \tilde{\epsilon}^o_{l,c,i}$ to produce an innovation vector for each member l. A 3D-Var (FGAT) analysis is then performed for each ensemble member using the appropriate innovation vector and a background-error variance matrix $\mathbf{D}_{(\widehat{\mathbf{w}}),c}$ that has been estimated from the ensemble of background initial states $\mathbf{x}^b_{l,c}(t_0)$. The unperturbed member ($l = 0$), which is not displayed, is also used to compute $\mathbf{D}_{(\widehat{\mathbf{w}}),c}$. The resulting analysis increment is then applied to the model to produce the analysis model state trajectory.

2.2 Development of the next generation variational ocean data assimilation system : NEMOVAR (A. Weaver, S. Ricci, I. Mirouze)

In early 2006 a collaborative project was initiated between CERFACS and ECMWF to develop a three- and four-dimensional variational assimilation (3D-Var and 4D-Var) system for the latest version of the OPA model : OPA9/NEMO. The new system is referred to as NEMOVAR. NEMOVAR inherits the basic incremental algorithmic structure of OPAVAR, the variational assimilation system developed at CERFACS for OPA8.2, but is being adapted to the NEMO framework and extended to run on distributed-memory (MPP) machines and to use dynamic memory. Achieving this objective has required a major rewrite of the different OPAVAR components. In addition, specific research activities have been initiated on the following algorithmic aspects of NEMOVAR : 1) the generalized diffusion model used for representing correlated background error (PhD topic of I. Mirouze) ; 2) the conjugate gradient minimization and preconditioning software (collaboration with the ALGO team at CERFACS) ; and 3) the incremental algorithm to allow for higher resolution in the outer loop compared to the inner (minimization) loop (collaboration with A. Vidard, INRIA). These improvements to the computer code and numerical algorithms are vital for future applications (research and operational) of variational assimilation with higher resolution, state-of-the-art NEMO configurations.

An MPP implementation of a 3D-Var system with NEMO in both the outer and inner loops has been developed. The system currently employs identical resolution in the inner and outer loops ; the multi-



(a) Correlation at 165°E (b) Correlation at 140°W (c) Correlation at 110°W

(d) RMS error at 165°E (e) RMS error at 140°W (f) RMS error at 110°W

FIG. 2.2 – Correlation (upper panels) and RMS error ($\mathrm{m\ s^{-1}}$; lower panels) between equatorial zonal currents from TAO data and those from the control (no data assimilation) experiment (dotted curves), and experiments with empirically-specified and enemble-generated background-error standard deviations (solid and dashed curves respectively) over the 1993-2000 period at 165°E (left panels), 140°W (middle panels) and 110°W (right panels).

incremental feature is still in development. The 3D-Var system has been tested with both the ORCA2° and ORCA1° global configurations. Validation experiments so far have mainly been conducted on a single cycle although the system has recently been adapted to perform multiple cycles as well. Additional assimilation data-sets have been included compared to those used in OPAVAR. The current NEMOVAR system can assimilate temperature and salinity profiles from the ENACT/ENSEMBLES (EN3v2) and CORIOLIS databases, along-track altimeter anomalies from the multiple satellite (Geosat, T/P, Jason-1, ERS-1, ERS-2, GFO) database from CLS/AVISO, gridded Mean Dynamic Topography (MDT) products (Rio-05, model-derived), and model-gridded sea surface temperature (SST) products (Reynolds OIv2, HadISST). Particular attention has been paid to computational efficiency and optimization : in this area significant improvements have been made over OPAVAR. Two notable features of OPAVAR yet to be fully transferred to NEMOVAR include 4D-Var (specifically the development of the NEMO Tangent-linear and Adjoint Models - NEMOTAM) and the capacity to generate ensembles of analyses (with and without adaptive background-error covariances). Work in developing these features for NEMOVAR is ongoing in collaboration with ECMWF and INRIA.

2.3 References

[1] N. Daget and A. T. Weaver, (2008), A three-dimensional ensemble variational data assimilation system for the global ocean : sensitivity to the observation- and background-error variance formulation, *Mon. Weather Rev.*, **In preparation**.

[2] S. Ricci, A. T. Weaver, J. Vialard, and P. Rogel, (2005), Incorporating state-dependent temperature-salinity constraints in the background-error covariance of variational ocean data assimilation, *Mon. Weather Rev.*, **133**, 317–338.

[3] J. Vialard, A. T. Weaver, D. L. T. Anderson, and P. Delecluse, (2003), Three- and four-dimensional variational assimilation with an ocean general circulation model of the tropical Pacific Ocean. Part 2 : physical validation, *Mon. Weather Rev*, **131**, 1379–1395.

[4] A. T. Weaver, J. Vialard, and D. L. T. Anderson, (2003), Three- and four-dimensional variational assimilation with an ocean general circulation model of the tropical Pacific Ocean. Part 1 : formulation, internal diagnostics and consistency checks, *Mon. Weather Rev.*, **131**, 1360–1378.

3 Data assimilation for atmospheric chemistry

In the 1990s, after long and major developments of meteorological data assimilation suites for Numerical Weather Prediction applications, the data assimilation techniques began to be applied to atmospheric constituents chemistry and transport modelling. Because of its relatively late application, initial efforts were focused on the data assimilation methodology.
Research activities on data assimilation for atmospheric chemistry have started at CERFACS some ten years later, when helping Météo-France on methodological aspects aimed to set up a data assimilation system. The first developments took place in the framework of the EC-FP5 ASSET project with a strong focus on stratospheric ozone.
Later, CERFACS took part in the French ADOMOCA (Assimilation de DOnnés pour les MOdèles de Chimie Atmosphérique) project with the objective of implementing a more general assimilation algorithm. Therefore, part of the work was dedicated to the generalization of the assimilation system initially designed for the ASSET project. Another important effort was dedicated to the enhancement of the assimilation overall algorithm and of single operators in order to improve the quality of the constituents' analyses. Moreover, the direct model used to provide constituents' background forecasts, namely the chemistry transport model (CTM) MOCAGE by Météo-France, was upgraded in some particular aspects. The quality of the analyses allows several scientific studies mainly dedicated to stratospheric ozone or upper troposphere carbon monoxide.

3.1 Generalization of the assimilation system

The aim of the ADOMOCA project is to gather the French atmospheric chemistry community working or planning to work on the assimilation of tropospheric and stratospheric chemistry species. Due to the large number of existing tools (models, observations, assimilation methods) in this field, the PALM software has appeared as the best way to set up an assimilation algorithm by coupling the needed operators and algebraic treatments. In the context of the ADOMOCA project, the structure of the original ASSET MOCAGE-PALM algorithm had to become more modular in order to admit other chemistry transport models and to assimilate new observations, not only stratospheric ozone profiles.

3.1.1 Non dependency of the assimilation system to the chemical transport model (A. Piacentini, H. Le Berre)

The orginal ASSET implementation of a variational 3D-VAR (in the First Guess at Appropriate Time or FGAT formulation) scheme was strictly bound to the MOCAGE Chemistry and Transport Model and was strongly oriented to the assimilation of stratospheric ozone profiles. From a technical point of view, it means that part of the assimilation suite data structures and memory management was shared with the stand alone forecast model and that the observation operator was mutuated from the model diagnostic routines.
This approach, while optimized for the ASSET studies, proved to be a limitation for the more general context of the ADOMOCA project. In order to apply the same assimilation algorithm to different models, it became necessary to make the assimilation specific treatments (observation handling, error statistics,

linear algebra, minimization and diagnostics) completely independent of the forecast model. The overall algorithmic approach did not change, but the suite was almost entirely rewritten. The new approach not only allowed the use of the same suite with different models (the parallelized and memory optimized version of MOCAGE on different regular or gaussian grids, MSDOL, LMDz – preliminary work – and even a NetCDF loader for off line studies), but also made easier to upgrade the assimilation components, as it will be briefly sketched in the following sections.

3.1.2 Algorithm evolution (A. Piacentini)

The variational 3D-FGAT scheme can be seen as a particular case of the most general incremental 4D-VAR algorithm. Respecting this feature in the suite design opens many evolution perspectives. The operators sequence now includes PALM units for the forward and backward increment propagation, for the model to control space two ways transforms, for the initialisation and modelling of the error statistics and for the observation screening. The role of this units is most relevant for the roadmap towards new ans more complex algorithms. The modular implementation allows to run production jobs with a stable configuration while working on the next schemes.

3.1.3 Observation operator (A. Piacentini, A. Klonecki)

The ASSET MOCAGE-PALM suite assimilated only stratospheric ozone profiles. Since the MOCAGE direct model already provided a diagnostic tool to compare the model field with observed profiles, the observation operator was based on the same routines. This natural choice required the explicit coding of the adjoint observation operator and introduce a strong limitation on the modularity of the system, because the ADOMOCA suite had to be able to take into account different model grids (and more generally different control space discretizations) and different observations, including nadir satellite profiles (inverted against an *a priori* profile with an averaging kernel), vertically integrated quantities and total columns.
For this reasons, the observation operator was integrally rewritten in collaboration with NOVELTIS and it is now able to compare fields on a general logically rectangular grid with all the above mentioned observations. Moreover, the sparse matrix formalism let us express the adjoint operator simply as the transposition of the linear direct one with a consistent reduction of the time spent in this part of the code.

3.1.4 Diagnostics (A. Piacentini)

A data assimilation suite produces a huge amount of output. It is therefore mandatory to standardize not only its format but also the criteria to quickly assess the quality of an assimilation experience. NetCDF was choosen as output format and the suite produces some relevant statistics files which can later on accessed by a number of NetCDF compliant analysis and plotting tools. We have in particular choosen the Ferret freeware (developed at the NOAA/PMEL) and we have realised a suite of diagnostic analyses that can be automatically run after each assimilation experiment. Two kinds of analyses have been implemented. A thourough comparison of dry run, forecast and analysis with the observations can run after each simulated day, while another set of diagnostics, more oriented to the assessment of the error statistics modelling and bias detection, can be executed after longer assimilations, typically on a monthly basis.

3.2 Improvment of the assimilation methodology

As the background error covariance matrix is a key component of any assimilation system, its modelling is an important step. Usually, this matrix is decomposed into correlations and variance matrices. An interesting and general method for modelling the correlation matrix of the background error for complex geometries (e.g. an ocean model masked and stretched grid) consists in approximating the correlation functions

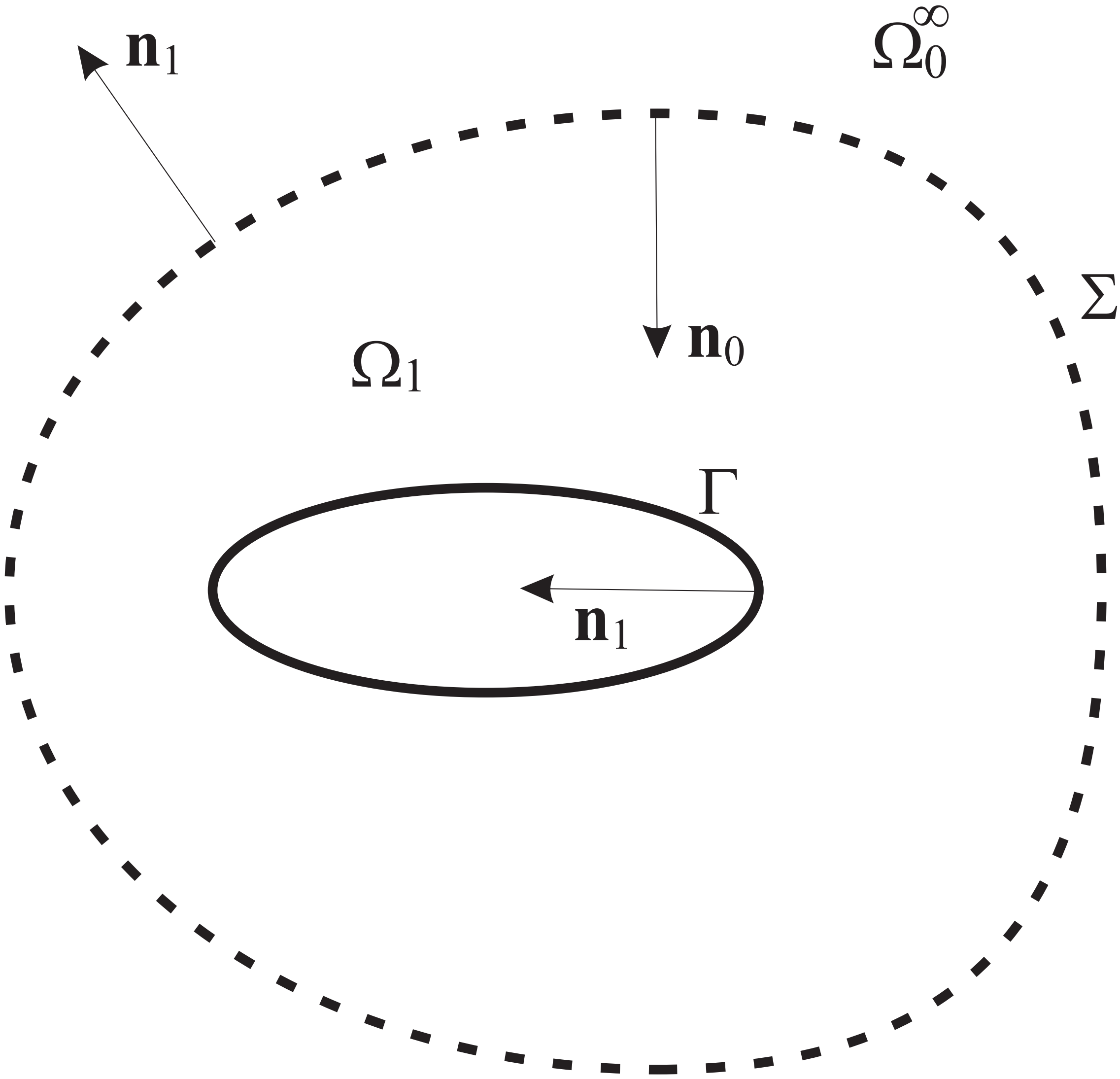


FIG. 3.1 – Example of daily diagnostic. On the left panel : ozone concentrations (ppbv) at 83hPa from a 3h forecast the 29 july 2003. On the right panel : ozone concentrations (ppbv) at 83hPa from the analysis at the same time. The color square represents the MIPAS assimilated observations.

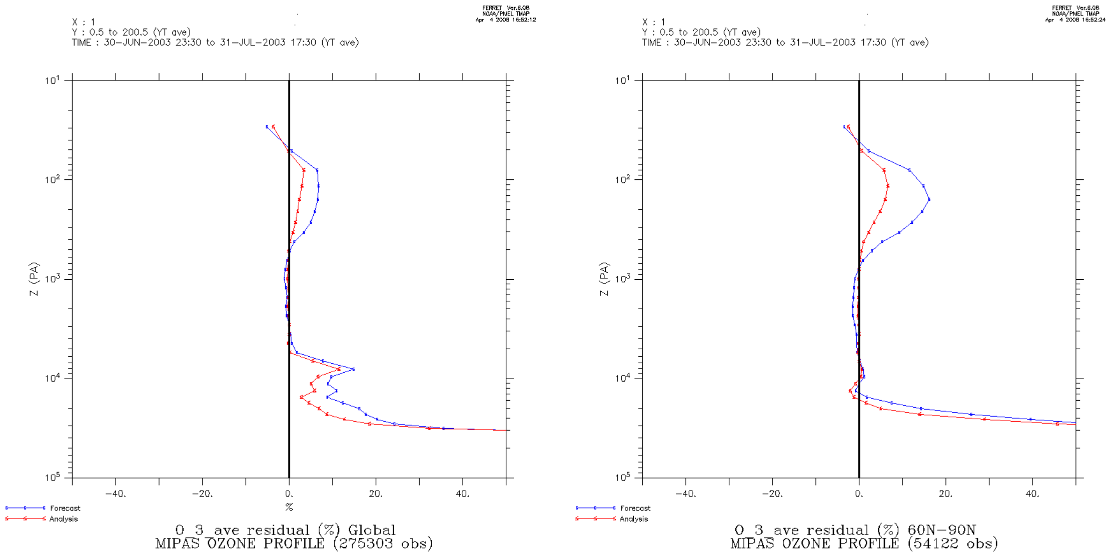


FIG. 3.2 – Example of monthly diagnostic. July 2003 monthly average (in %) of the diffence between the MIPAS observations and the 3h MOCAGE forecast (blue line) and of the diffence between the MIPAS observations and the MOCAGE-PALM analysis (red line). On the left panel : global spatial average. On the right panel : average over the North Pole Region $60°N - 90°N$.

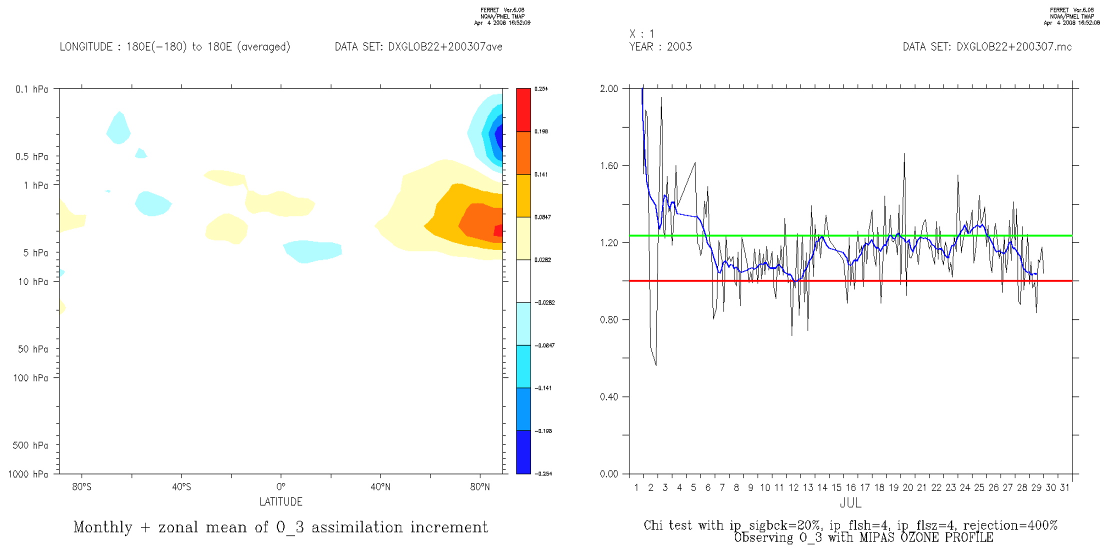


FIG. 3.3 – Example of monthly diagnostic. On the left panel : July 2003 monthly zonal average of the MIPAS assimilation increment. On the right panel : daily (blue line) and monthly (green line) average of the χ^2 test (black line) for the July 2003 MIPAS assimilation.

with the solution of a generalized diffusion operator. The horizontal correlation of the background errors of our assimilation system was computed by numerically solving such an equation but stability issues related to the time stepping scheme imposed a limitation on high latitude observation assimilation. A new numerical approach based on spherical harmonic representation was followed to bypass this restriction and it's constantly improved to take into account finer representations of horizontal correlations structures. Moreover, since in the ASSET assimilation scheme the vertical background error correlation was neglected, a simple formulation was introduced.

3.2.1 Horizontal correlation of the background errors (S. Massart, A. Piacentini)

The horizontal correlations of the background errors are modelled using a diffusion equation on the sphere on a $2^\circ \times 2^\circ$ grid. The original finite difference-time explicit implementation of the diffusion equation solver could not treat the polar regions on a rectangular longitude-latitude grid. As a consequence, the observations beyond 80° latitude were not assimilated. This was a major restriction for our assimilation system because it lead to the rejection of good quality data, and it prevented the detailed study of the ozone evolution within the polar latitudes, especially during the formation of the springtime ozone hole in the Southern Hemisphere.
In the new formulation, for each pressure level, the horizontal fields are projected onto the spherical harmonic basis. The diffusion equation is then solved, and projected back to the physical space. With this numerical approach for modeling the horizontal correlations of the background errors, we are now able to assimilate all the available observations.

3.2.2 Vertical correlation of the background error (S. Massart, A. Piacentini)

The vertical correlation of background errors were not taken into account in the original formulation of the assimilation algorithm. As a result, initial tests with assimilation of the Odin/SMR profiles given at fixed altitude levels showed that the analysis increments were different from zero only at the altitudes of the measurements. The correction was then propagated to the other levels by the vertical transport. Since the vertical motions are very slow in most of the altitude range where Odin/SMR data are available, the information brought by the SMR observations in the assimilation system did not cover the whole vertical domain. Therefore we have implemented a vertical correlation approximation in the background errors representation. Thus, the correlations μ_{ij} between two pressure levels i and j are approximated by a Gaussian function of the logarithm of their pressure ratio (p_i/p_j),

$$\mu_{ij} = \exp\left[-b \cdot \log^2\left(\frac{p_i}{p_j}\right)\right] . \quad (3.1)$$

The dimensionless parameter b was determined using the NMC method from a simulation covering July 2003 with the MOCAGE-PALM assimilation system used for the ASSET project (Manzoni, personal communication 2006). It was shown that the constant value $b = 4$ better characterizes the computed vertical correlations.

3.3 Chemistry transport model

3.3.1 Vertical resolution (S. Massart, H. Teyssedre)

The MOCAGE configuration used for the ASSET intercomparison exercise had a vertical grid bounded in altitude to a value of 5hPa. In addition, the model was forced by an ozone climatology in its first top level which extends from 10hPa to 5hPa. As a consequence, most of the information coming from the assimilation increment was lost above 10hPa. This constituted a severe limitation of our system, since a significant fraction of the stratospheric ozone is found above 10hPa. Therefore, in the new assimilation system the upper boundary of the model has been raised from 5hPa to 0.1hPa. The level distribution has been also enhanced from 47 to 60 levels. This configuration allows the direct use, without vertical interpolation, of the dynamical forcing supplied by the operational European Centre for Medium-Range Weather Forecasts (ECMWF) numerical weather prediction model.

3.3.2 Chemistry scheme (D. Cariolle, H. Teyssedre)

The latest version (version 2.8) of the linear ozone parameterization developed by [DA3] was included into the MOCAGE CTM. This scheme is implemented with activation of the ozone destruction due to PSC chemistry, with the simplest formulation that only uses local temperature. Compared to the implementation adopted for the ASSET project, the parameterization has been improved in the mesosphere and in the equatorial troposphere where there was a tendency to overestimate the ozone production by 50% at equatorial latitudes. The use of the linear scheme within the MOCAGE CTM forced by the ECMWF analyses for multiyear simulations, has shown that little biases and drift were present in the model results when compared to TOMS ozone data. This is an important advantage over complex chemical schemes which may not be free from drifts, and that are computationally more expensive.

3.4 Studies using the improved assimilation system

3.4.1 The ASSET intercomparison of ozone analyses (A. J. Geer, S. Massart *et al.*)

The EU-funded “Assimilation of Envisat data” (ASSET) project ([DA6]), aimed the assimilation of Envisat atmospheric constituent and temperature data into systems based on Numerical Weather Prediction (NWP) models and chemical transport models (CTMs). It has addressed several themes : enhancement of NWP analyses by assimilation of research satellite data ; studies of the distribution of stratospheric chemical species by assimilation of research satellite data into CTM systems ; objective assessment of the quality of ozone analyses ; studies of the spatial and temporal evolution of tropospheric pollutants ; enhanced retrievals of Envisat data ; and data archival and dissemination.
The performance of ozone data assimilation systems involved into ASSET were evaluated to show where they can be improved, and to quantify their errors ([DA4]). Thanks to the project, 11 sets of ozone analyses from 7 different DA systems were examined. Two were numerical weather prediction (NWP) systems based on general circulation models (GCMs) ; the other five used chemistry transport models (CTMs). The systems examined contained either linearised or detailed ozone chemistry, or no chemistry at all. In most analyses, MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) ozone data were assimilated. Two configurations of the MOCAGE-PALM assimilation system has participated the the comparison, one with a linearised ozone chemistry and one with a detailed stratospheric detailed chemistry. Analyses were compared to independent ozone observations covering the troposphere, stratosphere and lower mesosphere during the period July to November 2003. The analyses from the MOCAGE-PALM assimilation system were at least as good as the analyses from the other systems in the stratosphere.

3.4.2 Assessment of the quality of the ozone measurements (S. Massart, A. Piacentini, D. Cariolle, *et al.*)

Space-based remote sensing instruments providing atmospheric measurements have different time and space resolutions, and coverage. This makes the direct comparison of the measurements very difficult. Data assimilation has proven to be a far more powerful tool than simple interpolation techniques to create three-dimensional analysed fields for a given dataset. Thus, data assimilation can be used to assess instrument precision and bias. In this way, using the ASSET analyses as a transfer standard ([DA4]), it was estimated

that MIPAS is 5% higher than HALOE (Halogen Occultation Experiment) in the mid and upper stratosphere and mesosphere (above 30 hPa), and of order 10% higher than ozonesonde and HALOE in the lower stratosphere (100 hPa to 30 hPa).
To assess the quality of Odin/SMR ozone retrievals by MOLIERE-5 against ozonesondes, Envisat/MIPAS, Earth Probe/TOMS and UARS/HALOE data, the MOCAGE-PALM assimilation system was used in its lastest version ([DA8]). The Odin/SMR analysis and the other ozone datasets were in good agreement at mid and high latitudes, while in the lower tropical stratosphere a positive bias was found of the Odin/SMR, Envisat/MIPAS and Earth Probe/TOMS data compared to measurements from UARS/HALOE and ozonesondes. The precision of Odin/SMR ozone retrievals in terms of standard deviation is about 20% in the tropics, below 10% at high southern latitudes and below 5% at high northern latitudes.

3.4.3 Studies based on the assimilated fields (S. Massart, A. Piacentini, D. Cariolle, *et al.*)

Stratospheric ozone intrusion over the high Canadian Arctic UTLS region

An exceptional ozone increase in the upper troposphere–lower stratosphere region has been recorded by an ozone sounding performed over the high Canadian Arctic at the beginning of August 2003. Simultaneously observed low humidity and low tropopause height have suggested that this anomalous ozone enhancement is attributed to a downward transport from the stratosphere. This latter transport was investigated by using the Ertel potential vorticity field calculated from the ECMWF analyses ([DA10]). The occurrence of such high ozone concentrations was shown to be due to stratospheric ozone rich air intrusions. These latter mesoscale phenomena wre successfully captured using the assimilation of Envisat/MIPAS ozone profiles into MOCAGE-PALM. It was demonstrated that Envisat/MIPAS ozone profiles assimilation adds value in the sense that the analyses capture the whole stratospheric intrusion episode, whereas the raw model simulation does not.

Ozone loss in the 2002-2003 Arctic vortex

The evolution of the northern polar vortex during the winter 2002–2003 in the lower stratosphere was investigated by using assimilated fields of ozone (O3) and nitrous oxide (N2O) ([7]). Both O3 and N2O measurements used were obtained from the Sub-Millimetre Radiometer (SMR) aboard the Odin satellite and were assimilated into MOCAGE-PALM. O3 was assimilated into the full model including both advection and chemistry whereas N2O was only assimilated with advection since it is characterized by good chemical stability in the lower stratosphere.
The ability of the assimilated N2O field to localize the edge of the polar vortex was prooved. The O3 assimilated field has served to evaluate the ozone evolution and to deduce the ozone depletion inside the vortex. The chemical ozone loss was estimated using the vortex-average technique. The N2O assimilated field was also used to substract out the effect of subsidence in order to extract the actual chemical ozone loss. Comparisons to other results reported by different authors using different techniques and different observations have given satisfactory results.

The 2002 major warming in the southern hemisphere

Following an exceptionally active winter, the 2002 Southern Hemisphere (SH) major warming occurred in late September. It was preceded by three minor warming events that occurred in late August and early September, and yielded vortex split and break-down over Antarctica. Ozone (O3) and nitrous oxide (N2O) profiles obtained during that period of time (15 Aug.-4 Oct.) by the Sub-Millimetre Radiometer (SMR) aboard the Odin satellite were assimilated into MOCAGE-PALM ([DA1]). The assimilated O3 and N2O profiles were compared to groundbased measurements (LiDAR and balloon-sonde). It is found that O3 concentrations retrieved by the MOCAGE-PALM assimilation system shown a reasonably good agreement in the 20-28 km height range when compared with ground-based profiles. Moreover, comparison of N2O assimilated fields indicated that the dramatic split and subsequent break-down of the polar vortex, as well as the associated mixing of mid- and low-latitude stratospheric air, were well resolved and pictured by MOCAGE-PALM.

Transport pathways of CO in the African upper troposphere during the monsoon season

The transport pathways of carbon monoxide (CO) in the African Upper Troposphere (UT) during the West African Monsoon (WAM) was investigated through the assimilation of CO observations by the Aura Microwave Limb Sounder (MLS) into MOCAGE-PALM ([5]). Comparisons between the assimilated CO fields and in situ airborne observations from the MOZAIC program between Europe and both Southern Africa and Southeast Asia has shown an overall good agreement around the lowermost pressure level sampled by MLS ($\sim$215 hPa). The 4D assimilated fields averaged over the month of July 2006 have been used to determine the main dynamical processes responsible for the transport of CO in the African UT. The studied period corresponds to the second AMMA (African Monsoon Multidisciplinary Analyses) aircraft campaign. Using the high time resolution provided by the 4D assimilated fields, we gave evidence that the variability of the African CO distribution above 150 hPa and north of the WAM region is mainly driven by the synoptic dynamical variability of both the Asian Monsoon Anticyclone (AMA) and the Tropical Easterly Jet (TEJ).

3.4.4 Diagnostics of the background error covariance matrix (O. Pannekoucke, S. Massart)

The MOCAGE-PALM ozone background error correlation functions were estimated from an ensemble of perturbed forecasts ([8]). They appears to be heterogeneous and anisotropic. Such correlation functions are representable by a diffusion operator at a reasonable numerical cost. Thus, we have decided to build an heterogeneous and anisotropic diffusion operator on the sphere based on a local diffusion tensor. The first challenge resided in the determination of the local diffusion tensor corresponding to the local correlation function. Then the second challenge resided in the determination of the normalization in order to ensure the matrix modelled through the diffusion operator to be a correlation matrix. A validation within a randomization method illustrates the feasibility and the accuracy of the proposed method. In particular, it is shown that the local geographical variations of diagnosed correlation functions (through an ensemble of perturbed forecast) are well represented.

3.5 References

[5] B. Barret, P. Ricaud, C. Mari, J.-L. Attié, N. Bousserez, B. Josse, E. L. Flochmoen, N. J. Livesey, S. Massart, V.-H. Peuch, A. Piacentini, B. Sauvage, V. Thouret, and J.-P. Cammas, (2008), Transport pathways of CO in the African upper troposphere during the monsoon season : a study based upon the assimilation of spaceborne observations, *Atmos. Chem. Phys. Disc.*, **8**, 2863–2902.

[6] D. Cariolle, M. J. Evans, M. P. Chipperfield, N. Butkovskaya, A. Kukui, and G. Le Bras, (2008), Impact of the new HNO3 forming channel of the HO2 + NO reaction on the tropospheric budgets of HNO3, NOx, HOx and ozone, *Atmos. Chem. Phys. Discuss.*, **8**, 2695–2713.

[7] L. El Amraoui, V.-H. Peuch, P. Ricaud, S. Massart, N. Semane, H. Teyssèdre, D. Cariolle, and F. Karcher, (2008), Ozone loss in the 2002-2003 Arctic vortex deduced from the assimilation of Odin/SMR O3 and N2O measurements : N2O as a dynamical tracer, *Quart. J. Roy. Meteor. Soc.*, **134**, 217–228.

[8] S. Massart and O. Pannekoucke, (2008), Estimation of the local diffusion tensor and normalization for heterogeneous correlation modelling using a diffusion equation, *TR-AE-08-13*, **TR-AE-08-13**.

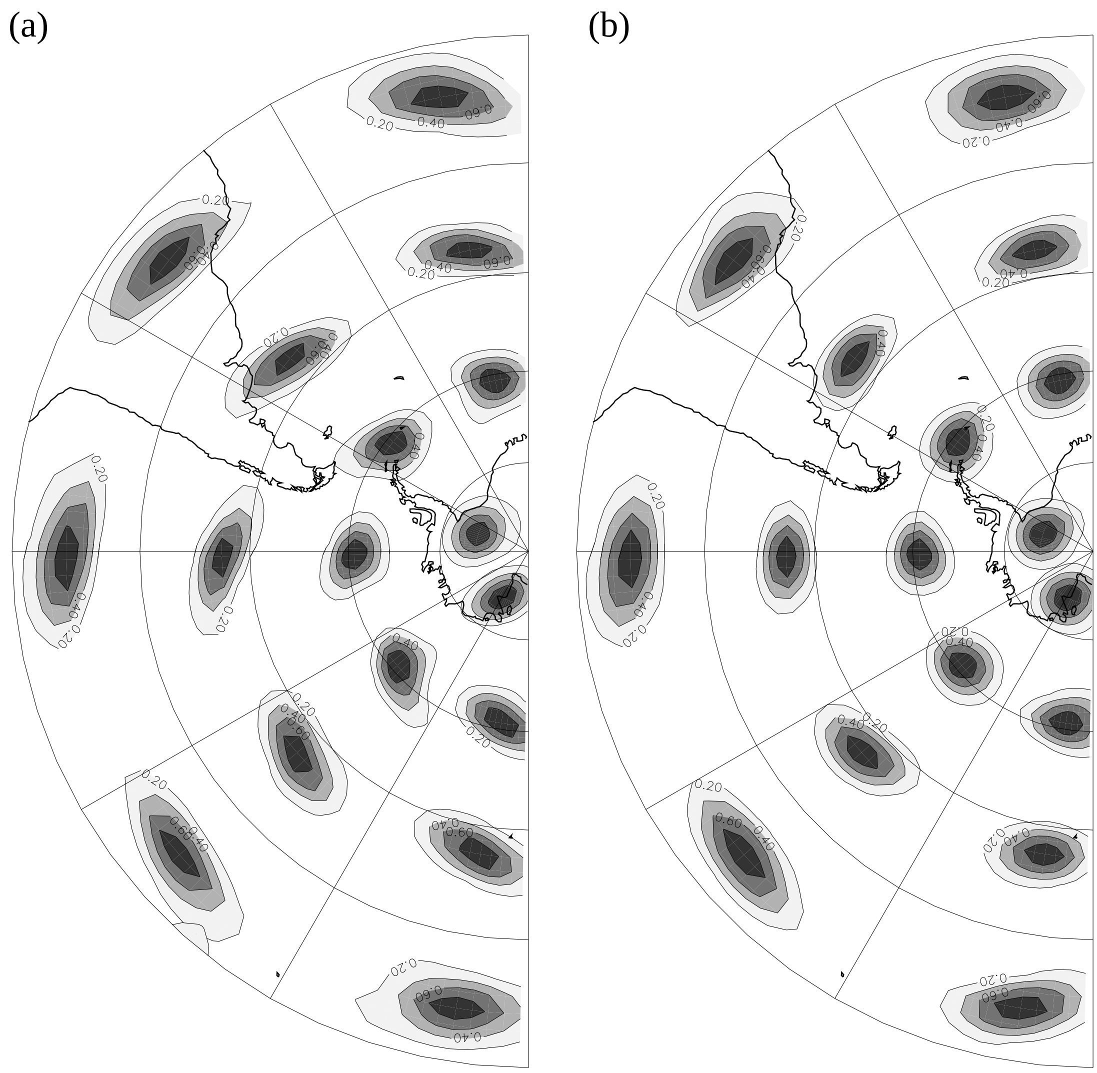


FIG. 3.4 – Examples of correlation functions of the background error viewed from the South Pole : (a) diagnosed from the ensemble of perturbed forecast and (b) from the correlation model diagnosed using a randomization method with 6400 samples. The contour lines correspond to values within the range 0.2 – 1, with an 0.2 increment. Parallel lines are plotted every 15 degrees from $90°S$ to $15°S$.

4 Data assimilation for nuclear plan modelling

Within a fruitful collaboration between EDF R& D and CERFACS, the tools improving nuclear core simulation progressed during the 2005-2008 period. The ADONIS project already proved the feasibility of the Data Assimilation (DA) use in nuclear core application. The prototypes MANARA and KAFEINE, that demonstrated that the DA is applicable in nuclear core physic, was extended and improved during the past years. We will detail further the evolution of each mock up.
On the level of MANARA, some developments were done in order to take into account information coming from the various instruments that are implanted inside the reactor.
For the KAFEINE prototype, several improvements were done to evaluate more precisely the evolution of model parameters along a core loading. A new common scientific project EDF/CERFACS has started for 3 years with the aim of DA applications to new EDF computing codes to evaluate the state of the core. Some details about the state of the project will be given as conclusion.

4.1 MANARA : a Modular Application for Neutronic Activity Reconstruction by Assimilation (B. Bouriquet, S. Massart, G. Gacon, P. Erhard, J. P. Argaud)

MANARA has been implemented to address the same problem as the EDF code CAMARET - that is to provide a fine estimate of the 3D power map (or neutron flux cartography) given some located measures and the simulation computed by a model. The CAMARET methodology is mainly focused on the exploitation of the data coming from CFM (Mobile Fission Chamber). This basic conception of CAMARET is not usable with heterogeneous instrumentation, as the information coming from several sources cannot be handled in the same framework. Here is the strong point of the DA that permits us to take into account all kind of information as soon as the error on this information is known [DA7].

Thus, developments have been taken to extend the basic MANARA prototype to a multi instrumented assimilation code. This new MANARA prototype is able to treat information coming from CFM, Low resolution CFM (LCFM), thermocouple and external chamber. Figure 4.1 presents the evolution of the accuracy of the reconstructed 3D neutron flux map as a function of the used instrument.
The curves on figure 4.1 show the root mean square diference to reference instruments for the various plans on the nuclear core (right to left from bottom to top). Within that figure the OMB (Observation Minus Background) curve represents the raw information coming from the COCCINELLE calculation. The OMA (Observation Minus Analysis) evolves as we add some instruments. It is easy to notice that the more instruments we have the best the agreement with reference value is. Moreover this behavior is compatible with the amount and accuracy of each instrument. We even notice that with information coming from integral measurements, such as thermocouple, some improvements appear.
The work done on the multi instrumentation enlightens even more the influence of the measurement on the data assimilation within the nuclear core. Thus, it has been decided to look after the influence of the

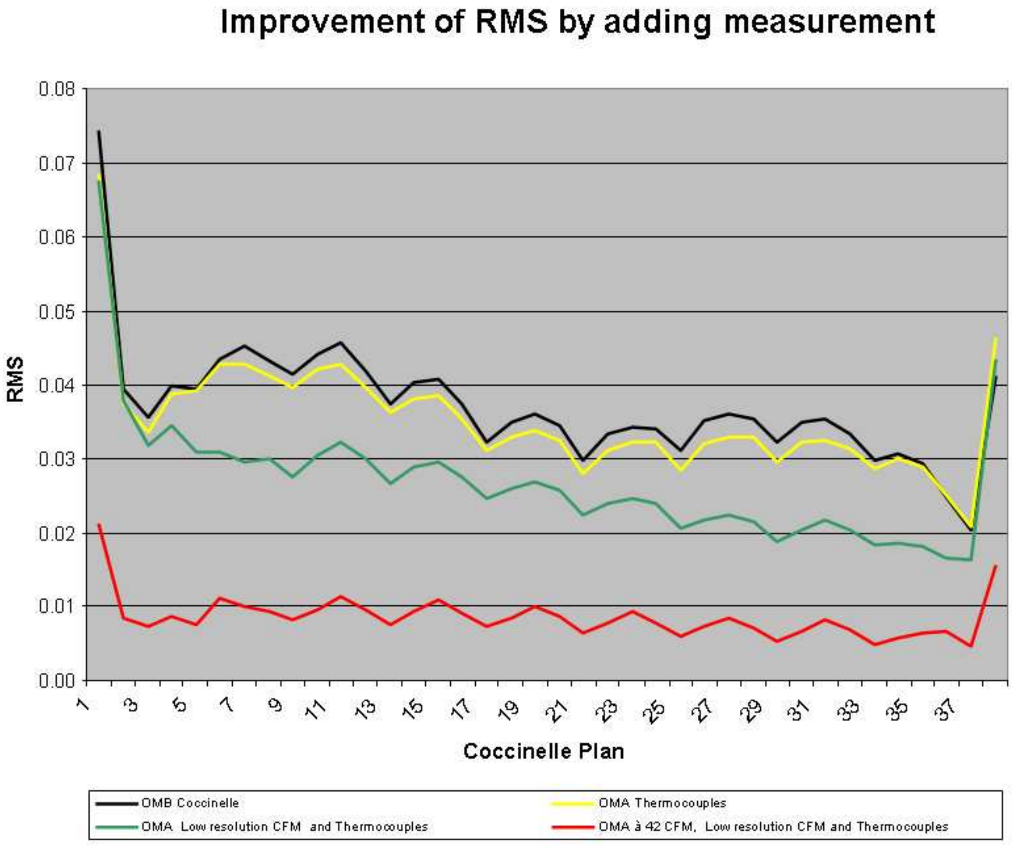


FIG. 4.1 – Evolution of the neutronic map flux with the instrumentations used

reducing of the number of available instruments on the quality of the 3D neutronic map. In order to evaluate this evolution, we will put ourselves in a configuration of 42 CFM available giving measurements on the 38 levels of the core. Thus, the 16 remaining locations are references to validate the reconstructed map of neutron flux.
There are C_{42}^p different way to remove p instruments from the 42 we have. This number of possibility can be very quickly huge. Nevertheless, we can take a sampling over all those possibilities to evaluate the mean accuracy when we loose p measurement locations. Thus, we take for each case 800 samples that is close to C_{42}^2. However, this is still a huge number of calculation that requires time consuming computation.
the computation was done on the IBM JS21 available at CERFACS. The next figure presents the results of the mean value of the disagreement with reference data as a function of the remaining instrumented locations. Those values are normalized by the estimation with all available measurements.

The curves on figure 4.1 presents two distinct behaviors as we reduce the number of instruments. The first part shows a low evolution of the reconstruction quality when only few instruments are missing. The second one shows a dramatic decrease of the quality of the evaluation of the core status when few instruments remain. This transition between the two behaviors is when around 6 to 10 CFM remains. This represents the critical level in the information necessary to reconstruct the core activity.

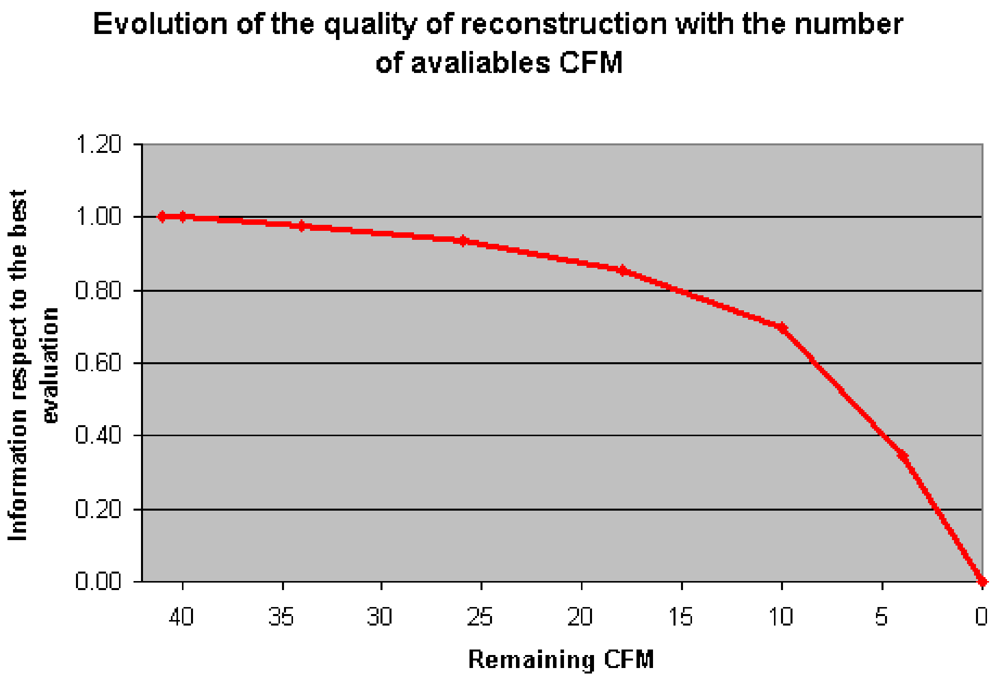


FIG. 4.2 – Evolution of the relative quality of the reconstruction of the nuclear core as a function of the remaining measurement instruments

The use of data assimilation has already been proved efficient to reconstruct the neutronic state of a nuclear core. In addition, we showed that, in the DA framework, information coming from heterogeneous sources can be collected to improve the quality of the evaluation of the neutronic state.
Refering to che work on multi-instumentation we noticed too that adding lower accuracy and a distribution in space that is not covering all the area give only a very thin improvement to a very well instrumented system.
Nevertheless looking more in detail the influence of the number of available instrument in the core, we notice a two-step evolution of the quality of the evaluation of the nuclear core is presistant event with addition of thermocouples. If the density of measurement is good enough the evaluation of the core is not very dependant of the number of instruments. Then above a critical value of available instruments, the addition of suppression of one more become critical on the quality of the evolution. Such behavior is the signal of a critical point in the information perquisite to evaluate the state of the nuclear core

4.2 KAFEINE KAlman Filter Estimation In NEutronic (S. Massart, B. Bouriquet, G. Gacon, P. Erhard, J. P. Argaud)

The KAFEINE prototype was developed in order to optimize the parameters of the COCCINELLE nuclear core model[DA7] . At first, this optimization was focused on the reflector modeling parameter. This is still a very important topic that was the object of several studies reported below. Nevertheless, modularity of PALM allows making some development in order to make the KAFEINE code was develloped to be able to perform DA on various parameters. Moreover some extra development was done on the prototype in order to have an external loop that are searching to an optimal convergence using the post validation methods developed by Derozier and Ivanov[10, 9] . The scheme of the new KAFEINE PALM prototype is shown in figure 4.2. This scheme exploits the parallel calculation capacity of PALM to optimize the calculation time.

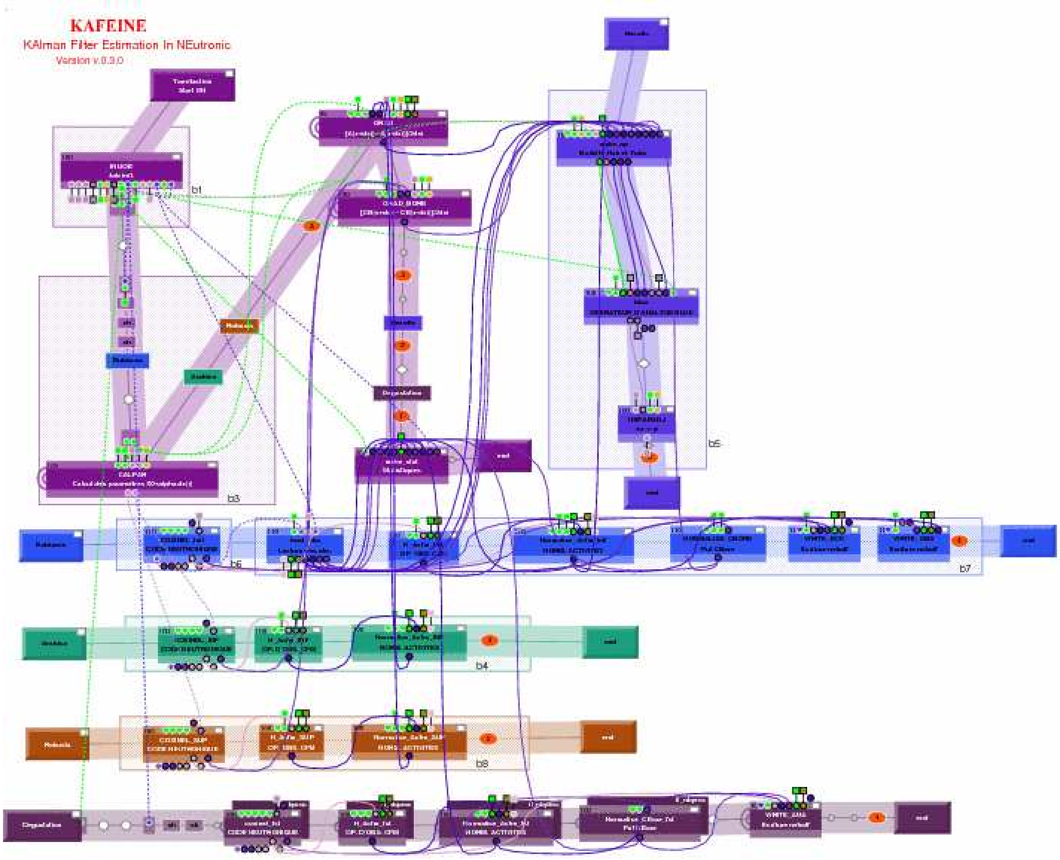


FIG. 4.3 – PALM scheme of the KAFEINE prototype

As mentioned above work focuses mainly on the reflector parameter. A careful study of this parameter showed that it may evolve along a nuclear core life. Thus, it was assumed an analytic profile for its evolution with time. The parameters have been computed by the KAFEINE prototype within a wide range of nuclear core experimental history. The results show that evolution depends of the loading pattern and the history of the assembly. Nevertheless, some interesting information on the nuclear core modeling was enlightened by this study. Moreover some new DA schemes were performed, enriching knowledge on opportunities and limits of Kalman filter technique.

The interesting results and the feasibility proof that was done by this mock up are pushing it towards industrial applications for EDF nuclear core.

4.3 conclusion

Globally speaking all the work done on the application of DA in nuclear core leads to interesting results and a proof of global usefulness in nuclear core physics. Thus, all those encouraging results conduced to a new project which aim is to apply DA within a more operational framework, especially in the new nuclear core modeling codes. Moreover, some generics tool of DA will be build in order to promote these methods in other fields of interest at EDF.

4.4 References

[9] G. Desroziers, L. Berre, B. Chapnik, and P. Poli, (2005), *Quaterly Journal of the Royal Meteorologival Society*, **131 (613)**, 3385–3396.

[10] S. I. G. Desroziers, (2001), *Quaterly Journal of the Royal Meteorologival Society*, **127 (574)**, 1433–1452.

5 Publications

5.1 Journal Publications

[DA1] H. Bencherif, L. El Amraoui, N. Semane, S. Massart, D. V. Charyulu, A. Hauchecorne, and V.-H. Peuch, (2007), Examination of the 2002 major warming in the southern hemisphere using ground-based and Odin/SMR assimilated data : stratospheric ozone distributions and tropic/mid-latitude exchange, *Can. J. Phys.*, **85**, 1287–1300.

[DA2] D. Cariolle and J.-J. Morcrette., (2006), A linearized approach to the radiative budget of the stratosphere : influence of the ozone distribution., *Geophys. Res. Lett.*, **33, L05806**, 10.29/2005GRL025597.

[DA3] D. Cariolle and H. Teyssèdre, (2007), A revised linear ozone photochemistry parameterization for use in transport and general circulation models : Multi-annual simulations, *Atmos. Chem. Phys.*, **7**, 2183–2196.

[DA4] A. Geer, W. Lahoz, S. Bekki, N. Bormann, Q. Errera, H. Eskes, D. Fonteyn, D. Jackson, M. Juckes, S. Massart, V.-H. Peuch, S. Rharmili, and A. Segers, (2006), The ASSET intercomparison of ozone analyses : method and first results, *Atmos. Chem. Phys. Disc.*, **6**, 5445–5474.

[DA5] A. J. Geer, W. A. Lahoz, D. R. Jackson, D. Cariolle, and J. P. McCormack, (2007), Evaluation of linear ozone photochemistry parameterizations in a stratosphere-troposphere data assimilation system, *Atmos. Chem. Phys.*, **7**, 939–959.

[DA6] W. A. Lahoz, A. J. Geer, S. Bekki, N. Bormann, S. Ceccherini, H. Elbern, Q. Errera, H. J. Eskes, D. Fonteyn, D. R. Jackson, B. Khattatov, S. Massart, V.-H. Peuch, S. Rharmili, M. Ridolfi, A. Segers, O. Talagrand, H. E. Thornton, A. F. Vik, and T. von Clarmann, (2007), The Assimilation of Envisat data (ASSET) project, *Atmos. Chem. Phys. Disc.*, **7**, 1773–1796.

[DA7] S. Massart, S. Buis, P. Erhard, and G. Gacon, (2007), Use of 3D-VAR and Kalman Filter Approaches for Neutronic State and Parameter Estimation in Nuclear Reactors, *NSE*, **105(3)**, 409–424.

[DA8] S. Massart, A. Piacentini, D. Cariolle, L. El Amraoui, and N. Semane, (2007), Assessment of the quality of the ozone measurements from the Odin/SMR instrument using model assimilation, *Can. J. Phys.*, **85**, 1209–1223.

[DA9] A. M. Moore, J. Zavala-Garay, Y. Tang, R. Kleeman, A. T. Weaver, J. Vialard, K. Sahami, D. L. T. Anderson, and M. Fisher, (2006), On the low-dimensionality of ENSO as evidenced by the optimal forcing patterns of coupled models, *J. Climate*, **19**, 4683–4699.

[DA10] N. Semane, V.-H. Peuch, L. E. Amraoui, H. Bencherif, S. Massart, D. Cariolle, J.-L. Attié, and A. R., (2007), A linearized approach to the radiative budget of the stratosphere : influence of the ozone distribution., *Quart. J. Roy. Meteor. Soc.*, **113 S2**, 171–178.

[DA11] T07, (2007), Teyssèdre, H. and Michou, M. and Clark, H.L. and Josse, B. and Karcher, F. and Olivié, D. and Peuch, V.-H. and Saint-Martin, D. and Cariolle, D. and Attié, J.-L. and Nédélec, P. and Ricaud, P. and Thouret, V. and van der A, R. J. and Volz-Thomas, A. and Chéroux, F., *A new tropospheric and stratospheric Chemistry and Transport Model MOCAGE-Climat for multi-year studies : evaluation of present-day climatology and sensitivity to surface processes*, **7**, 5815–5860.

[DA12] A. T. Weaver, C. Deltel, E. Machu, S. Ricci, and N. Daget, (2006), A multivariate balance operator for variational ocean data assimilation, *Quart. J. Roy. Meteor. Soc.*, **131**, 3605–3626.

5.2 Conference Proceedings and Book Chapters

[DA13] D. Cariolle and S. Massart, (2007), Ozone distributions derived from satellite data assimilation and their impact on the stratospheric temperatures., Technical Report TR/AE/07/45, ESA Proceedings of the second ”Atmospheric Science Conference”, Montreux, Suisse 23-27 April 2007.

[DA14] D. Cariolle, S. Massart, and H. Teyssèdre, (2007), Polar and midlatitude ozone, Technical Report TR/AE/07/27, Proceedings of the ECMWF workshop on Polar Meteorology, September 2006.

5.3 Technical Reports

[DA15] J.-L. Atié, D. Cariolle, S. Massart, and A. Piacentini, (2007), Dual assimilation of MOPITT and MLS carbon monoxide in the MOCAGE model. A contribution to ACCENT-TROPOSAT-2, Technical Report TR/AE/07/66.

[DA16] G. G. Bouriquet B. and M. S., (2006), Assimilation multi-instrumentée dans la maquette MANARA, Technical Report TR/CMGC/06/71, CERFACS. Cerfacs Restricted.

[DA17] D. Cariolle and H. Teyssèdre, (2007), A revised linear ozone photochemistry parameterization for use in transport and general circulation models : Multi-annual simulations, Technical Report TR/AE/07/26.

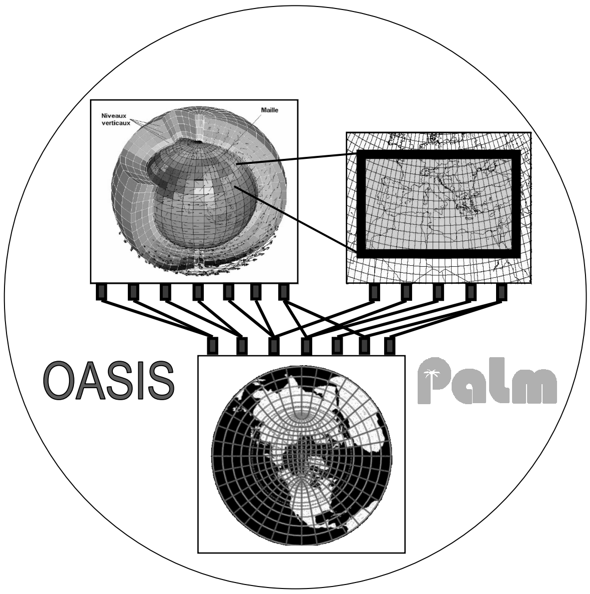
[DA18] D. Cariolle, T. H., and J.-J. Morcrette, (2006), Une approche linéarisée de la chimie de l'ozone et du transfert radiatif dans la stratosphère, Technical Report TR/AE/06/113, Atelier modélisation de l'atmosphère.

[DA19] M. Davey, M. Huddleston, B. Ingleby, K. Haines, P.-Y. Le Traon, A. T. Weaver, J. Vialard, D. Anderson, A. Troccoli, A. Vidard, G. Burgers, O. Leeuwenburgh, A. Bellucci, S. Masina, L. a. Bertino, and P. Korn, (2006), Multi-model multi-method multi-decadal ocean analyses from the ENACT project, CLIVAR Exchanges 38 11, No. 3.

[DA20] N. Ferry, Guérémy, J.-F. Troccoli, A. T. Weaver, and S. Gualdi, (2007), Within the GMES and towards the Marine Core Service at MERCATOR-OCEAN, Mercator-Ocean Quarterly Newsletter 24, January.

3

Code Coupling



1 Introduction

OASIS and PALM are two couplers, developped at CERFACS, that have climbed significant steps during the last two years.

The OASIS coupler, initiated at CERFACS in 1991 is now used by about 25 climate modelling groups around the world. This open source software is specialized in the coupling of climate modules such as ocean, atmosphere, sea-ice or land models. The development of this coupler is currently driven by the need of higher resolutions for climate models which are possible thanks to massively parallel platforms. These new architectures have imposed parallelism and efficiency while keeping OASIS basic concepts of portability and flexibility.

The PALM coupler, initiated at CERFACS in 1996 for the MERCATOR operational oceanography project, now counts about 80 users of various applications fields such as combustion, aerodynamics, nuclear plant modelling, atmospheric chemistry or land surface modelling. If several of these users appreciate this coupler for the design of their data assimilation applications, a growing number of those are seduced by the wide scope of its functionalities combined with its portability, flexibility and ergonomy features. Indeed, this coupler answers most of the requirements of simple to complex coupling algorithms : high level description of algorithms, parallel coupling, handling of computing resources, dynamic launching of components, graphical user interface, ...

During the last two years, the question of the coexistence of the PALM and OASIS couplers at CERFACS and in the scientific community has been adressed. Both couplers answer specific needs of distinct communities : static coupling with paralllel geophysicial interpolation for OASIS and dynamic coupling with complex algorithms for PALM. Thanks to its expertise, CERFACS can help users to choose to best coupler suited for their applications and, if needed, ensure the compatibility of both within a specific application. Based on its experience in development, user needs and requirements, CERFACS is one of the best place where the next generation of coupler can be matured.

2 The OASIS coupler and its applications

The OASIS coupler is open source software developed at CERFACS since 1991, used for coupling independent General Circulation Models (GCMs) of the atmosphere and the ocean as well as other climate modules (sea-ice, land, etc).

Today, OASIS is mainly supported and developed in the PRISM framework [CC3] in collaboration with the Centre National de la Recherche Scientifique (CNRS) from France and the IT division of NEC Laboratories Europe (NLE-IT) from Sankt-Augustin in Germany.

The PRISM concept (http ://prism.enes.org/), initially proposed as a Euroclivar recommendation and first funded by the European Community in 2001-2004, is to share the development, maintenance and support of software and metadata environment for Earth System Modelling. The objective is to lower the technical development efforts for the scientific teams assembling, running, monitoring, and post-processing Earth System Models (ESM) based on state-of-the-art component models developed in the different climate research centres in Europe and elsewhere.

Today, the PRISM Support Initiative (PSI) [CC2] has established a network of seven partners (CERFACS, NCAS, CNRS, ECMWF, NEC-CCRL, M&D, and the UK Met Office) and nine associate partners (CSC-Finland, IPSL, MPI-M, Météo-France, SMHI and computer manufacturers CRAY, NEC-HPCE, SGI and SUN) investing a total of about 8 persons-years per year (py/y) in the initiative.

Through OASIS support and development, CERFACS actively contributes to the PRISM Support Initiative into which CERFACS has committed 0.9 person-year/year for the 2005-2007 period, commitment that will most likely be renewed.

PRISM recently set-up the METAFOR project, gathering 11 partners and funded for 3 years starting in March 2008 under the European Community 7th Framework Plan for 2.2 MEuros.The main objective of METAFOR is to define a Common Information Model (CIM) that describes in a standard way climate data and the coupled models that produced the data. In close interaction with related initiatives at the international level, METAFOR will propose solutions to identify, access and use the climate data. METAFOR will build on existing metadata (data describing data) currently used in existing data repositories. The coupling metadata proposed in the new OASIS4 environment describing the coupling exchanges ensured by the coupler between the component models represent a first attempt to describe a coupled composition, and these coupling metadata need to be generalized and extended ; this task will be addressed in METAFOR.

Currently, the 3 versions of OASIS currently available, OASIS2, OASIS3 and OASIS4 are used by about 25 climate modelling groups around the world.

OASIS2 and OASIS3 are direct products of the coupler developments performed since more than 15 years at CERFACS. Portability and flexibility were their key design concepts. At run-time, OASIS2 or OASIS3 acts as a separate mono process executable, which main function is to interpolate the coupling fields exchanged between the component models, and as a communication library linked to the component models. For

OASIS3, a major evolution of the communication library lead to the release of the OASIS3 PRISM Model Interface Library (OASIS3 PSMILe). OASIS2/3 supports 2D coupling fields only.

As the climate modelling community is progressively targeting higher resolution climate simulations run on massively parallel platforms with coupling exchanges involving a higher number of (possibly 3D) coupling fields at a higher coupling frequency, a new fully parallel coupler, OASIS4, is currently developed within PRISM. The concepts of parallelism and efficiency drove OASIS4 developments, at the same time keeping in its design the concepts of portability and flexibility that made the success of OASIS3. OASIS4 supports 3D and 2D coupling fields.

The OASIS4 PSMILe Application Programming Interface (API) was kept as close as possible to OASIS3 PSMILe API. This ensures a smooth and progressive transition between OASIS3 and OASIS4 use in the climate modelling community, as is shown by the OASIS4 constantly growing community of users.

During the reporting period, some efforts were also devoted to demonstrating the OASIS and PALM compatibility ([CC10], [1], [CC14]) .

2.1 The OASIS2/3 coupler(S. Valcke)

2.1.1 Development and maintenance

The OASIS2 version is frozen since its last release in 2000. This version was however still used by some modelling groups during the past 2 years (see below). This inertia illustrates the length of the cycle needed to build and validate a coupled climate model.

The last version of the OASIS3 coupler ("prism_2-5") was released in september 2006 [CC16]. As most of the development efforts were devoted to OASIS4 during the preceeding period, that version did not contain any major modifications but only the following improvements :
- Few bugfixes already distributed to the OASIS mailing list during the preceeding period ;
- Some modifications regarding the options of the SCRIP interpolations ;
- A new PSMILe interface routine to retrieve the coupling period of field ;
- The phasing of the versions of the mpp_io library used in OASIS3 and OASIS4
- Diverse modifications for successful compilation with NAGW compiler ;
- Other minor modifications (automatic validation of options, etc.)

2.1.2 OASIS2/3 Users and applications

Today, OASIS2 or OASIS3 are used by about 20 climate modelling groups around the world. Among the main users, one can cite :
- CERFACS, Météo-France and IPSL, in France
- the European Centre for Medium range Weather Forecasts (ECMWF) at Reading
- the Max-Planck Institute for Meteorology (MPI-M) in Germany
- the National Centre for Atmospheric Science (NCAS) and the Met Office in the UK
- the "Koninklijk Nederlands Meteorologisch Instituut" (KNMI) in the Netherlands
- the Swedish Meteorological and Hydrological Institute (SMHI) from Sweden
- the "Istituto Nazionale di Geofisica e Vulcanologia" (INGV) and the"Ente Nazionale per le Nuove tecnologie, l'Energia el Ambiente" (ENEA) in Italy
- the International Research Institute for Climate Prediction, the NASA Jet Propulsion Laboratory, and the Oregon State University in the US

– the Canadian Meteorological Services in Canada
– the Japan Marine Science and Technology Center in Japan on the Earth Simulator super computer
– the International Center for Climate and Environment Sciences in China
– the Bureau of Meteorology Research Center (BMRC) and the University of Tasmania in Australia

In particular, we closely followed the assembling of the following coupled models :

– In the last years, the OASIS2 version was used by the Centre National de Recherches Météorologiques (CNRM) of Météo-France to assemble a Coupled GCMs (CGCM), based on the atmospheric model ARPEGE (from CNRM, Météo-France) and on the ocean model OPA (from Laboratoire d'Océanographie et du Climat, LOCÉAN, CNRS). This coupled models was validated and exploited through a series of climate experiments in the framework of various European projects (e.g. DEMETER, PREDICATE) and for the IPCC (Intergovernmental Pannel on Climate Change) Fourth Assessment Report (2007).
– OASIS2 was also used at CNRM to assemble a regional CGCM coupling ARPEGE medias and the Mediterranean configuration of OPA8, and is currently used to couple ARPEGE V4 and OPA8 for seasonal forecasting experiments on the IBM Power4 at the European Centre for Medium range Weather Forecasts (ECMWF).
– The Institut Pierre Simon Laplace (IPSL) also contributed to the last IPCC report in 2007 with global warming experiments using a coupled model based on the atmosphere model from the "Laboratoire de Météorologie Dynamique" (LMD), LMDZ, and on OPA8 coupled by OASIS2.
– OASIS3 is currently used at CERFACS in the framework of the European project ENSEMBLES and in the ANR project ESCARSEL, to couple ARPEGE V4, OPA9/NEMO and TRIP, a runoff model from University of Tokyo.
– OASIS3 is also used in the framework of the CICLE (Calcul Intensif pour le CLimat et l'Environnement) project, funded by the French "Agence Nationale de la Recherche" (ANR-05-GIGC-04) :
  – at IPSL, for their new global coupled model assembling the atmosphere and surface model LMDZ-ORCHIDEE with the ocean and sea-ice model OPA9/NEMO-LIM,
  – at Météo-France for its 4-model coupling between a regional atmosphere model, ALADIN-Climat, a regional meditteranean configuration of the OPA ocean model, the global atmosphere model ARPEGE-Climat V4, and the global ocean model OPA9.

2.2 The OASIS4 coupler(S. Valcke, L. Coquart)

The development of the OASIS4 coupler [CC15], started in 2002 during the EU project PRISM, implied to the complete rewritting of OASIS. This new fully parallel coupler now includes a Transformer, which performs the parallel interpolation of the coupling fields, and the OASIS4 PRISM System Model Interface Library (OASIS4 PSMILe), which insures fully parallel MPI-based exchanges of coupling data including automatic repartitioning and interpolation through the Transformer.

2.2.1 OASIS4 development

In 2006-2207, about 3 persons worked full time on the development and user support of OASIS4. In particular, the following tasks were realized in collaboration with CNRS and NEC Laboratories Europe, NLE-IT :

– Active user support to the 7 beta testers groups that started using it (see below)
– Implementation and validation of the 2D conservative remapping
– Implementation of the global parallel neighborhood search for the nearest-neighbour, bilinear, and bicubic interpolations
– Support of Gaussian Reduced grids (currently for mono-process applications only)
– Improvement and extensive validation of the interpolations needed for the CICLE project

– Migration from the CVS server to a Subversion server for source versionning, and use of TRAC, a issue tracking system for software development projects
– OASIS4 User Guide update for the release of the OASIS4_0_2 beta version in March 2006.

2.2.2 OASIS4 Users and applications

The OASIS4_0_2 beta version is currently used by the following groups for the following applications :
– the Global and regional Earth-system Monitoring using Satellite and in-situ data (GEMS) community (ECMWF, Meteo-France, and KNMI) for 3D coupling between atmospheric dynamic and atmospheric chemistry models ;
– the Swedish Meteorological and Hydrological Institute (SMHI)in Sweden for 2D coupling of regional ocean and regional atmosphere models ;
– the Nansen Environmental and Remote Sensing Center (NERSC) in Norway for a global Ocean-Ice-Atmosphere coupling between NCAR Community Atmosphere Model (CAM), the NERSC version of the Miami Isopycnic Coordinate Ocean Model (MICOM), and LANL's Community Ice CodE (CICE) ;
– the Institute for Marine Science at the Research Center for Marine Geosciences (IFM-GEOMAR) using OASIS4 with pseudo models to interpolate high resolution data onto high resolution model grids.
– The GENIE project for global ocean-sea ice-atmospher 2D coupling (GOLSTEIN ocean and IGCM atmosphere) at U. of Reading.

The migration from OASIS3 to OASIS4 is also under evaluation by the UK Met Office for its ocean-atmosphere coupled system and in the framework of the CICLE project for the IPSL coupled system and for the 4-model coupled system at Météo-France (see above).

2.3 PALM-OASIS compatibility (J.-M. Epitalon, S. Valcke, T. Morel)

The question of the compatibility between the two couplers developed at CERFACS, PALM and OASIS, naturally arose at some point during the last two years. Currently, those two couplers answer distinct needs of distinct communities, i.e. dynamic coupling vs static coupling with parallel geophysical interpolation. One can however foresee cases where the joint use of the two couplers will be considered, in particular for the merging of existing applications (e.g. the coupling of an oceanic data assimilation system using PALM with an atmosphere model already interfaced with the OASIS PSMILe library).

Even if it will always be recommended to use only one coupler, i.e the one best suited for the specific application, the compatibility between the PALM and OASIS couplers was investigated.

As a first step, and with minor modifications in PALM and OASIS, it was tested that the coupling by OASIS3 of two applications, one of those using PALM-Research, is indeed possible [CC10]. More theoretically, a technical and light solution was then proposed to ensure that PALM-MP could manage a dynamic coupled application into which one component would in fact be a coupled model using OASIS3 or OASIS4 [1].

With those practical and theoretical studies, we are now well prepared to address joint PALM and OASIS user needs that could appear in the future.

[1] J.-M. Epitalon, (2008), Intégration d'OASIS-3 avec PALM-MP - Analyse du problème et proposition de solution, Technical Report WN/CMGC/08/4, CERFACS. Available on Global Change web.

3 The PALM coupler and its applications

PALM is a software tool allowing the concurrent execution and the intercommunication of programs, even if they have not having been especially designed for that. In addition to the data exchange issues, the PALM coupler can take care of a number of services, such as intermediate computations on the exchanged data, grid to grid interpolations, parallel data redistribution. The couplings, therefore, span from simple sequential code assembling (chaining) to applications involving several models. Sometimes the codes must run in parallel, especially if the coupling takes place in the inner iterative processes of the computational entities.

PALM is a dynamic coupler : a coupled component can be launched and can release resources upon termination at any moment during the simulation. The originality of this coupler resides in the faculty of describing complex coupling algorithms. Programs, either parallel or not, can be executed in loops or under logical conditions. Computing resources such as the required memory and the number of concurrent processors, are handled by the coupler. A component of the coupled system starts only when it is active in the algorithm. For the rest of the time it can release memory and processors.

PALM applications are implemented via a graphical user interface (GUI) called PrePALM. In this interface, the programmer initially defines the coupling algorithm : number of components, sequential and parallel sections, loops and conditional executions, resources management.

3.1 Support and training (T. Morel, A. Piacentini, B. Bouriquet, S. Massart, S. Ricci)

Eight training sessions (three days each) have been held in the last two years, for a total of about one hundred trained new users. The training sessions are attended by researchers and engineers working in different domains, ranging from data assimilation to fluid dynamics model coupling.

Three specific training sessions have been organised on demand. The first one for the SEVE project (INRA CESBIO), the second one for ONERA in Châtillon and the last one for the NitroEurope European Project.

The user support, that consists mainly in helping the developers while setting up or porting their applications on different plate-forms including supercomputers, has been granted for CERFACS internal projects and for CERFACS' shareholders applications.

The training offer now includes a three days session on data assimilation with the PALM coupler. Two of such training sessions have already been held.

In order to increase the visibility of the PALM coupler and to help the users exchanging experiences and feedbacks, the PALM web site (www.cerfacs.fr/∼palm) has been entirely redesigned. In a restrained access section, the registered PALM users can find the description of the current PALM applications and some examples and hints for advanced PALM usage.

In addition to this standard PALM formation, a complementary one devoted to data assimilation with PALM has been developed. The goal of this formation is to give students the keys to realize an assimilation scheme within the PALM framework.

3.2 Development and maintenance (T. Morel, A. Thevenin, J. Latour)

In the last two years, the PALM team has worked on the optimisation of the coupler. The last stable release is version 2.5.1. This version can work in single processor mode (no need of MPI message passing) for the implementation of modular sequential applications not needing a strong coupling. The modular implementation is still enhanced by the use of the PALM application interfaces and of the Graphic User Interface PrePALM.

Another important new feature is the interface with NetCDF files : it allows NetCDF I/O without any changes in the user defined codes.

The 2Gb limit on the PALM work memory has been overcome to answer the requirements of the high resolution configurations used in the MERCATOR project.

According to the indications of the Scientific Council, a mid term strategic plan on the PALM development has been dressed in 2007. To fulfil the user needs, the development team has been provided with a second research engineer permanent position.

The PALM team is now working on a version oriented to the computers where the dynamic process spawning is not allowed. This version is due by the end of 2008 and will be used for code coupling on massively parallel plate-forms for which the full MPI2 standards has not been implemented yet (e.g. IBM Blue Gene).

3.3 Distribution policy

Since many years, CERFACS develops and maintains the PALM coupler and provides users support. The distribution policy changes for an operational or industrial usage, on one side, and the PALM use in a research centre, on the other side. The distribution policy is to a certain extent determined by considerations concerning CERFACS shareholding.

1. CERFACS shareholders have free access to the coupler sources, to the training sessions and to the users' support. Notice that the support does not cover the implementation of specific couplings, but it is bounded to questions on the coupler use.
2. Research centres in France and abroad can obtain the coupler after signing an agreement with CERFACS with the engagement of a mere "research" usage, excluding any commercial usage. The convention entitles the research centre to obtain a copy of the coupler sources. The installation is left to the users and support is not automatically provided. Help on these points depends on the direct implication of CERFACS in the research activity (joint participation in European or national projects, joint developments, publications, ...)
3. PALM is available for industrial use also for non CERFACS shareholders. In such a case, a contract has to be signed with CERFACS for the rights of use and for any specific development.

   In all the cases, the user accepts to fill and regularly updates a project description form. The project description will be accessible on line in a restrained access section of the PALM web site (unless confidentiality is explicitly required by industrial users, cf. case 3). This form is aimed to make information about PALM and knowledge sharing easier.

3.4 PALM Users and applications (T. Morel, A. Piacentini)

The PALM users community has largely increased in the last two years : it counts now approximately 80 users working in about thirty laboratories. The majority of the users are in France, but the number of European users is rapidly increasing.

The distribution policy, giving priority to CERFACS partners, determines the type of applications developed at CERFACS or in collaboration with the partners. Among these projects, described in more detail elsewhere in this report, let us mention :

- The ADOMOCA project for data assimilation in atmospheric chemistry
- Several coupling projects in computational fluids dynamics, like the MIPTO tool for the shape optimisation of combustion chamber, developed within the framework of the FP6 INTELLECT project
- The EDF/CERFACS ADONIS/ARTEMIS project for data assimilation in nuclear plant modelling.

Many other research projects have been able to adopt the PALM coupler, thanks to the PALM basic three days courses and the specialized Data Assimilation with PALM training sessions. For instance :

- The landscape scale land surface modelling project SEVE, which involves different laboratories from INRA, the CESBIO and Météo-France.
- The FLUBIO project, leaded by Antoine Dauptain
- The European project NitroEurope, that deals with the flows and transformations of nitrogen and the soil atmosphere interactions at a landscape scale.

[2] M. S. Bouriquet B., (2008), Assimilation de données avec le logiciel PALM : Manuel de formation, Working Note WN/CMGC/08/16, CERFACS.

4 Publications

4.1 Journal Publications

[CC1] S. Buis, A. Piacentini, and D. Déclat, (2006), A Computational framework for assembling high performance computing applications, *Concurrency Computat. : Pract. Exper.*, **18**, 247–262.

[CC2] S. Valcke, R. Budich, M. Carter, E. Guilyardi, M.-A. Foujols, M. Lautenschlager, R. Redler, S.-C. L., and N. Wedi, (2007), A European Network for Earth System Modelling, *EOS*, **88**, 143.

[CC3] S. Valcke, E. Guilyardi, and C. Larsson, (2006), PRISM and ENES : A European approach to Earth system modelling, *Concurrency Computat. : Pract. Exper.*, **18**, 231–245.

4.2 Conference Proceedings and Book Chapters

[CC4] J. Gattas, R. Reder, H. Ritzdorf, S. Valcke, and R. Vogelsang, (2006), OASIS : A code coupler for climate modelling, European Geosciences Union General Assembly 2006, Vienna, Austria.

[CC5] S. Valcke, L. Coquart, R. Redler, H. Ritzdorf, O. Marti, A. Caubel, J. Ghattas, S. Planton, S. Somot, and M. Lucas, (2006), OASIS4 : a code coupler for the climate modelling CICLE project, European Geosciences Union General Assembly 2007, Vienna, Austria.

[CC6] S. Valcke, T. Morel, and S. Buis, (2006), PALM : An efficient tool for dynamic coupled applications, European Geosciences Union General Assembly 2006, Vienna, Austria.

[CC7] S. Valcke, R. Redler, R. Vogelsang, and E. Guilyardi, (2006), PRISM et OASIS : une infrastructure logicielle pour la modlisation climatique en Europe, Proceedings of Ateliers de Modélisation de l'atmosphère MA 2006, Mto-France, Toulouse, France 2006.

4.3 Technical Reports

[CC8] S. Buis and M. T., (2006), Les espaces Dynamiques dans PALM_MP, Technical Report TR/CMGC/06/01, CERFACS. Available on Global Change web.

[CC9] L. Coquart and S. Valcke, (2006), Description du bance d'essai permettant de quantifier la qualit des interpolations avec le coupleur OASIS4, Technical Report TR/CMGC/07/102, CERFACS. Available on Global Change web.

[CC10] J.-M. Epitalon, (2007), Intégration des coupleurs OASIS-3 et PALM-Research, Technical Report WN/CMGC/07/93, CERFACS. Available on Global Change web.

[CC11] J. Ghattas and S. Valcke, (2006), Adaptation of OASIS4 and TOYOA4 to the PRISM Standard directory structure and Compile Environment, Technical Report TR/CMGC/06/75, CERFACS. Available on Global Change web.

[CC12] T. Morel, (2006), Etat des lieux du coupleur PALM, Technical Report WN/CMGC/07/36, CERFACS. Available on Global Change web.

[CC13] T. Morel, (2006), Manuel de formation au logiciel PALM_MP, Technical Report TR/CMGC/06/19, CERFACS. Available on Global Change web.

[CC14] S. Valcke and T. Morel, (2006), OASIS and PALM, the CERFACS couplers, Technical Report TR/CMGC/06/38, CERFACS. Available on Global Change web.

[CC15] S. Valcke and R. Redler, (2006), OASIS4 User Guide (OASIS4_0_2), Technical Report WN/CMGC/06/74, CERFACS. Available on Global Change web.

[CC16] S. Valcke, (2006), OASIS3 User Guide (prism_2-5), Technical Report WN/CMGC/06/73, CERFACS. Available on Global Change web.

4

Climate Modelling

1 Introduction

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

- To improve the understanding of climate processes underlying the natural variability of the main climate modes, such as the North Atlantic Oscillation (NAO), the Atlantic Meridional Overturning Circulation (AMOC) and the El Nino Southern Oscillation (ENSO) and of the response of the NAO, AMOC and ENSO to climate change.
- To detect, attribute and describe anthropogenic climate change on global to regional scales with a focus upon Europe and West Africa, using high resolution atmospheric models and long-term high quality observations.
- To assess the impacts of anthropogenic climate change at regional scale with specific interest in the changes of extreme events distribution and hydrological cycle properties with a focus upon Europe and West Africa and to provide uncertainty bounds in future climate projections.
- To study the potential of decadal predictability due to both external forcing and oceanic initial conditions. This may contribute to the assessment of the risk of abrupt climate change, with emphasis upon the possible slowdown of the thermohaline circulation and its regional impacts particularly over Europe.
- To explore and develop the appropriate tools to make the most efficient use of the new supercomputer architectures for climate modelling exercises.

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

2 Climate variability and predictability

2.1 Introduction

Climate exhibits considerable variability on a wide range of timescales. Fluctuations goes from synoptic events (weather) to decadal changes and have all strong economical and societal impacts. Interest in weather/climate fluctuations and their interaction have been rapidly growing over the last few years following, first the recent recurrence of *meteorological extremes* (2007 and 2003 summer heatwaves in eastern and western Europe respectively, 2002 central Europe flooding, Chrismas 1999 winter storms etc.), and second the more pressing evidence for anthropogenic influences on climate. In such a context, demand for predictability of climate variability logically emerged from the decision-makers sphere.
The concept of predictability and prediction is complex. For lead-time longer than 10 days or so, only a *probability forecast* that takes chaos into account can truly indicate determinism of the outcome. Long-range predictability comes (if it exists) from the boundary forcing (ocean, soil moisture etc on seasonal to decadal timescale, greenhouse gazes for climate changes). Climate predictability is tightly linked to the knowledge and the understanding of the mechanims that sustain its own existence. A long-range forecast, whatever its skill, is of scientifical value if we know **how** and **why** we can forecast. It thus appears that predictability and predictive skill measures need to be addressed with a systematic mechanistic approach of the variability. The activities of the “Climate Variability and Predictability” project directly takes place within this framework. Our goal is to better understand the physical origin of the low-frequency variability with the ultimate hope to improve its prediction. We thus combine a theoritical approach of the climate variability to its logical application in participating to the quasi-operational committee.

2.2 Climate variability and extremes

2.2.1 Towards a better understanding of the main modes of climate variability

2.2.1.1 Assessment of the role of individual ocean basins in forcing low-frequency variability in the North Atlantic European atmospheric circulation

Records of observed Sea Surface Temperatures (SSTs) show clear decadal variations especially in the Atlantic Ocean (see e.g. [2]), and in the Indo-Pacific tropical basin. Model coordinated experiments were designed within the FP6 DYNAMITE project, to assess the impact that such changes may have had on climate and on the North Atlantic Oscillation (NAO) in particular. Six Atmospheric General Circulation Models have been forced by anomalous SST patterns representing these SST trends. The ARPEGE model has been integrated in low-resolution standard mode (T63) and in stretched configuration with enhanced resolution over the North Atlantic.
In boreal winter (DJF), all models show that an Indo-Pacific (IP) warming leads to North Atlantic atmospheric changes projecting onto the positive phase NAO. Whilst the responses of each model are similar, the associated mechanisms appear to be different. In some models the response appears to involve propagation of Rossby waves from the North Pacific along the upper-level jet wave guide. In other models signal propagation is via the tropical Atlantic. The experiments in which warming is limited to the Indian Ocean show a much stronger response in midlatitude geopotential height anomalies, which shows that the

presence of concurrent warming in the west Pacific acts to weaken the Northern hemisphere response in boreal winter. These findings show that care must be taken when defining what is commonly referred to as the ”Indian Ocean” when assessing its related remote impacts. The Indo-Pacific warming leads, in boreal summer, to large-scale northern hemisphere warming with maximum loadings over Europe, projecting onto the so-called Blocking pattern (associated with anticyclonic conditions), and this signal is again consistent with observed trends. In contrast to boreal winter, the extratropical response in boreal summer is primarily excited by warming of the west Pacific rather than the Indian Ocean.
None of the models shows a significant response of the NAO in winter to a warming of the North Atlantic Ocean. These experiments were designed to use realistic forcings, and this may suggest that the Atlantic SST anomalies observed between 1950 and 1999 were not sufficient to significantly affect the NAO. However, feedbacks that may be present in a fully coupled ocean may be important in determining the complete response of the NAO, processes that are not fully captured in an AGCM. The response in boreal summer to Atlantic SST change is much clearer and more consistent between the models but the latter weakly projects on the observed trends.

2.2.1.2 Assessment of the role of individual ocean basins in forcing low-frequency variability in the African Monsoon

At decadal time-scale, a significant link has been highlighted between the observed Sahel drought that occurs after 1970 and an inter-hemispheric SST pattern associated with a warming (cooling) of the oceans in the Southern (Northern) hemisphere. ARPEGE experiments have been conducted both in standard and stretched resolution within the FP6-EU AMMA and ACI-DISCENDO projects to confirm these conclusions. They suggest that the basic structure of the Sahel drought can be simulated when the model only use the observed SST as a lower boundary conditions (however, the simulated precipitation decrease is mainly located over central and eastern Africa and underestimated due to a serious mean state error)[CM5]. The additional effect of enhanced greenhouse gases (GHG) and sulphate aerosols (SA) in the atmosphere upon African rainfall and dynamics variability is relatively weak and non significant over the 1950-1999 period. The sole significant effect related to GHG/SA changes is found in diurnal temperature range which is significantly diminished during the last two decades of the 20th century over Africa [CM4]. Over Northern and Southern Africa, this decrease is related to a significant increase of minimum temperatures mainly due to the additional greenhouse effect. Over West Africa, an increase of cloud albedo is responsible for cooler daily maximum temperature resulting in a weakening of the diurnal temperature range.
At inter-annual time scale, a significant relationship has been characterized between rainfall variability over the Sahel and El Nio Southern Oscillation (ENSO) on one hand and the tropical Atlantic Ocean on the other hand. Idealized experiments using ARPEGE confirm the role of both basins. Their combined action results in a longitudinal dipolar rainfall pattern over Africa associated with a global alteration of the Walker cells. Note that the latter results seem to be strongly model-dependant and are polluted by strong internal variability in the position of the Inter Tropical Convergence Zone. Note also that the relationship between West African monsoon and ENSO is only significant post-1970, suggesting a non-stationarity of the teleconnections.

2.2.2 Towards a better understanding of the climate and weather extremes

2.2.2.1 Relationship between wintertime drought conditions in southern Europe and subsequent summertime heat events

The risk of extreme heat waves in Europe like the unprecedented one of summer 2003 is likely to increase in the future, calling for increased understanding of these phenomena. From an analysis of meteorological records (ECA station-based data) over 58 years, we show that hot summers are preceded by winter rainfall deficits over Southern Europe [CM15]. Subsequent drought and heat spreads northward throughout Europe in early summer, due to atmospheric transport of anomalously warm and dry air from Southern Europe in southerly wind episodes. This is shown by the observations and supported by mesoscale meteorological sensitivity simulations (MM5) for summer 1994, used as a case study. Moreover previous winter and early spring rainfall frequency in the Mediterranean regions is correlated with summer temperature in central continental Europe. These results emphasize the critical role of the water reservoir in the soil of continental Mediterranean areas for the maintenance of European climate. This study has been conducted with the CHAMPION ANR project.

2.2.2.2 Fall/winter 2006-2007 : classical or atypical climate hot extreme over Europe ?

Europe witnessed unprecedented warmth persisting throughout fall and winter 2006-2007, with only a few cold breaks. Whether this anomaly and recent warming in Europe can be linked to changes in atmospheric dynamics is a key question in the climate change prospective. We show that despite the fall/winter atmospheric flow was favourable to warmth, it cannot explain alone such an exceptional anomaly [CM17]. Observed temperatures remained well above those found for analogue atmospheric circulations in other fall and winter seasons over 1950-to-present. Such an offset is detectable though during the last decade and culminates in 2006/2007. These observational results suggest that the main drivers of recent European warming are not directly changes in regional atmospheric flow and weather regimes frequencies, contrasting with observed changes before 1994. The other possibility is that the relationship between weather regimes and their thermo-dynamical properties is currently changing implying that the impacts of a given regime can not be directly (or linearly) assessed from past cases. Heat and moisture transport are potential candidates for explaining nonlinearities. Further investigation study are conducted with the CHAMPION ANR project.

2.2.2.3 Extreme precipitation events over southern-Europe and their relationship with intraseasonal atmospheric circulation

The atmospheric variability over the European-Mediterranean region is described using the weather regime paradigm applied on geopotential height at 500 hPa in autumn (season of highest probability of heavy precipitation episodes over the Mediterranean coasts). Results show that such an approach can discriminate the extreme precipitation events occurrence over several regions on the Mediterranean basin, in particular the Cevenol region [1]. Deeper analyzes suggest that rainfall extremes are associated with transitions between two specific large-scale regimes. We further show that the European-Mediterranean weather regimes can be related to the phases of some intra-seasonal atmospheric oscillation. By using Multi-Channel Singular Spectrum Analysis (MSSA), we identify a 50-day oscillation and the phases of this oscillation are found to be consistent with the preferred weather regimes transitions. This could influence intra-seasonal predictability and suggests that links between the episodic (weather regimes) and oscillatory (intra-seasonal oscillations) approaches may also apply to the regional scale. As an preliminary application, we present a statistical forecast scheme in which the knowledge of the phase of the oscillation can be used to forecast the probability of rainfall extremes occurrence over a given region.

2.2.2.4 Influence of anthropogenic forcings on the statistics of extremes

A common approach to estimate the probability of extreme events is based on the estimation of the so-called GEV distribution parameters inferred on the basis of historical data. Various studies show that usually the convergence of such a distribution is extremely slow. Here we used the Poisson-GDP model or the POT model based on a more efficient use of data to estimate GEV statistics. We have first estimated the parameters for these models using France daily data for temperature over 1873-2003 (dataset produced within the framework of the project IMFREX). We have started comparing these preliminary results to ensembles of model simulations carried out within the DISCENDO ACI-project in order to quantify the ability of the model to represent extreme events. The comparison between the different ensembles will allow to infer if the influence of the direct anthropogenic forcings (in addition to the effect arising from the oceanic boundary conditions) upon the distribution of extreme events can already be detected. Based on these results, we can estimate a relationship between observed and simulated distributions to discuss how extreme events are likely to behave in the future.

2.3 Climate predictability

2.3.1 Medium-range Forecast : role of the tropical intra-seasonal variability

Bridging the traditional gap between weather and climate spatio-temporal scales is one of the major challenges facing the atmospheric community. In particular, progress in both medium-range and seasonal-to-interannual climate prediction relies on our understanding of recurrent weather patterns and the identification of specific causes responsible for their favored occurrence, their persistence and/or their transition. Within this framework, we present evidence that the main climate intra-seasonal oscillation in the tropics (Madden-Julian Oscillation -MJO) controls part of the distribution and sequences of the four daily weather regimes classically defined over the North Atlantic-European region in winter. Regimes associated with the North Atlantic Oscillation (NAO) are the most affected allowing for medium-range predictability of their phase far exceeding the one week or so usually quoted as the limit. We built a very simple statistical model (GLM) to quantitatively assess the predictability level and find that the correct sign of the NAO regimes are successfully forecast in 70% of the cases based on the sole knowledge of the previous 12 day phase and amplitude of the MJO used as predictors.

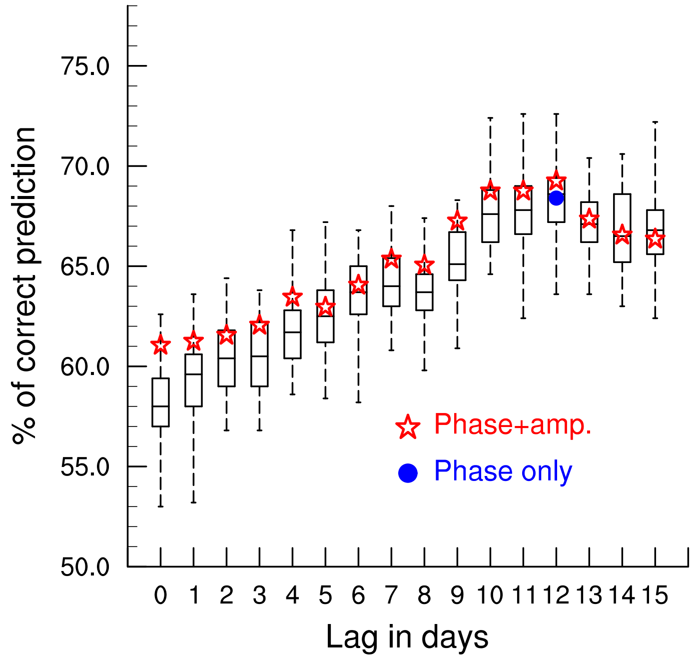


FIG. 2.1 – Percentage among a total of 3150 days of correct prediction of the sign of the NAO regimes as a function of lags based on the GLM model built from the MJO-NAO connection . Red stars (blue dot) correspond to the skill of the model when both phases and amplitude (only phases) of the MJO are used in the statistical model as predictors. Barplots show the model performance in a cross-validation mode.

Such a promising skill could be of great importance considering the tight link between weather regimes and both mean conditions and chances of extreme events to occur for European temperature and precipitation. The tropical-extratropical connection appears to be asymmetrical between the two NAO regimes. NAO+ regimes are favored about 10-day after a maximum convection MJO boost over the Indo-Pacific warmpool. The latter generates a rossby wave trains in the Pacific propagating eastward to the Atlantic, then favoring anticyclonic wave breaking leading in fine to NAO+ regimes. NAO- regimes are favored when MJO associated convection is maximum over the eastern-Pacific/western Atlantic warmpool. The moisture reservoir provides fuel for the North Atlantic storm track shifted southward and favoring cyclonic wave breaking leading in fine to NAO- regimes. Our findings are useful for further stressing the need to better initialize, simulate and forecast the tropical ocean-atmosphere coupled dynamics at the core of medium and longer range predictability in the northern hemisphere, and known as the Achilles' heel of the current seamless prediction suites.

2.3.2 Seasonal Forecast : towards an operational system

A seasonal forecast committee has been created at Mto-France including Mercator, Cerfacs, CNRM and DCLIM. The goal of this committee is to provide an expertise on operational seasonal forecasts produced within the EUROSIP project, and to produce a monthly bulletin based on the ensemble of products available worldwide from the main climate centres. Seasonal prediction for North Atlantic-European regimes has been tested and validated at Cerfacs based on the Meteo-France model and is now applied operationally on the new system including the latest versions of the ARPEGE and ORCA models and 40 perturbed members. Cerfacs also participates to the "seasonal forecast" briefing traditionally organized at the beginning of calendar seasons. An evaluation of the past-forecast is presented together with the prediction for the new forthcoming season.

2.3.3 Decadal Forecast : ocean variability and initial conditions

Following the experience of initialising the ocean part of seasonal forecast systems (FP5 DEMETER EU project), the use of ocean reanalyses has been extended to the initialisation of decadal hindcast experiments, in particular within the framework of the FP6 ENSEMBLES EU-project. A set of ensemble simulations has been carried out based on the of the ArpegeV4.6/Oasis3/NemoV1 coupled model, including the Lim sea-ice component. The embedded Trip model for runoff was replaced by climatological data because of systematic errors leading to unacceptable biases in the Mediterranean Sea.

Ensembles of 3 members are initiated on Nov. 1st every 5 years from 1960 to 2005, each member differing by their initial ocean states, and are integrated over 10 years.

The design of ensembles of reanalyses has been carefully described [CM16]. The perturbation scheme for the ensemble generation has been changed relative to former experiments designed for seasonal hindcasts. It now consists in a continuous set of daily perturbed fields (winds, SST) and includes water flux perturbations. This implies that the perturbation process has a longer influence in time, and can introduce spread in the buoyancy initial conditions of regions sensible for decadal variability. The sea-ice initialisation has also been developed, which was needed because no sea-ice model is used for the ocean reanalyses. Technical developments have been carried out to ensure the archiving of ocean data on the ECMWF data base. Very preliminary results show that the correlation skill of the prediction of ten-year mean sea-surface-temperatures a decade in advance is well above the persistence.

At the same time, ocean variability over the ERA40 period (1960-2006) has been analysed based on the reanalyses. Globally averaged heat content and sea-level variations show decadal scale fluctuations, but their interpretation must be done with care as they depend on the evolution of the observation network. Low frequency modes of variability in the tropics have also been characterized though. In the tropical Atlantic, inter-annual (3 to 7 years) and quasi-decadal signals have been evidenced in the upper ocean heat content, as well as in the Indian basin (2-to-5-year band). The statistical characteristics of these modes of variability are used to evaluate their predictability in the ENSEMBLES hindcasts.

2.4 References

[1] E. SanchezGomez, L. Terray, and B. Joly, (2008), Intraseasonal atmospheric variability and extreme precipitation events in the European-Mediterranean region, **in revision**.

[2] R. Sutton and D. Hodson, (2005), Atlantic Ocean Forcing of North American and European Summer Climate, *Science*, **309**, 115–118.

3 Climate change and related impacts

3.1 Introduction

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 recent Intergovernmental Panel for Climate Change (IPCC) fourth assessment report (AR4). However, there are still large uncertainties related to the fate of regional temperatures and to the global or continental evolution of other variables as those related to the hydrological cycle (precipitation). In order to optimally define the adaptation and mitigation strategies needed to cope with the potential impacts of this expected climate change, a deeper understanding of regional and local scale changes is needed as these scales are the appropriate ones for the impact community and stakeholders. Our first objective is thus to quantify the influence of anthropogenic causes upon recent regional climate change versus the role of intrinsic variability of the climate system (the detection and attribution question). Our second objective is to develop new methodological tools to tackle the difficult question of climate change and associated impacts at sub-regional to country scale, including the assessment of the various sources of uncertainties (regional climate projections and associated uncertainties).

3.2 Detection and attribution of recent climate change over France

The first regional-scale attribution studies were carried out as part of the Discendo project on the detection and attribution of climate change at the regional scale. The approach taken in this project is based on the use of variable resolution atmospheric models (with high resolution over the area of interest) and the consideration of the boundary oceanic conditions (sea surface temperatures - SST) as an additional forcing to anthropogenic forcings (greenhouse gases - GHG - and sulfate aerosols - SUL) and natural forcings (solar - SOL - and volcanism - VOL). The first step is to detect climate changes in relation to internal atmospheric variability and to variability linked to ocean fluxes (whether of an internal nature or linked to anthropogenic and/or natural factors). In other words, this method aims to detect a direct response of the forcings considered (GHG, SUL, SOL, VOL) on the atmosphere, in addition to the one potentially associated with ocean warming due to the same forcings.

The second step concerns the attribution methodology : it is based on the performance of ensemble simulations that differ in terms of the combination of forcings applied. The first ensemble is forced only by SSTs observed over the 1950-1999 period and the other forcings (GHG, SUL, NAT - SOL + VOL) are constant and fixed at their 1950 value. For the other ensembles, the observed changes in anthropogenic and natural forcings are added sequentially. The ensemble averages of the simulations performed constitute the climate signals and the internal variability - noise - is built from the intra-ensemble variability (the differences between each simulation and the corresponding ensemble average). These two ingredients are then used in the optimal fingerprint method, which can also be seen as a simple regression method with several parameters.

The methodology has been applied to decadal anomalies in minimum and maximum summer temperatures over the 1950-1999 period ([CM13]). The observed warming for minimum temperatures can be explained by the combination of the oceanic signal with the direct effects due to GHGs and SULs. It should also be noted that here the SUL forcing is essential to detecting a combination of signals. The oceanic signal seems to be strongly linked to a variability mode known as the Multidecadal Atlantic Oscillation (AMO) whose origin is probably internal to the ocean. The shift to a positive phase of this oscillation in the last decades of the 20th century contributed to a slight increase in the main warming due to anthropogenic effects (GHG + SUL). The detection of maximum temperatures is less robust, but the combined effects of SSTs and GHGs are detected even if the model seems to slightly underestimate the response of these forcings in relation to observations. The physical interpretation of the detection and attribution method relies upon the hypothesis that via changes in evapotranspiration, the spatial variation of soil water content could amplify warming in the drier regions and limit it in wetter regions. This mechanism is present in the present climate simulation of the regional climate model as well as in pseudo-observations such as the SAFRAN mesoscale analysis and its application to an hydro-meteorological model.

3.3 Development of downscaling techniques based on weather types

Many impact studies often require climate data at a very fine scale (1-10 km, and even less), far beyond what the current global or even regional climate models can deliver. In order to study the impact of climate change over France on river flows or on wind power, meteorological variables at a resolution lower than 10 km are needed whereas the typical resolution of regional and global climate models is currently about 25-50 and 250 km, respectively. This scale issue known as downscaling has been extensively studied in recent years and many dynamical and statistical methods have been developed to bridge this scale gap. Here we report on recent developments using weather-type methods and applied to the fine-scale projections derived from the Coupled Model Intercomparison Project (CMIP3) multi-model (widely used in the IPCC AR4). A methodology allowing the statistical downscaling of a large number of climate models has been developed ([CM2],[8]) to bridge the scale gap between climate models and impact studies. The methodology is based on the links that exist between the large scale circulation (LSC), represented by a small number of weather types computed on mean sea level pressure, and the regional climate properties see [5]. The weather types are explicitly determined to be discriminant for the climate variable of interest(for instance precipitation or 10m-wind). To do so, we apply mathematical classification tools simultaneously to both variables (for instance, mean sea level pressure and precipitation). Intra-type dynamical variability and non-dynamical temperature changes are also taken into account through a multivariate regression step. The algorithm has been constructed using the NCEP reanalysis and observed datasets (such as the meso-scale SAFRAN analysis or the Météo-france wind dataset) to build the transfer function between the large scale circulation predictors and the predictands (the variables needed by the impact model), respectively. The methodology has been intensively validated and sensitivity studies to key parameters have been carried out ([CM3],[8]). In the following, we only report here results about hydrological and wind changes. Other impacts (agro- and ecosystems) are currently studied with similar methods and results should be available soon. The methodology has been also used in the downscaling and bias correction of atmospheric forcing for high-resolution ocean models. There are still large uncertainties as to the future evolution of the thermohaline circulation, partially due to coupled model biases and ocean model resolution used in the CMIP3 exercise. A complementary approach is to use atmospheric LSC predictors to infer the surface atmospheric variables needed to force an ocean model. This atmospheric forcing function is then used to force a higher resolution ocean model for the period of interest. The approach has been validated with the NEMO 0.25 degree regional Atlantic model for the 1979-2002 period by comparing oceanic diagnostics between the control simulation (observed atmospheric forcing) and the one with forcing obtained by the weather type statistical downscaling.

3.4 Climate change impacts : hydrology and wind ressources

3.4.1 Hydrological changes

As shown by the studies performed within the ESCRIME project ([CM23]), the 21st century projected climate changes in France are important and may thus have serious socio-economical consequences. The potential impacts linked to the hydrological cycle (affecting river flows, soil moisture, snow cover etc.) are probably among the more worrying.
The downscaling method described previously has been applied to 14 climate models from the CMIP3 multi-model dataset for the sres-A1B scenario (2046-2065 period) and the present climate (1971-2000 period). Then, the hydro-meteorological system ISBA-MODCOU over France (Habets et al., 2007) has been forced by downscaled meteorological forcing to realize an ensemble of hydrological scenarios and obtain a probabilistic estimation of changes of different hydrological variables in France ([CM18], [3]). Figure 3.1 depicts the relative changes of the discharges for several French rivers.

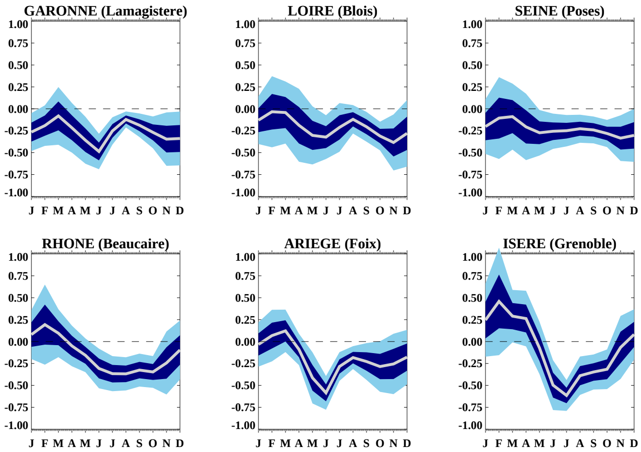


FIG. 3.1 – Relative seasonal changes of discharges for several french rivers between the 2046-2065 and 1971-2000 periods. The black line is the multi-model average. The light (dark) grey shading is delimited by the multi-model average +/- one (two) inter-model standard deviation. Note that the effect of dam is not taken into account by the hydro-meteorological model in both present and future climate.

Even if the uncertainty is large, some clear signals are emerging as earlier as in the middle of the 21st century. The decrease of discharges in summer and autumn, resulting from a decrease of precipitation and increase of evapotranspiration during winter and early spring is quasi-generalized. As an example, the discharge of the Rhne at Beaucaire (Seine at Poses) decreases by around 35% (25%) in the ensemble mean. The results for the Arige and the Isre illustrate the importance of the changes linked to snow. The earlier snowmelt and/or decrease of snowfall during winter results in a strong decrease of late spring/early summer discharges. During winter, the inter-model spread is larger than in summer for the majority of the rivers and the sign of the multi-model mean changes is often not clear. Other analyses indicate that if the occurrence of drought is very likely to largely increase in the future climate, the changes of high flow and floods are much more uncertain ([CM18]).

3.4.2 Wind changes

Because wind energy is a fast growing renewable energy, there is a high interest in assessing the impact of climate change on wind energy resources. In this perspective, a refinement to the downscaling methodology based on weather typing has been undertaken. The additional step requires the use of mesoscale modeling. First, 850hPa wind weather types have been defined, and mesoscale simulations with the MesoNH model (Lafore et al. 1998) have been performed for a sample of days selected into those weather types. Then, 10m wind distributions at high spatial resolution have been estimated by weighting each simulation by the corresponding changes in weather type occurrence frequency. This method has been applied to thirteen climate models from the CMIP3 multi-model dataset : changes in the occurrence frequency of the 850hPa wind weather types have been calculated in order to assess potential changes in the 10m wind distributions ([8]). Two time periods have been focused on : a control period (1961-1990) from the climate of the twentieth century experiment and one climate projection period (2046-2065) from the IPCC SRES A1B experiment. Figure 3.2 shows the relative changes of the 10m winds over France in winter.

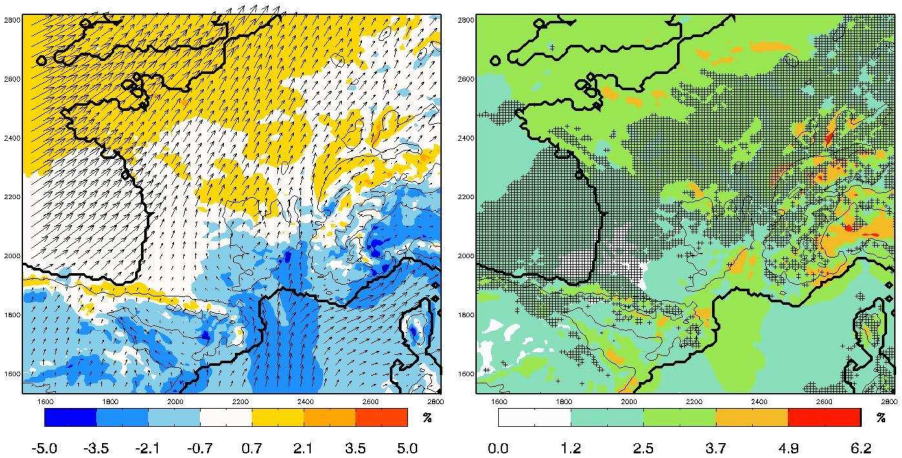


FIG. 3.2 – Left Panel : Multimodel mean 10m wind changes in winter. Color shading indicates multimodel changes in the 10m wind speed (in percent) and vectors represent the associated vector anomalies. Right Panel : Color shading represents the inter-model dispersion (1 inter-model standard deviation) and non shadow areas indicate areas where at lest 75% of the models provide changes of the same sign.

The South-East of France experiences a decrease of the mean wind speed. This decrease is associated with a decrease of the northerly and northwesterly winds (Mistral and Tramontane events). On the contrary, the North, the North-West and the Centre of France experience a weak increase of the mean wind speed. This increase is associated with an increase of the southwesterly winds. The sign coherence of the models is high in those regions since at least 75% of the models provide changes of the same sign. However, the dispersion of the models is large. This indicates that while there is good agreement between the models with regard to an increase or a decrease of the mean wind speed, any estimation of the amplitude of those changes remains uncertain. In the South-West and the East of France, there is no significant change in the multimodel mean 10m wind speed and the sign of the multimodel mean changes is not clear. Finally, although changes in the 10m wind speed are weak (maximum of 5%), changes in the mean wind power density (which is proportional to the cube of the wind speed) are much larger (maximum of 20%, not shown) and may be of interest for wind energy development in France.

3.5 Uncertainties in climate change projections : a process-based approach

Many studies have recently tried to better understand and quantify the different sources of uncertainties in global climate projections for the 21st century. The problem is even more difficult if one is interested in regional and sub-regional scale projections. When analyzing fine-scale projections, the full cascade of uncertainty through the chain of external forcing, global and regional models and/or statistical techniques has to be considered. We have begun to work on a better quantification of the various sources of uncertainties at regional scale. We have focused on the climate model uncertainty (the epistemic uncertainty) which is due to incorrect, incomplete or missing representation of key processes of the climate system (clouds, soil-atmosphere feedbacks, ocean eddies ...). We have proposed a new approach to better quantify and eventually reduce the epistemic uncertainty. The approach is based on the concept of process-based metrics. The idea is to first identify a set of key physical processes in the present climate which are responsible for the projection spread of a given variable in the future climate. The second step is to compare the representation of these key processes in the current climate between the models and the observations. In a first application of the approach, [4] have shown that an important fraction of the spread in CMIP3 projections of European summer evapotranspiration is likely to be due to the unrealistic representation of evapotranspiration control mechanisms in some models for the current climate. Using this process-based metrics to constrain regional future climate change leads (in this case, but not necessarily always) to a reduction of the modeling uncertainty and to a best guess (ensemble mean) temperature regional projection of slightly larger amplitude for the European summer.

3.6 References

[3] J. Boé and L. Terray, (2008), Régimes de temps et désagrégation d'échelle, *La Houille Blanche*, **2-2008**, doi :10.1051/lhb :2008016.

[4] J. Boé and L. Terray, (2008), Uncertainties in European summer climate change : role of evapotranspiration, **35**, L05702, doi :10.1029/2007GL032417.

[5] J. Boé and L. Terray, (2008), A weather type approach to analysing France winter precipitation : twentieth century trends and influence of anthropogenic forcing, **in press**.

[6] Habets, F., A. Boone, J. Champeaux, P. Etchevers, E. Leblois, E. Ledoux, P. L. Moigne, E. Martin, S. Morel, Q. Segui, F. Rousset-Regimbeau, and P. Viennot, (2008), The SAFRAN-ISBA-MODCOU hydrometeorological model applied over France, *J. Geophys. Res.*, in press.

[7] J. P. Lafore, J. Stein, N. Asencio, P. Bougeault, V. Ducrocq, J. Duron, C. Fischer, P. Héreil, P. Mascart, V. Masson, J. P. Pinty, J. L. Redelsperger, E. Richard, and J. V.-G. de Arellano, (1997), The Meso-NH Atmospheric Simulation System. Part I : adiabatic formulation and control simulations, *Annales Geophysicae*, **16**, 90–109.

[8] J. Najac, J. Boé, and L. Terray, (2008), A multi-model ensemble approach for assessment of climate change impact on surface winds in France, **in revision**.

4 Prospective tools for climate modelling

The consideration of new scientific questions such as regional climate impacts or scale interaction issues etc requires more and more computer resources. These resources are in constant and rapid evolution. Designing, porting and maintaining climate models on appropriate platforms is therefore a more and more demanding issueand even more a real challenge. This heavy task is done in strong synergy between researchers, engineers in geosciences and the scientific computing community.
To prepare the new important rendez-vous, our activity is partitioned in two items :

– Porting climate modelling tools, and particularly Cerfacs CGCM, on new architectures (scalar and massively parallel)
– Develop higher resolution CGCM on world's most powerful supercomputers

4.1 Coupled models on new architectures

A new configuration of the Cerfacs CGCM has been developed since June 2005. It includes the latest version of ARPEGE V4 atmospheric model (T63 resolution), OPA V9 (NEMO configuration, 2 degrees resolution) oceanic model including LIM sea-ice and TRIP runoff models. Coupling was done using OASIS3 library. Evolution of world HPC market leads us to port the model on other computing platforms than traditional vector ones. We first have made an important effort to implement, in a ready-to-use environment, the first Linux version of ARPEGE-NEMO CGCM. Gained flexibility and efficiency were good enough to be part of the so-called Leage for Efficient Grid Operations (LEGO) Grid-related ANR project[CM30]. The coupled model version was configurated with project partners to allow its equivalent use on any nodes of the heterogeneous Grid'5000 platform [CM26]. We also helped our partners to integrate the coupled model on a parallel software component configuration and optimize simulation/post-processing scheduling on a hierarchical platform [9]. We began testing network-based data migration solutions across the Grid to permit a cross-node simulation. Using Grid5000 Linux-heterogeneous clusters platform helps us to launch a first parametrization test on embarrassingly parallel experiments, requiring a huge number of independent processors.
In addition, climate modelling research will soon require a higher number of communicating processors because of increased resolution and new components. We took a step forward possible use of massively parallel architectures for climate simulations : both atmospheric and oceanic CGCM components have been installed and optimized on the new Cerfacs IBM Blue Gene/L machine [10] ; coupled configuration porting problems and bottlenecks (I/O, communication libraries) have been identified.

4.2 High resolution coupled model assembling

New CGCM generation combines finer resolution in both atmospheric (typically spectral truncation T106 or higher) and oceanic (typically half degree or higher) general circulation models and more frequent coupling time step (every hour instead of daily basis) to fully resolve the diurnal cycle. These requirements heavily load the most powerful computer currently available.
To anticipate and prepare the future CGCM version to be used for the next challenging IPCC AR5 exercise, the implementation of such CGCM began with a training period at the Earth Simulator Center (Japan).

Our main objective was to optimally configurate our CGCM oceanic component and to evaluate the implementation issues of such configuration [CM29].
We then assembled the high resolution version of the oceanic component (OPA9 + LIM sea-ice, half degree horizontal resolution, higher vertical resolution 45 to 90 vertical levels) with a high resolution version of ARPEGE (version 4) [CM28], on the new Météo-France supercomputer (based on NEC SX8R processors which closely match the Earth Simulator ones). The sea-ice model behaviour with high frequency coupling time step and combined effects of surface layer fine resolution and diurnal cycle has been preliminary investigated.

4.3 References

[9] Y. Caniou, E. Caron, E. Charrier, A. Chis, F. Desprez, and E. Maisonnave, (2008), Ocean-Atmosphere Model Scheduling over the Grid, International Conference on Parallel Processing (ICPP 2008).

[10] E. Maisonnave, (2008), Portage d'ARPEGE/NEMO sur IBM Blue Gene/L, Working Note WN/CMGC/08/07, CERFACS. Available on Global Change web.

5 Publications

5.1 Journal Publications

[CM1] M. Alexander, J. Yin, G. Branstator, A. Capotondi, C. Cassou, R. Cullather, Y.-O. Kwon, J. Norris, J. Scott, and I. Wainer, (2006), Extratropical Atmosphere-Ocean Variability in CCSM3, *J. Climate*, **19**, 2496–2525.

[CM2] J. Boe, L. Terray, F. Habets, and E. Martin, (2006), A simple statistical-dynamical downscaling scheme based on weather types and conditional resampling, *J. Geophys. Res.*, **111**, D23106, doi :10.1029/2005JD006889.

[CM3] J. Boe, L. Terray, F. Habets, and E. Martin, (2007), Statistical and dynamical downscaling of the Seine basin climate for hydro-meteorological studies, *Int. J. Clim.*, **27**, 1643–1655.

[CM4] C. Caminade and L. Terray, (2006), Influence of increased greenhouse gases and sulphate aerosols concentration upon diurnal temperature range over Africa at the end of the 20th century, *Geophys. Res. Letters*, **33**, L15703, doi :10.1029/2006GL026381.

[CM5] C. Caminade, L. Terray, and E. Maisonnave, (2006), West African Monsoon System response to greenhouse gas and sulfate aerosols forcing under two emissions scenarios, *Clim. Dyn.*, **26(5)**, 531–547.

[CM6] C. Cassou and C. D. ans M. A. Alexander, (2007), Investigating the impact of reemerging sea surface temperature anomalies on the winter atmospheric circulation over the North Atlantic, *J. Climate*, **20**, 3510–3526.

[CM7] C. Cassou and E. Guilyardi, (2007), Modes de variabilité et changement climatique, *La météorologie*, **59**, 22–30.

[CM8] C. Cassou, (2007), Été 2003 : La Fièvre du mercure, *Lettre PIGB-PMRC*, **20**, 3–13.

[CM9] M. Collins, N. Botzet, A. F. Carril, H. Drange, A. Jouzeau, M. Latif, S. Masima, O. H. Otteraa, H. Pohlmann, A. Sorteberg, R. Sutton, and L. Terray, (2006), Interannual to Decadal Climate Predictability in the North Atlantic : A Multimodel-Ensemble Study, *J. Climate*, **19**, 1195–1203.

[CM10] B. Dewitte, S.-W. Yeh, B.-K. Moon, C. Cibot, and L. Terray, (2007), Interaction between near-annual and ENSO modes in a CGCM simulation : Role of the equatorial background mean state, *J. Climate*, **20(6)**, 1035–1052.

[CM11] H. Douville, J.-C. André, and G. de Marsily, (2007), Les impacts des changements climatiques sur le cycle hydrologique, *Responsabilité et Environnement (Srie trimestrielle des Annales des Mines)*, **47**, 49–53.

[CM12] S. Paz, Y. M. Tourre, C. Cassou, and H. Kutiel, (2006), Atmospheric dynamics over Northwest Africa and Linkages with Sahelian Rainfall, *Geophys. Res. Letters*, **33**, L14808, doi :10.1029/2006GL026695.

[CM13] S. Planton and L. Terray, (2007), Détection et attrinution à l'échelle régionale : le cas de la France, *La météorologie*, **58**, 25–29.

[CM14] P. Rogel, Y. M. Tourre, V. Benoit, and L. Jarlan, (2006), Tropical Atlantic moisture availability and precipitation over West Africa, *Geophys. Res. Letters*, **33**, L21711, doi :10.1029/2006GL027178.

[CM15] R. Vautard, P. Yiou, F. D'Andrea, N. de Noblet, N. Viovy, J. C. Cassou, Polcher, P. Ciais, M. Kageyama, and Y. Fan, (2007), Summertime European heat and drought waves induced by wintertime Mediterranean rainfall deficit, *J. Geophys. Res.*, **34**, L07711, doi :10.1029/2006GL028001.

[CM16] A. Weisheimer, F. Doblas-Reyes, P. Rogel, E. D. Costa, N. Keenlyside, M. Balmaseda, J. Murphy, D. Smith, M. Collins, B. Bhaskaran, and T. Palmer, (2007), Initialisation strategies for decadal hindcasts for the 1960-2005 period within the ENSEMBLES project, *ECMWF Technical Memorandum*, **521**.

[CM17] P. Yiou, R. Vautard, P. Naveau, and C. Cassou, (2007), Inconsistency between atmospheric dynamics and temperatures during the exceptional 2006/2007 fall/winter and recent warming in Europe, *Geophys. Res. Letters*, **34(21)**, L21808, doi :10.1029/2007GL031981.

5.2 PhD Thesis

[CM18] J. Boé, (2007), Changement global et cycle hydrologique : Une étude de régionalisation sur la France, thèse de doctorat de l'université paul sabatier.

[CM19] C. Caminade, (2006), Rôle de l'océan et influence des émissions d'origine anthropique sur la variabilité climatique en Afrique, thèse de doctorat de l'université paul sabatier.

5.3 Conference Proceedings and Book Chapters

[CM20] J.-C. André, (2006), Données et connaissances environnementales : Quelques remarques d'ordre éthique sur un patrimoine à protéger, In *Cienca y Etica en la Globalization*, Cienca y Etica en la Globalization, Mexico, 25-26/10/2006, in press.

[CM21] J.-C. André, (2007), *Sur quelques impacts du changement climatique en Europe et sur l'Atlantique*, Odile Jacob.

[CM22] H. Douville, K. Laval, D. Cariolle, S. Planton, and J. C. André, (2006), Eau et Climat, In *Les eaux continentales*, vol. 25, Rapport sur la science et la technologie de lAcadmie des sciences, Editions EDP Sciences, 201–238.

[CM23] L. Terray and P. Braconnot, (2007), INSU - ONERC - IDDRI.

5.4 Technical Reports

[CM24] P.-A. Auger, (2007), Variabilité et prévisibilité décennale de l'état thermique des océans tropicaux Atlantique et Indien à partir de réanalyses océaniques et d'expériences couplées de prévision décennale, Technical Report TR/CMGC/07/67, CERFACS. available on Global Change web.

[CM25] P.-Y. Guillerm, (2007), Influence du couplage haute-fréquence sur la variabilité climatique mensuelle à interannuelle à l'aide de modèles couplés océan-atmosphère, Technical Report TR/CMGC/07/65, CERFACS. available on Global Change web.

[CM26] E. Maisonnave, T. Morel, and S. Valcke, (2007), Portage et déploiement du modèle couplé OCC17 sur la plateforme distribuée Grid 5000, Working Note WN/CMGC/07/44, CERFACS. Available on Global Change web.

[CM27] E. Maisonnave, (2006), Oceanic Part of OCC17 Coupled Model : Physical Interface, Technical Report TR/CMGC/06/36, CERFACS. available on Global Change web.

[CM28] E. Maisonnave, (2007), Expériences couplées frontières (Earth Simulator / Météo France) : Performances, Working Note WN/CMGC/07/02, CERFACS. Available on Global Change web.

[CM29] E. Maisonnave, (2007), Implémentation du modèle couplé ECHAM5-NEMO-LIM sur le Earth Simulator, Mission Report CRM/2006/5, IPSL, Paris, France.

[CM30] E. Maisonnave, (2007), LEGO : Grid Compliant Climate Model Analysis, Technical Report TR/CMGC/07/16, CERFACS. available on Global Change web.

5

MERCATOR project

1 CERFACS contribution to the MERCATOR project

This report summarizes CERFACS' contributions to the Mercator Ocean project.

1.1 Introduction

Mercator Ocean is the french contribution to the international Global Ocean Data Assimilation Experiment (GODAE) which is first international experiment of operational oceanography. Mercator Ocean must achieve an operational exploitation of a global ocean based upon primitive equation with a high resolution and the data assimilation of *in situ* and satellite observations ocean data. Different main research axis have been selected. The integration of the SAM2 data assimilation scheme into the global (1/4^o) and regional (1/12^o) NEMO ocean configurations is a new challenge. The data assimilation of future SSS (Sea Surface Salinity) satellite data is also a key challenge and offers new perspectives to monitor ocean circulation. The developpment of a global system with OPA-VAR (3D-Var) to perform ocean reanalyis is also investigated. The sensitivity of the medium range surface ocean predictability has also been investigated into the northern Atlantic. Mercator Ocean uses the full range of NEMO ocean circulation models developed at LOCEAN and particularly develops a high resolution global ocean model (1/12^o). This new configuration will be the basis for the the next ocean operational system.

1.2 Two operational ocean forecasting systems (regional and global) (M. Drevillon, J.M. Lellouche, and B. Tranchant)

The previous regional ocean forecasting system covered Atlantic and Mediterranean at 1/12^o and was named PSY2v2. This system offered a way to investigate the characteristics and evolution of the ocean meso-scale. An evaluation of this system to forecast the Loop Current and Eddy Frontal Positions in the Gulf of Mexico has been performed and an article entitled "The High Resolution Real Time Mercator Forecasting System : Description and evaluation in the Gulf of Mexico" has been submitted to the *Journal of Marine System* and is currently under review [MER2].

The target MERSEA V2 ocean forecasting system includes a global 1/4^o horizontal resolution system (called PSY3V2 at Mercator), see [4] and a Atlantic and Mediterranean 1/12^o horizontal resolution system (called PSY2V3 at Mercator). It is planned to be launched operationally in early 2008 for the end of the MERSEA project.
In addition to the improvement of the assimilation technique, new ocean model configurations have been defined for both the 1/4^o global system and the 1/12^o Atlantic and Mediterranean system. The model configurations now include coupling with a sea ice model and bulk formulae atmospheric forcing fields, aiming at the future high resolution global forecasting system at 1/12^o. They use the NEMO (Nucleus for European Models of the Ocean) modelling system which presently includes the latest version of OPA, coupled to the thermodynamic-dynamic sea ice model LIM2 (Louvain sea Ice Model 2). The configurations

that are used was built within the framework of the DRAKKAR (www.ifremer.fr/lpo/drakkar) work group. The combination of recent implementation of an energy-enstrophy conserving scheme for momentum advection with a partial steps representation of the bottom topography yields significant improvements in the mean circulation and in the representation of western boundary currents such as the Gulf Stream and the downstream flow of the North Atlantic Current. Moreover, the 1/4^o model solution is often comparable to solutions obtained at 1/6^o or 1/10^o resolution on some aspects concerning mean flow patterns and distribution of eddy kinetic energy. In order to better resolve the upper layers, the vertical grid, now with 50 z-levels, has been refined at the surface ending with a discretization of 1m until 20m depth and of 500m for the bottom layers. With this surface refined-mesh, this new vertical grid has been designed to improve the circulation in the coastal shelves and to represent more adequately the impact of the atmospheric diurnal cycle, which is planned to be explicitly modelled in the near future. The atmospheric forcing fields which drive the V2 system are calculated using empirical bulk parameterisation. Efforts are currently being made to improve these formulations in order to reduce surface systematic biases. The sea ice is fully comprehensive with the implementation of the LIM2 model. With sea ice concentration, sea ice/snow thicknesses, sea ice drift and sea ice thermal content prognosed by this multi-layer model with visco-plastic formulations, forecasts will handle most of the processes linked to the sea ice lifecycle.

The data assimilation technique named SAM2v1 used in the V2 ocean forecasting system is a multi-data and multivariate assimilation algorithm is based on a Singular Extended Evolutive Kalman (SEEK) filter analysis method. The SEEK filter is a reduced-order Kalman filter introduced by [13] in the context of mesoscale ocean models. This method assimilates jointly satellite SLA and SST, and in situ profiles of temperature and salinity. The error statistics are represented in a sub-space spanned by a reduced number of dominant 3D error directions. This data assimilation technique was validated in a 29 year (1979-2007) reanalysis experiment performed with a low resolution (2^o) global forecasting system.

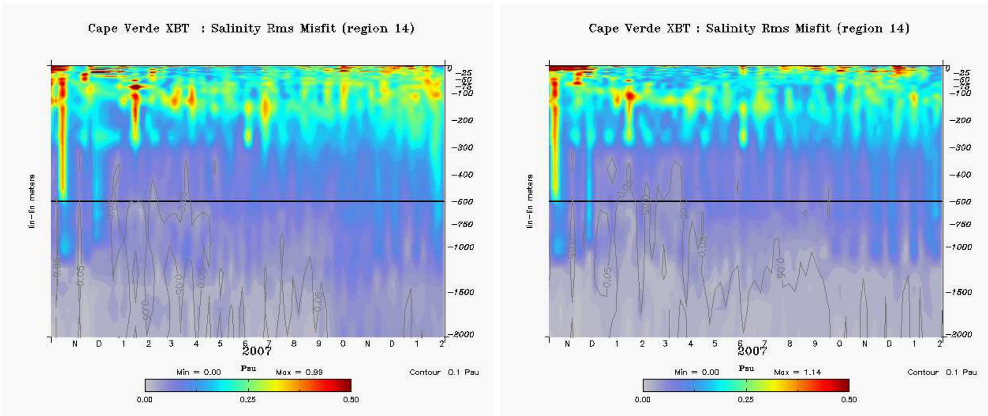


FIG. 1.1 – RMS of the misfit between observations salinity profiles and model forecast calculated for the Atlantic Subtropical Gyre over the year 2007 with the global 1/4^o (left) and the regional 1/12^o (right).

These improvements altogether prepare another MERSEA step : the development of the future global forecasting system at eddy resolving resolution (1/12^o) which will constitute the global component of the MyOcean European project. Two numerical experiments of the ”Global V2” global 1/4^o systems were run over the MERSEA TOP2 test time period (from April 2007 to September 2007). They are called the ”Global V2-old” and ”Global V2-new”. Indeed, flaws in the global 1/4^o V2-old system have been diagnosed at the end of the period. The model flaws were mainly impacting the temperature, salinity and velocity variables around Islands (i.e. for the North Atlantic area, Canaries, Azores, Green Cape, Caribbean). It was due to a problem in the barotropic velocity correction applied. Various adjustments of the data assimilation

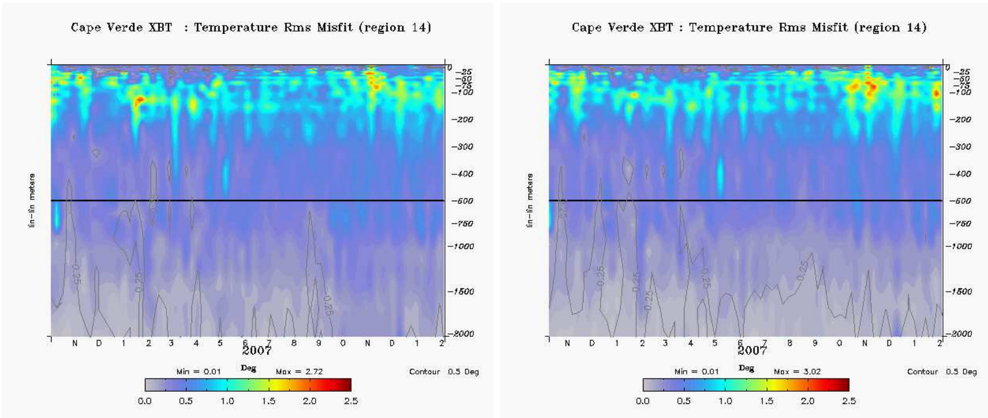


FIG. 1.2 – RMS of the misfit between observations temperature profiles and model forecast calculated for the Atlantic Subtropical Gyre over the year 2007 with the global 1/4° (left) and the regional 1/12° (right).

system were also necessary such as the use of a 3D temperature and salinity representativity error. These improvements finally lead to the current ”Global V2-new” version, and to the first version of the 1/12° V2 Atlantic and Mediterranean zoom. Fig.1.1 and Fig.1.2 illustrate the evolution in time of the Root Mean Square errors of the temperature and salinity misfits for the global 1/4° and for the Atlantic and Mediterranean 1/12° systems in the region of the Atlantic Subtropical Gyre (here called ”Cape Verde XBT”). The latter is one of the geographical regions on which the statistics are computed for both the global and regional systems. The behaviours of the systems are quite similar, and the Atlantic zoom obtains slightly better statistics with depth, as expected. Note that a salinity drift occurs in the global system at the end of the period (not shown). This problem is partly due to the use of incorrect error covariances in summer 2007 for the global system, which slightly alters the statistics of the global experiment. The V2 system is currently being validated, showing general good performances, and still some room for improvements such as enhancing the corrections between 1000m and 2000m.

1.3 Expected impact of the future Ocean surface salinity missions in the Mercator Ocean operational systems (B. Tranchant)

Sea Surface Salinity (SSS) has never been observed from space. The SSS from planned satellite missions such as Soil Moisture and Ocean Salinity (SMOS) and Aquarius is a key to better understanding how ocean circulation is related to water cycle and how both these systems are changing through time. Observing System Simulation Experiments (OSSEs) have been carried out with an ocean forecasting system developed at Mercator Ocean. They consist in hindcast experiments assimilating an operational dataset (Sea Surface Temperature (SST), in-situ profiles of temperature and salinity and Sea Level Anomalies (SLA)) and various simulated SMOS and Aquarius Sea Surface Salinity (SSS) data. generated by [MER3]. These experiments use an eddy permitting model (1/3°) covering the North Atlantic from 20°S to 70°N. The new generation of fully multivariate assimilation system referred to as SAM2v1 which is being developed from the SEEK (Singular Evolutive Extended Kalman) algorithm is used, see [13]. This scheme is a Reduced Order Kalman Filter using a 3D multivariate modal decomposition of the forecast error covariance. The OSSEs enabled us to show the positive impact of SSS assimilation on the Mercator Ocean operational forecasting system. These experiments particularly show the importance to specify appropriated observation errors and the impact of having and/or combining different observing system. Several conclusions can be highlighted such as the importance of the space/time scales consistency between the data products and our ocean prediction systems. This study has to be considered as an important step for assimilation of SSS measured from space. Further studies have to be conducted with other simulated data, other oceanic configurations and other improved assimilation schemes. To illustrate this study, the following section shows the importance of having SSS data with time and space scales close to those found in the ocean forecasting system. Different types of simulated SSS data have been generated and assimilated into our operational system. An example of simulated daily SMOS and Aquarius measurements along tracks are shown on Figure 1.3 for July 6, 2003. All data assimilation experiments are similar to the REF experiment which consist of a hindcast simualtion using a 7-day assimilation cycle and assimilating operational data over one year (2003). Figure 1.4 show the impact of assimilating different observing systems. It shows the time evolution of mean and variance of differences for four experiments :REF (no SSS data assimilation), SMOS L2(assimilation of SMOS L2 products), Aquarius L2 (assimilation of Aquarius L2 products) and Aquarius+SMOS L2 (assimilation of two L2 products). The impact of the Aquarius L2 products is weak compared to the SMOS L2 products. The combination of the two L2 products had thus a small effect on final results.Indeed, even if the observation error See [16] and [15] for more details.

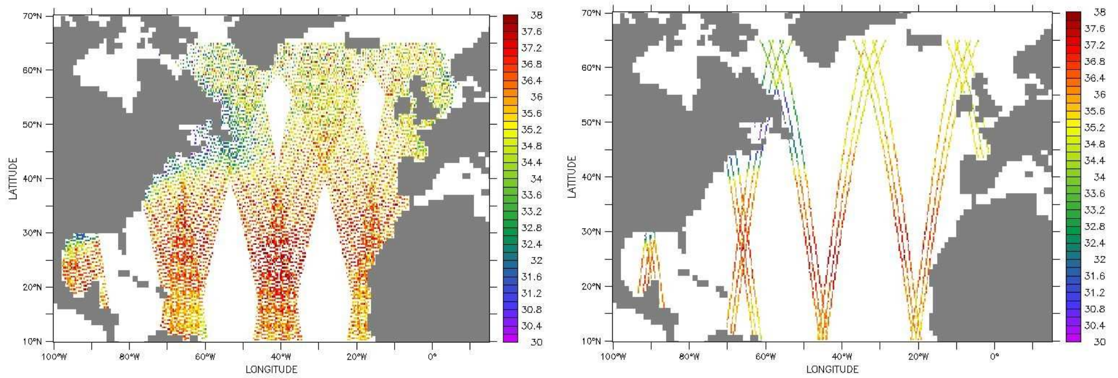


FIG. 1.3 – Pixel location on July 6th 2003 for SMOS L2 (top) and Aquarius L2 (bottom) : salinity in PSU.

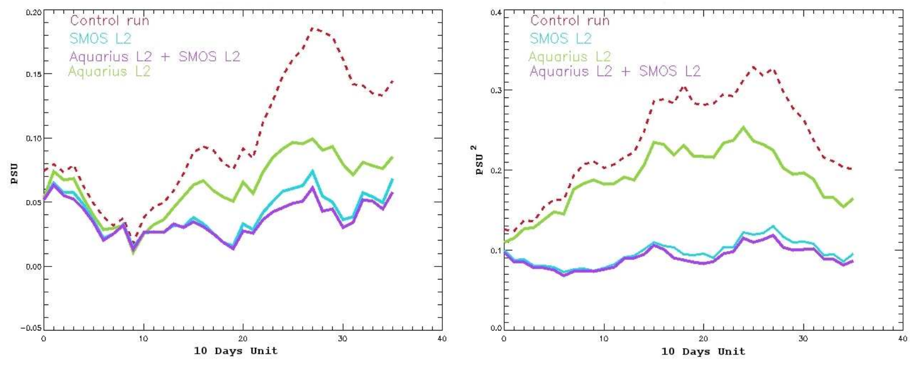


FIG. 1.4 – Spatial average of the mean in PSU (left) and variance in PSU2 (right) of difference between three different estimates control run or REF (red dashed line), SMOS L2 (blue solid line), Aquarius L2 (green solid line), SMOS L2+Aquarius L2 (purple solid line) and ”truth” every ten days during the year 2003 for the overall domain.

1.4 Reanalysis with OPAVAR (E. Rémy)

Besides its operational activities, advanced assimilation techniques are explored at MERCATOR-OCEAN. The variational technique is applied to global low resolution ocean state estimation in the context of reanalysis and ocean climate monitoring. A reanalysis was produced over the period 1960-2005 using the ORCA 2° model configuration (OPA, LODYC) and the OPAVAR assimilation code (A. Weaver, CERFACS) in its 3DFGAT version [17]. This is the first attempt to combine in situ and altimetry observations in a long term reanalysis made with ORCAVAR. In situ temperature and salinity observations are assimilated with along track Sea Level Anomalies. The problem of combining those observations is addressed : both data sets contain different information about the heat and salt content and this can lead to incoherencies due to misspecification of observation error, model error or to the choice of the Mean Dynamical Topography. The benefit of using a realistic MDT was demonstrated, as the synthetic one computed by M.H. Rio, compared to the use of a model MDT. The ability of the assimilation to reproduce the observed interannual variability of the heat content and sea level variability was demonstrated. The model acts as a spatial interpolator and gives us access to the entire water column properties, allowing us to get an estimation of the deeper changes in the heat content of the ocean and their spatial repartition. Contribution of the thermosteric, halosteric effects and mass fluxes to the sea level changes were also estimated. There is still some bias in the estimation of the salinity field which should be fully understood. Figures 1.5 show sea level trend estimation over the 1993-2001 period from the satellite observations and from the reanalysis.

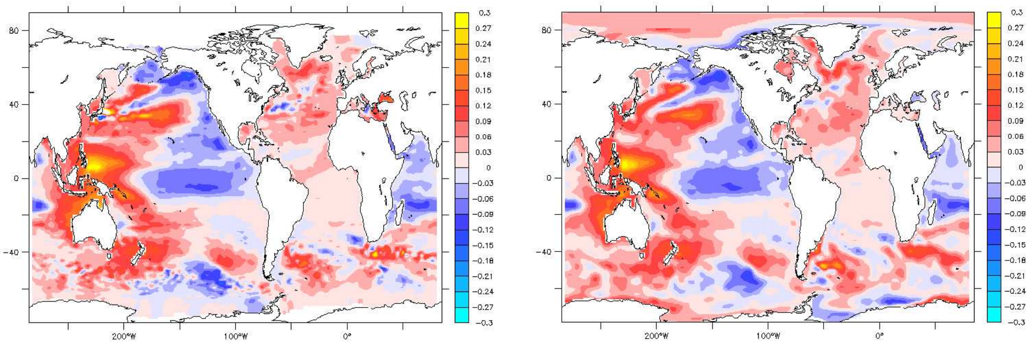


FIG. 1.5 – Sea level trend between 1993 and 2001 : on the left from the merged observed satellite products, on the left from the reanalysis

1.5 Medium range surface ocean predictability dependency of the atmosphere forecast in the northern Atlantic (Y. Drillet and R. Bourdallé-Badie)

The Mercator-Ocean system provides a weekly analysis and a 14-days forecast of the ocean with a 1/3° North Atlantic model coupled assimilating altimetry, in situ and climatology data sets. This forecast is better than the persistency but the ECMWF monthly ensemble atmospheric forecast allows an extension to 1 month forecast. This study shows a equivalence of the 7-days ocean forecast with the two atmospheric data set, an improvement of the 14-days ocean forecast using the ECMWF ensemble mean forecast and a

28-days ocean forecast always better than the persistency with significant correlation especially between SST forecast and best estimate. ovement for the 14-day ocean forecast forced by the ensemble atmospheric forecast is important for all ocean surface variables with a large difference in the evolution of the skill score. For the SST (Figure 1.6), the skill score stays stable around 0.36 when it decreases under 0.3 with the operational atmospheric forecast. This decreasing of the skill score is clearly linked to the total heat flux which has the same comportment. The persistency of the atmospheric forecast during the last 4 days of forecast has a direct impact on the performance of the ocean forecast system. For the sea surface height, the skill score for the two forecasts decreases between 7 and 14-days time, with a faster decreasing for the forecast forced by the operational atmospheric forcing linked to wind forecast which have a negative skill score for the 14-days time.

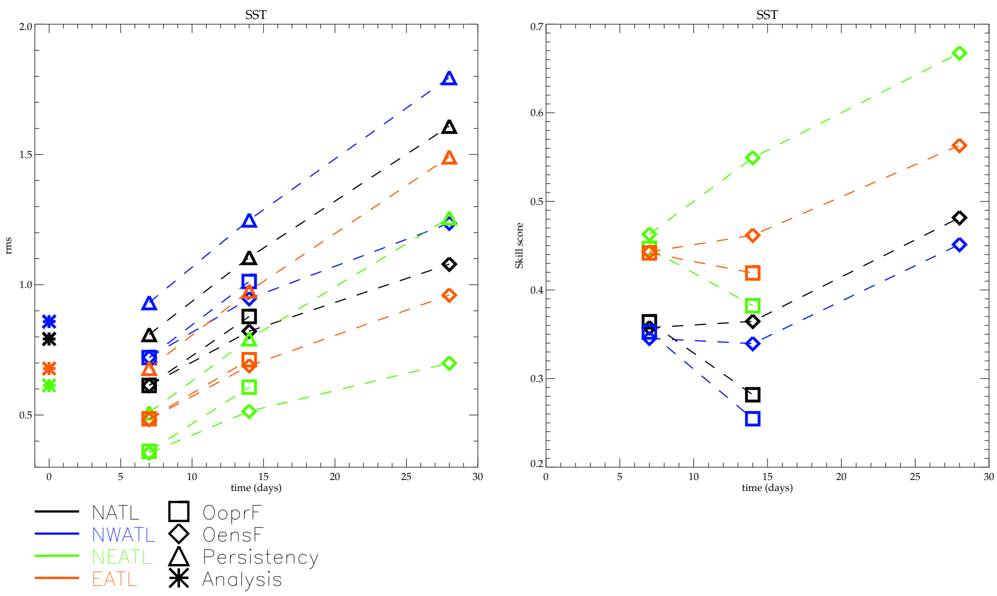


FIG. 1.6 – Annual mean of the SST RMS error (left panel) and skill score (right panel) for the 7-days, 14-days and 28-days forecasts computed over the global North Atlantic domain (NATL in black), the North West Atlantic (NWEATL in blue), the North East Atlantic (NEATL in green), the East Atlantic (EATL in red). Square represents the operational ocean forecast, lozenge the ensemble mean forecast and triangle the persistency. The stars are the RMS error computed between best analysed and Reynolds SST.

1.6 Evaluation of the meso-scale activity in the mercator-ocean global eddy resolving model (R. Bourdallé-Badie, C. Derval, O. LeGalloudec and Y. Drillet)

1.6.1 Model Description

The eddy resolving Mercator-Ocean OGCM (there after called ORCA12) is based on NEMO code [11], which includes the OPA9 ocean model coupled to the LIM2 sea ice model [5]. The grid is a global quasi isotropic tripolar ORCA grid, 2 poles in the northern hemisphere [10], with resolution from 9.3 to 1.8 km (Fig. 1.7). Vertical coordinate is z-levels type with partial cells parameterization [2].The vertical resolution is based on 50 levels with layer thickness ranging from 1m at the surface to 450 at the bottom. The thickness is lower than 2 m in the 10 m upper layers of the ocean to increase around 20 m at 100 m depth and 170 m at 1000 m depth.

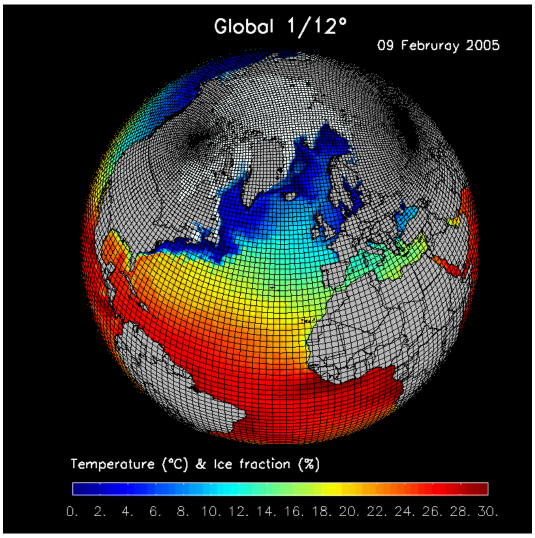


FIG. 1.7 – ORCA12 grid ; 1 point on 24 is plotted

A free surface that filters high frequency features is used for the surface boundary condition [14]. The closure of the turbulent equation is a turbulent kinetic energy mixing parameterization. TVD advection scheme [9] is used for the tracer fields combine to an enstrophy and energy conserving scheme [2] and [1]. An isopycnal laplacian operator is used for the lateral diffusion on the tracers (125 m2.s-1) and a horizontal bilaplacian operator is used for the lateral diffusion on momentum. (-1.25e10 m2.s-2) on the largest meshes (at the equator). On the momentum part, laplacian diffusion is added at the equator, between $2^oS - 2^oN$. This is a function nullify at 2^o and maximum at the equator $(20m^2.s^{-1})$. In this simulation, a partial slip condition is applied at the coast in the entire domain expect in Mediterranean Sea where a no slip one is applied. A nonlinear bottom friction is applied.

The global bathymetry is processed from ETOPOV2g bathymetry. Monthly climatological runoffs, from the Dai & Trenberth database [3], are prescribed [MER14]. A runoff along the Antarctic [7] coast has been added with an annual value of 2613 kg/year. The model is initialised with the Levitus temperature and salinity climatology [8]. Two restoring zones toward climatological temperature and salinity are prescribed, one in the Gulf of Cadiz and the other in the Babel Mandeb strait. ORCA12 is forced by the CLIO bulk formulae [6] using wind stress, evaporation, precipitation, net heat and solar fluxes. Atmospheric forcing fluxes are daily temporal mean of the 6-hours operational analyses provided by the European Center for Medium-range Weather Forecasts (ECMWF). The ORCA12 simulation covers the period from the 01 January 1999 to the 31 december 2006

The ORCA12 simulation has been performed on 158 processors of the mercator-ocean computer (SGI scalar computer). The memory cost of this model is 370 Go and 30500 CPU hours are needed for 1 year of simulation. 3-days mean outputs have been stored.

To evaluate to improvement due to the resolution a simulation with the mercator-ocean "eddy permitting" OGCMS (thereafter call ORCA025) [2] have been performed. The code, the parameterisations, the bulk formulae and the initialisation and forcing files are the same than for the ORCA12 experiment. The differences are : 1) the grid resolution ($1/4^o$ at the equator versus $1/12^o$ for ORCA12) 2) the values of diffusion coefficients (laplacian isopycnal for the tracers at $300m^2.s-1$; bilaplacian for the momentum at $-3^{e11}m^2.s^{-2}$ and maximum laplacian added at the equator for momentum at $200m^2.s^{-1}$.

1.6.2 Data description

Three data bases have been used in this study : the sea surface height simulated by ORCA12 (eddy resolving global model)), simulated by ORCA025 (an eddy permitting global model) and the altimetry data combining several satellites available. All these data covered the period 2004 to 2006. The horizontal resolution and the temporal sampling of these data bases are not homogeneous. The output models are 3 days mean each 3 days when the altimetry maps combined every 7 days the data collected by almost 3 satellites (Jason, Envisat, GFO). The time scale that we are talking about in the following is largely larger than the sampled of these data, so we considered that the biases which can be introduce by this sampling is negligible. The horizontal resolutions of the data bases are also different. The two model outputs are respectively for ORCA025 and ORCA12 at the $1/4^o$ and at the $1/12^o$. The altimetry data is on a regular $1/3^o$ grid. The differences between these grids can also introduced some biases than we also considered as negligible compare to the space scale considered in this study.

1.6.3 Sea surface height Variability

A 7 years simulation has been performed with the ORCA12 model. The firsts years are not studded, they are considerate as a ”spin-up” period. The studding period covered the years 2004 to 2006. The mean general circulation is, in both models ($1/4^o$ and $1/12^o$), in good agreement compare to the altimetry observation (Figure 2) : Western boundaries currents pathways are correct, particularly the Gulf Stream separation well simulated in the $1/12^o$ model. The overshoot, present in the eddy-permitting models, like ORCA025, is not present in ORCA12. Figure 1.8 shows the Root Mean Square (rms) of sea surface height, over the period 2004 to 2006, for both models and for altimetry data. The global pattern of both models is correct. The models are able to reproduce the ocean variability observed in major currents with a realistic level of energy. Nevertheless, in some places, the global $1/4^o$ simulation shows a lake of intensity compare to the observations. The $1/12^o$ simulation reproduces very well the observed variability with a good level of intensity at all latitudes. The penetration of western boundaries currents is more realistic $1/12^o$ than in the $1/4^o$ (kuroshio extension, North Atlantic Current). The meso-scale activity around Australia is improved in the global $1/12^o$ compare to the $1/4^o$ global model. The Leeuwin current extension is very well represented in the $1/12^o$ model. High resolution is a necessity to resolve the first Rossby radius and so well represent meso-scale activity and variability at these latitudes [12].

[1] A. Arakawa and P. J. Lamb, (1980), A potential enstrophy and energy conserving scheme for the shllow water equations, *Monthly Weather Review*, **109**, 18–36.

[2] B. Barnier and et al., (2006), Impact of partial steps and momemtum advection schemes in a global ocean circulation model at eddy permitting resolution, *Ocean Dynamics*, **DOI : 10.1007/s10236-006-0082-1**.

[3] Dai and Trenberth, (2003), New estimates of continental discharges and ocean freshwater transport, *AMS Symposium on Observing and Understanding the Variability of Weather and Climate, Long Beach*.

[4] M. Drevillon and et al., (2008), The GODAE/Mercator-Ocean global ocean forecasting system : results,applications and prospects, *accepted to appear in Journal of Operational Oceanography*, **1**, 51–57.

[5] H. Goosse, J.-M. Campin, E. Deleersnijder, T. Fichefet, P.-P. Mathieu, M. A. Morales Maqueda, and B. Tartinville, (2001), Description of the CLIO model version 3.0.

[6] H. Goosse, J.-M. Campin, E. Deleersnijder, T. Fichefet, P.-P. Mathieu, M. A. Morales Maqueda, and B. Tartinville, (2001), Description of the CLIO model version 3.0.

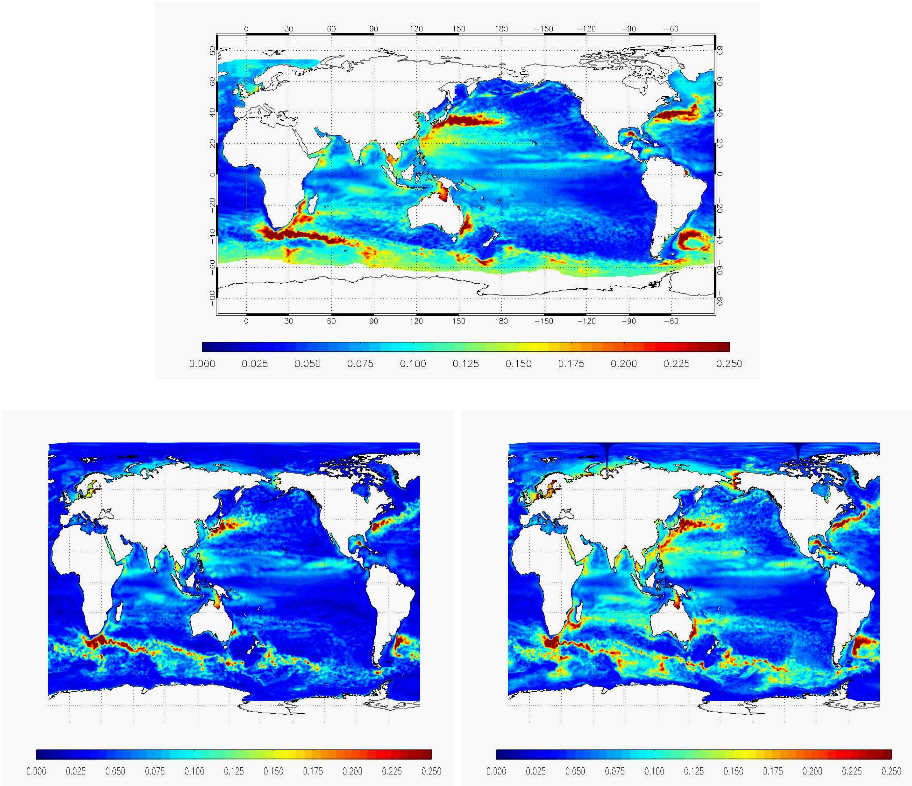


FIG. 1.8 – Sea surface height variability over the year 2004-2006 for the altimetric data (high) ; ORCA025 (bottom left) ; ORCA12 (bottom right)

[7] S. Jacobs and et al., (1992), Melting of ice shelves and mass balance of Antarctica, *Journal of Glaciology*, **38**, 375–387.

[8] S. Levitus, J. Antonov, and T. Boyer, (2005), Warming of the world ocean, 1955-2003, *Geophy. Res. Lett.*, **32**.

[9] M. Lévy and et al., (2000), Choice of an advection scheme for biogeochemical models, *geophysical Research Letter*, **28**.

[10] G. Madec and M. Imbard, (1996), A global ocean mesh to overcome the North Pole singularity, *Clim. Dyn.*, **12**, 381–388.

[11] G. Madec, P. Delecluse, M. Imbard, and C. Levy, (1998), OPA8.1 : Ocean general circulation model reference manual, *Notes du pole de modélisation, Institut Pierre-Simon Laplace (IPSL)*.

[12] M. E. Maltrud and J. L. McClean, (2005), An eddy resolving global $1/10^o$ ocean simulation, *Ocean Modelling*, **8**, 31–54.

[13] D. Pham, J. Verron, and M. Roubaud, (1998), A Singular Evolutive Extended Kalman Filter for data assimilation in oceanography, *J. Marine Syst.*, **16(3-4)**, 323–340.

[14] G. Roullet and G. Madec, (2000), Salt conservation, free surface and varying volume : a new formulation for ocean GCMs, *J. of Geophysical Research - Oceans*, **105, 23,927-923,942**.

[15] B. Tranchant, C. Testut, L. Renault, and N. Ferry, (submitted in 2007), Data assimilation of simulated SSS SMOS products in an ocean forecasting system, *Journal of operational Oceanography*.

[16] B. Tranchant, C. Testut, L. Renault, N. Ferry, F. Birol, and Brasseur, (2008), Expected impact of the future SMOS and Aquarius Ocean surface salinity missions in the Mercator Ocean operational systems : New perspectives to monitor ocean circulation, *accepted to appear in Remote Sensing of Environment*, **112**, 1476–1487.

[17] A. Weaver, J. Vialard, and A. L.T., (2003), Three- and Four-Dimensional Variational Assimilation with a General Circulation Model of the Tropical Pacific Ocean ;, Part I : Formulation, Internal Diagnostics, and Consistency Checks, *Mon. Wea. Rev.*, **131**, 1360–1378.

2 Publications

2.1 Journal Publications

[MER1] B. Barnier, T. Madec, G.and Penduff, J.-M. Molines, A.-M. Treguier, J. Le Sommer, A. Beckmann, C. Boning, J. Dengg, C. Derval, E. Durand, S. Gulev, E. Remy, C. Talandier, S. Theerren, M. Maltrud, J. McClean, and B. de Cuevas, (2007), Impact of partial steps and momentum advection schemes in a global ocean circulation model at eddy-permitting resolution, *Ocean Dynamics*, **56**, 543–567.

[MER2] J. Lellouche, S. Giraud, L. Crosnier, E. Greiner, and M. Benkiran, (2007), The High Resolution Real Time Mercator Forecasting System : Description and evaluation in the Gulf of Mexico, *submitted to J. Marine Syst.*

[MER3] E. Obligis, C. Boone, S. Philipps, G. Larnicol, B. Tranchant, and P. Le Traon, (accepted for publication in 2007), Benefits of the future Sea Surface Salinity measurements from SMOS. generation and characteristics of SMOS geophysical products, *IEEE trans. geoscience and remote Sensing*.

2.2 Conference Proceedings and Book Chapters

[MER4] M. Drévillon and the Mercator Team, (May 13-18, 2006), The PSY3v1 GODAE Mercator ocean foreacsting system, a global eddy permitting (1/4°) ocean model assimilating altimetry data, 15 years of progress in radar altimetry,symposium, Venice, Italy, p. 114.

[MER5] M. Drévillon and the Mercator Team, (2007), The GODAE/Mercator-Ocean global ocean analysis and forecasting system assimilating ARGO data, UGG XXIV General Assembly, Perugia, Italy, July 2–13.

[MER6] M. Drévillon and the Mercator Team, (2007), THE MERSEA / MERCATOR-OCEAN GLOBAL 1/4° ANALYSIS AND FORECASTING SYSTEM V2, Proceedings of the MERSEA Meeting, Roma, Italy, April.

[MER7] N. Ferry, B. Tranchant, C.-E. Testut, M. Rémy, E. Drévillon, E. Greiner, M. Benkiran, J. Lellouche, and P. Brasseur, (May 13-18, 2006), Fifteen Years of Altimetry and Satellite Data : Benefits for Mercator Ocean Operational Forecasting System, 15 years of progress in radar altimetry,symposium, Venice, Italy, p. 182.

[MER8] J. Lellouche and the Mercator Team, (2007), The regional Mercator-Ocean high resolution analysis and forecasting system : a benchmark for the future global high resolution forecasting system, UGG XXIV General Assembly, Perugia, Italy, July 2–13.

[MER9] J. Lellouche, M. Benkiran, L. Crosnier, and E. Greiner, (May 13-18, 2006), Assesment and validation of the new multivariate Mercator high resolution forecasting system, 15 years of progress in radar altimetry,symposium, Venice, Italy, p. 113.

[MER10] E. Remy, A. Weaver, and N. Daget, (May 13-18, 2006), Controling the large-scale ocean circulation using a multivariate 3D-Var approach ; the complementary role of altimetry and in situ measurements, 15 years of progress in radar altimetry,symposium, Venice, Italy, p. 113.

[MER11] E. Remy, A. Weaver, and M.-H. Rio, (2007), Combining in-situ and altimetry observations in a low resolution global ocean reanalysis, UGG XXIV General Assembly, Perugia, Italy, July 2–13.

[MER12] B. Tranchant, C.-E. Testut, N. Ferry, and P. Brasseur, (May 13-18, 2006), Interest of combining satellite altimeter data with temperature and salinity data on the new assimilation MERCATOR System, 15 years of progress in radar altimetry,symposium, Venice, Italy, p. 114.

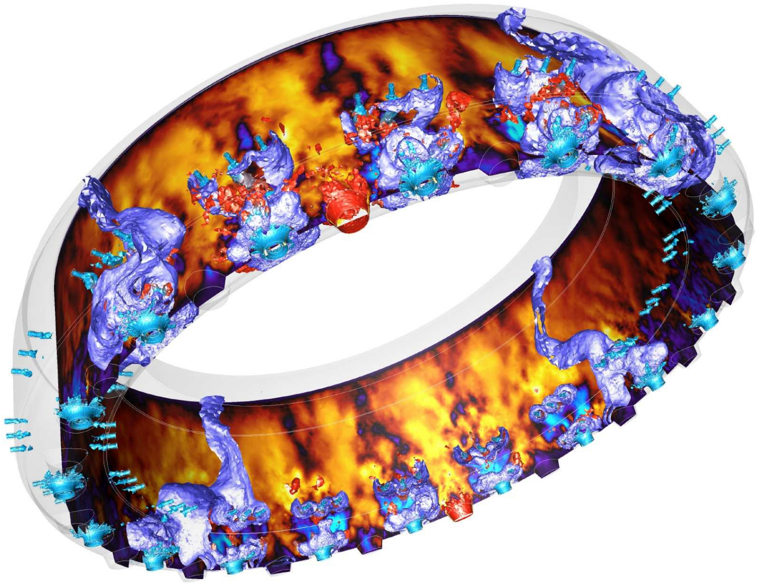
[MER13] B. Tranchant, C.-E. Testut, L. Renault, N. Ferry, and P. Brasseur, (2007), Interest of assimilating future Sea Surface Salinity measurements from SMOS and Aquarius missions in the Mercator Ocean operational systems, UGG XXIV General Assembly, Perugia, Italy, July 2–13.

2.3 Technical Reports

[MER14] R. Bourdallé-Badie and A.-M. Treguier, (2006), A climatology of runoff for the global ocean-ice model ORCA025, technical report, Mercator-Ocean.

6

Combustion



1 Introduction

Thierry Poinsot

The combustion activity at CERFACS takes place within the CFD team. 25 to 30 researchers (including PhD students and post doctoral students) participate to the combustion research. Even though RANS (Reynolds Averaged Navier Stokes) and DNS (Direct lSimulation) activities continue in this field at CERFACS, the LES (Large Eddy Simulation) revolution is now driving the activity of the combustion group because LES bridges the gap between simulation tools used for research and required for industry. The software developed by CERFACS and IFP (AVBP) is a standard tool for reacting flows at many places in Europe (CNRS laboratories, ONERA centers, Universities in Spain, England, Netherlands or Germany, etc) but is also industrialized for industrial partners (SNECMA, Turbomeca, PSA, Renault). Numerical studies of combustion instabilities and combustion noise are growing areas. More generally, LES is now receiving multiple additional submodels to fully demonstrate their potential in realistic configurations : flow near multiperforated plates, radiation, acoustic boundary conditions for turbines and compressors. LES tools are also being coupled to other solvers to predict acoustic fields or structure mechanical and thermal loading. For the first time in 2007, CERFACS has simulated a full annular combustion chamber on massively parallel machines, setting up new references in the field.
The combustion activity covers all fields linked to modern research organization : research, teaching, formation, interaction with industry. The academic quality of combustion research at CERFACS is well established through numerous publications in refereed journals and invited conferences : the very strong investment in AVBP over the last years (approximately 200 man year) has made it a unique research tool and a strength for all students and researchers who want to study combustion and publish their results. In terms of man-power, the team is organized around 5 permanent scientists and more than 20 researchers staying less than 4 years. Most combustion scientists leaving CERFACS find positions right away and keep in touch with CERFACS. The collaboration with french laboratories is also excellent : CERFACS provides codes to IMF Toulouse, CORIA in Rouen, EM2C in Ecole Centrale Paris and participates to multiple contracts with other research institutions. European support is very strong with multiple FP'6 and FP'7 programmes (Fluistcom, Intellect, Molecules, Quantify, Timecop, Eccomet, Aether, Myplanet, Limousine, TLC...). The EST Marie Curie projects Eccomet and Myplanet are examples of recent CERFACS successes : these two projects coordinated by CERFACS have provided support to hire 15 European PhD students between 2006 and 2011 as well as 10 visitors. These scientists will be working on two-phase flow combustion and combustion instablities at CERFACS, ONERA and IMFT and contribute to the advancement of fundamental research in this field.

2 Basic phenomena

The combustion team at CERFACS has now a long experience in turbulent combustion modelling and simulation. Fundamental issues are addressed, related to flame dynamics, chemistry, thermodynamics, interaction with walls, heat transfer, radiation, phase change, flame / acoustic interactions, etc ... as well as numerical schemes and high performance computing. The numerical approaches go from Direct Numerical Simulation to Large Eddy Simulation and RANS.
The models and computational methodologies developed in the team are validated against academic or generic laboratory configurations, simpler than the real ones but still representative and allowing a detailed experimental characterisation. This is a crucial step before the application to the large variety of real industrial configurations considered in the team. Aeronautical gas turbines for both aircrafts and helicopters are the main class of application, but piston engines and rocket engines are also treated.
The simulation of complex industrial systems requires efficient numerical techniques as well as accurate physical submodels. This is the purpose of a series of activities devoted to numerical schemes and the understanding and modelling of physical mechanisms. To facilitate the studies these mechanisms are isolated in simplified generic configurations.

2.1 Direct and Large Eddy Simulations of Effusion Cooling (S. Mendez, F. Nicoud, T. Poinsot)

One crucial but complex physical issue is linked to wall phenomena. Turbulent gaseous flows along walls become very complex in the presence of a flame or hot gases. Moreover industrial burners use walls that are perforated with numerous and submillimetric holes. These multiperforated walls play a key role in the burner cooling but have also a non negligible effect on the flow inside the burner. Consequently they must be taken into account in simulations and, because their direct computation would be too costly, they require specific modelling. This was the objective of the PhD work of S. Mendez (defended in fall 2007) who realized Direct Numerical Simulations (DNS) of one hole of such multiperforated plates (Fig. 2.1) and built a model to represent their dynamic and cooling effect. This work was published in [1]. It is now continued to take into account the coupling between the internal and external flows through the multiple holes on the walls, and to study the effect on acoustics.

[1] S. Mendez and F. Nicoud, Large-eddy simulation of a bi-periodic turbulent flow with effusion, *J. of Fluid Mech.*, in press, 2008.

2.2 Interaction of a flame with liquid fuel on a wall (G.Desoutter, B. Cuenot, C. Habchi)

Another important wall phenomenon in piston engines or in injection systems of gas turbines is the formation of liquid films on the walls that may lead later to unburnt hydrocarbons, smoke, and a reduced engine efficiency. In piston engines, this is particularly true for Direct Injection Engines (IDE). Using DNS, G. Desoutter studied during his PhD (defended in spring 2007) the interaction between a liquid film and a

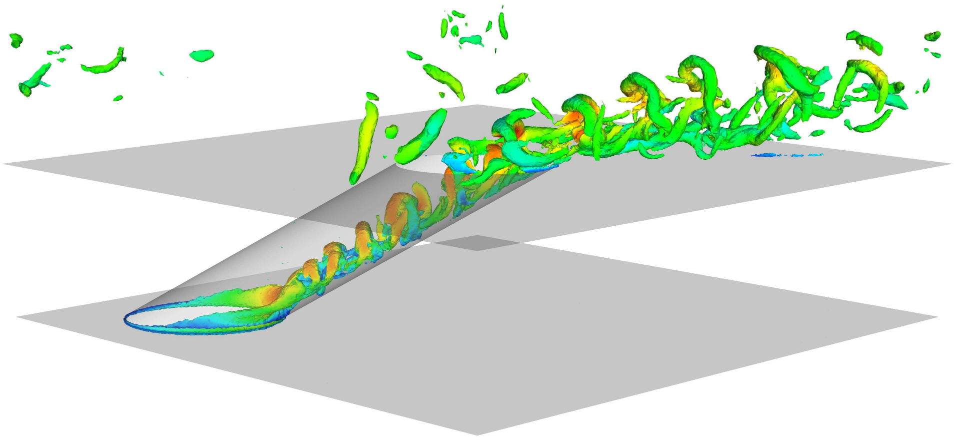


FIG. 2.1 – Visualization of the structure of the flow around a perforated plate obtained by Direct Numerical Simulation (velocity iso-surface) [1].

flame. His detailed analysis allowed to develop a model for RANS, in the form of a modified law of the wall that predicts the evaporation of the film. Implemented in the code of IFP, the new law of the wall was tested and evaluated in engine simulations.

2.3 Chemistry (G.Albouze, G.Boudier, B. Cuenot, T. Poinsot)

Although strongly linked to the flow, combustion remains chemically controlled and this aspect must be treated with great care. One and two-step reduced chemical schemes are useful and are used routinely at CERFACS [COMB4, COMB9, COMB1]. However, they are not sufficiently accurate when the mixture is too rich or when ignition mechanisms or pollutant levels must be predicted. To overcome this difficulty one promising method is the use of tabulations that represent with sufficient detail the chemical behavior of the system. CERFACS tests this technique in collaboration with EM2C Paris, CORIA Rouen and IFP. For example, the FPI method, originally developed by O. Gicquel [2] reconstructs the flame structure from only two variables (the mixture fraction and the progress variable) and a tabulation. The FPI approach may be either used with the Thickened Flame model or with a Pdf approach for turbulent combustion. It was implemented in AVBP, and tested on 1D laminar flames as well as on the turbulent premixed burner of PRECCINSTA [3], where it gave encouraging results.

[2] B. Fiorina, O. Gicquel, L. Vervisch, S. Carpentier and N. Darabiha, Premixed turbulent combustion modeling using a tabulated detailed chemistry and PDF, *Proc. of the Comb. Inst.*, **30**-1, 867-874, 2005.
[3] S. Roux, G. Lartigue, T. Poinsot, U. Meier and C. Bérat, Studies of mean and unsteady flow in a swirled combustor using experiments, acoustic analysis and Large Eddy Simulations, *Combustion and Flame*, **141**, 40-54, 2005.

2.4 Euler modelling of particle dispersion (E. Riber, B. Cuenot, T. Poinsot, O. Simonin)

In the Euler - Euler approach for the liquid disperse phase, the droplet velocity represents the statistical average of the velocities of all droplets present in the cell. As a consequence the true droplet velocities, not explicitly known, contribute to a non zero standard deviation from the mean. In her PhD thesis (CERFACS and IMF Toulouse, defended early 2007) E. Riber has studied the role of this velocity deviation, the so-called ”Random Uncorrelated” (RU) velocity, in the cases of the two-phase jet flow of Ishida [4] and of Borée et al [5]. If its impact on the mean velocity is limited, the RU velocity contributes significantly to the liquid phase velocity fluctuations as measured in experiments. In two-phase combustion these fluctuations have an important role as they contribute to the mixing of the reactants. It is therefore necessary to reconstruct this quantity in the Eulerian formulation, which is still an open problem. One possible way is to solve a conservation equation for the corresponding kinetic energy, which has been implemented in AVBP. The challenge is to write the correct models for the production and destruction terms of this equation (paper to appear in J. Comp. Phys. in 2008).

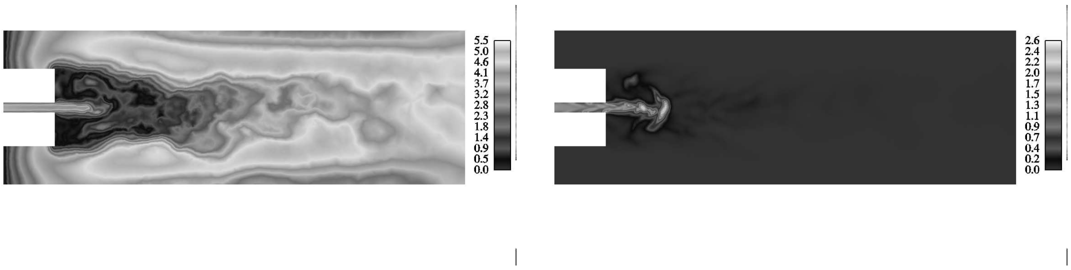


FIG. 2.2 – Instantaneous fields of particle velocity modulus (left) and particle volume fraction (right)obtained with the Euler-Euler approach in the cutting plane $y = 0$ of the configuration of Borée et al. [5].

[4] K. Hishida, K. Takemoto and M. Maeda, Turbulent characteristics of gas-solids two-phase confined jet, *Japanese Journal of Multiphase Flow*, **1**-1, 56-69, 1987.
[5] J. Borée, T. Ishima and I. Flour, The effect of mass loading and inter-particle collisions on the development of the polydispersed two-phase flow downstream of a confined bluff body, *J. of Fluid Mech.*, **443**, 129-165, 2001.

2.5 Numerical aspects (M. Porta, N.Lamarque, J.-M. Senoner, B. Cuenot, T. Poinsot, R. Abgrall)

The quality of Large Eddy Simulation of turbulent flows is strongly conditioned by the accuracy and robustness of numerical schemes. This is even more critical for compressible flows and reacting flows, where sharp velocity or density gradients may appear. Finally the performance of the numerical schemes is also altered near boundaries where the mathematical problem may not be well posed. Therefore a compromise must be found between accuracy and stability, that depends on the numerical scheme, the geometry and the flow considered. This has been extensively studied in the PhD thesis of N. Lamarque and M. Porta (both defended in 2007). To increase stability while keeping accuracy, one possible alternative to the centered schemes used today in AVBP is the distributed residuals method, that leads to partially upwinded schemes. The difficulty is to determine the best distribution of nodes weight to reach the accuracy and stability target. This is an on-going work, in collaboration with the group of R. Abgrall (MATMECA) who developed this class of schemes.
Another numerical issue is the implementation of time implicit integration. Up to now only explicit methods

have been used in AVBP, essentially due to the complexity of implicit methods and the uncertainty about the true computing time reduction when it comes to calculate reacting compressible flows with high accuracy. CERFACS and Stanford studied this question together in the last two years, comparing AVBP and the LES code of Stanford, CDP which is implicit. The conclusion was that the gain offered by the implicit solver in the stabilized phases of the flow was not large but that in most configurations, a significant computing time was devoted to transient phases during which the physical solution is built. These phases do not have any physical meaning and are systematically removed from the analysis. As a consequence the required level of accuracy during these phases is reduced and must be just enough to lead to the correct solution after stabilisation. Moreover the details of the time evolution of the flow are of no interest and may be skipped. In this context implicit methods have a clear interest as they will allow to install physical solutions much faster and save substantial computing time. Work has started towards the implementation of such methods in AVBP, and first basic tests have been conclusive.

3 LES of two-phase reacting flows

3.1 LES of two-phase flames based on Euler-Euler formulation (M. Boileau, N.Lamarque, J. Lavédrine, G. Lacaze, M. Sanjosé, B. Cuenot, T. Poinsot)

The Euler-Euler model for the simulation of two-phase reacting flows has been integrated in the current version of AVBP (AVBP6.0) and is used today in production mode. Most projects involve the simulation of the liquid disperse phase and the team is currently accumulating experience in the behavior of such flows in complex geometries.

The two-phase flow model has been applied to the configuration installed on the MERCATO test facility of ONERA (Fauga), with an injector system of Turbomeca. The simulation results have been compared to the measurements for both phases in evaporating regimes without combustion. Agreement for the liquid phase is not as excellent as for the gas phase but is already satisfactory even though polydisperse effects are not accounted for. The same methodology has been applied to the simulation of two other configurations with injectors from Snecma and Turbomeca (TLC project). Again the comparison with measurements for the liquid phase is very encouraging and was published in FLow, Turb. Combustion [6].

The robustness of the code even allowed to compute a very large scale geometry, namely an annular combustor of Turbomeca in an ignition regime (to appear in Comb. Flame 2008). Computing the entire annular burner instead of one sector only is crucial for at least two phenomena. First azimutal acoustic modes are correctly captured only if the whole geometry is taken into account. Second the ignition mechanism of the full burner involves specific processes that are totally different from the ignition mechanism of one single burner : for the first burner, an igniter (either a spark plug or a torch flame) is used to initiate combustion, whereas all other sectors of a full chamber are ignited by the propagation of the flame from its closest neighbor. As the flame propagation is submitted to the surrounding turbulent flow, itself very sensitive to the geometry, only the full chamber computation gives a correct overview of the ignition process. During his PhD (defended in 2007) M. Boileau succeeded in setting up and running such a simulation, which still constitues a World Premiere (Fig. 3.1). The detailed analysis of the results confirmed the interest of computing the fulll geometry and allowed to identify key mechanisms that were never isolated before.

The Euler-Euler model has also been applied successfully to another type of application, namely the two-phase combustion in a rocket engine. The PhD work of G. Lacaze focuses on the study of the ignition and burning of the VINCI engine that is currently under development at Snecma. In such burners the oxygen is injected as liquid whereas hydrogen, previously used as a cooler fluid, is gaseous. The oxygen liquid jet does not atomize as droplets but more as ligaments and the Euler Euler approach is well suited to this very complex regime where droplets can not be identified. The evaporation, mixing and flame ignition mechanisms must be closely controlled to reach the required levels of reliability and robustness for such engines. Another particularity of the VINCI engine is that is is a stage engine that is operated in a very low pressure environment (almost void). This implies high compressibility effects (shocks) that add to the complexity of the system. Nevertheless the two-phase reacting simulations have been performed and first results show a correct and physical behaviour of the model (Fig. 3.2).

FIG. 3.1 – Temperature field in the combustor at one instant of the ignition sequence (grey : cold - white : hot). The black line is the iso-level T=1500 K locating the flame front which propagates in the azimuthal direction close to the injectors outlets.

[6] M. Boileau, S. Pascaud, E. Riber, B. Cuenot, L. Y. M. Gicquel, T. J. Poinsot and M. Cazalens, Investigation of Two-Fluid Methods for Large Eddy Simulation of Spray Combustion in Gas Turbines, *Flow Turb. Comb.*, **80**, 291-321, 2008.

3.2 LES of two-phase flows based on Euler-Lagrange formulation (M. Garcia, F. Jaegle, J.M. Senoner, B. Cuenot, T. Poinsot)

In parallel to the Euler-Euler model, CERFACS is developing an Euler-Lagrange version for two-phase flow simulations with AVBP. The main difficulties linked to the Lagrangian approach are (1) the efficient computation of the individual droplets in the context of massively parallel computing and (2) the accurate and robust calculation of the mass and heat transfer between the phases. Indeed the droplets act as individual point source terms, that may be destabilizing for non dissipative numerical schemes used in LES, and not statistically representative if a sufficient number of droplets in the cell is not reached. Moreover the coupling between the phases requires the use of interpolators that may alter the accuracy of the solution. On the other hand the Lagrangian formulation allows to calculate in a direct way (i.e. without modelling) important effects such as droplet dispersion or interaction with walls. Today the question of the best approach (either Eulerian or Lagrangian) for the disperse phase is still widely open. CERFACS and Stanford collaborated actively on this issue at the CTR Summer Program of 2006 [COMB50] where a Lagrangian solver from Stanford was compared to Eulerian and Lagrangian solvers from CERFACS (using AVBP) for the experiment of Borée et al [4]. The two methods have a clear potential and CERFACS now develops both.
The efficient implementation of a Lagrangian parallel solver in AVBP has been realized by M. Garcia during her PhD (to be defended end of 2008). Using specific domain partitioning methods and load balancing it is possible to keep a very good scalability of the code and reach high efficiencies even on an important number of processors. The extension to combustion was performed by F. Jaegle and J.M. Senoner, both

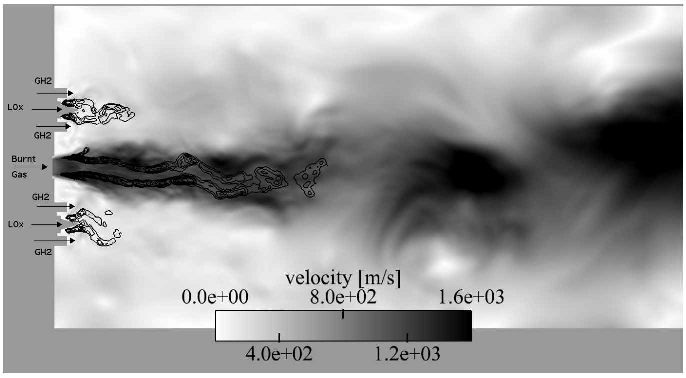


FIG. 3.2 – Instantaneous view of the velocity and reaction rate isocontours in the vicinity of the igniter in a VINCI type engine.

PhD students of the Marie Curie project ECCOMET, coordinated by CERFACS. They implemented models for evaporation and mass transfer to the gas phase and tested the final combustion model on simple one-dimensional laminar flames where they obtained results very similar to the results obtained in the Eulerian formulation. Finally the model was applied to the MERCATO configuration mentioned in the previous section, which demonstrated the feasability of such simulations (Fig 3.3).

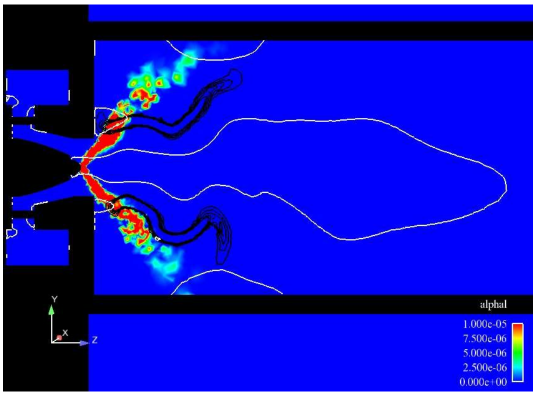


FIG. 3.3 – Instantaneous view of the volume fraction field and reaction rate isolines (black lines) in the configuration MERCATO obtained with Euler-Lagrange AVBP solver. White lines inidicate zero axial velocity.

4 Unsteady combustion

4.1 LES of combustion instabilities (A. Giauque, G. Staffelbach, A. Roux, L. Gicquel, N. Lamarque, G. Boudier, T. Poinsot)

The main driving force behind the development of LES tools in the last five years at CERFACS has been the study of combustion instabilities. Initiated first for Siemens and Alstom, these studies are now performed for SNECMA and TURBOMECA. In 2006 and 2007, multiple studies have been devoted to LES of combustion instabilities. This sections summarizes some of the recent results obtained in this field.

The baseline solver for unsteady combustion studies at CERFACS is AVBP. It is used with various submodels for combustion (one and two-step reduced schemes, FPI methods for more complex kinetics), subgrid scale tensor (WALE [7], dynamic model, one-equation model), gray gas models for radiation, law-of-the-walls for heat transfer. Since 2005, it was applied to industrial gas turbines [COMB10, COMB4, COMB9], laboratory burners [COMB2, COMB13], aero gas turbines [COMB1] or ramjets [8]. The most important results which come out consistently from these studies are the following :

- LES of reacting flows is reaching maturity and can be done in complex geometries, provided high-order spatial schemes and small time steps are used. A compressible solver is also mandatory to capture acoustic waves [9].
- LES captures the unstable modes exhibited by real combustors both in frequencies and amplitudes but results remain very sensitive to numerical parameters (scheme order), acoustic parameters (impedances) and models. For example, taking into account radiation and heat losses at walls modifies the frequency and the amplitude of modes [COMB13, COMB9].
- Present computer capacities allow to reach resolution in small gas turbine chambers which are sufficient to ensure mesh independent results or more precisely for LES, mesh convergent results. This was shown by Boudier et al [COMB34] who compared reacting flow results in a complex geometry burner for three levels of refinement ranging from 1.5 million to 44 million elements and showed that results on the medium and fine grid were quite similar in terms of mean values. However, for RMS values, this is true only for the flow variables (velocity field) ; the temperature and the species which are controlled by subgrid scale phenomena continue to present more and more small scales and wrinkling as the mesh is refined [COMB34].
- Analyzing LES results can be difficult and additional tools are useful to understand the unsteady activity appearing in the LES results. This includes tools to construct maps of spectral activity, POD (proper orthogonal decomposition) [8] which have been coupled to AVBP but also acoustic solvers such as AVSP described in Section 4.2.
- Unmixedness has been identified in multiple burners as a major and often neglected source of instability [10]. Predicting instabilities in real combustors will require the computation of the mixing process between air and fuel even if this one is often supposed to be perfect.
- The role of azimutal modes in annular chambers has also become a theme of major importance. These modes have been out of reach of LES for a long time because most LES codes were able to compute only one sector of the real turbine instead of the 15 to 24 which compose the turbine. A major breakthrough achieved at CERFACS in 2007 is the first LES of a complete gas turbine chamber.

As an example, Fig. 4.1 displays the temperature field (right picture) in a complete TURBOMECA combustion chamber in which an azimutal mode appears under certain extreme conditions. This LES was

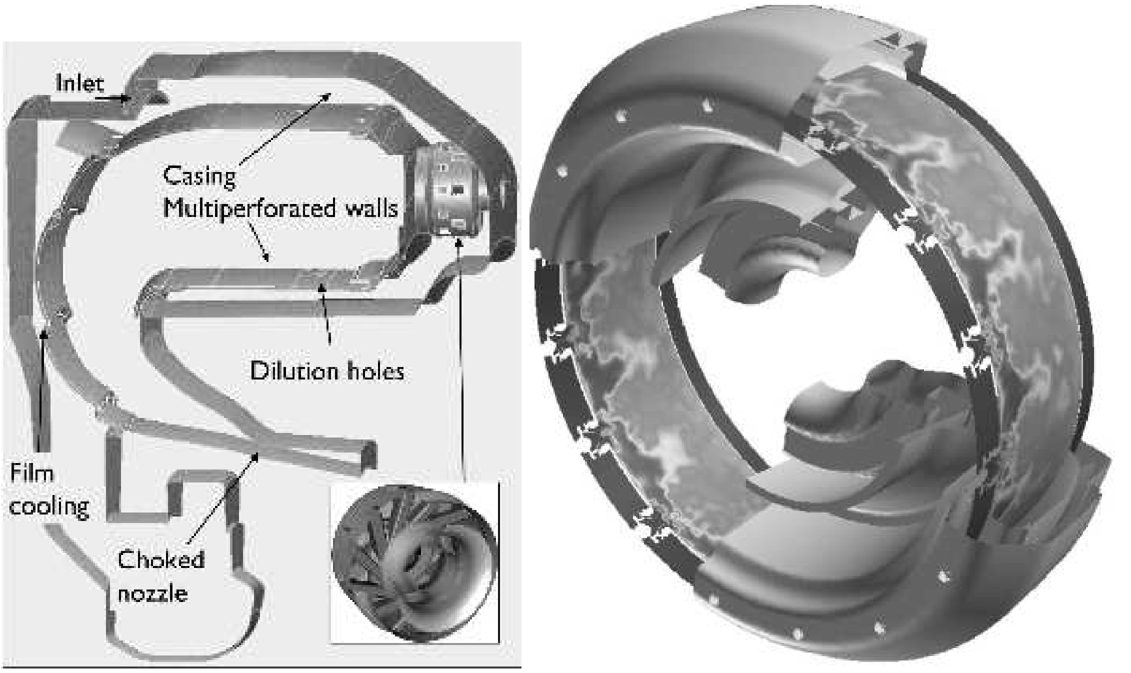


FIG. 4.1 – The first LES of a complete gas turbine. Parallel computation on 700 processors. The geometry of one sector (left) is copied 14 times to create the complete chamber (right).

performed on 700 processors of a Cray XT 3 machine. The left figure shows the geometry of one sector : it contains the casing, the multiperforated walls, all geometrical details of the swirler, film cooling and the chocked nozzle. The full geometry is obtained by copying 14 times the mesh of one sector. It contains 42 million elements. The time step is 0.067 microsecond.

[7] F. Nicoud and F. Ducros, Subgrid-scale stress modelling based on the square of the velocity gradient, *Flow Turb. and Combustion*, **62**, 183-200, 1999.
[8] A. Roux and L.Y.M. Gicquel and Y. Sommerer and T. Poinsot, Large eddy simulation of mean and oscillating flow in side-dump ramjet combustor, *Combustion and Flame*, **152**, 154-176, 2008.
[9] V. Moureau, G. Lartigue, Y. Sommerer, C. Angelberger, O. Colin and T. Poinsot, High-order methods for DNS and LES of compressible multi-component reacting flows on fixed and moving grids, *J. of Comp. Physics*, **202**, 710-736, 2005.
[10] S. Roux and G. Lartigue and T. Poinsot and U. Meier and C. Brat, Studies of mean and unsteady flow in a swirled combustor using experiments, acoustic analysis and Large Eddy Simulations, *Combustion and Flame*, **141**, 40-54, 2005.

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

Acoustics play a key role in combustion and must be accounted for both experimentally and numerically. To understand confined flames, the LES codes presented in Section 4.1 are powerful tools but they are also extremely expensive. An alternative and complementary path is to to develop acoustic codes solving the wave equation in complex geometries for reacting flows. CERFACS is developing a full three-dimensional Helmholtz solver (called AVSP) solving the Helmholtz equation in the frequency domain. It is coupled to the LES code AVBP : they use the same data structure ; the fields of mean temperature, mass fraction and local flame transfer function required by AVSP are obtained by post-processing AVBP simulations. As an

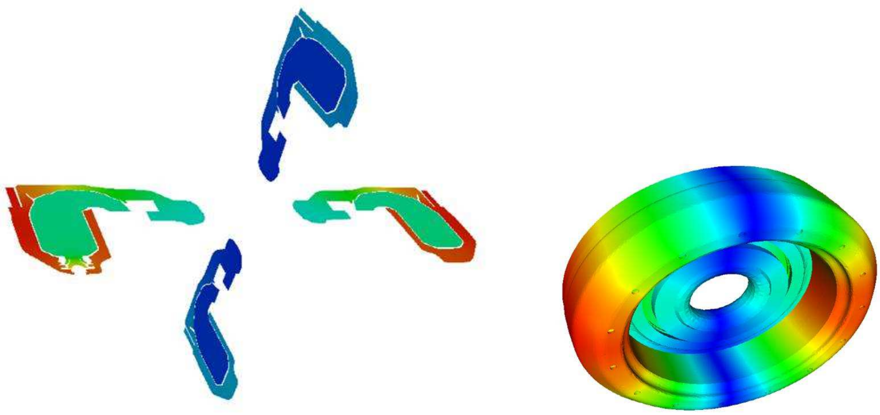


FIG. 4.2 – Acoustic pressure field at 565 Hz in a gas turbine annular chamber. Left : solution in four cutting planes Right : solution over the outer boundary .

example, Fig. 4.2 shows a geometry of a single gas turbine burner and the structure of the second annular mode evidenced by AVSP in a fulll annular chamber with 15 burners. These modes are often crucial for the stability of the combustor and for its noise emission. Note that the analysis includes the geometrical details of the 15 swirlers, the combustion chamber and the casing. The AVSP code has now been used to study a variety of academic [COMB6] and industrial [COMB10, COMB4, COMB9], [11] configurations. Recent developments include a generalization of the flame transfer function model to account for pressure fluctuations (and not only acoustic velocity fluctuations), the effect of casing on the thermo-acoustic modes [COMB53], the prescription of appropriate boundary conditions for accounting for upstream/downstream elements in a gas turbine [COMB44] and the numerical algorithm used to solve the large scale non-linear eigenvalue problem [12] arising from the discretization of the Helmholtz equation.
More recently, AVSP has been adapted to handle propagation issues related to the combustion noise thematic. This AVSP-forced version of the code (as opposed to the AVSP-modal tool used for thermo-acoustic modes analysis) uses acoustic sources from AVPB to compute the acoustic spectrum in the near field region. As an illustration, Fig. 4.3 shows a typical map of sources from a swirled stabilized turbulent flame and the corresponding computed power spectrum at the outlet section of the combustion chamber.
The indirect noise generation (noise generated from entropy spots interacting with regions of strong mean velocity gradient) has also been addressed at CERFACS and a simple analytical model has been developed to assess the direct-to-indirect noise ratio [COMB45]. In this respect, the difficult task of including non-zero Mach number effects in AVSP has also been initiated.

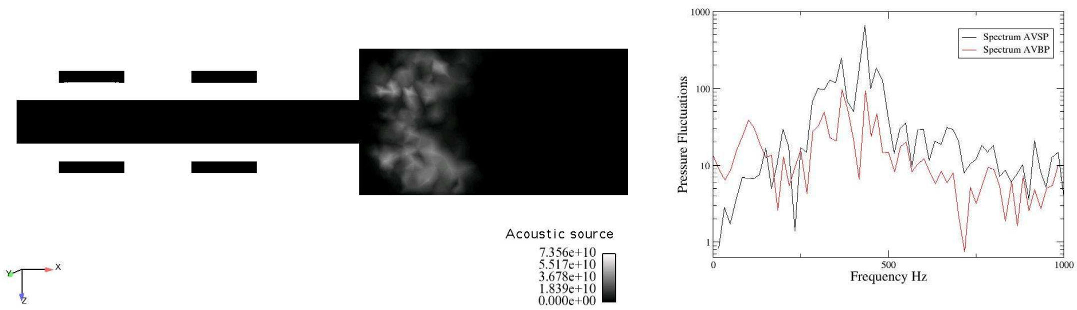


FIG. 4.3 – Left : acoustic sources at 400 Hz from a swirled stabilized turbulent flame (experiment studied at Ecole Centrale Paris) as computed from AVBP. Right : acoustic spectrum computed from AVSP-forced and compared to the LES result of AVBP.

[11] A. Roux, L.Y.M. Gicquel, Y. Sommerer and T. Poinsot, Large eddy simulation of mean and oscillating flow in side-dump ramjet combustor, *Combustion and Flame*,**152**, 154-176, 2008.
[12] C. Sensiau, F. Nicoud, M. VanGijzen, J.W. VanLeeuwen, A comparison of solvers for quadratic eigenvalue problems from combustion, *International Journal of Numerical Methods in Fluids*, in press, 2008.

4.3 LES of ignition in rocket and piston engines (G. Lacaze , B. Enaux, B. Cuenot, T. Poinsot)

As the capacities of LES progress, the requests for more precise predictions of unsteady phenomena such as ignition increase too. In 2006 and 2007, a new model for ignition using LES was developed in AVBP : this model (called ED for Energy Deposition) tries to avoid the classical approaches based on the use of an external model used during the first instants of ignition (where the flame kernel is too small to be resolved on the LES mesh) coupled to the LES code when the kernel is large enough. In the ED model, energy is simply deposited on the grid and ignition takes place when the kinetics get fast enough for reaction to occur. The ED approach is only possible when an increased resolution near the spark or the laser used for ignition is available. The ED model was tested in rocket engines in the PhD of G. Lacaze and in piston engines in the PhD of B. Enaux.

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

Following the first LES applied to rocket engines (PhD of A. Dauptain and now G. Lacaze), the necessity to take into account the real thermodynamics of the fluids encountered in such systems has been identified : in rocket engine burners the reactants are stored at very high pressure levels, that are above the critical point. In this case there is no more surface tension, i.e. no interface between dense and light phases of the fluid that are separated by very high density gradients. The critical point itself is a singular point with particular properties such as infinite specific heat. To inject the correct mass flow at the prescribed pressure and temperature conditions, it is necessary to use a real gas equation of state that gives the correct density under these conditions. This implies fully different thermodynamics. These new thermodynamics then affect the

numerics of the code, either directly in the jacobian matrices or in the boundary conditions, or indirectly through accuracy and stability problems.
In AVBP the cubic equation of state of Peng-Robinson has been chosen : preliminary tests showed that it was the best model to represent real gas thermodynamics in the target conditions. Its implementation in AVBP by T. Schmitt (who will defend his PhD thesis end of 2008), also required numerous developments to adapt the code. After validation on simple test cases, the model AVBP-GR has been applied to supercritical jets studied experimentally at DLR. The comparison with the measurements shows that the model captures the main effects of dense fluid, as for example the longer potential core. Application to more realistic configurations such as the Mascotte configuration of ONERA is underway, where the calculation is performed for reacting regimes.

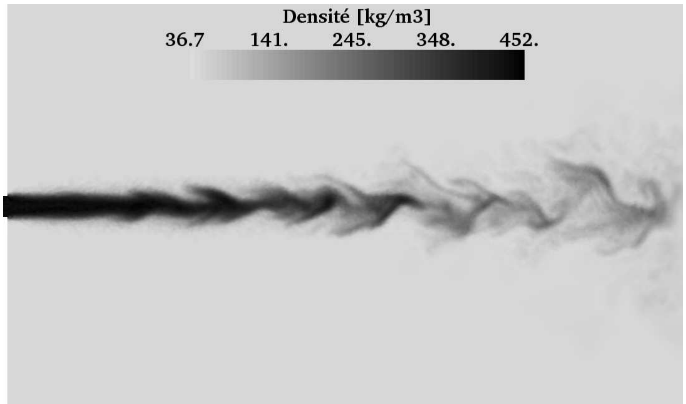


FIG. 4.4 – Instantaneous view of the density field obtained for a dense supercritical N2 jet injected at 100K, 40 bars in a subcritical N2 environment at 298K, 40 bars.

5 Software engineering

5.1 High performance computing (G. Staffelbach, O. Vermorel, M. Porta)

As LES techniques become more precise, the requests to apply LES to more complex and larger devices increase. CERFACS has already shown that AVBP was able to make use of machines up to 4000 processors and exhibited almost linear scaling on multiple architectures (Fig. 5.1). This opens the path to more ambitious computations : in 2007, a project dedicated to the computation of a four-cylinder engine with LES has started with IFP, CINES, PSA and Renault. Another one dedicated to the computation of complete gas turbine chambers also started with CORIA, EM2C, Turbomeca and Snecma at the end of 2007. These projects require significant efforts in software engineering to generates meshes, decompose them, optimize the computation and perform the post processing of the solutions.

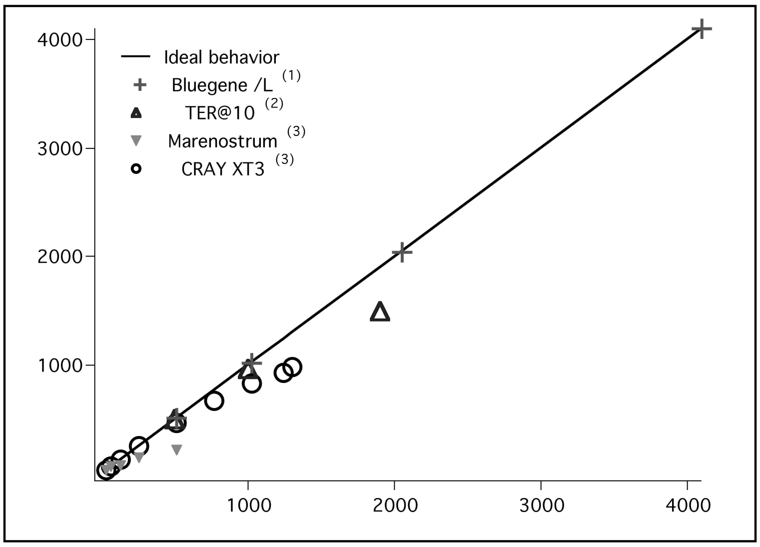


FIG. 5.1 – AVBP speed up on various architectures for cases from 10 to 40 million cells.

5.2 Code coupling and multiphysics (F. Duchaine, J. Amaya, A. Sengissen)

Another major challenge for the coming years is linked to multiphysics and the efficient coupling of multiple solvers that simulate very different physical problems. To this purpose CERFACS continues to develop code coupling using the PALM software. In the CFD team, several projects are now underway to couple AVBP with other softwares : a steady heat transfer solver (TMG), an unsteady heat transfer solver (a CERFACS evolution of AVBP for heat transfer in solids), and a radiation solver (DOMASIUM, Ecole des Mines d'Albi). Fluid / structure interaction studies were also performed during the DESIRE project and showed that the LES results can be coupled to a structure code to predict liner deformations [COMB2]. In the framework of the INTELLECT project, PALM was used to couple a flow solver with mesh generation tools in an optimisation chain (Fig.5.2). The aim was to develop an efficient tool able to guide gas turbine manufacturers in decision-making, implying high performance computing (through massively parallel architectures) and flexibility to the application.

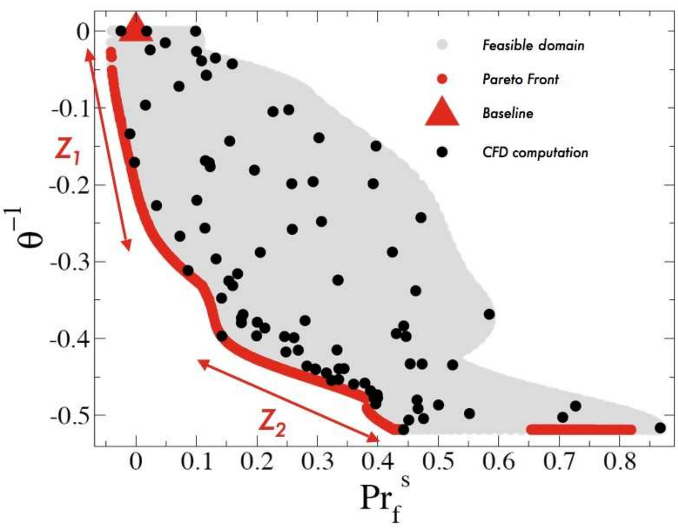


FIG. 5.2 – Optimisation in the PALM environment.

6 Publications

6.1 Journal Publications

[COMB1] G. Boudier, L. Gicquel, T. Poinsot, D. Bissières, and C. Bérat, (2007), Comparison of LES, RANS and Experiments in an Aeronautical Gas Turbine Combustion Chamber, *In Proc. of the Combustion Institute*, **31**, 3075–3082.

[COMB2] R. Huls, P. VanderHoogt, A. Sengissen, T. Poinsot, and A. DeBoer, (2007), Prediction of vibration by coupling finite elements and large eddy simulations, *Journal of Sound and Vibration*, **304**, 224–229.

[COMB3] C. Jimenez and B. Cuenot, (2007), DNS study of stabilisation of turbulent triple flames by hot gases, *In Proc. of the Combustion Institute*, **31**, 1649–1656.

[COMB4] C. Martin, L. Benoit, Y. Sommerer, F. Nicoud, and T. Poinsot, (2006), LES and acoustic analysis of combustion instability in a staged turbulent swirled combustor, *AIAA Journal*, **44**, 741–750.

[COMB5] S. Mendez, F. Nicoud, and T. Poinsot, (2006), Large-Eddy Simulations of a Turbulent Flow around a Multi-Perforated Plate, *Lecture Notes in Computational Science and Engineering - Complex effects in Large Eddy Simulations*, **56**, 289–303.

[COMB6] F. Nicoud, L. Benoit, C. Sensiau, and T. Poinsot, (2007), Acoustic modes in combustors with complex impedances and multidimensional active flames, *AIAA Journal*, **45**, 426–441.

[COMB7] D. Poitou, H. El, and B. Cuenot, (2007), Diagnosis of turbulence radiation in turbulent flames and implications for modeling in Large Eddy Simulation, *Turkish Journal of Engineering and Environmental Sciences*, **31**, 371–381.

[COMB8] K.-U. Schildmacher, A. Hoffman, L. Selle, R. Koch, C. Schulz, H.-J. Bauer, and T. Poinsot, (2007), Unsteady Flame and Flow Field Interaction of a Premixed Model Gas Turbine Burner, *In Proc. of the Combustion Institute*, **31**, 3197–3205.

[COMB9] P. Schmitt, T. Poinsot, B. Schuermans, and K. Geigle, (2007), Large-eddy simulation and experimental study of heat transfer, nitric oxide emissions and combustion instability in a swirled turbulent high pressure burner, *Journal of Fluid Mechanics*, **570**, 17–46.

[COMB10] L. Selle, L. Benoit, T. Poinsot, F. Nicoud, and W. Krebs, (2006), Joint use of Compressible Large-Eddy Simulation and Helmholtz solvers for the analysis of rotating modes in an industrial swirled burner, *Combustion and Flame*, **145**, 194–205.

[COMB11] A. Sengissen, A. Giauque, G. Staffelbach, M. Porta, W. Krebs, P. Kaufmann, and T. Poinsot, (2007), Large Eddy Simulation of piloting effects on turbulent swirling flames, *In Proc. of the Combustion Institute*, **31**, 1729–1736.

[COMB12] A. Sengissen, T. Poinsot, J. VanKampen, and J. Kok, (2006), Response of a swirled non-premixed burner to fuel flow rate modulation, *Lecture Notes in Computational Science and Engineering -Complex effects in LES*, **56**, 337–351.

[COMB13] A. Sengissen, J. VanKampen, R. Huls, S. G., J. Kok, and T. Poinsot, (2007), LES and experimental studies of cold and reacting flow in a swirled partially premixed burner with and without fuel modulation, *Combustion and Flame*, **150**, 40–53.

[COMB14] G. Staffelbach, L. Gicquel, and T. Poinsot, (2006), Highly parallel large eddy simulations of multiburner configurations in industrial gas turbines, *Lecture Notes in Computational Science and Engineering - Complex effects in Large Eddy Simulations*, **56**, 326–336.

6.2 Theses

[COMB15] L. Artal, (2006), *Modélisation des flux de chaleurs stationnaires pour un mélange multi-espèce avec transfert de masse à la paroi - TH/CFD/06/12*, PhD thesis, Université de Montpellier II.

[COMB16] V. Auffray, (2007), *Etude comparative de schémas numériques pour la modélisation de phénomènes diffusifs sur maillages multiéléments - TH/CFD/07/14*, PhD thesis, Institut National Polytechnique de Toulouse, France.

[COMB17] M. Boileau, (2007), *Simulation aux grandes échelles de l'allumage diphasique des foyers aéronautiques -TH/CFD/07/103*, PhD thesis, INSTITUT POLYTECHNIQUE NATIONAL DE TOULOUSE.

[COMB18] G. Boudier, (2007), *Application de la méthode LES à la combustion instationnaire dans les foyers d'hélicoptère - TH/CFD/07/123*, PhD thesis, Institut National Polytechnique de Toulouse.

[COMB19] A. Dauptain, (2006), *Allumage des moteurs fusées cryotechniques - TH/CFD/06/85*, PhD thesis, INSTITUT NATIONAL POLYTECHNIQUE DE TOULOUSE.

[COMB20] G. Desoutter, (2007), *Etude numérique de la propagation d'une flamme sous l'influence d'un film liquide de carburant sur la paroi - TH/CFD/07/72*, PhD thesis, Institut National Polytechnique de Toulouse, France.

[COMB21] F. Duchaine, (2007), *Optimisation de Forme Multi-Objectif sur Machines Parallèles avec Méta-Modèles et Coupleurs. Application aux Chambres de Combustion Aéronautiques - TH/CFD/07/96*, PhD thesis, Institut National Polytechnique de Toulouse.

[COMB22] A. Giauque, (2007), *System identification and disturbance energies in reacting flows -TH/CFD/07/15*, PhD thesis, Institut National Polytechnique de Toulouse, France.

[COMB23] L. Gicquel, (2007), *Habilitation à Diriger des Recherches - TH/CFD/07/64*, PhD thesis, Institut National Polytechnique de Toulouse.

[COMB24] N. Lamarque, (2007), *Schémas numériques et conditions limites pour la simulation aux grandes é chelles de la combustion diphasique dans les foyers d' hélicoptère - TH/CFD/07/117*, PhD thesis, Institut National Polytechnique de Toulouse, France.

[COMB25] S. Mendez, (2007), *Simulation numérique et modélisation de l'écoulement autour des parois multi-perforées - TH/CFD/07/104*, PhD thesis, Université Montpellier II.

[COMB26] S. Pascaud, (2006), *Vers la simulation aux grandes échelles des écoulements turbulents diphasiques réactifs : application aux foyers aéronautiques - TH/CFD/06/44*, PhD thesis, Institut National Polytechnique de Toulouse.

[COMB27] M. Porta, (2007), *Développement, vérification et validation des outils LES pour l'étude du bruit de combustion et de l'interaction combustion/acoustique/turbulence - TH/CFD/07/46*, PhD thesis, Institut National Polytechnique de Toulouse, France.

[COMB28] E. Riber, (2007), *Développement de la méthode de simulation aux grandes échelles pour les écoulements diphasiques - TH/CFD/07/41 turbulents*, PhD thesis, INSTITUT NATIONAL POLYTECHNIQUE DE TOULOUSE.

[COMB29] S. Roux, (2007), *Influence de la modélisation du mélange air/carburant et de l'étendue du domaine de calcul dans la simulation aux grandes échelles des instabilités de combustion. Application à des foyers aéronautiques - TH/CFD/07/38*, PhD thesis, InstitutNational Polytechnique de Toulouse.

[COMB30] A. Sengissen, (2006), *Simulation aux grandes échelles des instabilités de combustion : vers le couplage fluide/structure - TH/CFD/06/30*, PhD thesis, Institut National Polytechnique de Toulouse, France.

[COMB31] G. Staffelbach, (2006), *Simulation aux grandes échelles et analyse acoustique de turbines à gaz industrielles multi-brûleurs - TH/CFD/06/31*, PhD thesis, Institut National Polytechnique de Toulouse, France.

[COMB32] L. Thobois, (2006), *Intérêt et faisabilité de la simulation aux grandes échelles dans les moteurs automobiles - TH/CFD/06/3*, PhD thesis, Institut Polytechnique National de Toulouse.

6.3 Conference Proceedings and Book Chapters

[COMB33] G. Boudier, N. Lamarque, C. Sensiau, G. Staffelbach, L. GIcquel, T. Poinsot, and V. Moureau, (2007), Investigating thermo-acoustic stability of a real gas turbine combustion chamber using Large-Eddy Simulations, In *11th CEAS-ASC Workshop of X3-Noise*, Lisbon, Portugal.

[COMB34] G. Boudier, G. Staffelbach, L. GIcquel, and T. Poinsot, (2007), Mesh dependency of turbulent reacting Large-Eddy Simulations in a gas turbine combustion chamber, In *QLES (Quality and Reliability of LES) workshop*, Leuven, Belgium, ERCOFTAC, Ed 1.

[COMB35] O. Cabrit, L. Artal, and F. Nicoud, (2007), Direct numerical simulation of turbulent multispecies channel flow with wall ablation, In *39th AIAA Thermophysics Conference*, Miami, USA, AIAA Paper 2007–4401.

[COMB36] B. Cuenot, M. Boileau, S. Pascaud, J.-B. Mossa, E. Riber, T. Poinsot, and C. Bérat, (2006), Large Eddy simulation of two-phase reacting flows, In *ECCOMAS CFD 2006*, Egmond Aan Zee, The Netherlands.

[COMB37] B. Cuenot, Y. Sommerer, L. Gicquel, and T. Poinsot, (2006), LES of reacting flows, In *3rd International Workshop on Rocket Combustion Modeling*, Paris, France.

[COMB38] G. Desoutter, C. Habchi, B. Cuenot, and T. Poinsot, (2006), Single-component liquid film evaporation model development and validation using direct numerical simulationsS, In *ICLASS 2006*, Kyoto, Japan, Paper ID ICLASS06–079.

[COMB39] F. Duchaine, L. Gicquel, T. Poinsot, D. Bissières, and C. Bérat, (2006), Optimization Loop based on a CFD RANS code, In *ICAS 2006*, Munich, Germany.

[COMB40] M. García, E. Riber, O. Simonin, and T. Poinsot, (2007), Comparison between Euler/Euler and Euler/Lagrange LES approaches for confined bluff-body gas-solid flow, In *International Conference on Multiphase Flow*, Liepzig, Germany, CD–ROM – S3–Fri–A–62.

[COMB41] A. Giauque, T. Poinsot, M. Brear, and F. Nicoud, (2006), Budget of disturbance energy in gaseous reacting flows, In *Proceedings of the Summer Program*, Center for Turbulence Research, NASA AMES, Stanford University, USA, 285–297.

[COMB42] L. Gicquel, Y. Sommerer, B. Cuenot, and T. Poinsot, (2006), LES and Acoustic Analysis of Turbulent Reacting Flows : Application to a 3D Oscillatory Ramjet Combustor, In *ASME 2006*, RENO, USA.

[COMB43] G. Lacaze, B. Cuenot, and T. Poinsot, (2006), LES of Laser ignition in a micro-combustor, In *3rd International Workshop on Rocket Combustion Modeling*, Paris, France.

[COMB44] N. Lamarque and T. Poinsot, (2007), Determination of boundary conditions for acoustic eigenmodes, In *11th CEAS-ASC Workshop of X3-Noise*, Lisbon, Portugal.

[COMB45] M. Leyko, F. Nicoud, and T. Poinsot, (2007), Comparison of indirect and direct combustion noise in aircraft engines, In *11th CEAS-ASC Workshop of X3-Noise, Lisbon, Portugal.*

[COMB46] S. Mendez and F. Nicoud, (2007), Numerical investigation of an anisothermal turbulent flow with effusion, In *5th International Symposium on Turbulence and Shear Flow Phenomena*, TU Munich, Germany.

[COMB47] S. Mendez, J. Eldredge, F. Nicoud, T. Poinsot, M. Shoeybi, and G. Iaccarino, (2006), Numerical investigation and preliminary modeling of a turbulent flow over a multi-perforated plate, In *Proceedings of the Summer Program*, Center for Turbulence Research, NASA AMES, Stanford University, USA, 57–72.

[COMB48] D. Poitou, H. El, and B. Cuenot, (2007), Diagnosis of turbulence radiation in turbulent flames and implications for modeling in Large Eddy Simulation, In *5th Mediterranean Combustion Symposium*, Monastir (Tunisia).

[COMB49] M. Porta, N. Lamarque, and F. Nicoud, (2007), Analysis of the effects of artificial boundary terms in Taylor-Galerkin schemes, In *Conference on Numerical Methods for Fluid Dynamics*, The Institute for Computational Fluid Dynamics, University of Reading - UK.

[COMB50] E. Riber, M. García, V. Moureau, H. Pitsch, O. Simonin, and T. Poinsot, (2006), Evaluation of numerical strategies for LES of two-phase reacting flows, In *Proceedings of the Summer Program*, Center for Turbulence Research, NASA AMES, Stanford University, USA, 197–211.

[COMB51] E. Riber, M. Moreau, O. Simonin, and B. Cuenot, (2006), Development of Euler-Euler LES approach for gas-particle turbulent jet flow, In *ASME - European Fluids Enigneering Summer Meeting*, Miami, Florida - USA.

[COMB52] P. Ryzhakov, M. Porta, R. Rossi, and T. Schoenfeld, (2007), On the FSI for combustion chambers, In *Int. Conf. on computational methods for coupled problems in science and engineering -coupled problems 2007*, Santa Eulalia, Ibiza, Spain, 618–622.

[COMB53] C. Sensiau, F. Nicoud, L. Gicquel, T. Poinsot, and V. Moureau, (2007), Acoustic analysis of industrial gas turbines, In *11th CEAS-ASC Workshop of X3-Noise*, Lisbon, Portugal.

[COMB54] G. Staffelbach and T. Poinsot, (2006), High Performance Computing for Combustion Applications, In *Super Computing 2006*, Tampa, Florida, USA.

[COMB55] G. Staffelbach, G. Boudier, N. Lamarque, C. Sensiau, L. Gicquel, and T. Poinsot, (2007), Azimuthal Thermo-Acoustic Stability of a Full Gas Turbine Combustion Chamber Using Large-Eddy Simulations, In *11th CEAS-ASC Workshop of X3-Noise*, Lisbon, Portugal.

6.4 Technical Reports

[COMB56] J. Amaya, (2006), Modélisation du fonctionnement d'une chambre de combustion aéronautique : vers une étude des instabilités de combustion, Stage de Master Recherche - Dynamique des Fluides WN/CFD/06/72, Ecole Nationale Supérieure de l' Aéronautique et l' Espace.

[COMB57] S. Ayache, (2007), Validation of numerical tool : AVBP, Rapport de stage WN/CFD/07/84, CERFACS.

[COMB58] L. Benoit, (2006), Manuel Théorique de la chaîne QUIET, Contract Report CR/CFD/06/109, CERFACS.

[COMB59] L. Benoit, (2006), Spécifications de la chaîne QUIET, Rapport contractuel CR/CFD/06/45, CERFACS.

[COMB60] L. Benoit, (2007), Dossier de validation de la chaîne QUIET, Tech. Rep. CR/CFD/07/19, CERFACS.

[COMB61] L. Benoit, (2007), Dossier technique sur l'interface AVSP preprocessing1.2.py de la chaîne QUIET, Tech. Rep. CR/CFD/07/20, CERFACS.

[COMB62] L. Benoit, (2007), Manuel utilisateur QUIET, Contract report CR/CFD/07/9, CERFACS.

[COMB63] L. Benoit, (2007), Manuel utilisateur QUIET, Tech. Rep. CR/CFD/07/21, CERFACS.

[COMB64] L. Benoit, (2007), Tutorial de la chaîne QUIET, Tech. Rep. CR/CFD/07/22, CERFACS.

[COMB65] M. Boileau, J. Jouhaud, and J.-F. Boussuge, (2007), Simulation LES de l' expérimentation E - Livrable 1 : rapport intermédiaire relatif aux lots 1.1.a, 1.1.b et 1.1.c, contract report CR/CFD/07/94, CERFACS.

[COMB66] M. Boileau, J. Jouhaud, and J.-F. Boussuge, (2007), Simulation LES de l'expérimentation E - Livrable 2 : Rapport intermédiaire relatif au lot 1.1.d, Contract report CR/CFD/07/95, CERFACS.

[COMB67] G. Boudier, N. Lamarque, C. Sensiau, L. Gicquel, and T. Poinsot, (2007), Simulation LES 3D à chaud du contournement et de la chambre ARDIDEN - géometrie 1, pt 115 - Deliverable 2 : Lot 2 - tâche 2, Contract report CR/CFD/07/74, CERFACS.

[COMB68] G. Boudier, N. Lamarque, C. Sensiau, L. Gicquel, and T. Poinsot, (2007), Simulation LES 3D à froid du contournement et de la chambre ARDIDEN - mise en place des calculs et géometries - Deliverable 1 : Lot 1 - tâche 1.1, Tech. Rep. CR/CFD/07/73, CERFACS.

[COMB69] M. Brear, F. Nicoud, and A. Giauque, (2006), Transport of energy by disturbances in gaseous combustion, Tech. Rep. TR/CFD/06/88, CERFACS.

[COMB70] O. Cabrit, (2006), Modélisation des flux de chaleur sur une tuyère ablatée par un mélange multi-espèces, Rapport de stage - Master de recherche dynamique des fluides énergétique et transferts WN/CFD/06/52, INSA.

[COMB71] B. Cuenot, (2007), ECCOMET- First periodic report, Contract report ECCOMET CR/CFD/07/92, CERFACS.

[COMB72] B. Cuenot, (2007), ECCOMET-First Annual Report, Contract report CR/CFD/07/105, CERFACS.

[COMB73] J. Dassé, (2006), Simulation numérique directe de la combustion turbulente avec NTMIX3D, rapport de stage de fin de 2ème année Ingénieur WN/CFD/06/79, ENSEEIHT, Département Hydraulique et Mécanique des Fluides.

[COMB74] J. Dassé, (2007), Caractérisation acoustique d'une plaque multiperforée, stage de Master recherche DET WN/CFD/07/87, CERFACS.

[COMB75] J. Dassé, (2007), Caractérisation de l'impédance acoustique d'une plaque multi-perforée, Rapport de stage de fin d'étude WN/CFD/07/59, Institut National Polytechnique de Toulouse - ENSEEIHT.

[COMB76] F. Duchaine, (2006), Guide d'utilisation de la chaîne de calcul thermique N3SNatur-ASTRE-Abaqus pour la prédiction des températures de parois, Tech. Rep. CR/CFD/06/51, CERFACS.

[COMB77] F. Duchaine, (2006), Mise en place d'une chaîne de calcul N3S-Natur - ASTRE - Abaqus en vue de la prédiction des températures de parois des chambres de combustion à l'aide du coupleur PALM MP, rapport contractuel CR/CFD/06/118, CERFACS.

[COMB78] B. Enaux, (2006), Simulation aux grandes échelles d'un jet en écoulement transverse, Master Recherche DET (filière Energétique et Transferts) WN/CFD/06/56, Institut National Polytechnique de Toulouse.

[COMB79] A. Eyssartier, (2007), Mise en place de l'interface de pré-processing pour le code de calcul AVBP - (partie conditions aux limites), Stage 2ème année d'ingénieur - Hydraulique et Mćanique des Fluides, ENSEEIHT WN/CFD/07/85, CERFACS.

[COMB80] L. Gicquel, G. Boudier, and T. Poinsot, (2006), Evaluation de la méthode Large Eddy Simulations pour la prédiciton de l'extinction d'un moteur d'hélicoptère - Deliverable 1 : ARRIUS extinction 9/1000, contract repont ARRIUS CR/CFD/06/53, CERFACS.

[COMB81] L. Gicquel, G. Boudier, and T. Poinsot, (2006), Evaluation de la méthode Large Eddy Simulations pour la prédiciton de l'extinction d'un moteur d'hélicoptère - Deliverable 2 : ARRIUS extinction 9/1000 et 10/1000, Tech. Rep. CR/CFD/06/54.

[COMB82] L. Gicquel, G. Boudier, and T. Poinsot, (2006), Evaluation de la méthode Large Eddy Simulations pour la prédiction du profil FRT, Contract report CR/CFD/07/8, CERFACS.

[COMB83] K. Grau, (2007), Applications of the Proper Orthogonal Decomposition Method, Internship report WN/CFD/07/97, CERFACS.

[COMB84] E. Gullaud, (2007), Instabilités thermoacoustiques, Rapport de fin d' études à l' ENSMA WN/CFD/07/79, CERFACS.

[COMB85] G. Lacaze and B. Cuenot, (2007), Rapport d'avancement - Thèse sur l'allumage moteur fusée cryotechnique, Rapport contractuel CR/CFD/07/49, CERFACS.

[COMB86] G. Lacaze, B. Cuenot, and T. Poinsot, (2007), Rapport d'avancement - Thèse sur l'allumage des moteurs fusée cryotechnique, Rapport contractuel CR/CFD/07/114, CERFACS.

[COMB87] G. Lacaze, (2006), Rapport d'avancement - Thèse sur l'allumage moteur fusée cryotechnique, Contract report CR/CFD/06/91, CERFACS.

[COMB88] G. Lacaze, (2007), Arrhenius kinetic parameters for a reversed equilibrium reaction, Tech. Rep. WN/CFD/07/39, CERFACS.

[COMB89] N. Lamarque and T. Poinsot, (2007), Inlet and outlet boundary conditions for acoustic eigenmodes computation in gas turbines combustion chambers, Preliminary version of an article submitted to AIAA Journal TR/CFD/07/142, CERFACS.

[COMB90] N. Lamarque, G. Boudier, C. Sensiau, L. Gicquel, and T. Poinsot, (2007), Simulation LES 3D à chaud du contournement et de la chambre ARDIDEN - géometrie 2, pt 115 - Deliverable 3 : Lot 3 - tâche 3, Contract report CR/CFD/07/75, CERFACS.

[COMB91] N. Lamarque, (2006), Rapport d'avancement annuel 2006, contract report - CIFRE TURBOMECA CR/CFD/06/97, CERFACS.

[COMB92] J. Lavedrine and B. Cuenot, (2006), TLC- Deliverable Report : D4.1.2a - Predictions of multi-point injection systems : LES simulations, contract report CR/CFD/06/93, CERFACS.

[COMB93] S. Mendez and F. Nicoud, (2007), LES results for RANS modelling and recommendations on LES models for multi-perforated plates, Tech. Rep. CR/CFD/07/60, CERFACS.

[COMB94] M. Myrczik, (2006), Determination of inlet impedances for acoustic eigenmode computation in combustion chambers, Rapport de stage de fin d'études d'ingénieur WN/CFD/06/58, ENSICA.

[COMB95] T. Pedot, (2007), Dossier technique sur l'interface quiet V1.0 de la chaîne QUIET, rapport contractuel TR/CFD/07/31, CERFACS.

[COMB96] T. Pedot, (2007), Réalisation d'une interface graphique pour la chaîne Quiet - Rapport de stage de fin de deuxième année, Tech. Rep. WN/CFD/07/33, CERFACS.

[COMB97] M. Porta, (2006), Validation of unsteady boundary conditions for LES applications, FLUISTCOM report TR/CFD/06/104, CERFACS.

[COMB98] E. Riber, V. Moureau, M. García, T. Poinsot, and O. Simonin, (2007), Evaluation of numerical strategies for Large Eddy Simulation of particulate two-phase recirculating flows, Preliminary version of an article submitted to Journal of Computational Physics TR/CFD/07/135, CERFACS.

[COMB99] A. Roux, J. Lavedrine, C. Sensiau, Y. Sommerer, and T. Poinsot, (2006), Définition de la pratique de calcul pour la caractérisation acoustique d'un système d'injection, Rapport contractuel SNECMA CR/CFD/06/27, CERFACS.

[COMB100] S. Roux, (2006), Application de la décomposition en modes propres à des calculs de simulations aux grandes échelles, Rapport de stage 2ème année Ingénieur - ENSEEIHT WN/CFD/06/61, CERFACS.

[COMB101] S. Roux, (2006), Manuel d'utilisation de la POD au CERFACS, rapport de stage 2ème année Ingénieur WN/CFD/06/60, ENSEEIHT - INPT.

[COMB102] M. Sanjosé, (2006), Etude numérique et application de la LES diphasique, Rapport de stage de fin d'études WN/CFD/06/57, Institut National Polytechnique de Toulouse.

[COMB103] M. Sanjosé, (2006), Etude numérique et application de la LES diphasique, rapport de stage Master WN/CFD/06/59, Institut National Polytechnique de Toulouse.

[COMB104] T. Schmitt, (2006), Simulation aux grandes échelles de la combustion en régime supercritique, Rapport avancement des travaux de thèse WN/CFD/06/96, CERFACS.

[COMB105] T. Schmitt, (2007), Simulation aux grandes échelles de la combustion en régime supercritique, Rapport contractuel CR/CFD/07/115, CERFACS.

[COMB106] J.-M. Senoner, M. García, S. Mendez, G. Staffelbach, O. Vermorel, and T. Poinsot, (2007), The growth of rounding errors and the repetitivity of Large Eddy Simulations on parallel machines, Tech. Rep. TR/CFD/07/127, CERFACS.

[COMB107] C. Silva, (2007), First Step of Development of a Numerical Tool for Combustion Noise Analysis, Stage de fin d'études d'ingénieur - Ecole Nationale Supérieure de l'Aéronautique et de l'Espace WN/CFD/07/86, CERFACS.

[COMB108] Y. Sommerer, C. Sensiau, A. Roux, S. Roux, and T. Poinsot, (2006), Analyse du comportement acoustique du foyer DEM21 avec prise en compte du distributeur, rapport contractuel SNECMA CR/CFD/06/26, CERFACS.

[COMB109] R. Vicquelin, (2006), Calcul LES d'une Combustion Sans Flamme, rapport Master Recherche Energie, Aéronautique et Spatial WN/CFD/06/70, Ecole Centrale de Paris, France.

[COMB110] R. Vicquelin, (2006), Calcul LES d'une Combustion Sans Flamme, Rapport de stage de fin d' études WN/CFD/06/82, Ecole Centrale de Paris, France.

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 CO2, 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 3 for green house potential factor from aircraft emission : a molecule of CO2 emitted from a jet airplane is a factor of 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 project 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 have been developed and they both include the microphysic needed to describe the ice particle formation and evolution for about 30 minutes after injection in the atmosphere. The NTMIX model also includes the minimum gas-phase chemistry scheme to compute the evolution of the nitrogen species. The next steps will be the introduction of gas-phase and heterogeneous chemistry within the Méso-NH model, and the implementation of a radiative code to compute the perturbation of the radiative fluxes brought by the ice particles.

For the large scale, a linearized approach to the atmospheric chemistry has been further developed to account for the injection of NOx, H_2O and CO from air traffic. It has been introduced in the chemical transport model (CTM) MOCAGE, and will be used for the assessment of the atmospheric chemical perturbations due to the present and future aircraft traffic. In addition, a new parameterization to account for the non-linearities of the chemistry during plume dilution has been developed. It has been introduced in the LSCE CTM and used to assess the effect of the small scale effects on the evaluation of ozone formation due to the NOx injection by the present day fleet. It is found that introduction of the plume dilution processes diminishes the ozone formation by about 15% at the global scale. Similar effects are expected for the case of plume formed by ships, and mesoscale simulations of plumes dispersion have been performed using the Méso-NH model coupled to a particle trajectory model. Results show that the dilution time scales can be derived from the general characteristics of the marine boundary layer, our parameterization can therefore be easily adapted to treat the chemical impact of ship traffic.

We have establish numerous cooperations within the present project. 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, with the ECMWF for validation of our linearized ozone parameterization, and at the european level within the QUANTIFY project coordinated by the DLR in which CERFACS is responsible of the activity II ”Dilution and Processing”.

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

2 Small-scale simulations of aircraft and ship emissions

2.1 Near-field wake chemistry (R. Paoli, D. Cariolle)

This activity aims at developing in the NTMIX solver a chemical and microphysical model of gas and particle emissions in the near-field of an aircraft wake. Two approaches have been followed. The first one is an *on-line* coupling where the three-dimensional flow equations are solved together with conservation equations of each chemical species. This allows detailed knowledge of the dynamics/chemistry interactions that are important especially in the early expansion of the jet in the wake. The first results are encouraging, for example Fig. 2.1 shows that the reaction rate between ozone and NO occurs at the edge of the jet as a consequence of mixing between exhaust and ambient air. Current extension of this study are the inclusion of heterogeneous chemistry in the model via a coupling with the Lagrangian particle module of NTMIX ; and the initialization of flow-field using real aircraft wake pre-computations.

The second approach is an *off-line* coupling in that the output of Lagrangian fluid-particle trajectories (time histories of temperature, mixing ratio, etc.) serve as input of box models with complex chemistry and particle microphysics. Averaging over a large number of particle provides a detailed representation of the thermodynamic properties of the wake and allows precise (and fast) evaluation of the microphysical properties (see Fig. 2.2). For example, we showed the importance of accounting for plume mixing and heterogeneities to correctly initialize box models or larger-scale models. This study was carried out in collaboration with ONERA and lead to a publication in Meteorol. Z. [2].

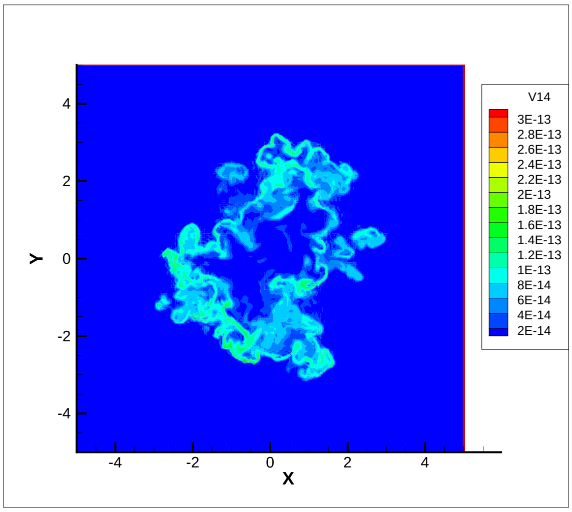


FIG. 2.1 – Plane cut of the product of concentrations $NO_x \times O_3$ that is proportional to the rate of the reaction responsible for ozone destruction.

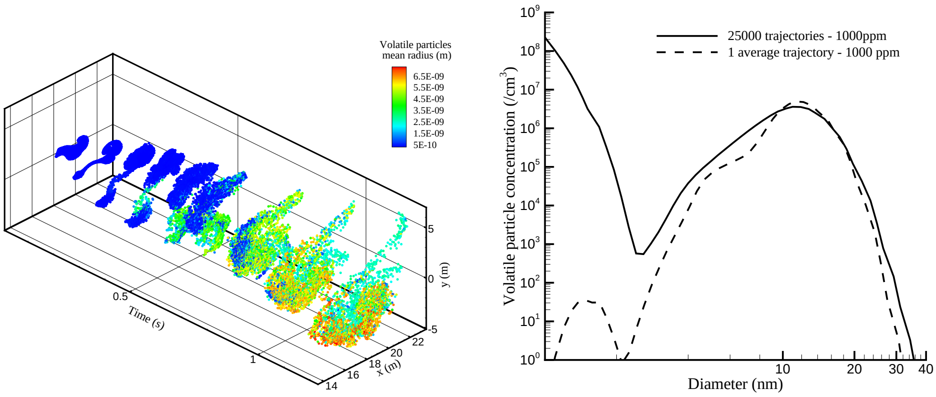


FIG. 2.2 – Left panel : example of two-dimensional slices of volatile particles mean radius as a function of plume age. Right panel : example of volatile particles size distribution 1 sec. after engine exit. Comparison between one simulation along a mean trajectory and average results of 25000 trajectories run.

2.2 Simulation of contrail evolution in the atmosphere (R. Paugam, R. Paoli, D. Cariolle)

This section describes the results of one of the core activities of the team. The main goals of this study were (i) to develop a model for the simulation of the contrail evolution from its formation up to its interaction with the atmosphere ; (ii) to quantify coefficients of the parameterizations that are needed to include the aircraft emissions into large scale models ; and (iii) to predict the distribution of ice particles inside a contrail for the evaluation of its radiative impact. These objectives were fulfilled by carrying out extensive numerical simulations of contrail using Meso-NH model coupled with a microphysical scheme specifically developed for this issue. The dynamics of a contrail is controlled by the aircraft wake vortices during the initial phase of its evolution, and by the atmospheric processes in the late regime. In this study, we focused on the contrail behavior between 20 s and 30 min after emission time, i.e. from the formation of ice particles (end of the jet-vortex interaction) to the time when the radiative forcing effects on the dynamics are no longer negligible. During this period, the wake evolves through a wide range of scales, from 50 m for the early phases (vortex and dispersion regime) to 1 km when atmospheric processes dominate (diffusion regime). Thus, a simulation strategy based on two successive steps have been developed, with a first simulation until vortex break down ($t \simeq 320\,\mathrm{sec}$), followed by a second one modeling the interaction between the contrail and the atmosphere up to a contrail age of 30 min. To our knowledge, current available measurements performed during the vortex regime are not sufficiently accurate to completely validate our model. However indirect validation of our simulations has been done by comparisons with previous modeling works reported within the literature. Our modeling approach, that consists in forcing of Crow instability, gives results in agreement with previous published works, thought slightly overestimating the vortex descent, and the vertical spreading of the contrail. Nevertheless, the simulations of the vortex and dispersion regimes recover the main dynamical characteristics of the aircraft wake (i.e. formation of vortex ring, linear growth of the short and long wavelength instabilities, formation of a secondary wake induced by the barcolinic torque), and give an ice particles behavior consistent with the measurements performed on young contrails (see Fig. 2.3). Based on these results, we point out the competition between the short and long wavelength instabilities in the formation of the vortex ring, and the importance of the vertical distribution of ice particles at the end of the vortex regime. Finally, we obtain the spatial distribution of ice particles for a contrail aged

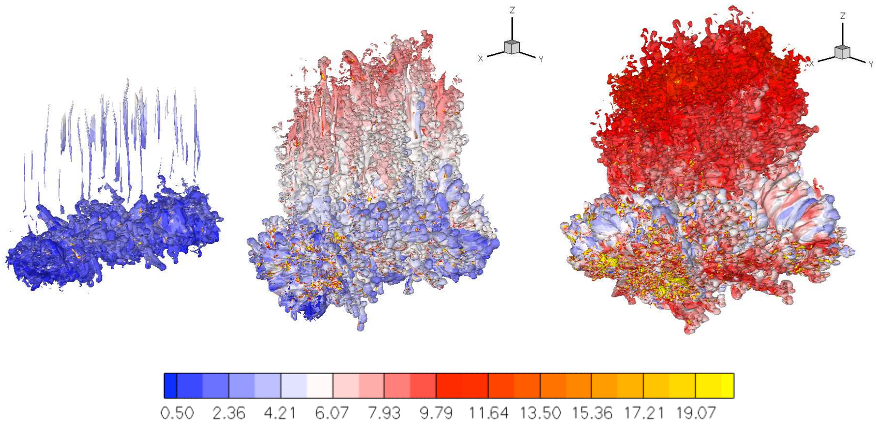


FIG. 2.3 – Perspective view of the isosurface of ice density $\rho_i = 2\,10^{-6}\,\mathrm{kg\,m^{-3}}$ with isocontours of the average ice particle radius (μm) for the vortex and dispersion regime at $t = 160,\ 220,\ 320\ \mathrm{sec}$.

of 320 s that can be used as initial condition for the following simulation of the diffusion regime. The challenge of the diffusion regime is to model the atmospheric processes that affect the contrail evolution, such as wind shear, radiative forcing, and atmospheric turbulence. Previous works in the literature studied the impact of wind shear and radiative forcing on the contrail behavior, but less emphasis was placed on atmospheric turbulence. Therefore, we developed a new strategy to simulate a synthetic turbulent flow that has the same integral properties as the measured turbulence at the tropopause level. To our knowledge, our study constitutes the first simulation of the diffusion regime with an early transition of a contrail into young cirrus. For this regime there are more experimental data, and the numerical results reproduce quite well the measurements. We simulate a contrail aged of 30 min which has cross-sectional dimensions of the same order of magnitude of the observations, with similar ice mass per meter of flight and similar mean size of ice particles (see Fig. 2.4). For such initial conditions, and imposing moderate turbulent fluctuations, we observed the contrail has a life time of about $t = 2.3\,\mathrm{hours}$. A scientific manuscript is in preparation based on the results of this activity. Future directions in this activity include the sensitivity analysis of contrail evolution to the strength of the atmospheric turbulence, and the simulation in the far-field regime up to the complete transformation of contrail into a cirrus cloud. At this stage, it could be possible to evaluate the optical thickness and the radiative forcing of a contrail expanding at the scales of the global climate model. Another perspective for our study is the implementation of a module of kinetic chemistry to simulate ozone non-linear chemistry in the wake. The coefficients of the aircraft emissions parameterization in GCM should then be improved, and in particular the role of the heterogeneous chemistry acting on the ice particles.

2.3 Ship plume simulations (F. Chosson, R. Paoli)

This activity was developed in the framework of European Integrated Project QUANTIFY and consists in two sub-activities that are devoted to the analysis of ship plume dispersion and ship tracks, respectively.

Plume dispersion. Detailed ship plume simulations in various convective boundary layers have been performed using a modified version of the Lagrangian Dispersion Model DIFPAR (EDF R&D ; Wendum, 1998) driven by the atmospheric model Meso-NH in Large Eddy Simulation mode. The simulations (see Fig. 2.5) focus on early stage (1-2 hours) of plume dispersion regime and take into account the effects of plume rise on dispersion. Results are presented in an attempt to provide to chemical modelers a

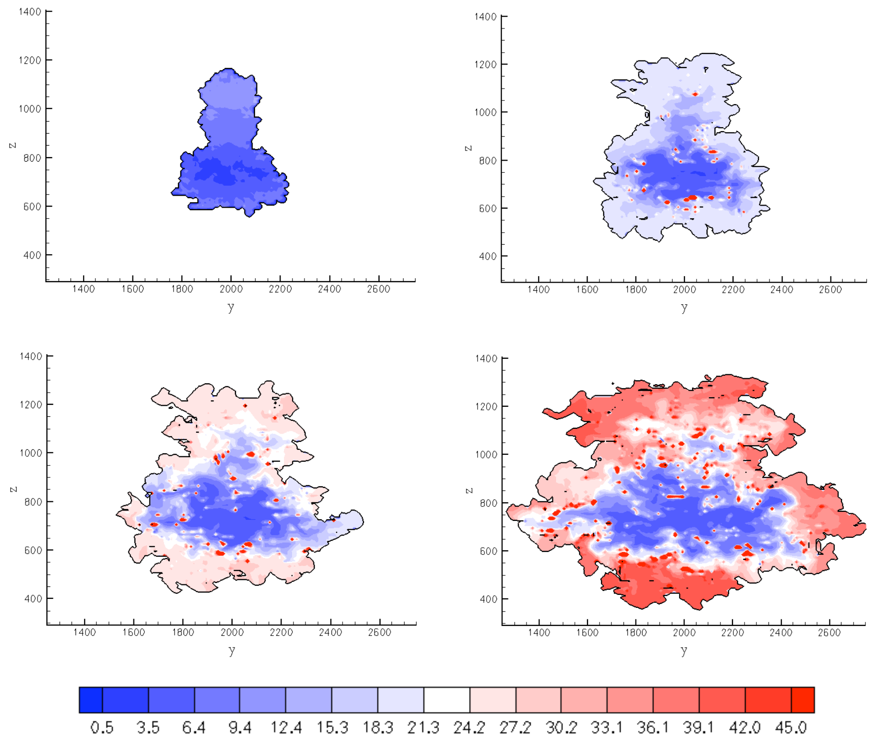


FIG. 2.4 – Cross sectional view of the isocontours of the average ice particle radius (μm) for the diffusion regime at $t = 320,\ 720,\ 1120,\ 2120\,\mathrm{s}$.

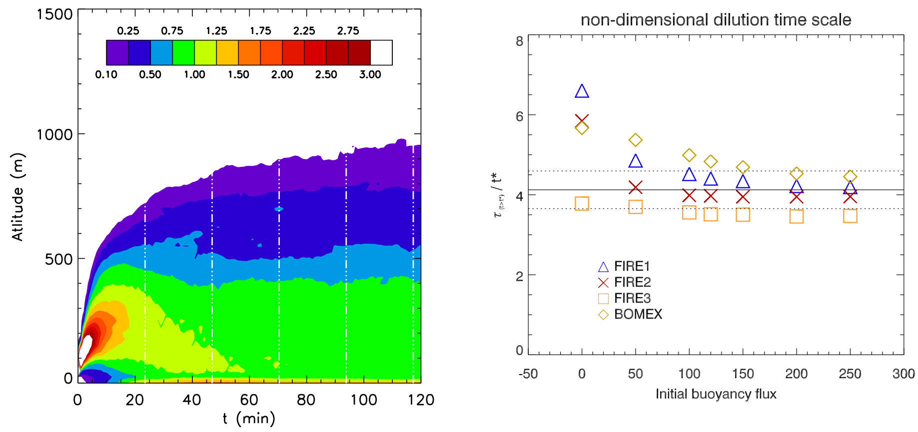


FIG. 2.5 – Left panel : time evolution of normalized mean vertical concentration of a ship plume case with stable boundary layer situation. The vertical dashed-dotted lines represent the characteristic turnover time scale t^* of the boundary layer. Right panel : dilution rate estimate as best fit results of non-dimensional (divided by t^*) constant dilution time scale for steady dilution regime, as a function of initial buoyancy flux at ship stack for four boundary layer cases.

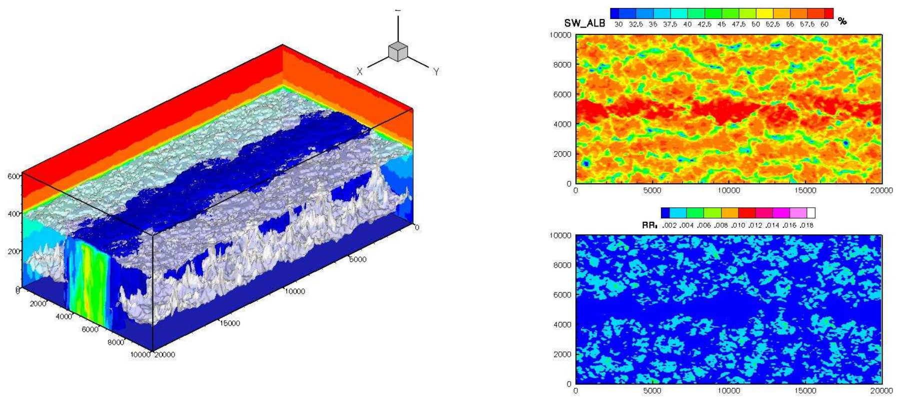


FIG. 2.6 – Ship track at $t = 30\,\mathrm{min}$. Left panel : isosurface of cloud water mixing ratio of $0.01\,\mathrm{g/kg}$. Also shown is the ship exhaust plume particles concentration isosurface of $100\,\mathrm{cm}^{-3}$ (blue shape) ; Right panel : shortwave integrated albedo at $z = 1080\,\mathrm{m}$ (top) and corresponding within-cloud precipitation water mixing ratio at $z = 350\,\mathrm{m}$ (bottom).

realistic description of characteristic dispersion impact on exhaust ship plume chemistry. Plume dispersion simulations are used to derive analytical dilution rate functions. Even though results exhibit striking effects of plume rise parameter on dispersion patterns, it is shown that initial buoyancy fluxes at ship stack have minor effect on plume dilution rate. After initial high dispersion regimes a simple characteristic dilution time scale are used to parameterize the subgrid plume dilution effects in large scale chemistry models. The results show that this parameter is directly related to the typical turn-over time scale of the convective boundary layer (Fig. 2.5). This work served as a basis for a scientific paper submitted in February 2008 to Atmospheric Chemistry and Physics, and accepted in march 2008 for ACP Discussion[1]).

Ship tracks. The objective of this study was to analyze the modification of cloud radiative microphysical and precipitation properties due to the passing of a vessel. To that end, a new aerosol activation scheme, based on the work of Cohard et al. (2000), was developed and implemented in the Meso-NH atmospheric model. Several cloud-topped marine boundary layer situations (derived from FIRE experiment, stratocumulus cloud, Duynkerke et al., 2004) have been simulated using the atmospheric model MesoNH. Furthermore, the microphysical model for activation of aerosols and condensational growth of Cloud Condensation Nuclei (CCN) has been set-up. This allows us to perform simulations with multi aerosol modes and multi aerosol types (chemical composition and dimensional properties). For each boundary layer situation, a coupled LES/Lagrangian simulation has been performed in order to simulate the early dispersion regime of ship plume, taking into account the initial plume rise due to buoyancy fluxes release at ship stack. The resulting cross-wind ship exhaust aerosols concentration fields are then injected into the main LES domain, yet simulating different ship tracks situations. Two complete reference simulations have been performed with a domain size of $20 \times 10 \times 10\,\mathrm{km}^3$ with a mesh size of $50 \times 50 \times 10\,\mathrm{m}^3$, for a simulation period of 4 hours (see Fig. 2.6) and 24 hours (not shown). The ship tracks characteristics were successfully simulated, i.e. increasing cloud droplet number concentration within plume, with a perturbed cloud that exhibits the expected aerosol indirect effects. Hence, results show enhanced integrated shortwave albedo and drizzle suppression within ship plume (see Fig. 2.6). Those effects decrease with time in respect to the dilution processes. In cooperation with the Laboratoire d'Aérologie de Toulouse, the number of simulations will be extended to other cases in order to test the impact of the boundary layer height, the ship exhaust particles concentration and the background aerosol type on the ship track properties and their evolution. The results will be processed and compiled for a future publication expected before the end of 2008.

[1] F. Chosson, R. Paoli, and B. Cuénot, (2008), Ship plume dispersion rates in convective boundary layer for chemistry models, *Atmospheric Chemistry and Physics Discussions*, **8**, 6793–6824.

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

3 Large scale ozone distribution and aircraft emissions

3.1 Linearization of the atmospheric chemistry (D. Cariolle, H. Teyssèdre)

A linearized ozone scheme is used in the ARPEGE/Climat model. It has been developed by Cariolle and Déqué (1986) in order to study the interactions between the ozone distribution and the climate evolution. It is computationally efficient and can be used for first rapid assessment of impacts without the need to use more sophisticated chemical transport models such as MOCAGE [PAE7], which is much more resource demanding.
The ozone scheme has been first updated to remove as much as possible the bias of the parameterization and to better take into account the effects of the heterogeneous chemistry. This version [PAE2] is now included in the MOCAGE-PALM assimilation suite [PAE3], in the Arpège/Climat model, and in the ECMWF operational forecating suite. The latter gives routine forecasts of the ozone evolution, and was able to predict in Autumn 2007 the deepening of the ozone hole ten days in advanced (figure 3.1). This work has been performed in cooperation with the ECMWF research department (A. Dethof, J.J. Morcrette, A. Untch).

In order to use the linearized scheme to study the impact of aircraft emissions on the ozone content, the scheme has been further developed to include the influence on ozone chemical production and destruction rates of the perturbations due to NOy species (mainly $NO + NO_2$ and HNO_3), CO and H_2O. To this end the MOBIDIC model has been used and comparison with the MOCAGE model has been performed using emissions and/or distributions of perturbed species from the FP5 SCENIC project. This task was undertaken by D. Cariolle in collaboration with the CAIAC team (H. Teyssèdre and D. Olivié) of the CNRM. The results show that the linear approach fits well the full chemical computations. It is now included within the Arpège/Climat model and will be used to explore the climate impact of various forcing scenarios from the transport sectors, aviation and ship notably. This work is undertaken within the FP 6 QUANTIFY project.

3.2 Impact of the new HNO_3-forming channel of the $HO_2 + NO$ reaction on tropospheric HNO_3, NO_x, HO_x and ozone (D. Cariolle)

We have studied the impact of the reaction $NO + HO_2 \rightarrow HNO_3$ on atmospheric chemistry [3]. A pressure and temperature-dependent parameterisation of this minor channel of the $NO + HO_2 \rightarrow NO_2 + OH$ reaction has been included in both the 2-D MOBIDIC model and the 3-D tropospheric chemical transport model (CTM) of the Leeds University.
Significant effects on the nitrogen species and hydroxyl radical concentrations are found throughout the troposphere, with the largest percentage changes occurring in the tropical upper troposphere (UT). Including the reaction leads to a reduction in NO$_x$ everywhere in the troposphere, with the largest decrease of 25% in

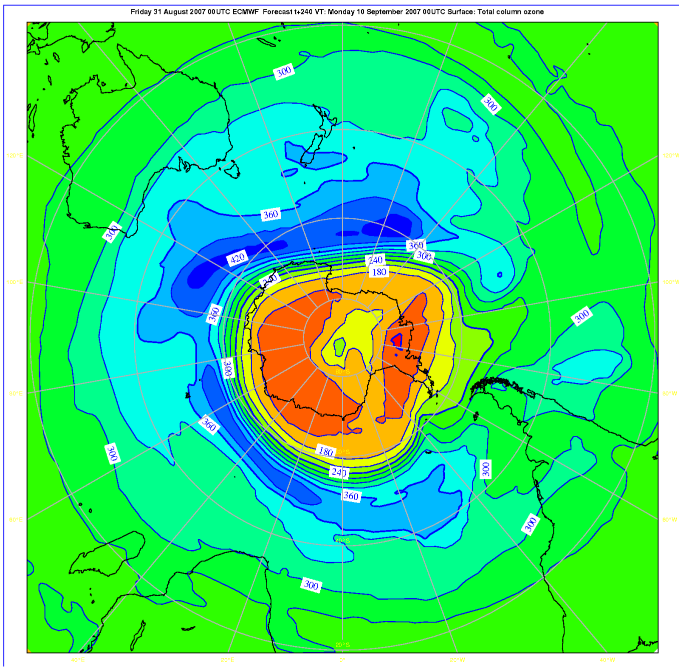


FIG. 3.1 – 10 day ECMWF forecast of the total ozone column for September 10 using the linearized scheme. An ozone hole is predicted with lowest values close to 150 DU, in agreement with observations.

the tropical and southern hemisphere UT. The tropical UT also has a corresponding large increase in HNO_3 of 25%. OH decreases throughout the troposphere with the largest reduction of over 20% in the tropical UT. Mean global decreases in OH are around 13% which leads to a increase in CH_4 lifetime of 5%. The impact on tropospheric ozone is a decrease in the range 5 to 12%, with the largest impact in the tropics and southern hemisphere. Only small changes are calculated in the minor species distributions in the stratosphere.
It is therefore anticipated that this reaction might play an important role when calculating the impact of aircraft NOx emissions on ozone. This new reaction will be introduced in the MOCAGE CTM and new evaluations of the ozone formation by aircraft will be performed in the near future. This work has been performed in cooperation with the Institute for Atmospheric Science, University of Leeds, UK (M. Chipperfield,M. Evans) ; the Institut de Combustion, Aérothermique, Réactivité et Environnement, CNRS (N. Butkovskaya,G. Le Bras) ; and the Service d'Aéronomie, IPSL, CNRS (A. Kukui).

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

We have developed a new method to account for the non-linear chemical effects during plume dispersion. The method is suitable for isolated emissions from local sources and leads to a parameterization which is implemented in a global model and use to evaluate the impact of aircraft emissions. Compared to previous approaches that introduce corrected emissions or corrective factors to account for the non-linear chemical effects, our parameterization is based on the description of the plume effects via a fuel tracer and a lifetime during which the non-linear interactions between species are important and operate with effective reaction rates. The implementation of the parameterization insure mass conservation and allows the transport of non-diluted emissions in plume-form by the model dynamics.

3.3.1 Basic Formulation

During the dilution phase the concentrations of the species have concentrations of several orders of magnitude superior to that of the background atmosphere, so that the same reaction operating inside a plume can see its effects amplified with regard to its influence in the plume free atmosphere. This arises from the calculation of the rates of production/destruction of the chemical reactions which are obtained by the product of the concentrations of the reacting species. The chemical system shows therefore strong nonlinearities, so the injection at high concentration of a chemical species or particle will have a variable impact depending on the degree of dilution of the plume. We have first addressed this problem from a theoretical point of view [4], and establish the set of equations and methods required to account for the non-linear terms in the continuity equations of the minor species. In a second step we have derived the simplifications of the system of equations that can be used within large scale models when injected and produced species can be treated separately.

One of the key parameters is the time τ needed to achieve plume dispersion. If this time is short compared to the rates of the reactions which drive the non-linearity of the chemical processes the plume induced effects will be unimportant, on the other hand they will be significant if the reaction rates are lower or of the same order. This timescale is mainly driven by the dilution rate of the plumes which is a function of the characteristics of the atmospheric turbulence.

Once this parameter is set it is then possible to determine the fraction of the injected species remaining within the plume for which the chemical system has characteristics different from that of the surrounding atmosphere. To represent this process a "fuel tracer" is added to the CTM variables. This tracer gives the quantity of injected material not yet diluted at large scale. Denoting by r_f the mixing ratio of this tracer, its continuity equation reads :

$$\partial r_f/\partial t = < F_f > + I - \frac{1}{\tau}.r_f \tag{3.1}$$

where $< F_f >$ denotes the divergence of the transport fluxes of the tracer, I is the injection rate obtained from emission data, and τ the plume lifetime.

Thus, the mixing ratio at the large scale of a non-diluted emitted species is obtained by multiplying r_f by its emission index. For the NOx ($= NO + NO_2$) species, one can write :

$$r_{NOx} = r_f.EI_{NOx} \tag{3.2}$$

where r_{NOx} is the mixing NOx ratio in the non-diluted phase, and EI_{NOx} the emission index for the NOx.

After dilution, the NOx in the non-diluted phase are restored in the diluted phase noted as $\overline{NOx}$. Thus, the mixing ratio of $\overline{NOx}$ is obtained by solving the following equation :

$$\partial r_{\overline{NOx}}/\partial t = < F_{\overline{NOx}} > + \frac{1}{\tau}.r_f.EI_{NOx} + large\ scale\ chemical\ sources\ and\ sinks \tag{3.3}$$

Knowing the fraction of the injected species between the diluted and non-diluted states it is then possible to calculate the rates of production of the secondary formed species. These rates will be modified within the non-diluted air masses because of the strong concentrations of the injected species. The modified rates are introduced via the determination of effective reaction rates K_{eff} which are used to compute secondary formed species within the plume. For instance ozone would have chemical source and sink terms from the large scale, and similar terms from the non-diluted phase. The continuity equation for the ozone mixing ratio r_{O_3} would be :

$$\partial r_{O_3}/\partial t = ... - K.\overline{NOx}.r_{O_3} - K_{eff}.NOx.r_{O_3} + ... \tag{3.4}$$

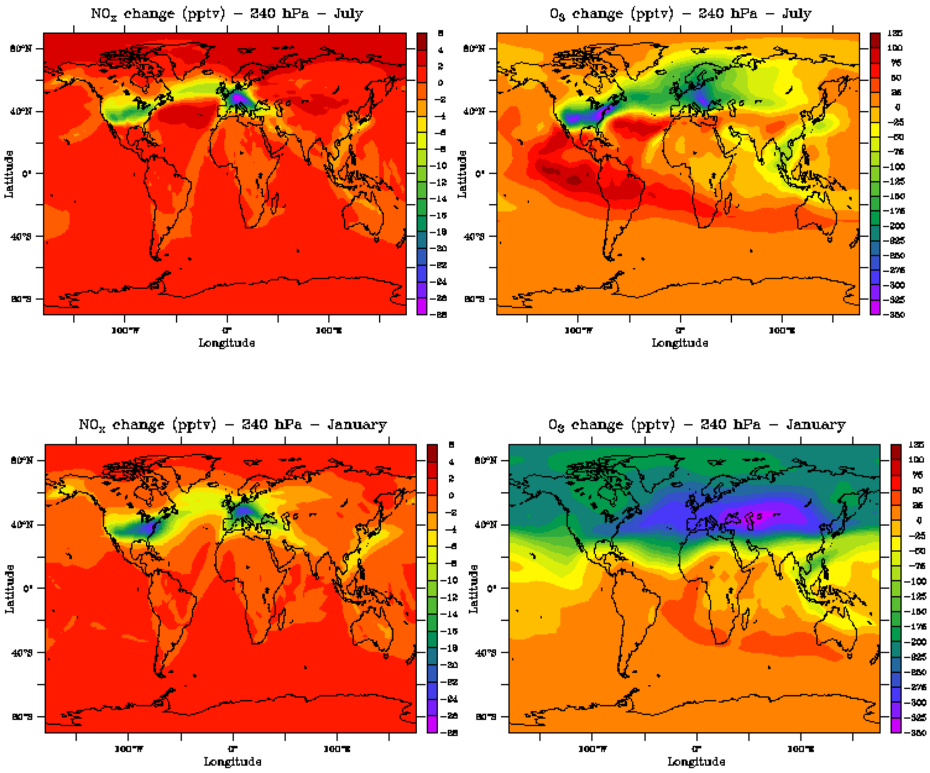


FIG. 3.2 – Distribution of NOx and O_3 variations due to aircraft plume effects at 240 hPa for July (top) and January (bottom).

where K_{eff} is the effective reaction rate for the ozone reaction with the non-diluted fraction of the NOx, a reaction that goes in addition to the reactions already accounted within the large scale model for background species concentrations.

This approach is derived from the methods of "segregation" that has been developed in studies of formation by NOx emission in boundary layers.

3.3.2 Impact of aircraft NOx emissions on the ozone distribution

With inclusion of the plume effects, the simulations with the LSCE model of the impact of aircraft emissions are in rather good agreement with previous work. We found that the ozone production is decreased by 10 to 15 % in the northern hemisphere with the largest effects in the north Atlantic corridor when we account for plume effects on the chemistry (figure 3.2). These figures are consistent at the global scale with evaluations made with corrected emissions, but regional differences are noticeable due to the possibility offered by our parameterization to transport emitted species in plume-form before operating at large scale.

This work has been performed in cooperation with the Laboratoire des Sciences du Climat et de l'Environnement, CEA-CNRS (D. Caro, A. Cozic, D. Hauglustaine) within the QUANTIFY project.

Our method will be further improved to account for the local temperature and turbulence properties diagnosed within the large scale model, and to more complex chemical cycles that can have multistep regimes during the plume dilution processes. In particular the transformation of NOx into HNO_3 within the plume has a very significant impact and should be better quantified. We expect to obtained more accurate transformation rates from the Meso-NH contrail simulations.

[3] D. Cariolle, M. J. Evans, M. P. Chipperfield, N. Butkovskaya, A. Kukui, and G. Le Bras, (2008), Impact of the new HNO_3-forming channel of the HO_2+NO reaction on tropospheric HNO_3, NO_x, HO_x and ozone, *Atmospheric Chemistry and Physics Discussions*, **8**, 2695–2713.

[4] R. Paoli, D. Cariolle, B. Cuénot, R. Paugam, and F. Chosson, (2008), Modeling chemical reactions and emissions from concentrated sources into global models, *Comptes Rendus Mechanique*, submitted.

4 Publications

4.1 Journal Publications

[PAE1] Cariolle, D. and J.-J. Morcrette. A linearized approach to the radiative budget of the stratosphere : influence of the ozone distribution. *Geophys. Res. Lett.*, 33, L05806, doi :10.29/2005GRL025597, 2006.

[PAE2] Cariolle, D. and Teyssèdre, H. : A revised linear ozone photochemistry parameterization for use in transport and general circulation models : Multi-annual simulations, *Atmos. Chem. Phys.*, *7*, 2183-2196, 2007.

[PAE3] Geer, A.J., W.A. Lahoz, D.R. Jackson, D. Cariolle and J.P. McCormack. Evaluation of linear ozone photochemistry parameterizations in a stratosphere-troposphere data assimilation system. *Atmos. Chem. Phys.*, 7, 939959, 2007.

[PAE4] Massart, S., A. Piacentini, D. Cariolle, Laaziz El Amraoui, N. Semane. Assessment of the quality of the ozone measurements from the Odin/SMR instrument using model assimilation. *Can. J. Phys.*, 85, 1209-1223, 2007.

[PAE5] Geer, A. J., Lahoz, W. A., Bekki, S., Bormann, N., Errera, Q., Eskes, H. J., Fonteyn, D., Jackson, D. R., Juckes, M. N., Massart, S., Peuch, V.-H., Rharmili, S., and Segers, A. : The ASSET intercomparison of ozone analyses : method and first results. *Atmos. Chem. Phys.*, 6, 5445-5474, 2007.

[PAE6] Lahoz, W. A., Geer, A. J., Bekki, S., Bormann, N., Ceccherini, S., Elbern, H., Errera, Q., Eskes, H. J., Fonteyn, D., Jackson, D. R., Khattatov, B., Marchand, M., Massart, S., Peuch, V.-H., Rharmili, S., Ridolfi, M., Segers, A., Talagrand, O., Thornton, H. E., Vik, A. F., and von Clarmann, T. : The Assimilation of Envisat data (ASSET) project. *Atmos. Chem. Phys.*, 7, 1773-1796, 2007.

[PAE7] Teyssèdre, H., M. Michou, H.L. Clark, B. Josse, F. Karcher, D. Olivié, V.-H. Peuch, D. Saint-Martin, D. Cariolle, J.-L. Attié, P. Nédélec, P. Ricaud, V. Thouret, R.J. van der A, A. Volz-Thomas, and F. Chéroux. A new tropospheric and stratospheric Chemistry and Transport Model MOCAGE-Climat for multi-year studies : evaluation of present-day climatology and sensitivity to surface processes. *Atmos. Chem. Phys.*, 7, 5815-5860, 2007.

4.2 Technical reports

[PAE8] Atié, J.-L., ..., D. Cariolle, S. Massart and A. Piacentini. Dual assimilation of MOPITT and MLS carbon monoxide in the MOCAGE model. A contribution to ACCENT-TROPOSAT-2.*CERFACS Technical Report*, TR/AE/07/66, 2007.

[PAE9] Cariolle, D., H. Teyssèdre and J.-J. Morcrette. Une approche linéarisée de la chimie de l'ozone et du transfert radiatif dans la stratosphère. Atelier modélisation de l'atmosphère.*CERFACS Technical Report*, TR/AE/06/113, 2006.

[PAE10] Cariolle, D.. Parameterization into large scale models of the nonlinearities of the atmospheric chemistry during plume dispersion.*CERFACS Technical Report*, TR/AE/07/24, 2007.

[PAE11] Cariolle, D., and H. Teyssèdre. A revised linear ozone photochemistry parameterization for use in transport and general circulation models : Multi-annual simulations.*CERFACS Technical Report*, TR/AE/07/26, 2007.

[PAE12] Cariolle, D., S. Massart and H. Teyssèdre. Polar and midlatitude ozone. Proceedings of the ECMWF workshop on Polar Meteorology, September 2006. *CERFACS Technical Report*, TR/AE/07/27, 2007.

[PAE13] Cariolle, D. and S. Massart. Ozone distributions derived from satellite data assimilation and their impact on the stratospheric temperatures. ESA Proceedings of the second Atmospheric Science Conference, Montreux, Suisse 23-27 April 2007.*CERFACS Technical Report*, TR/AE/07/45, 2007.

[PAE14] Paugam, R., R. Paoli, D. Cariolle and B. Cuenot. Numerical simulation of aircraft plume evolution using a mesoscale code. *CERFACS Technical Report*, TR/AE/07/30, 2007.

8

Aerodynamics and Multiphysics

ADVANCED AERODYNAMICS
AND MULTIPHYSICS

CERFACS

1 Introduction

Jean-François Boussuge

The ”Advanced Aerodynamics and Multiphysics” team 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 team is to develop efficient numerical solvers for the resolution of fluid dynamics problems on industrials configurations. Most of the efforts are dedicated to implement numerical methods, however complex simulations play also an important role. The considered applications can be splitted in two domains : civil aircraft and turbomachinery.

The main part of our activity concerns the multiblocs structured solver called *elsA*. This solver belongs to Onera, and Cerfacs has an official agreement to participate to its development. Besides *elsA*, others codes are available (in-house codes : AVBP, NTMIX and an external code from DLR : Tau) which enable to study different applications ranging from wake vortex to aerothermal simulation.

During the past two years, the group has been more and more involved in the field of turbomachinery either in development of numerical methods or in complex simulations. It has to be noticed that this activity impacts now an important part of the team in term of research, contract and people involved.

All the work described in the following sections have been done in close collaboration with industrials partners such as Airbus, Snecma and Turboméca and also with research centers among which Onera, IRPHE and Paris VI. In addition to these strong and old links, the team has started a joint effort with ECL concerning the turbomachinery activity.

2 Numerical aerodynamics

2.1 Numerical methods

2.1.1 Harmonic Balance Technique : an efficient Fourier-based algorithm for time periodic flows (F. Sicot, G. Puigt, M. Montagnac)

Even if three-dimensional steady turbulent flow simulations begin to be handled routinely in aircraft industry, three-dimensional unsteady turbulent flow simulations still require large amounts of computing time and a substantial acceleration of the calculations is needed in order to reduce design cycles.
To build an efficient method for unsteady flows, it is interesting to take into consideration all flow characteristics. As an example, a large range of applications leads to time periodic flows : turbomachinery, pitching wings, helicopter blades, wind turbines... These flows are intrinsically unsteady and in the recent years, a more efficient time-domain method dedicated to time-periodic flows has been developed. The Harmonic Balance Method (HBT) [1], which casts the unsteady governing equations in a set of coupled steady equations corresponding to a uniform sampling of the flow within the time period. These steady equations can then be solved using standard steady RANS methods (see Fig. 2.1) with convergence acceleration techniques such as local time stepping and multigrid. The convergence of a steady computation is better mastered than the transient needed by an unsteady computation to reach the periodic state.

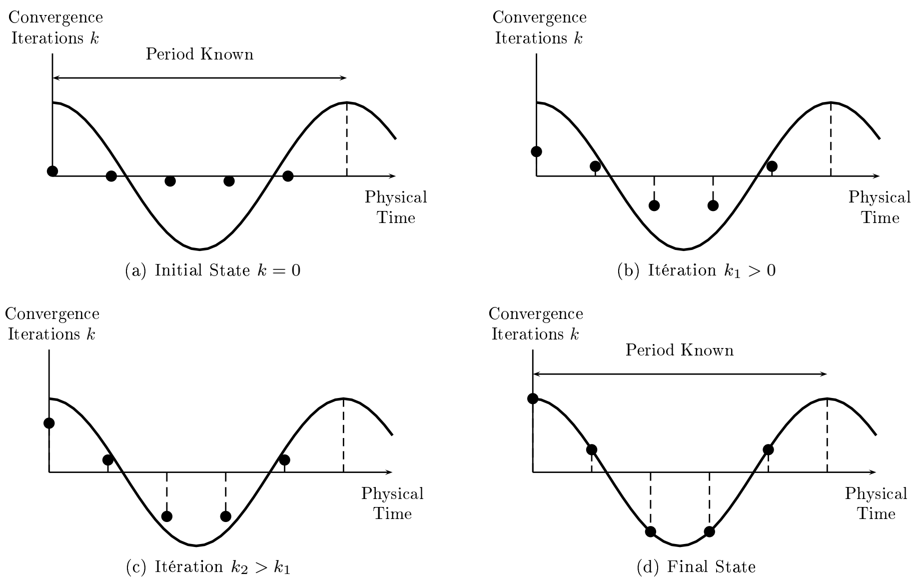


FIG. 2.1 – Principle of the HBT.

Up to now, explicit algorithms such as Runge-Kutta methods were used to advance the calculations in pseudo-time. This makes the pseudo-time steps relatively small and therefore requires a large number of iterations to reach the steady state of all the instants. Furthermore it has been observed that the convergence

rate decays as the number of harmonics is increased [2]. To circumvent this, a specific implicit time integration scheme has been derived. Based on a block-Jacobi approach, its larger stability criterion enables much larger time steps and makes the HBT more robust.
The method has been validated on pitching airfoil and wings for different flow conditions (subsonic up to transonic, with or without separation). See following section for an example.

[1] K. C. Hall, J. P. Thomas, W. S. Clark, *Computation of Unsteady Nonlinear Flows in Cascades using a Harmonic Balance Technique*, AIAA Journal, Vol. 40, No. 5, pp. 879-886, 2002
[2] A. Gopinath and A. Jameson, *Time Spectral Method for Periodic Unsteady Computations over Two- and Three- Dimensional Bodies*, 43rd Aerospace Sciences Meeting and Exhibit, AIAA Paper 2005-1220, Reno, Nevada, 2005

2.1.2 Harmonic Balance Technique : Extension to ALE with mesh deformation (G. Dufour, F. Sicot)

In the field of aeroelasticity, an important class of periodic aerodynamics problems is the forced motion of structures in airflows. The simulation of these flows with the *elsA* software is usally performed within the Arbitrary Lagrangian Eulerian (ALE) formulation on deforming meshes, with unsteady time-integration. Using the periodic nature of these flows, the HBT method can be used in place of unsteady simulations in order to reduce the computational time. To apply the HBT method to such problems, several developments have been made. First, a modified version of the HBT source term has been implemented, to account for mesh deformation. Secondly, some terms specific to the ALE formulation of the Navier-Stokes equations have been modified to ensure compatibility with the method. Finally, the integration of the method has been done through the development of a python module, in such a way that it can be used in a modular context. The results have been verified against the reference simulations of the previous part (2.1.1) for the Lann ct5 test case (pitching in transonic flow, without separation), see Fig. 2.2.

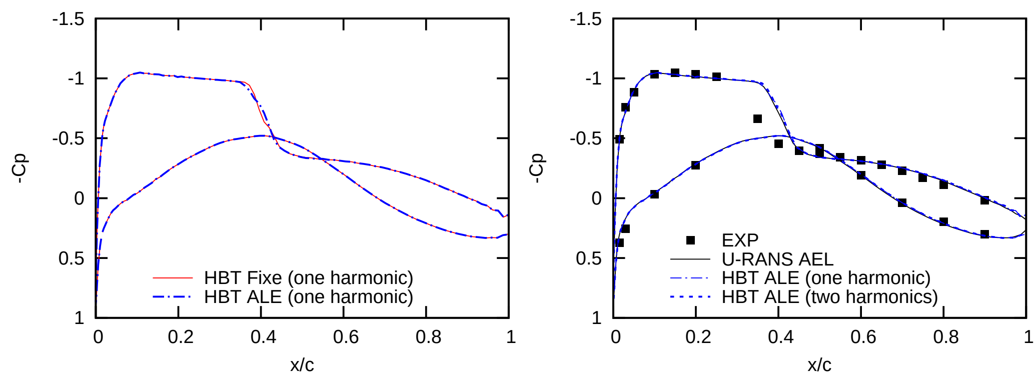


FIG. 2.2 – Lann wing, ct5 test case : HBT-ALE simulations with deformed meshes.

The slight differences are due to the use of different (deformed *vs* fixed) meshes. The simulations have also been validated with the unsteady simulations (U-RANS AEL) of Delbove [1] and the experimental results of Davies [2], showing fair agreement (Fig. 2.2-b). The target application for the method is the prediction of blade flutter in compressors.

[1] Julien Delbove, *Contribution aux outils de simulation aéroélastique des aéronefs : prédiction du flottement et déformation statique des voilures*, PhD Thesis, École Nationale Supérieure de l'Aéronautique

et de l'Espace, 2005
[2] Davis, S. S., *NACA 64A010 (NASA Ames Model) Oscillatory Pitching*, AGARD report no 702, 1982

2.1.3 Spatial DNS Simulation of a Co-Rotating Vortex System (H. Deniau, L. Nybelen)

The present numerical study is motivated by the challenge to simulate the three-dimensional spatial dynamics of a co-rotating vortex system, through the development of an elliptic instability, using a high order solver of the compressible Navier-Stokes equations. This phenomenon was previously studied by temporal simulations. The interest of spatial simulation is first to analyse the effect of the axial velocity on the merging process which are neglected with the temporal approach, and to study interaction with jet flows.

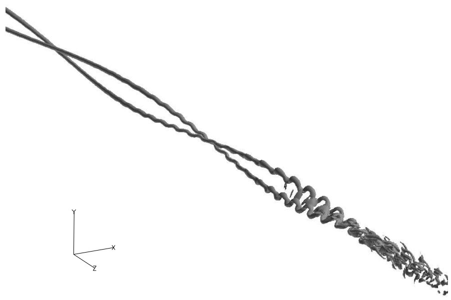


FIG. 2.3 – Selected isosurface of vorticity magnitude, $W_{axial} = 0.2$; $V_\theta = 0.1$.

The numerical problem is the choice of the boundary conditions : inflow and outflow conditions and also lateral boundary conditions. A special attention has been paid on the latter due to the difficulty induced by the non zero circulation of the considered vortex system. The classic boundary conditions of Poinsot and Lele based on the characteristics wave approach have been modified to be more adapted to the physics considered here. This new boundary condition is based on the assumption of an irrotational flow close to the borders (in order to determine the magnitude of the waves), or a serie expansion for the transversal velocity component in term of perturbated potential flow.
A special corner treatment is also proposed to reduce perturbation generated in this area. After a validation of these improved boundary conditions and of all numerical tools used such as selective artificial dissipation, spatial simulations of the vortex breakdown phenomenon have allowed validating our solver for a three-dimensional case. Thus, the merging process of equal co-rotating vortices through the development of elliptic instability with axial velocity was simulated. Three vortex flow configurations were considered with different vortex systems and velocity peaks ratio (azimuthal and axial velocities). The first results show on the one hand the ability to compute spatial instability development in vortex flow, on the other hand the influence of the axial velocity on the instability dynamics. However, spatial simulations are limited by the computational resources (linked to the resolution and axial domain length to capture the merging process) and restricted to academic vortex flow configurations.

2.1.4 High order schemes in *elsA* (A. Fosso-Pouangué, H. Deniau)

In order to assess jet noise by coupling *elsA* with a wave propagation model, it is needed to capture properly the turbulent structures which are noise sources of the jet, and to convect pressure waves by minimizing

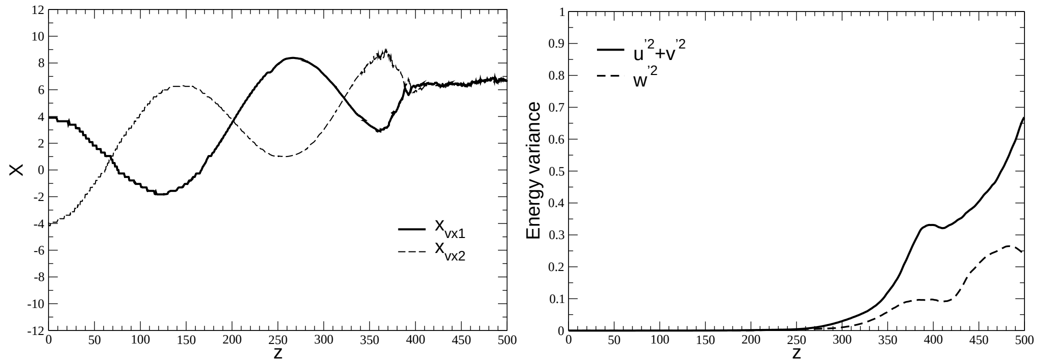


FIG. 2.4 – Horizontal vortex core positions as function of the axial distance (left) and variance of the cross -flow and axial kinetic energy (right).

schemes-due dissipation and dispersion effects. Therefore, it is necessary to implement high order schemes in *elsA*. Compact high order schemes have the advantage to use a smaller stencil compared to explicit ones of the same order. Implementation of a sixth-order compact scheme have been introduced in *elsA* by the work of Sicot which apply Lacor and Smirnov ideas [1] to stretched meshes. The present activity focuses on three aspects : implementation of join boundary closures, generalization to curvilinear meshes and filtering. Numerical tests have highlighted the instability of the Sicot join boundary closure on stretched meshes. A new boundary closure has been considered using implicit upwind compact schemes. Another important part of the work has consisted in realizing a sixth-order compact scheme on curvilinear meshes also based on ideas developed by Lacor and Smirnov. This approach has been validated on Cartesian meshes since it is exactly equivalent to the Sicot approach and gives the same numerical results. When using high order schemes, it is often necessary to apply a filter in order to stabilize computations.

To keep the approach consistance, the filter chosen is a high order compact filter proposed by Gaitonde and Visbal [2]. It is applied on conservative fields for each substep of the time advance scheme. The test case used is the convection of a vortex in an uniform flow in a domain with periodic boundary conditions. Figures 2.5 and 2.6 shows results for the different schemes on an uniform mesh and on a wavy mesh.

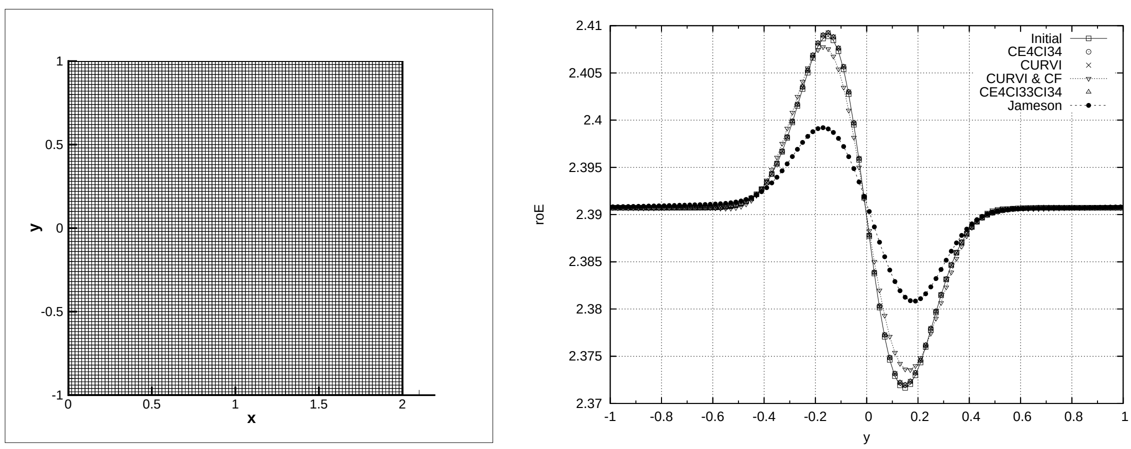


FIG. 2.5 – Uniform cartesian mesh, total energy after 20 turnover periods.

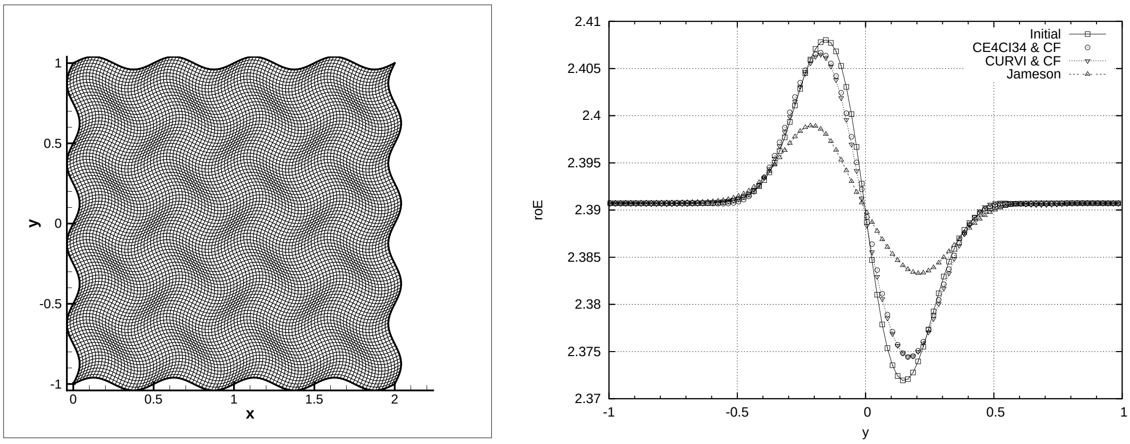


FIG. 2.6 – Wavy mesh, total energy after 22 turnover periods.

[1] C. Lacor, S. Smirnov and M. Baelmans, *A Finite Volume Formulation of Compact Schemes on Arbitrary Structured Grids*, J. of Comput. Phys., Vol 198, pp 535-566, 2004
[2] D. Gaitonde and M. Visbal, *Further development of a Navier-Stokes solution procedure based on higher-order formulas*, AIAA Paper 1999-557, Reno, Nevada, 1999

2.1.5 POD based surrogate model for parametric aerodynamic design (T. Braconnier, J.-C. Jouhaud)

For analysing complex systems, data reduction has become a real challenge in many scientific areas (turbulent fluid flows, optimization, control design, structural vibrations, numerical imaging...). This is especially true in the context of aerodynamic studies where the amount of data has considerably increased this last decade. At this time, surrogate models appear as one of the most efficient tools for achieving data reduction and to perform aerodynamic optimization. Different approaches are available, but the one used at Cerfacs is based on the **P**roper **O**rthogonal **D**ecomposition model.
First, a POD data reduction is performed by computing a database built on the matrix containing the CFD computations (snapshots) at chosen parameters of the flight domain. The POD basis is obtained either by an eigenvalue decomposition of the correlation matrix or by a singular values decomposition of the snapshot matrix. Then, the quality of the model is estimated by the leave-one-out method and new flight parameters inside the flight domain are automatically determined by a quad-tree algorithm.

Next, a reconstruction step allows us to predict either the conservative variables or aerodynamic quantities, using an interpolation scheme such as cubic splines, Kriging method or radial basis functions.

For illustrating the use of the POD model, the C_p distribution on the RAE2822 airfoil at the flight parameter $\pi_0 = (2.79^o, 0.73)$ has be predicted (see right part of Fig. 2.7). The studied flight domain is defined by $\{\pi = (\alpha, M_\infty) \in [0^o, 4^o] \times [0.6, 0.8]\}$, the starting sampling domain contains the four corresponding corners and the POD model automatically selects the 20 more relevant parameters inside the flight domain in order to correctly mimic the subsonic-transonic transition (see Fig. 2.7).

The POD model has been proved to be an efficient (in term of CPU time and memory requirement) and a reliable approach to implement data compression in order to use the results of previous heavy CFD computations and to avoid to perform such computations any time aerodynamic quantities are needed for

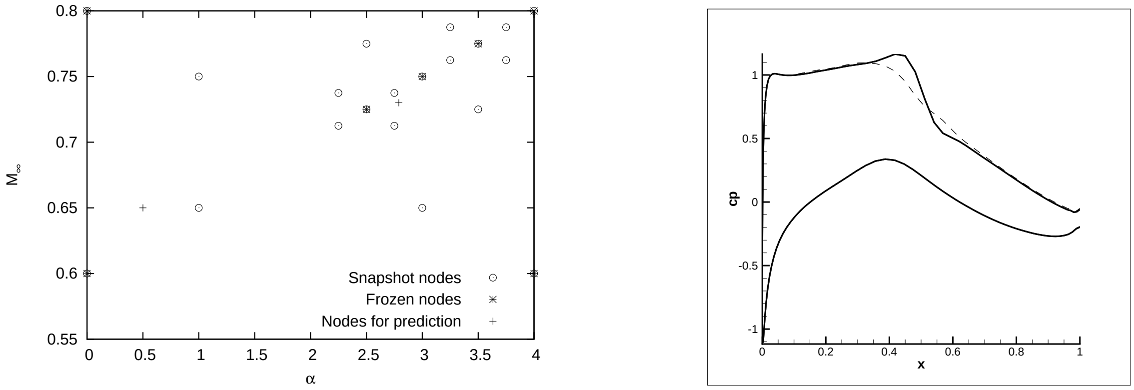


FIG. 2.7 – CFD computation (solid line) and POD model prediction (dashed line) at $(2.79^o, 0.73)$.

new flight parameters. For aircraft manufacturers, it is a crucial issue and this strategy can be applied to numerous applications : aerodynamic control and design, aeroelasticity, multidisciplinary optimization or simply exchange of data between different disciplines.

2.1.6 Development of a response surface based optimization algorithm (J. Laurenceau)

In the field of high-fidelity aerodynamic shape optimization, the choice of the optimization algorithm is heavily constrained by the computational cost implied by one function evaluation. Thus, gradient descent algorithms are particularly appreciated for their speed of convergence. Coupled with an adjoint method to inexpensively compute the gradient vector (sensitivity of the drag with respect to the shape variables for instance), these methods require the least computational cost. Despite that, these local optimizers can not avoid the multiples local optima of typical aerodynamic functions and are sensitive to numerical noise.

Global optimizers such as genetic algorithms can not directly drive the expensive CFD evaluator, but it appears that the use of response surfaces to inexpensively approximate the CFD solver based on a limited sample database of calculation is promising. The response surface build with only a few hundred samples can not accurately represent the function depending on several tens variables, but it proves to give correct trends. Then, by iteratively refining the surrogate model at promising locations it is possible to largely outperform a gradient based optimizer.

A comparison of different sampling refinement criteria was done using aerodynamic test cases and the *OPTaliA* framework of *Airbus* to finally establish an optimizer capable of proposing a population of three new shapes per process iterations. The refinement at the predicted minimum on the Kriging surrogate model $\hat{F}(x)$, proved to converge too prematurely whereas the use of Kriging standard error $\hat{S}(x)$, to explore zones of high uncertainty enables to ensure a more global convergence (Fig. 2.8).

2.1.7 Application of the response surface based optimizer on a 3D test case (J. Laurenceau)

Typical industrial shape optimization problems usually consider several hundreds design variables whereas it is not possible to perform more than two hundreds functions evaluations for computational cost issues. As the accuracy of a Kriging surrogate model decreases when dimension increases, a Cokriging model interpolating the information given by the gradient vector was used. By using the discrete adjoint method

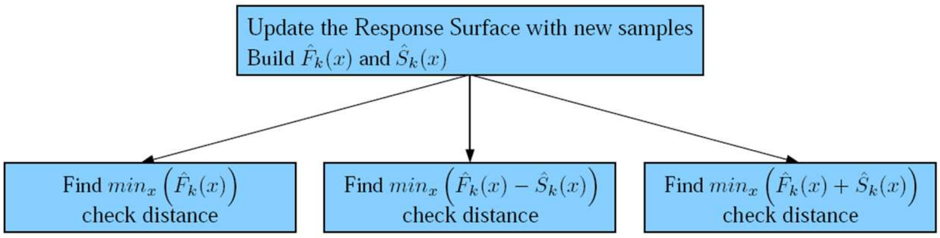


FIG. 2.8 – Kriging based optimization algorithm.

of *elsA*, it is possible to obtain this vectorial information on the function at the same cost of one function evaluation (scalar information).

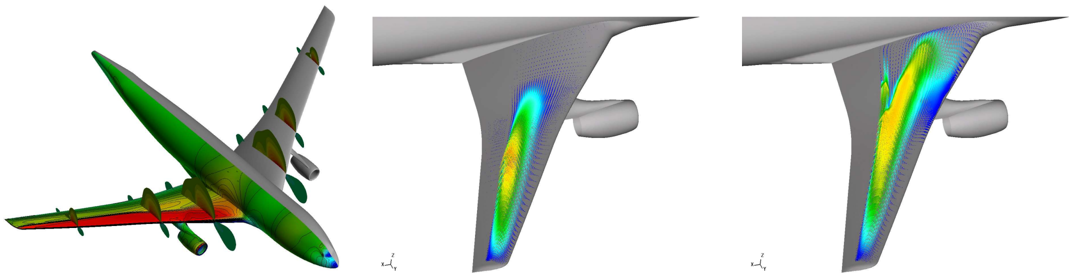


FIG. 2.9 – Optimisation of the AS28G configuration. Left : Baseline configuration. Middle : Optimal deformation field given by the gradient optimizer. Right : Optimal deformation field given by the Cokriging based optimizer.

It was then possible to demonstrate the efficiency of the Cokriging based optimizer to reduce the drag of an AS28G WBPN configuration (Wing Body Pylon Nacelle) using the *OPTaliA* framework of *Airbus*. For this problem depending on 48 design variables driving amplitude, position and width of 16 Hicks-Henne bumps, one function evaluation takes 5 hours using 10 Opteron scalar processors. Despite the fact that the Cokriging based optimizer requires 65% more function evaluations to converge than the gradient based reference, it finally achieves a better function improvement in less process iterations. Moreover, this optimizer proves to perform more exploration of the design space than the gradient algorithm. It converges to a shape far from the baseline configuration and more complex than the shape given by the gradient reference (Fig. 2.9).

2.2 Meshing techniques

2.2.1 Chimera IHC : A highly automated method for overset grids (B. Landmann)

The Chimera grid methodology uses a set of overlapping grids to discretise the solution domain. In the overlapping regions certain grids are prioritised for the calculation of the flow field. The Chimera technique facilitates the block-structured grid generation process and enables the simulation of bodies in relative movement. However, for complex configurations the prioritisation of certain grids to other ones, that is also known as Chimera grid setup, can become a tedious task, because most of the existing setup techniques work in an iterative (trial and error) manner and require a high degree of user input. Therefore a different setup approach is favoured in this work package. It works in a completely automated manner and requires no user input. The algorithm is based on the implicit hole cutting (IHC) algorithm firstly presented by Lee and Bader [1]. It was enhanced by several methodologies, in order to eliminate shortcomings in the original method. The resulting over-all algorithm is more general than the original one, while preserving the high automatism of the original method. An easy example (without loss of generality) is shown in Fig. 2.10.

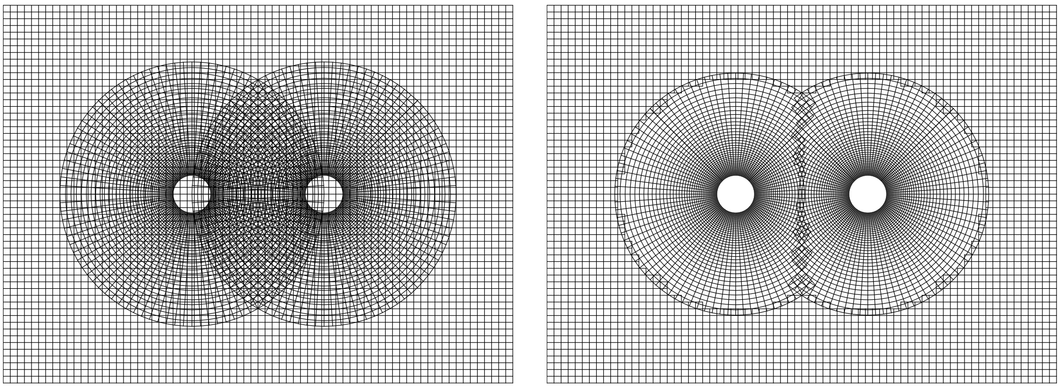


FIG. 2.10 – Example for implicit hole cutting method : Two cylinder grids embedded in a background grid.

The modified IHC method is implemented into the *elsA* flow solver. Several complex industrial test cases have been successfully passed. The method is moderately more expensive than the standard methods included in *elsA* but due to its automatic manner it has the potential being used extensively in order to ease the simulation of complex aerodynamic configurations at Airbus France.

[1] Y. Lee and J. Bader, *Implicit Hole Cutting - A New Approach to Overset Grid Connectivity*, AIAA Paper 2003-4128, Reno, Nevada, 2003

2.2.2 Automated assembly algorithm for patched Chimera grids (F. Blanc)

The possible configurations of Chimera grids are numerous. Designing an automated algorithm able to deal with each specific configuration is an exhausting and possibly endless task. That is the reason why a new Chimera grid assembly algorithm, called "patch assembly algorithm" has been developed. This algorithm does not aims at being able to assemble all type of Chimera grids but aims at assembling efficiently and robustly a specific type of Chimera grid. It includes all the grids where the Chimera technique is used for adding to a geometry, defined in a background grid, a new geometrical feature meshed in a patched Chimera grid. A spoiler added over a wing is a simple example : the background grid is the airfoil mesh and the spoiler mesh would be the patched Chimera grid. This type of Chimera grid has been chosen since it covers a wide range of applications of the Chimera technique. Examples can be : stores under an airplane, adding blades to an helicopter or tail surfaces on a fuselage... The patch assembly algorithm automatically blanks as much cells as possible in the background grid. As no mask definition is required, the user workload for using the Chimera technique is greatly reduced. Moreover, the algorithm does not use any geometrical feature, as a consequence, it does not face any of the threshold setting problems generally associated to the use of such entities. The algorithm, developed in *elsA* flow solver, has been tested on a lot of industrial configurations on which it has proved its efficiency and its robustness (see Fig. 2.2.2).

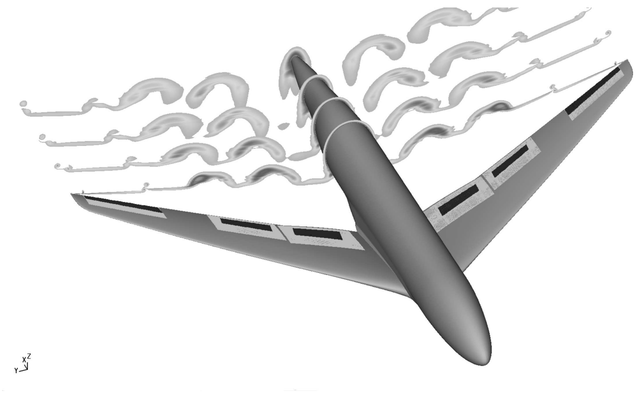


FIG. 2.11 – Computation on a Chimera grid automatically assembled by the “patch assembly algorithm”. The aileron and two deployed spoilers have been added to the airplane using the Chimera technique.

2.2.3 Association of local and global multigrids (M. Montagnac)

Local multigrid and global multigrid were implemented independently in the *elsA* software. The main difference was that fluxes were stored at interface centers for the local approach to provide the refluxing function and only the flux balance was stored at cell centers in the global approach. The merging of the two techniques has led to choose the lowest storage of data and as a consequence to develop a special process to impose the refluxing function. Now, steady flows for AMR configurations can benefit from a full multigrid acceleration.

2.2.4 Sliding Mesh Boundary Condition (M. Montagnac)

The non coincident interface boundary condition is the core of the sliding mesh feature. The former was developed by Cerfacs to avoid the propagation of grid points through block interfaces in the meshing process. At the end, grid lines through an interface may be not continuous. For configurations with an axial symmetry, the interface between blocks is moving during the motion period and connectivities between interfaces have to be computed at each time step. This functionality was available for flows around advanced $360°$ high-speed propellers in an absolute frame and it has been extended for turbomachinery activities (cf. section 3.2.1 and 3.2.2) especially for axisymmetric configurations in relative frames.

2.2.5 Extension of the *elsA* code to hybrid meshes (G. Puigt, A. Fosso-Pouangué)

In the framework of structured meshes as for the *elsA* code, obtaining a blocking and then a mesh can be a difficult task when the geometry is complex. Even if Chimera technique can relax the mesh constraints, there are still configurations which are difficult to handle with a structured approach. This is particularly the case for high lift configurations for planes (presence of flaps and slats) or for blade cooling (presence of several hundreds of small gaps which inject “cold air” in the main flow). For such applications, the unstructured meshes can be an interesting solution.

They can be obtained easily with automatic mesh generators, even if the geometry is very complicated. However, unstructured solvers are known to be less efficient than structured ones : for a given mesh, the classical CPU loss is higher than 25%. Thus, in order to assess complex configurations with a limited CPU time penalty, the best way to proceed is to extend *elsA* to multi-blocks hybrid meshes : some blocks are treated by the structured part of *elsA* and others by the unstructured one.

This tedious task has been started in a strong collaboration with Onera. As far as the Cerfacs is concerned, our work focused on the definition of diffusion schemes for both structured and unstructured meshes. In particular, the choice of the diffusion scheme was not straightforward, the main difficulty being the order of accuracy of the gradients at the interface position.
Some results for laminar flows have been obtained for 2D and 3D cases and in particular, solutions are quite similar on structured and unstructured meshes composed of hexahedron (Fig. 2.12). Future works will include the extension to turbulent flows and also the transfert information between structured and unstructured blocks.

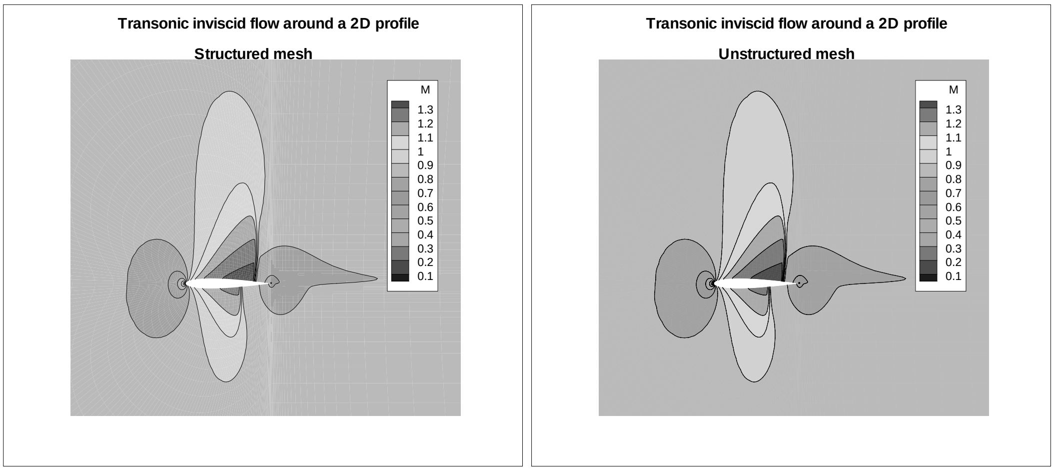


FIG. 2.12 – Two dimensional transonic computation : iso-Mach contours obtained on the same structured (left hand side) and unstructured (right hand side) meshes.

3 Applications

3.1 Aircraft

3.1.1 Large Eddy Simulations for aerothermal applications (M. Boileau, J.-C. Jouhaud)

In order to optimize air cooling systems, the aeronautical industry is looking for reliable computational tools for the prediction of heat transfer between the solid components and the turbulent air flow. Previous work at Cerfacs proved the accuracy of Large Eddy Simulation (LES) for such applications ([AAM4]). As a result, Airbus France has renewed its support in 2007 for the use of the LES code AVBP in the framework of flow and heat transfer simulation in industrial configurations. Two main flow configurations have been studied. The first one corresponds to the well-known case of the flow past a square cylinder at Reynolds $22\,000$. A wall-resolved LES has been performed using a huge hybrid grid (7.6 millions cells). Both the aerodynamics (compared with a reference experiment [1,2]) and the global heat flux (compared with an empirical correlation) have been correctly reproduced. This calculation has provided reference data in order to validate a LES with a wall modeling approach. Using this wall model, the AVBP code has been coupled with the industrial code TMG which solves the thermal conduction inside the solid cylinder (cf. Fig. 3.1).

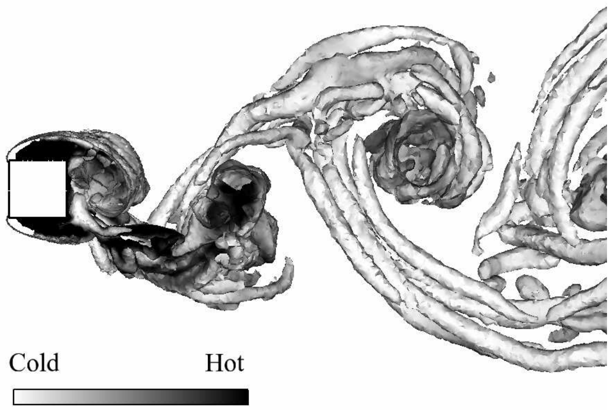


FIG. 3.1 – LES of the flow past a square cylinder with conjugate heat transfer inside the solid. Iso-surfaces of instantaneous vorticity coloured by the air temperature.

The second configuration is the flow inside the experimental model of an aero-engine nacelle cooling (cf. Fig. 3.2). LES is particularly well suited for this case where the heat transfer from the engine casing walls to the air flow is strongly dependent on the large turbulent scales generated by the cooling jets (Reynolds $144\,000$) impinging the walls and some obstacles. The methodology of wall modeling developed in the first configuration has been applied to several LES.

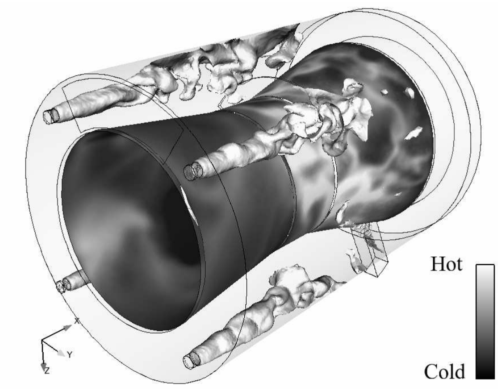


FIG. 3.2 – LES of the flow and heat transfer in the experimental model of an aero-engine nacelle cooling. Instantaneous temperature field on the engine casing walls and iso-levels of temperature showing the four cooling jets.

[1] D.A. Lyn and W. Rodi. The flapping shear layer formed by flow separation from the forward corner of a square cylinder. *Journal of Fluid Mechanics*, 267 :353–376, 1994.
[2] D.A. Lyn, S. Einav, W. Rodi, and J.H. Park. A laser-Doppler velocimetry study of ensemble-averaged characteristics of the turbulent near wake of a square cylinder. *Journal of Fluid Mechanics*, 304 :285–319, 1995.

3.1.2 VITAL project : numerical simulation of nozzle flows (F. Blanc, G. Joubert, G. Puigt)

In the framework of VITAL project (enVIronmenTALly Friendly Aero Engine), the Cerfacs jointly works with Airbus France on the simulation of engine nozzles and on comparison with experimental data. The main goal is to choose the parameter values suitable to reproduce as better as possible the experimental data for both axi-symmetric two-dimensional and three dimensional cases. In particular, this work focuses on the use of the third-order upwind Roe's scheme with low speed preconditioning while the same computations are done with JST scheme at Airbus.

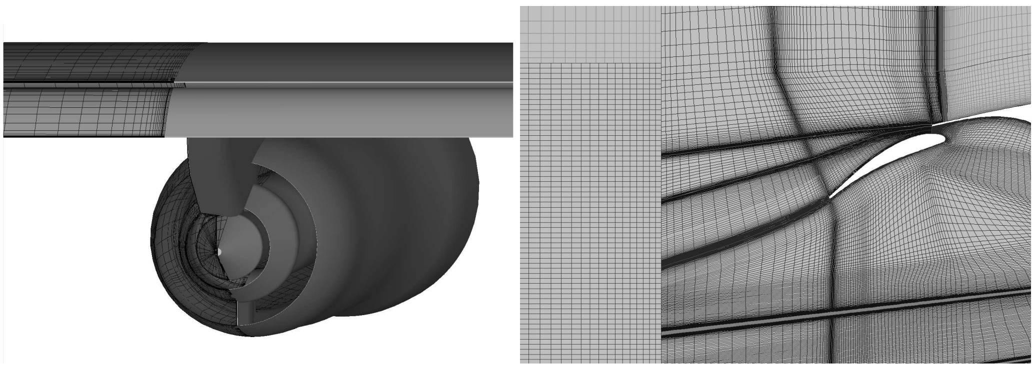


FIG. 3.3 – VITAL project : view of one of the considered geometries for the simulations and partial view of the mesh around a no-match join between blocks.

Inflow data and considered geometries reproduce faithfully the experimental process. The considered geometry consists in a nozzle, a nacelle, a pylon and a flap-extended wing (Fig. 3.3). In order to decrease as much as possible the number of mesh nodes without losing accuracy, no-match joins have been chosen during the mesh construction process.

3.1.3 Air intake : Numerical Simulation of the Distortion generated by Crosswind Inlet Flows (Y. Colin)

An issue related to the development of subsonic aircraft engine nacelles is the design of efficient air intakes which have to fulfill both geometrical constraints and engine requirements. One of the engine requirements is focused notably on the homogeneity of the flow in front of the fan which is quantified by the distortion levels of the total pressure in this plane as shown in Fig. 3.4. Airplane on the ground with crosswind is a critical case for the nacelle design. Subsonic or supersonic separations occur in the inlet, according to the engine mass flowrate. The resulting heterogeneity of the flow may account for the outbreak of aerodynamic instabilities of the fan blades and, if the distortion is large enough, the fan might stall.

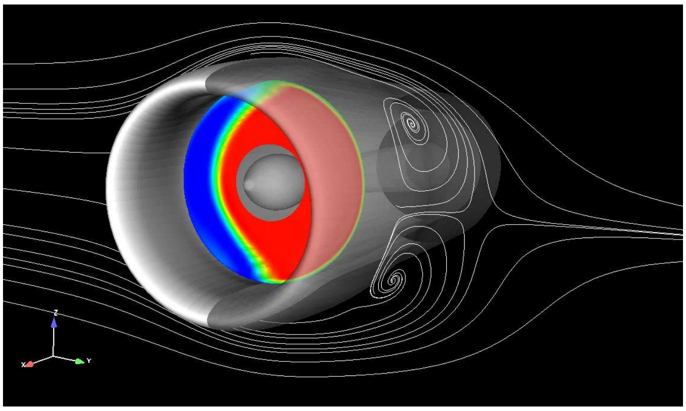


FIG. 3.4 – Flow heterogeneity in the fan plane.

The goal of this study was to have a robust, accurate and efficient tool capable of simulating complex flows around and inside a nacelle in a crosswind and to predict the distortion levels. It was successfully achieved with unsteady RANS simulations (even for a steady physics) using low speed preconditioning technique and transition modelling.

3.1.4 Wake Vortex : active participation in the European project FAR-Wake (L. Nybelen)

Cerfacs has developed a strong expertise on the topic of wake vortex dynamics, which is now widely recognized in the scientific community. Numerous studies have been conducted investigating the stability of different vortex systems, by means of Direct Numerical Simulations (DNS) or Large-Eddy Simulations (LES). These studies are both a mean of characterizing the wake of an aircraft in the near-field and a way to determine the decay in the far-field, which is important in predicting the behaviour of a large transport aircraft wake. Cerfacs investigates wake vortex dynamics through a collaboration with IMFT (Institute of Fluid Mechanics of Toulouse) though a PhD Thesis. Cerfacs is active in the framework of European program called FAR-Wake (leading to fives Technical Reports). During the period $2006 - 2007$, Cerfacs has been

involved in studying the waves propagations and their collisions (vortex bursting) along a single vortex, as they contribute to the wake vortex decay in the far-field.
An appearance criterion of the vortex bursting phenomenon has been established as function of the waves amplitudes. Moreover a second wake vortex dynamics has been extensively studied : the interaction between a cold or a hot jet with a vortex in realistic flight conditions. A parametric study was conducted and permitted to show the influence of the jet position and its intensity. In cases of a short separation distance with the vortex and a strong axial flux of the jet (take-off or approach phase), the interaction resulted to the complete loss of vortex coherency. These results showed that the merging process of the co-rotating vortices (generated at the wing tip and flap) in the extended near-field, might lead to a smaller vortex than the one without the flow jet, as one vortex was destroyed by the interaction with the jet flow.

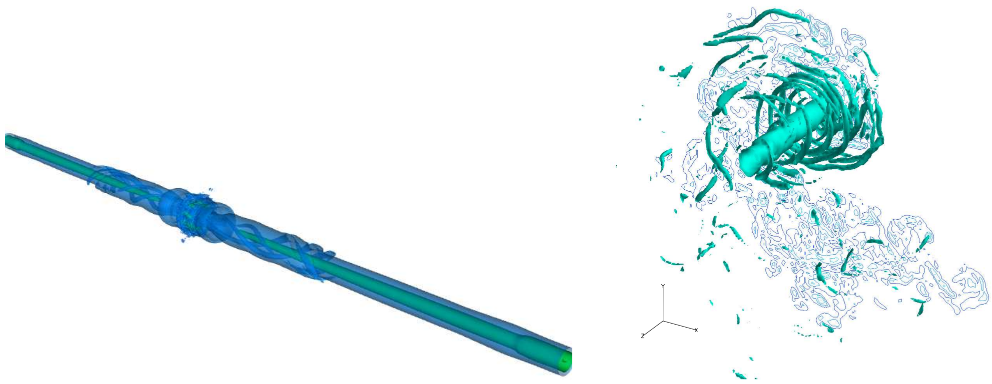


FIG. 3.5 – Vortex bursting through the waves collisions (left), Jet/vortex interaction at cruise flight condition (right).

3.2 Turbomachinery

3.2.1 Unsteady Simulation of an Axial Compressor Stage with Passive Control Strategies (N. Gourdain)

Mainly two ways can be found in literature for the enhancement of compressor performances. Active control like blowing or air injection are flexible but not easy to implement in a modern gas turbine engine, since cost and weight are increased by the control installation. Passive methods are another solution to increase compressor performances. Different designs of passive methods have been proposed like axisymmetric grooves or non axisymmetric casing treatment. It is now well established that passive treatments represent a very promising way for industrials applications since the integration cost is moderate with respect to the benefits of the technology. Unfortunately, some studies also show that some compressors exhibit no increase of the performance even with an optimization of the casing treatment geometry. In this context, the present work focuses on the investigation of the flow control in the tip region with passive control methods. The studied configuration is a stage of an axial compressor designed by Snecma for research applications. Two kinds of passive methods are tested. The first one consists of a casing treatment with non axisymmetric slots and the second one is based on a longitudinal groove in the head of each rotor blade (Fig. 3.6). The design of the first device is based on previous works [1] whereas the longitudinal groove approach has never been tested in literature. Numerical simulations of the flow are done thanks to the *elsA* software for the three cases (no control and with the two control devices). The results show that two regions are critical for the compressor stability when no control is performed. Firstly, the development of a large flow blockage region near the rotor leading edge has a strong destabilizing effect. Secondly, a separation of the rotor suction side boundary layer is also observed at near stall conditions. The non axisymmetric casing treatment configuration shows a good ability to control the tip leakage flow but failed to reduce the boundary layer separation on the suction side. However, an increase of the operability is observed but with a penalty for the efficiency. The simulation with the second approach (longitudinal groove) pointed out that the device is able to control partially all the critical flows with no penalty for the efficiency. These results are sum up on Fig. 3.7 that shows the blocked flow regions (white color) for the three configurations.

[1] I. Wilke and H. P. Kau, *A Numerical Investigation of the Flow Mechanisms in a High Pressure Compressor Front Stage with Axial Slots*, J. of Turbomachinery, Vol. 126, No 3, pp. 339-349, 2004

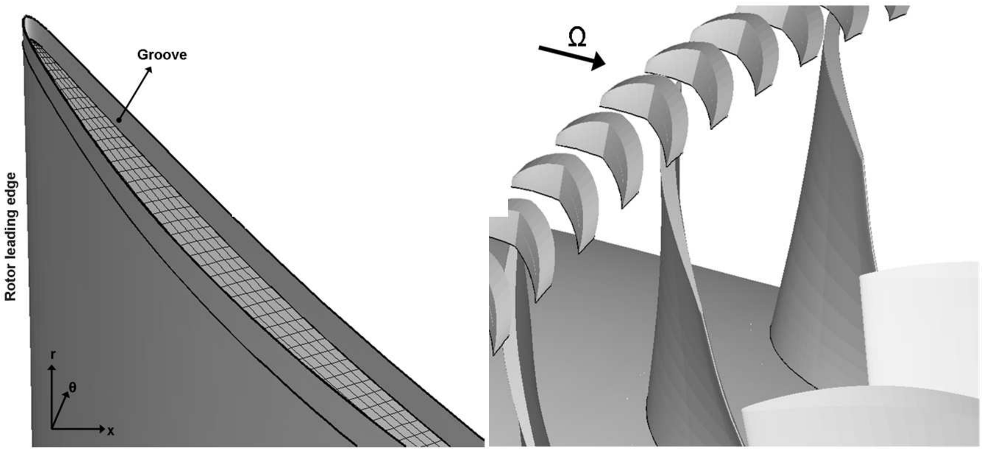


FIG. 3.6 – Technologies studied to extend the operability of the compressor : non axisymmetric casing treatment (left) and longitudinal groove (right).

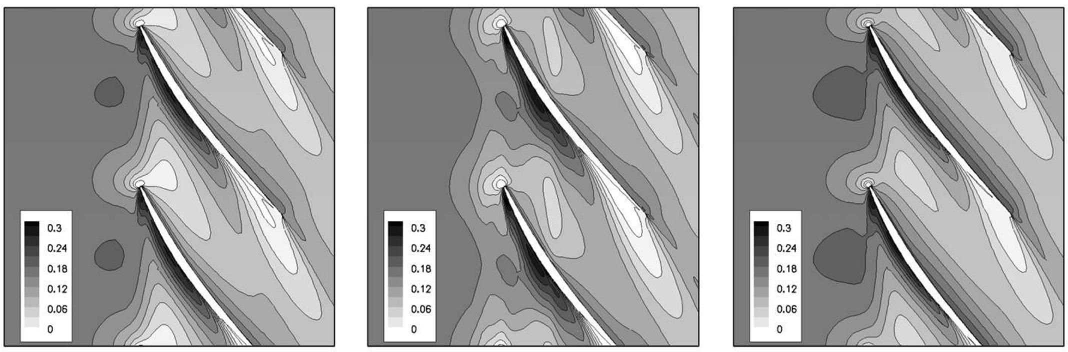


FIG. 3.7 – Comparison of the time averaged axial flow field : smooth wall (left), casing treatment (middle) and longitudinal groove (right).

3.2.2 Casing Treatment Simulations for a Supersonic Axial Compressor (M. Roumeas, N. Gourdain)

Casing treatment with non axisymmetric slots are applied on a supersonic compressor developed by Snecma (NEWAC project). The aim of this work is to investigate the ability of such passive devices to control the tip leakage flow and to improve the compressor efficiency. The study is performed by the mean of steady and unsteady 3D numerical simulations on a single rotor channel with the *elsA* software. For this application a special boundary condition has been developed by Cerfacs to simulate this kind of configuration (unsteady fully non matching point condition). Then a major work has been done to evaluate the mechanisms induced by this passive control method and many configurations have been tested. Numerical results indicate that the non axisymmetric slots extend significantly the compressor stable operating range, and increase the pressure ratio. Some configurations can also reduce total losses in the compressor and thus increase the efficiency. The main effect of casing treatments is based on the tip leakage flow impact and the reduction of the resulting vortex. Indeed, flow circulation in the slots allows weakening the rolling-up of the tip leakage flow. Hence, the induced blockage zone that leads to surge development at high pressure and near high efficiency operating points is strongly reduced. This contribution can be highlighted by a comparison between the axial velocity flow fields of the smooth wall case and the casing treatment case (Fig. 3.8).

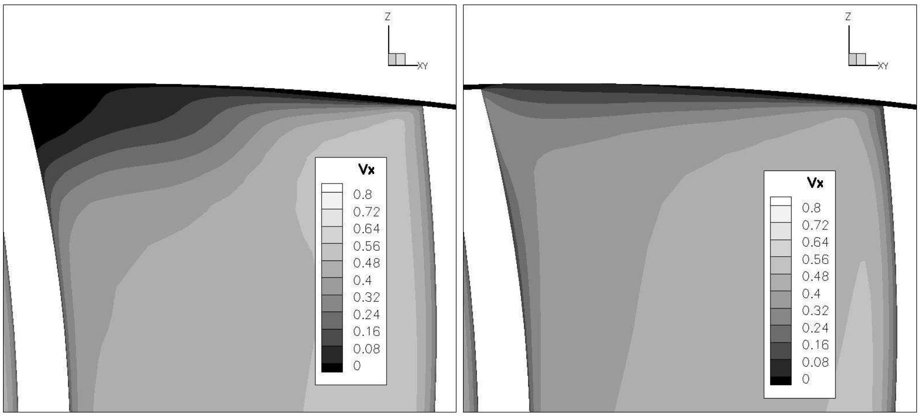


FIG. 3.8 – Non dimensional axial velocity, smooth wall configuration (left) and casing treatment configuration (right).

3.2.3 Unsteady Simulation of a Full High Pressure Compressor (N. Gourdain, M. Stoll)

Objectives in term of pollutant emissions and costs are now responsible of new constraints for motorists. An increase of the efficiency of the compression system allows a reduction of the system weight and the specific consumption, and thus can be used to achieve these challenging goals. Today, the design of a new generation of compressors is essentially based on numerical simulations. The main difficulty is that the flow in a multistage compressor is 3D and highly unsteady. Indeed only very costly approaches can be used to simulate all the flow phenomena. In order to limit the simulation cost, two restrictions are usually used in the literature. The first one is that only a spatial periodicity of the system is considered (i.e. a periodic sector). It means that rotor/stator periodicities are not correctly reproduced and unsteady effects are not well taken into account. The second restriction is that a steady approach is often considered with a mixing plane method at the rotor/stator interfaces. This technique is mainly used for industrial applications that

need a very fast calculation. The main limitation of these simulations is that the blade load variation can not be efficiently estimated. To overcome these limitations, an unsteady computation of the full geometry is required. At the moment, only few authors have already performed such a simulation of a full multistage compressor (Schluter [1]).
In this context, the objective of the current project is to compute the flow in a full high pressure compressor. The results will be used to validate available prediction models and for further research. The simulated test case is a transonic compressor with three stages and one inlet guide vane. This machine designed by Snecma for aerodynamic and thermal studies is representative of a part of the CFM-56 high pressure core. The total number of points for the whole compressor is about 134 millions. The RANS equations are solved with the structured multi-blocks flow solver *elsA*. As a first step, an unsteady RANS approach is used to perform simulations on a part of the geometry (a 22.5 degrees sector). No restriction is applied for the rotor/stator interaction flow structures since a natural periodicity can be found for the present compressor. This calculation will be used as a reference calculation for the full compressor. Thanks to recent developments in the *elsA* code, the unsteady simulation of the full geometry is now in progress on massively parallel plateforms (see Fig. 3.9) , like a Blue Gene supercomputer (up to 2048 processors) and a Bull supercomputer (up to 512 Itanium2 processors).

FIG. 3.9 – Whole simulation of the three stages compressor, Instantaneous Axial Velocity Flow Field (black : low velocity, white : high velocity).

[1] J.Schluter, S.Apte, G.Kalitzin, E.Van der Weide, *Large-scale integrated LES-RANS simulations of a gas turbine Engine*, Annual Research Briefs, Stanford University, 2005

4 Software engineering

4.1 Massively parallel (M. Montagnac)

Cerfacs has acquired a massively parallel processing system with an IBM BlueGene/L machine. The *elsA* software has been successfully ported on this architecture and results on academic and industrial configurations have shown a good scalability of the software.

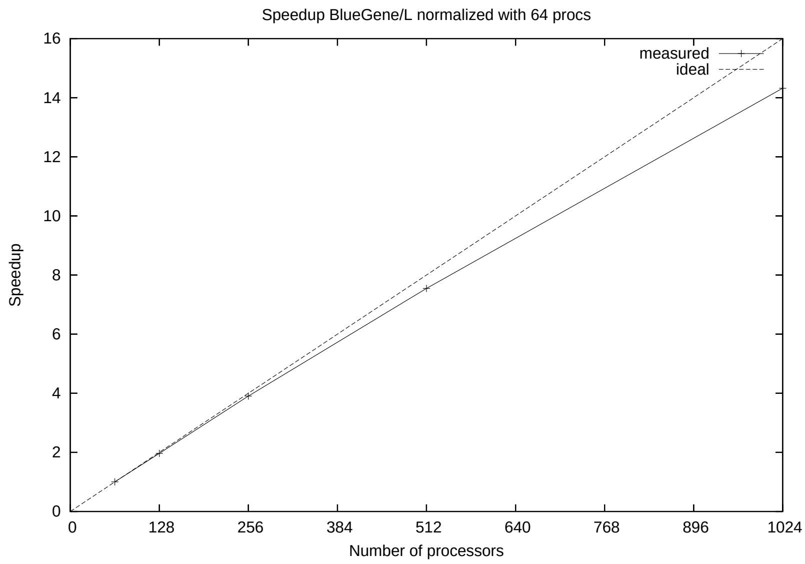


FIG. 4.1 – Speedup on BlueGene/L with a full aircraft configuration.

For example, Fig. 4.1 shows the performance measured on a typical industrial configuration of civil aircraft composed of 1037 blocks with 28 millions of mesh points. Numerical options were the classical ones including convergence acceleration techniques as a 3-level multigrid algorithm and a full implicit approach. The turbulence model was the one-equation model of Spalart-Allmaras.

Cerfacs has also redesigned some parts of the code in order to decrease data traffic over the communication network. Two main points were developed. The first idea was to integrate mean flow equations and turbulent equations at the same time. On the previous Airbus configuration, the gain can go up to 40 % depending on the machine and the number of processors used. The second idea was to remove the exchange of some variables between blocks, thus avoiding parallel communications.

Cerfacs has performed parallel performance evaluations for complex turbomachinery configurations on different architectures (CRAY XD1, NEC SX-8, IBM BlueGene). Unfortunately, the initial small number of large blocks leads to a significant load balancing error. The use of the splitter and merger tools of the *elsA* software allowed to change the cases topologies and optimize the load balance. This study demonstrated the possibility of massive parallel computations for such industrial cases.

4.2 Code performance (M. Montagnac)

Nowadays, most of parallel computers are composed of scalar processor nodes. These architectures are characterized by a hierarchy of memories, named cache memories, to optimize data access. To fully benefit from the processor power, a software must be coded in a special manner so as to provide data at the right time to the central processing unit. To this end, works have been done in the *elsA* software in order to reduce load and store operations. The first topic has concerned the integration of mean flow and turbulent equations at the same time so some variables can be used simultaneously and not sequentially anymore. The second idea has been to remove the notion of fictitious grid in the non coincident boundary condition. Indeed, previously, blocks sharing a non coincident border were connected by means of an overlapping grid. Data from blocks were transferred to this grid and fluxes at this interface were computed on this grid. This required a lot of data copies back and forth. Therefore, this fictitious grid was removed and fluxes are directly computed on block interfaces. Performance has been observed to be improved by 30 % on the example of section 4.1 but this figure depends on numerous factors as for example the number of non coincident boundary used.

4.3 CFD environment (M. Montagnac, G. Puigt)

Airbus France has defined a proprietary common software architecture to perform parallel multi-physics simulations. All external codes used, such as *elsA*, must conform to data specifications imposed. In that context, Cerfacs has made the extensively used non coincident boundary condition compatible with the Airbus data manager.
In addition, numerical experts often write multidisciplinary computation scenarii that obviously couple third-party tools and legacy tools and dispatch them to end-users. Therefore, a scenario can be seen as a succession of calls of different modules. Most of scenarii include a module that represents an aerodynamic calculations. For us, the module is the *elsA* software that performs many iterations until the solution is converged. There was an emerging need to only perform a single iteration of an aerodynamic calculation in order to call another module between two successive iterations. Therefore, Cerfacs has implemented an alternative *elsA* interface to give access to the iteration loop in the python steering file. This way, Airbus experts can now simulate a few iterations of a flow around a configuration and call afterwards a new python module, for example a mesh deformation module, to modify data that are shared by memory through the data manager.

5 Publications

5.1 Journal Publications

[AAM1] G. Alleon, S. Champagneux, G. Chevalier, L. Giraud, and G. Sylvand, (2006), Parallel Distributed Numerical Simulations in Aeronautic Applications., *Journal of Applied Mathematical Modelling*, **30**, 714–730.

[AAM2] L. Debiane, B. Ivorra, B. Mohammadi, F. Nicoud, T. Poinsot, A. Ern, and H. Pitsch, (2006), A low complexity global optimization algorithm for temperature and pollution control in flames with complex chemistry, *International Journal of Computational Fluid Dynamics*, **20**, 93–98.

[AAM3] A. Devesa, J. Moreau, J. Hélie, V. Faivre, and T. Poinsot, (2007), Initial conditions for Large Eddy Simulations of piston engine flows, *Computers and Fluids*, **36**, 701–713.

[AAM4] J. Jouhaud, L. Gicquel, B. Enaux, and M.-J. Esteve, (2007), LES Modeling for Aerothermal Predictions Behind a Jet In Cross-Flow, *AIAA Journal*, **45**, 2438–2447.

[AAM5] J. Jouhaud, P. Sagaut, and B. Labeyrie, (2006), A kriging approach for CFD/Wind tunnel data comparison, *Journal of Fluid Engineering*, **128**, 847–855.

[AAM6] J. Jouhaud, P. Sagaut, M. Montagnac, and J. Laurenceau, (2007), A surrogate-model based multi-disciplinary shape optimization method with application to a 2D subsonic airfoil, *Computers and Fluids*, **36**, 520–529.

5.2 Theses

[AAM7] Y. Colin, (2007), *Simulation numérique de la distorsion générée par une entrée d'air de moteur civil par vent de travers - TH/CFD/07/128*, PhD thesis, ENSAE Toulouse , France.

[AAM8] A. Devesa, (2006), *Modélisation de paroi pour la simulation d'écoulements instationnaires non-isothermes - TH/CFD/06/103*, PhD thesis, Université de Montpellier II.

5.3 Conference Proceedings and Book Chapters

[AAM9] Y. Colin, B. Aupoix, J.-F. Boussuge, and P. Chanez, (2007), Numerical Simulation and analysis of crosswind inlet flows at low mach numbers, In *8TH ISAIF*, LYON FRANCE.

[AAM10] Y. Colin, B. Aupoix, J.-F. Boussuge, and P. Chanez, (2007), Numerical Simulation of the distorsion generated by crosswind inlet flows, In *18th ISABE 2007*, Beijing, China.

[AAM11] A. Devesa and F. Nicoud, (2006), On Unsteady Effects in Wall Modeling, In *5th International Symposium on Turbulence, Heat and Mass Transfer*, Dubrovnik, Croatia.

[AAM12] N. Gourdain, M. Montagnac, and J.-F. Boussuge, (2007), Numerical Simulation of an axial compressor with non axisymetric casing treatment, In *2nd EUCASS conference for Aerospace Sciences*, Bruxelles, Belgique, Paper 124.

[AAM13] S. Mouton, J. Laurenceau, and G. Carrier, (2007), Aerodynamic and Structural Optimisation of Powerplant Integration under the Wing of a Transonic Transport Aircraft, In *42ème colloque d'aérodynamique appliquée*, Sophia Antipolis, France.

[AAM14] L. Nybelen, H. Moët, and R. Paoli, (2006), Simulations of merging in a two co-rotating vortex system, In *ECCOMAS CFD 2006*, Egmond Aan Zee, The Netherlands.

[AAM15] D. Panara, M. Porta, and T. Schoenfeld, (2006), Unsteady Boundary Layer Strategies for Pulsating and Oscillating Turbulent Channel Flow Application, In *ECCOMAS Conference CFD*, Egmond aan Zee, The Netherlands.

[AAM16] D. Panara, M. Porta, R. Dannecker, and B. Noll, (2006), Wall-functions and boundary layer response to pulsating and oscillating turbulent channel flows, In *5th International Symposium on Turbulence, Heat and Mass Transfer*, Dubrovnik, Croatia, 209–212.

[AAM17] T. Schoenfeld, J.-F. Boussuge, S. LeDizés, and T. Leweke, (2007), FUNDAMENTAL VORTEX PHENOMENA : INSTABILITIES AND INTERACTIONS WITH JETS AND WAKES, In *1st European Air and Space Conference*, Berlin, Germany, Paper CEAS–2007–7.

5.4 Technical Reports

[AAM18] F. Benahmed, (2007), Simulation aérothermique instationnaire, Rapport de stage WN/CFD/07/83, CERFACS.

[AAM19] F. Blanc, J.-P. Boin, J.-F. Boussuge, M. Montagnac, and G. Puigt, (2006), Programme FLOWSIM II : Réponse au cahier des charges du 30/05/2006, Number 06012906, WP2 : Flow Simulation System development, Contract report CR/CFD/06/105, CERFACS.

[AAM20] Y. Colin and J.-P. Boin, (2006), Driving state definition and normalization within elsA-Python script, Rapport technique TR/CFD/06/29, CERFACS.

[AAM21] A. Devesa and F. Nicoud, (2006), Assessment of a Two-Layer Wall Model for Large Eddy Simulations of Highly Non-isothermal Turbulent Flows, Tech. Rep. TR/CFD/06/68, CERFACS.

[AAM22] E. Etienne, (2006), Création d'une base de données de Travaux pratiques en calcul numérique, rapport de stage de 2ème année d'ingénieur WN/CFD/06/76, ECOLE NATIONALE SUPERIEURE DE MECANIQUE ET D'AEROTECHNIQUE.

[AAM23] A. Fosso-Pouangé, (2007), Mise en oeuvre d'une approche non structurée dans elsA, Stage Master WN/CFD/07/88, CERFACS.

[AAM24] E. Germaine, (2007), Modélisation de la couche limite turbulente instationnaire pour les simulations aux grandes échelles : construction et mise en oeuvre d'une approche lois de paroi dans le logiciel elsA, Stage Master WN/CFD/07/82, CERFACS.

[AAM25] N. Gourdain and F. Leboeuf, (2007), Unsteady simulation of an axial compressor stage with passive control strategies, Preliminary version of an article submitted to Journal of Turbomachinary TR/CFD/07/134, CERFACS.

[AAM26] N. Gourdain, S. Burguburu, F. Leboeuf, and G. MIchon, (2007), Numerical simulation of rotating stall inception in an axial compressor, Preliminary version of an article submitted to AIAA Journal TR/CFD/07/133, CERFACS.

[AAM27] N. Gourdain, M. Montagnac, and J.-F. Boussuge, (2006), Calcul de démonstration d'une configuration de rotor isolé avec traitement de carter non axisymétrique, Contract report CR/CFD/06/81, CERFACS.

[AAM28] N. Gourdain, M. Montagnac, and J.-F. Boussuge, (2007), Etude de traitement de carter non axisymétrique -Compte rendu de l'action WP3- Evaluation de la validité d'une approche loi de paroi, Contract report CR/CFD/07/11, CERFACS.

[AAM29] N. Gourdain, M. Montagnac, and J.-F. Boussuge, (2007), Evaluation des performances du compresseur NEWAC avec traitements de carter, Rapport contractuel CR/CFD/07/32, CERFACS.

[AAM30] J. Laurenceau and M. Montagnac, (2007), Rapport technique d'avancement deuxième année. Optimisation multidisciplinaire préliminaire de l'installation motrice avec la chaîne d'optimisation de formes aérodynamiques OPTALIA, rapport contractuel CR/CFD/07/62, CERFACS.

[AAM31] T. Marger, (2006), Simulations numériques d'interaction entre un jet moteur et un tourbillon de sillage, Rapport de Projet de fin d'études - ENSICA WN/CFD/06/62, CERFACS.

[AAM32] M. Montagnac and B. Landmann, (2007), Rapport technique d'avancement T0+18, DTP - modèles aérodynamiques - phase 3, Rapport contractuel CR/CFD/07/132, CERFACS.

[AAM33] M. Montagnac, J. Jouhaud, and B. Landmann, (2007), Rapport technique d'avancement T0+12, DTP - Modèles aérodynamiques - phase 3, Rapport contractuel CR/CFD/07/47, CERFACS.

[AAM34] M. Montagnac, J. Jouhaud, B. Landmann, and J.-F. Boussuge, (2006), Rapport Avancement T0+6 DTP Modèles de Données Aérodynamiques Phase 3, contract report CR/CFD/06/106, CERFACS.

[AAM35] M. Montagnac, (2007), Rapport technique de synthèse PRC ANANAS Phase 2, Rapport technique CR/CFD/07/34, CERFACS.

[AAM36] L. Nybelen, (2006), CFD simulations for DFS 32/10 and deflected spoiler case, Contract report AWIATOR CR/CFD/06/102, CERFACS.

[AAM37] L. Nybelen, (2006), LES of turbulent cold jet/vortex interaction, Contract report CR/CFD/06/117, CERFACS.

[AAM38] L. Nybelen, (2007), LES of hot jet/vortex interaction, Contract report CR/CFD/07/111, CERFACS.

[AAM39] L. Nybelen, (2007), Temporal DNS on end-effects and vortex waves, contract report CR/CFD/07/110, CERFACS.

[AAM40] G. Puigt, N. Gourdain, and J.-F. Boussuge, (2006), Premier rapport d' avancement du projet AITEC Fiche A5, Phase 1 : Time Harmonic Balance T0+3mois, Contract report CR/CFD/06/14, CERFACS.

[AAM41] G. Puigt, N. Gourdain, and J.-F. Boussuge, (2006), Second rapport d'avancement du projet AITEC Fiche A5, Phase 1 :Time Harmonic Balance T0+9 mois, contract report AITEC CR/CFD/06/66, CERFACS.

[AAM42] G. Puigt, F. Sicot, N. Gourdain, and J.-F. Boussuge, (2007), Dernier rapport contractuel du projet AITEC Fiche A5, Phase 1 : Time Harmonic Balance - T0+18 mois, Rapport contractuel CR/CFD/07/57, CERFACS.

[AAM43] G. Puigt, F. Sicot, N. Gourdain, and J.-F. Boussuge, (2007), Dernier rapport technique du projet AITEC Fiche A5, Phase 1 : Time Harmonic Balance - T0+18 mois, Rapport contractuel CR/CFD/07/58, CERFACS.

[AAM44] G. Puigt, F. Sicot, N. Gourdain, and J.-F. Boussuge, (2007), Troisième rapport d'avancement du projet AITEC Fiche A5, Phase 1 : TIme Harmonic Balance T0+15 mois, Contract report CR/CFD/07/29, CERFACS.

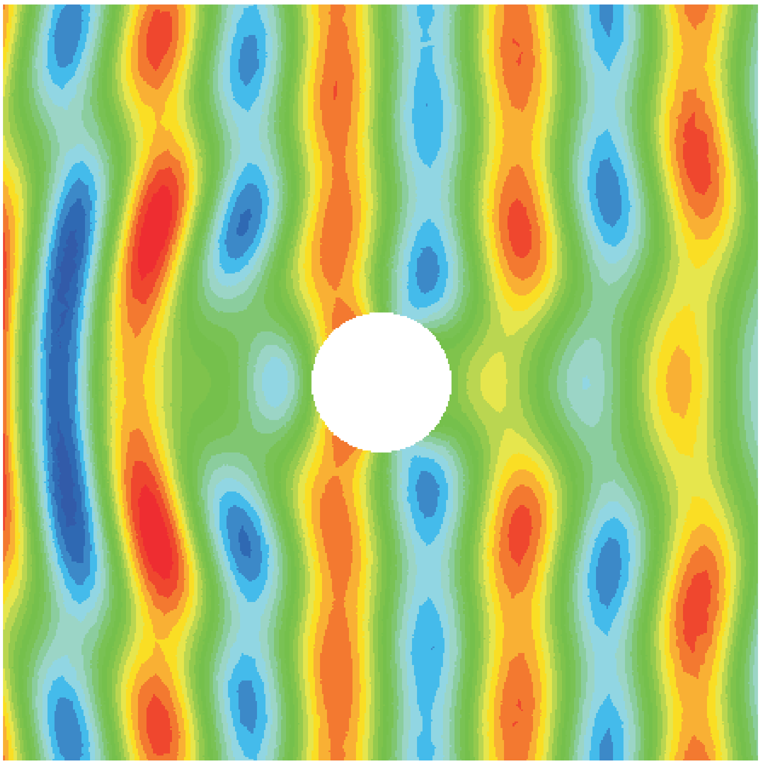
[AAM45] G. Puigt, (2006), Première note de conception de la THB projet AITEC Fiche A5, Phase 1 : Génération des scripts python - T0+6 mois, rapport contractuel CR/CFD/06/39, CERFACS.

[AAM46] G. Puigt, (2006), Second rapport d'avancement du projet AITEC Fiche A5, Phase 1 : Time Harmonic Balance T0+6 mois, rapport contractuel CR/CFD/06/40, CERFACS.

[AAM47] F. Sicot, (2006), High Order Schemes on Non-Uniform Meshes in a Finite Volume Formulation, Rapport de stage fin d'études TR/CFD/06/21, CERFACS.

9

Electromagnetism and Acoustics Team



1 Overview presentation

The main expertise of the *Electromagnetic and acoustic* team concerns the numerical solution of problems related to the scattering of time-harmonic electromagnetic waves. The methods which have been developed in the CESC code (CERFACS Electromagnetism Solver Code) combine integral equations and finite elements. Large size problems arising at high frequency are now tractable, thanks to the Fast Multipole Method. Appropriate Domain Decomposition techniques have been also developed to increase the efficiency of the algorithms in the presence of heterogeneous regions.

We present below two examples of computations for realistic industrial cases, which have been performed to answer specific demands of our industrial partners (respectively here CNES and AIRBUS).

During the last two years, a part of our activity was devoted to the solution of electromagnetic scattering problems, when the nature of the scatterer is modeled by a (possibly non uniform) impedance condition. We have developed for this case new formulations, whose performances have been already verified on large size problems. This has been partly supported by a PEA and is now the subject of a collaboration with ONERA.

The CESC code can be used to provide synthetic data for validating inverse scattering algorithm. Our contribution in this domain which is the object of a collaboration with the INRIA Project DEFI concerns the Linear Sampling Method (LSM). Synthetic data have been obtained and the LSM algorithm has been efficiently implemented for various cases, including that of an embedded scatter.

Finally, the *Electromagnetic and acoustic* team has initiated for two years a new activity, relative to the numerical simulation in aeroacoustics. An original finite element approach has been proposed and implemented in 2D to simulate acoustic scattering in presence of an arbitrary mean flow.

2 Integral equations for electromagnetism scattering

2.1 New formulations for partially coated scatterers

F. Collino, F. Millot and S. Pernet

Using a boundary element method to solve electromagnetic scattering by coated obstacles is not straightforward. Indeed, the impedance boundary relation (modeling the presence of the coating) which relates the electric and the magnetic currents $\mathbf{J}$ and $\mathbf{M}$ is difficult to take into account numerically.
To treat this difficulty, there are several possibilities. The solution proposed by Bachelot, Gay and Lange consists in writing an integral formulation which only ensures the impedance boundary relation when the convergence is achieved (i.e. when the spatial step tends toward zero). It will be referred to in the sequel as the BGLF method. Unfortunately, this formulation degenerates to an Electric Field Integral Equation (EFIE) on the perfectly metallic parts of the boundary of the obstacle, and it is well-known that the convergence rate of most of the iterative solvers is very slow for the EFIE.
The first idea to solve this difficulty is to use an equation like a so called Combined Field Integral Equation (CFIE) (see section 2.1.1). The second idea is to construct a new type of integral equations which are inherently well-conditioned (see section 2.1.2).

2.1.1 A Combined Field Integral Equation

We have derived a Combined Field Integral Equation for an impedance boundary condition [3]. This formulation can be written with two terms, one which is directly linked to the classical CFIE term when the obstacle is perfectly conducting $A_{cfie}\mathbf{J}$ and an additional unusual term which is related to $\mathbf{n}\times A_{cfie}\mathbf{M}$. This choice allows anyone who possesses a metallic CFIE solver to implement the impedant CFIE at lower cost.
For the numerical implementation :
– Two approaches have been proposed in order to treat correctly the additional term $\mathbf{n}\times A_{cfie}\mathbf{M}$.
– After discretization, the final system is solved with an iterative solver coupled with a FMM algorithm.
– The construction of a SPAI preconditioner for this formulation has also been proposed.
The numerical results obtained with this new formulation are very close to those obtained with BGLF (see figure 2.1). Moreover, when the impedance value is small or variable, our algorithm converges faster and a CPU time gain is observed. In particular, we have shown that our method allows us to treat efficiently the partially coated objects.

For example, we consider a cylinder of height $360m$ and radius $120m$. The mesh is composed of 347324 triangles that corresponds to 520986 degrees of freedom for the electric current (the number of points per wavelength is about 10).
We have considered two configurations. The first one corresponds to a constant impedance while, in the second one, we have divided the cylinder in three sections with three distinct values of the impedance. In particular, one of the sections is assumed to be perfectly conducting. Note that the number of iterations does not depend very much on the value of the impedance. On the contrary, BGLF is very sensitive to the variations of impedance and particularly when there is a perfectly conducting part on the surface of

the obstacle. Moreover, an important gain in CPU time (related to a significant decrease of the number of iterations) is obtained with our formulation.
Figure 2.1 shows the Radar Cross Sections for the two configurations : all curves are very close.

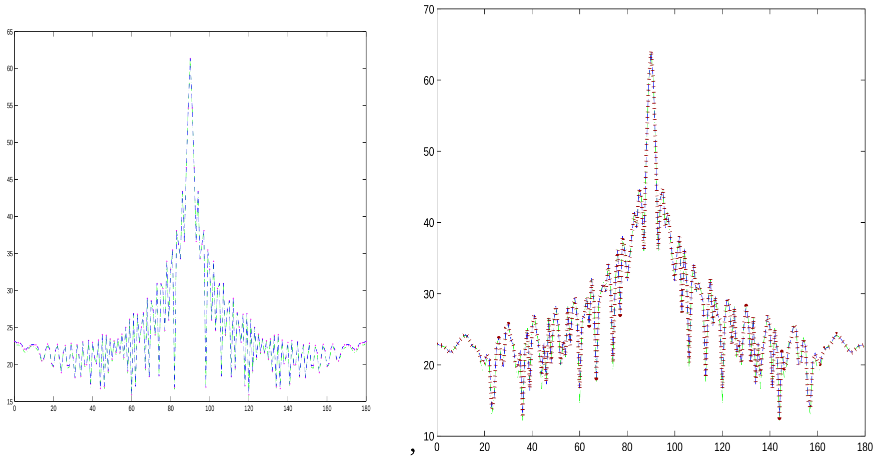


FIG. 2.1 – RCS of the cylinder when the cylinder : constant (up) and varying (down) impedance value (-. : BGLF, – : ICFIE1)

2.1.2 An inherently well-conditioned integral equation

Note that even if the Fast Multipole Method (FMM) allows to treat complex situations possessing several millions of degrees of freedom, the use of a preconditioner is primordial in order to reduce the cost of these techniques. Indeed, even the CFIE method becomes ill-conditioned and leads to a linear system whose the condition number deteriorates when the frequency increases or if the mesh is very fine in comparison to the wavelength. An alternative to the use of the classical algebraic preconditioners is the construction of Fredholm integral equations of second kind which decompose under the form “Identity + C” where C is a compact operator. In recent years, it turned out that one was able to construct such integrals in a more or less systematic way in the context of the perfectly conducting objects ([1], [2], [4]). In particular, they have shown that the convergence rate is wavenumber (k) and mesh-size (h) independent. All these inherently well-conditioned integral equations are based on the adequate construction of an approximation $\tilde{Y}$ of the so-called admittance operator Y of the scatterer defined by $Y\ :\ \mathbf{M}\ \rightarrow\ \mathbf{J}$. What particularizes these equation is the way used to derive $\tilde{Y}$. There are essentially two ways : the first one is based the Calderón projector ([1], [2]) and the second used a micro-local approximation of Y [4].

We have recently extended these results to impedance problems [5]. In particular, we have proposed a Fredholm integral equation of second kind to iteratively solve the scattering problems with a variable impedance boundary condition. This equation is based on a micro-local approximation of a particular operator O. In a first step, we have proved that the new integral equation is well-posed by using the pseudo differential calculi. Next, we have proposed a way to compute numerically the action of O on a tangential vector field. The technique is based on a Pade approximant and a discrete Helmholtz decomposition. Finally, we have used the FMM to compute the matrix-vector products coming from the classical integral operators. The numerical experiments have confirmed the robustness and the stability of the method. In particular, it is less costly than the Combined Field Integral Equation described in the previous section. Let us point out that it exists few numerical experiments using this kind of techniques because they are difficult to implement.

Figure 2.2 shows the Radar Cross Sections for the almond case : all curves are very close. So, this study also allowed to prove that these techniques can be attractive to treat industrial problems and that it is interesting to continue their developments.

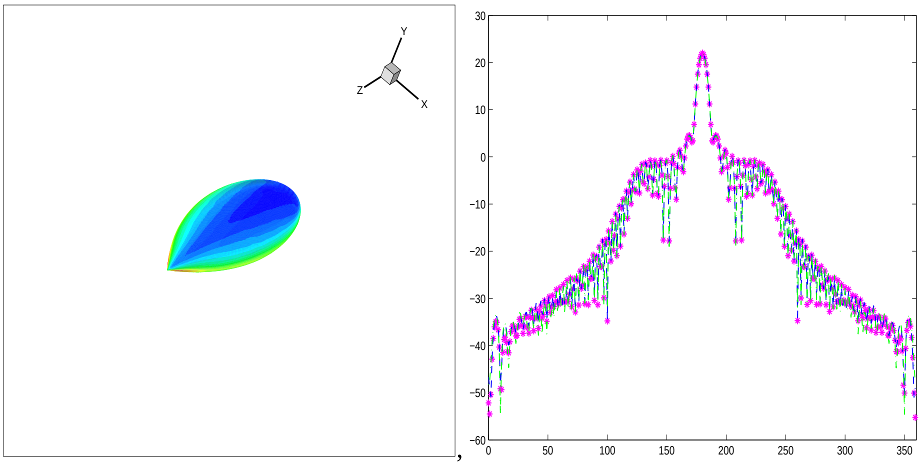


FIG. 2.2 – Geometry of the almond and its RCS

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

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

[3] F. Collino, F. Millot, and S. Pernet, (2008), Boundary-Integral Methods for Iterative Solution of Scattering Problems with Variable Impedance Surface Condition, *Progress In Electromagnetics Research*, **PIER 80**.

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

[5] S. Pernet, A well-conditioned integral equation for iterative solution of scattering problems with a variable Leontovitch boundary condition, *submitted*.

2.2 Solving Real Life Scattering Problems

F. Collino and M'B. Fares

2.2.1 Computation of the far field pattern of a micro-satellite

In the framework of a grant with CNES, we developed some new functionalities in the CESC_FMM code : mesh with wires structures, multi delta-gap sources, ...We also optimized the code in order to be able to treat 100000 unknowns problems on a simple laptop (optimization of the SPAI preconditionner). All this work was done to make possible the treatment of a micro-satellite of the *Myriad* class with two spiral antennas fed by delta-gaps at 2.032 GigaHertz. Such an example requires a quite powerfull machine when a direct solver is used : the run, performed on one hundred processors and twenty-five nodes of the IBM machine EGEE, requires nearly two hundred GigaBytes and two hours of CPU times (times 100, when the numbers of processors is taken into account). The CESC_FMM code was run on a simple station Pentium 2.8 GH with two Gigabytes ; it took thirty-one hours to perform one hundred iterations of flexible GMRES and achieve a 0.00025 residual. The comparison of the far fields obtained by the two methods are in good agrement.

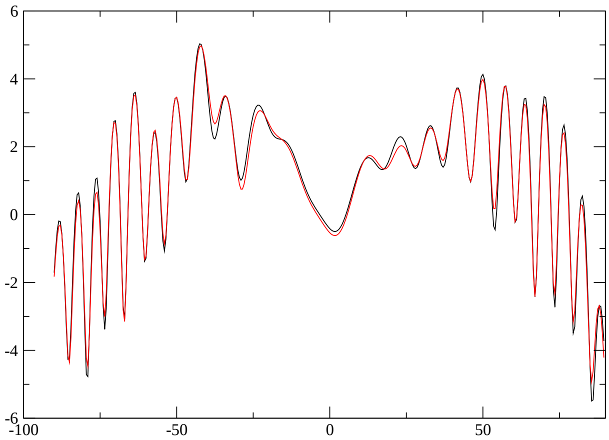


FIG. 2.3 – Comparison of the right polarization of the far field pattern at 2.0332 GigaHertz. Solution of the direct `LU` code is in black lines, solution obtained with `CESC-FMM` after 100 iterates and 31 CPU times in red lines.

2.2.2 Scattering by the A380 stabilizer nearly an Instrument Landing System

The Instrument Landing System (ILS) is an instrument approach system which provides precise guidance to an aircraft approaching a runway.
The objective of the study is to compare the diffraction computations for the A380 stabilizer nearly the ILS which are obtained by three methods **(1)** Integral equation method (EI) is the reference method **(2)** the Physical Optics (PO) **(3)** the uniform theory of diffraction (UTD) for frequencies 110 and 330 Mhz.
Computations are performed for several incidence and observation angles. First on a simplified model which replaces the stabilizer by a thin plate. Then on the exact CAO for the stabilizer.
The aims is to test if the results with PO and UTD remain valid on the simplified model. If this is the case, one could avoid the use of the direct method EI which is time and memory expensive.
In applications, such computations are used to estimate the perturbation that would be caused by the stabilizer in the neighborhood of ILS.

Here are some of the conclusions of the study :
(1) The simplified model is not suited to get accurate results by asymptotic methods.
(2) However, the 2 asymptotic methods give similar results for the 110 Mhz frequency and a satisfactory accuracy for the non grazing incidence angles.
(3) For the 330 Mhz frequency, UTD gives better results than PO for the grazing incidence angles.
(4) To get enough accuracy for all angles (0 or not), the use of an exact method with an accurate CAO model is recommanded.
This work has been conducted in cooperation with the team of B. Souny, ENAC (Ecole National de l'Aviation Civile) and was supported by `Airbus Industrie`.

3 Domain decomposition for acoustic scattering

A. Bendali and M'B. Fares

3.1 The motivation

The problem, addressed in this part, concerns the numerical computation of a radiated or a scattered time-harmonic acoustic field in the presence of a rigid obstacle surrounded by a finite region inhomogeneoulsy filled with penetrable materials. A second characteristic of the problem is that it deals with relatively high-frequency configurations, and thus it becomes necessary to resort to High Performance Computing (HPC), that is, computing on massively parallel platforms, to be able to perform the actual computations.

Such an important problem for the applications has given rise to several works. The main issue herein, arguably, is to find a suitable way to efficiently treat the unbounded region beyond the finite element mesh. Two classes of such treatments have been developed and intensively used. The first class can be called "approximate methods" in the sense that, an inherent error remains present even without any error of discretization. The main advantage of these methods lies in the fact that they lead to a linear system with a purely sparse matrix. However, these methods have a major disadvantage. It is not possible in general to control the accuracy of the solution they deliver in the end. For the second class of methods, the only errors are coming from the discretization. They are hence called "exact methods" and are generally based on a coupling of Finite Element Method (FEM) with a Boundary Element Method (BEM) like this is done in the works reported here. A major disadvantage of these methods, in the context of HPC, is that they lead to a matrix which is partly dense, due to the part of the discrete equations related to the FEM, and partly sparse, for the ones concerning the discretization by a BEM. More precisely the general linear system solvers in HPC are tailored for either one of these two types of matrices. Neither a suitable method nor a HPC code specially adapted to deal with a matrix partly dense and partly sparse seem to exist. To overcome this difficulty, a quite obvious approach is to use a Domain Decomposition Method (DDM) to uncouple the part of the equations related to the BEM from that concerning the discretization by the FEM by means of an iterative procedure. However, the most natural procedures which consist of transmitting either Dirichlet or Neumann data from one domain to the other, do not work in the framework of problems with weak coerciveness properties like those related to waves propagation. The correct way to deal with this kind of problems was introduced by Després [11] (see also [10] for a detailed description and some improvements).

In a first work, we followed this way to proceed since, at least at the level of the continuous problem, that is, without considering any discretization error, the convergence of the algorithm can be established theoretically [11, 10, 8]. However, we depart from this previous work in two fundamental directions :

1. only standard BEM are used instead of those doubling the unknowns based on another principle than the utilization of the usual Green kernel [9, 6],
2. the procedure we develop is a FETI-like method in the sense that the DDM can be interpreted exactly as an efficient iterative process to solve the coupling of the FEM and the BEM formulation.

3.2 The method under investigation

We first give the statement of a model problem incorporating the main features of the class of scattering problems which can be solved through the procedures that have been developed. It is a boundary-value problem of transmission type. Particularly, in order to introduce the DDM on which is based the solving procedure, we point out how the transmission problem can be stated as a system of two boundary-value problems, one, with variable coefficients, posed on a bounded domain, and the other posed in terms of the Helmholtz equation endowed with a radiation condition at infinity, coupled by appropriate boundary conditions at their common interface.
The acoustic scattering problem can be written as the following system

$$\begin{cases} \Delta u_0 + k^2 u_0 = 0 \text{ in } \Omega_0^\infty, \\ \text{Rad. Condition.} \end{cases} \quad \begin{cases} \nabla \cdot \chi \nabla u_1 + k^2 n^2 \chi_1 u_1 = 0 \text{ in } \Omega_1, \\ \chi \nabla u_1 \cdot \mathbf{n}_1 = 0 \text{ on } \Gamma, \end{cases} \quad \begin{cases} u_1|_\Sigma = u_0|_\Sigma, \\ \chi \nabla u_1 \cdot \mathbf{n}_1|_\Sigma + \partial_{\mathbf{n}_0} u_0|_\Sigma = 0. \end{cases} \tag{3.1}$$

where χ and n are varying functions characterizing the acoustic properties of the non homogeneous medium filling the part of the obstacle Ω_1 (cf. FIG. 3.1).

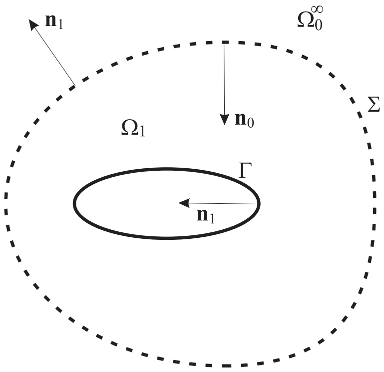


FIG. 3.1 – The rigid obstacle and its surrounding layer

One issue in the construction of a coupling of a FEM with a BEM is to discretize the equation in Ω_1 by using a FEM. Limiting oneself to a nodal FEM, a first step is to introduce the auxiliary unknown

$$p := \partial_{\mathbf{n}_0} u_0|_\Sigma = -\chi \nabla u_1 \cdot \mathbf{n}_1|_\Sigma \tag{3.2}$$

The discretization of the equation in Ω_0^∞ is based on an integral representation of u_0 (see [EMA3] which includes the description of the full procedure). We are then led to solve the following linear system

$$\begin{bmatrix} [A_{\Omega_1}] & [M_\Sigma] \\ [C] & [S] \end{bmatrix} \begin{bmatrix} [u_1] \\ [p] \end{bmatrix} = \begin{bmatrix} 0 \\ [f] \end{bmatrix} \tag{3.3}$$

It is the combination of sparse blocks $[A_{\Omega_1}]$ and $[M_\Sigma]$, related to the FEM, with dense blocks $[C]$ and $[S]$, associated to the BEM, that prevents from dealing with system (3.3) by means of usual HPC solvers.
The description of the domain decomposition approach to overcome this difficulty can be given through the following iterative procedure :

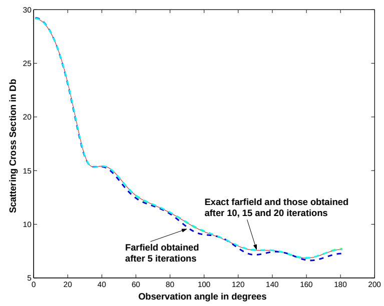


FIG. 3.2 – Exact cross-section and those obtained during the iterations

- do an LU decomposition of $\left([A_{\Omega_1}] + \beta\widetilde{[M_\Sigma]}\right)$ and $([C] + \beta\,[S])$
- set $[g_1]^{(0)} := 0$, $[g_0]^{(0)} := 0$,
- iterate until convergence for $m = 0, 1, 2, \ldots$
  - solve a sparse linear system by a forward and a backward substitution :

$$\left([A_{\Omega_1}] + \beta\widetilde{[M_\Sigma]}\right)[u_1]^{(m+1)} = \widetilde{[M_\Sigma]}\,\widetilde{[g_1]^{(m)}}, \tag{3.4}$$

  - solve a dense system in the same way :

$$([C] + \beta\,[S])\,[u_0]^{(m+1)} = [S]\,[g_0]^{(m)} + [f]\,, \tag{3.5}$$

  - transmit data to Ω_0^∞ :

$$[g_0]^{(m+1)} := -\,[g_1]^{(m)} + 2\beta\,[u_1]_\Sigma^{(m+1)}\,,$$

  - transmit data to Ω_1 :

$$[g_1]^{(m+1)} := -\,[g_0]^{(m)} + 2\beta\,[u_0]^{(m+1)}\,.$$

- end of loop

The convergence properties of the iterative process can be significantly improved by using a Krylov method instead of the above simple successive approximations procedure (see [EMA3] where the effective implementation on HPC platforms is also described).
The results depicted in FIG. 3.2 validate the iterative procedure and show that only 10 iterations are sufficient to obtain the scattering cross section.
For large-scale problems, solving sparse system (3.4) by mean of a direct method may become impracticable due to the blowing up in fill-ins. It is then necessary to resort to a DDM at the level of the sparse system also. But application of a DDM to a sparse systems related to a nodal FEM has faced a blocking difficulty : the way to deal with cross-points, that is, nodes shared by more than two sub-domains. In [EMA2], we have introduced a way to proceed with such a difficulty and proved the stability and the convergence of the related algorithms in a very large theoretical framework. Finally, we have shown in a paper [7] which was very recently published that using one iteration of this algorithm instead of completely solving sparse problem (3.4) yields an efficient method converging in almost the same number of iterations than the initial procedure.
Finally, let us mention a paper [EMA1] published by the team which provides several techniques borrowed from this circle of methods to efficiently solve the scattering of an electromagnetic wave by a deep cavity inside a large perfectly conducting structure.

[6] N. Bartoli and F. Collino, (2000), Integral equations via Saddle Point Problems for Acoustic Problems, *Mathematical Modelling and Numerical Analysis*, **34**, 1023–1049.

[7] Y. Boubendir, A. Bendali, and M. Fares, (2008), Coupling of a non-overlapping domain decomposition method for a nodal Finite Element Method with a Boundary Element Method, *International Journal for Numerical Methods in Engineering*, accepté pour publication, **73(11)**, 1624–1650.

[8] Y. Boubendir, (2002), *Techniques de décomposition de domaine et méthode d'équations intégrales*, PhD thesis, CERFACS–INSA–MIP.

[9] F. Collino and B. Després, (2003), Integral equations via saddle point problems for time-harmonic Maxwell's equations, *Journal of Computational and Applied Mathematics*, **150**, 157–192.

[10] F. Collino, S. Ghanemi, and P. Joly, (2000), Domain Decomposition Method for Harmonic Wave Propagation : a General Presentation, *Computer methods in applied mechanics and engineering*, **184**, 171–211.

[11] B. Després, (1991), Domain decomposition method and the Helmholtz problem., *Mathematical and numerical aspects of wave propagation phenomena*, 44–52.

4 Electromagnetic imaging by the Linear Sampling Method

F. Collino and M'B. Fares

4.1 Description

The research topic is related to wave imaging techniques, which aim at reconstructing various features of a scatterer (localization, shape, nature) from multi-static data (resulting from wave emission and records at several locations). Among inversion methods that underwent significant progress in recent years, the so-called sampling methods have become popular since they provide quick and simple inversion algorithms that are not iterative and do not rely on any linearization assumption (Kirchhoff, Born). Contrary to usual optimization techniques, they do not involve any solution of the direct scattering problem but they amount to solve, for each sampling point, a small ill-posed linear system. Moreover, no a priori knowledge on the physical nature of the imaged inclusion is required. The first non academic works about validation of the LSM method were realized at CERFACS on electromagnetism problems. They were published in the journal Inverse Problems [12]. They are at the origin of the survey paper on LSM [13].

4.2 Development

To validate the LSM method, one needs synthetic data corresponding to the values of the scattering field by the object to be reconstructed. The CESC code (parallel code for solving Maxwell equations by the Boundary Integral method) which was developed at CERFACS was used to generate these data.

Two variants of LSM have been validated :

(I) LSM in far field : the object is illuminated by plane waves on a sphere (or part of a sphere) around the object.

(II) LSM in near field (also called RG-LSM, reciprocity gap LSM) [EMA5]. In this case one computes the reponse of the object to dipole excitations :

- (a) in free space, on a surface (closed or not) around the object.
- (b) in a two-layer space : on a surface situated at the interface between the two media.

The inversion principle is the same for each method :

1. Build the matrix F of LSM via synthetic data.
2. Compute a Singular Values Decomposition of F.
3. For each x in a box containing the object, invert the system of matrix F and compute the norm of the solution $g(x)$ which serves as step function for the object support. (Let us point out that the system of matrix F is ill-posed and Tikhonov regularization has to be used).

An efficient parallelization has been developed for this inversion algorithm.

Finally the main steps of the software design and development are summarized below :

(1) adaptation of the CESC code to generate the entries for the LSM code into the appropriate format.
(2) enrichment of the CESC code to compute the Green function for a two layer space. Such a computation is very expensive (Sommerfeld integrals). An optimization and a parallelization were required to achieve the goal. The classical LSM in a two layer space relies on this computation. This was one of the reason which motivated the use of the RG-LSM which is free from this expensive computation.
(3) optimization and parallelization of the LSM code.

The LSM method has been successfully applied to reconstruct one or several dielectric objects with different dielectric constants, see Figures 4.1 and 4.2. The numerical experiments have demonstrated the ability of LSM to recover the geometry of the scatterers with rather good accuracy in various situations. However, further investigations are needed to control the quality of the reconstruction. This will be the topic of further studies.

[12] F. Collino, M. Fares, and H. Haddar, (2003), Numerical and analytical studies of the linear sampling method in electromagnetic inverse scattering problems, *Inverse Problems*, **19**, 1279–1298.

[13] D. Colton, H. Haddar, and M. Piana, (2003), The linear sampling method in inverse electromagnetic scattering theory, *Inverse Problems (Special section on imaging)*, **19**, S105–S137.

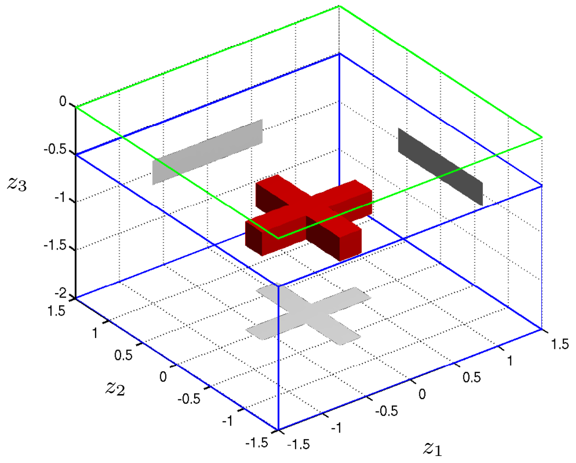


FIG. 4.1 – Exact geometry of the dielectric object embedded in a substrate. The receptors are located in the air on the green plane.

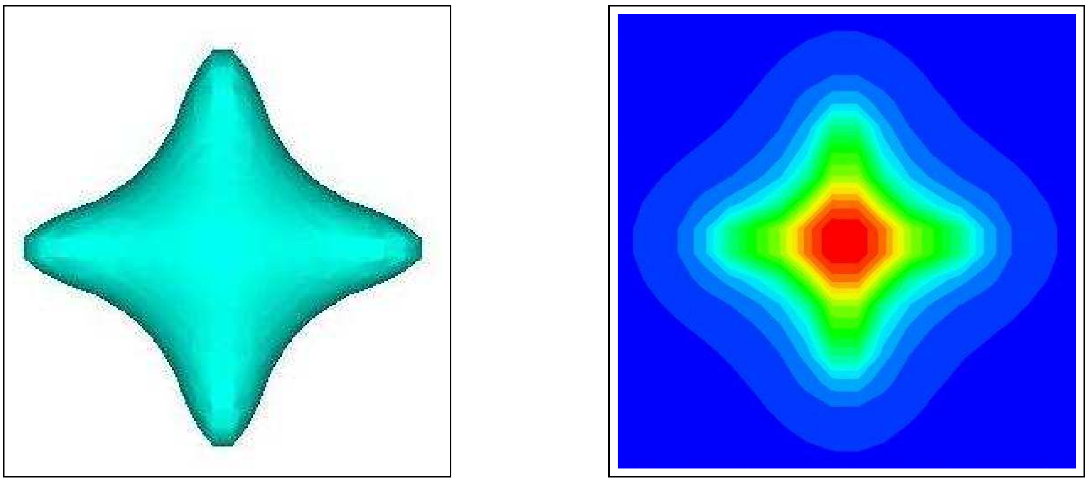


FIG. 4.2 – RG-LSM reconstructed geometry with an added 1% random noise. The wavelength in the air is $\lambda = 1$. Left : 3D representation. Right : horizontal cross section.

5 Finite element simulation of acoustic scattering in a subsonic flow

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

5.1 The motivation

The reduction of noise in aeronautics and car industry is currently driving an intensive research in aeroacoustics. In particular, numerical tools of simulation are developed, which should provide a better understanding of the complex phenomena resulting from the interaction between acoustics and flow. Beside the simulation of noise generation by turbulent flows which has been significantly improved in the past few years - in particular with the progress of the Direct Numerical Simulation-, the seemingly simpler problem (linear equations) of acoustic propagation in a known mean flow has been less investigated. Let us emphasize that although the propagation of sound in the presence of a flow has some analogies with (acoustic or electromagnetic) wave propagation in a heterogeneous medium (a simplified model leads to considering that the presence of the flow changes the local speed of the wave), it is a significantly more difficult problem because it couples acoustic and hydrodynamic phenomena (convection of vortices, instabilities).

We are interested in the numerical simulation of acoustic scattering in presence of a subsonic flow, in the frequency regime that has been much less investigated than the transient regime. Up to our knowledge, only the potential case (when the flow and the source are irrotational) which leads to a Helmholtz like scalar equation has been completely handled. Our objective, in collaboration with POEMS (UMR 2706 CNRS-INRIA-ENSTA), is the design of a general finite element method, able to solve the time harmonic problem in the realistic cases that arise in industry. Such a tool would be very useful for the engineer by providing him intrinsic quantitative data (radiation pattern, resonance frequencies...) helpful for the optimum design of the industrial setup.

5.2 An original approach based on the equation of Galbrun

Acoustic propagation in an arbitrary subsonic flow is generally modelized by the Linearized Euler Equations whose unknowns are the perturbations of velocity $\mathbf{v}$ and pressure p. An alternative is the less well known equation of Galbrun. Galbrun's equation corresponds to a mixed Euler-Lagrange representation : the unknown is the perturbation of Lagrangian displacement $\mathbf{u}$ and it is expressed as a function of the Eulerian variables (the position x and the time t). Classical Eulerian quantities ($\mathbf{v}$ and p) can be easily recovered a posteriori by simple expressions which relate Eulerian and Lagrangian perturbations.

A main advantage of Galbrun's equation comes precisely from this unusual unknown : indeed, most of the boundary conditions involved in the applications (impedance wall, fluid-structure coupling, transmission through shear layers etc...) express some continuity of the perturbation of the normal displacement ; such conditions are therefore very easy to handle in Galbrun's framework while the counterpart is almost impossible with Euler equations.

The main point, which led several teams to give up Galbrun's equation, is that a direct discretization by Lagrange Finite Elements does not work, due to a lack of coerciveness. A solution consists in writing an augmented equation by adding to the original equation a term which does not change the value of the solution (the additional term vanishes for the solution) and which restores coerciveness. This term is related to hydrodynamic phenomena : it requires the evaluation of the curl of the solution $\psi = \mathbf{curl}\,\mathbf{u}$ (called for convenience *vorticity* in the following). This approach has been validated by Bonnet-Ben Dhia et al. [EMA4, EMA20] in the case of a parallel shear flow.

5.3 The results

5.3.1 Derivation of a Low Mach model

Our contribution concerns the extension of the method to a non parallel flow. We have first derived the so-called hydrodynamic equation, which relates ψ and $\mathbf{u}$. Solving the coupled problem (the augmented Galbrun's equation + the hydrodynamic equation) for the two variables ψ and $\mathbf{u}$ would be very expensive. Moreover, the hydrodynamic equation degenerates when the flow vanishes. We have proposed a simplified approach based on a low Mach approximation of the hydrodynamic equation, which provides a differential expression of ψ as a function of $\mathbf{u}$. This way, the unknown ψ can be eliminated and the final problem for $\mathbf{u}$ is proved to be of Fredholm type for slow variations of the flow.

5.3.2 Numerical validation

The method has been validated in the two-dimensional case of an incompressible potential flow around an obstacle. The flow is supposed to be uniform far from the obstacle (of Mach M_∞). For such flows, we can use an exact potential model for comparison. Both models (the potential equation and the augmented Galbrun's equation) are solved by using Lagrange finite elements and Perfectly Matched Layers (located in the area where the flow is uniform). We have considered two configurations :

– First we have considered a flow around a cylinder, perturbed by an incident plane wave. In this case we have used the analytical expression of the flow. Fig. 5.1 shows the Mach field of the mean flow for $M_\infty = 0.1$ (its maximum is located near the circle). Fig. 5.2 shows the result obtained with Galbrun's approach (x-component of the perturbation of the Euler speed) and the difference of the same quantity obtained with both approaches. There is a very good agreement ; the difference can be detected only in a small area where the velocity takes its largest values.

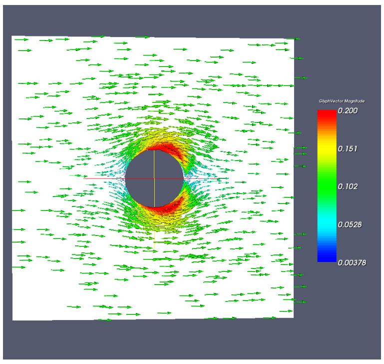


FIG. 5.1 – Incompressible potential flow around a cylinder

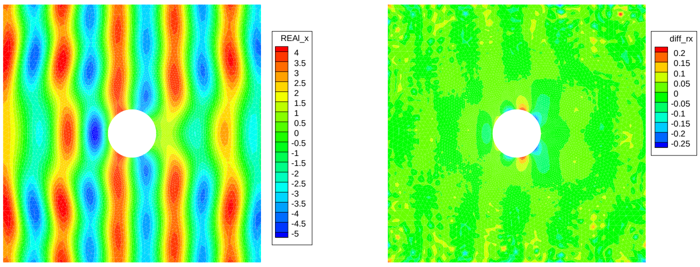


FIG. 5.2 – Euler horizontal velocity : Galbrun's approach (left) and difference with the potential approach (right)

– Then we have considered a flow around a 2D model of aircraft nacelle and an acoustic source located inside the nacelle (see fig. 5.3). The flow is computed numerically via the finite elements solution of a Laplace problem. Again, we have compared the two methods and observed a good agreement between them. Simulations for $M_\infty = 0.1$ and $M_\infty = 0.2$ clearly show the effect of the flow on the directivity of the sound. Fig. 5.4 shows the far-field patterns obtained from the Galbrun solution and compared to the one corresponding to the no-flow experiment.

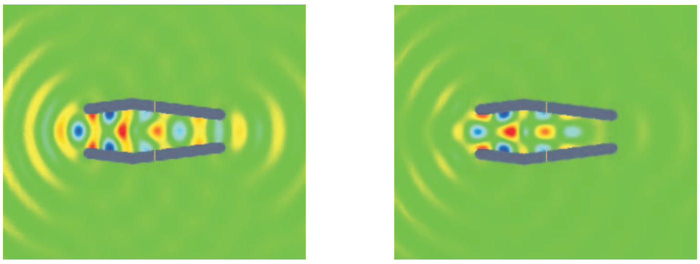


FIG. 5.3 – Euler horizontal velocity obtained with Galbrun's approach : $M_\infty = 0.1$ (left) and $M_\infty = 0.2$ (right)

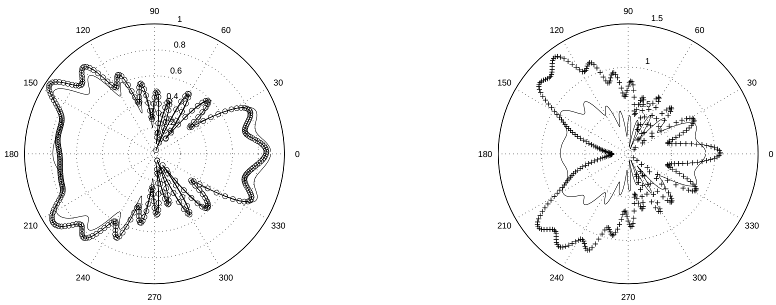


FIG. 5.4 – Far-field pattern : $M_\infty = 0$ (-), $M_\infty = 0.1$ (o) and $M_\infty = 0.2$ (+)

6 Publications

6.1 Journal Publications

[EMA1] N. Balin, A. Bendali, M. Fares, F. Millot, and N. Zerbib, (2006), Some applications of substructuring and domain decomposition techniques to radiation and scattering of time-harmonic electromagnetic waves , *C. R. Physique*, **7**, 474–485.

[EMA2] A. Bendali and Y. Boubendir, (2006), Non-Overlapping Domain Decomposition Method for a Nodal Finite Element Method, *Numerisch Mathematik*, **103**, 515–537.

[EMA3] A. Bendali, Y. Boubendir, and M. Fares, (2007), A FETI-like domain decomposition method for coupling finite elements and boundary elements in large-size problems of acoustic scattering, *Computers & Structures*, **85, Issue 9**, 526–535.

[EMA4] A.-S. Bonnet-BenDhia, E.-M. Duclairoir, G. Legendre, and J.-F. Mercier, (2007), Time-harmonic acoustic propagation in the presence of a shear flow, *J. Comput. Appl. Math*, **204(2)**, 428–439.

[EMA5] F. Cakoni, M. Fares, and H. Haddar, (2006), Analysis of two linear sampling methods applied to electromagnetic imaging of buried objects, *Inverse problems*, **22**, 845–867.

[EMA6] B. Collard, M. Fares, and B. Souny, (2006), A new formulation for scattering by impedant 3D bodies, *J. of Electromagn. Waves and Appl.*, **20**.

[EMA7] F. Collino, T. Fouquet, and P. Joly, (2006), Conservative space-time mesh refinement methods for the FDTD solution of Maxwell's equations, *Journal of Computational Physics*, **211**.

[EMA8] K. Mer-Nkonga, M. Mandallena, D. Goudin, B. Stupfel, and F. Collino, (2006), A numerical strategy for a high frequency electromagnetic scattering problem in a mixed formulation, *C. R. Physique*, **7**.

[EMA9] S. Pernet and X. Ferrieres, (2007), HP a-priori error estimates for a non-dissipative spectral discontinuous Galerkin method to solve the Maxwell equations in the time domain, *Mathematics of Computation*, **76**.

[EMA10] J. Poirier, A. Bendali, and P. Borderies, (2006), Impedance boundary conditions for the scattering of time-harmonic waves by rapidly varying surfaces, *IEEE Transactions on Antennas and Propagation*, **54**.

6.2 Technical reports

[EMA11] A. BENDALI and M. FARES, (2007), Boundary Integral Equations Methods in Acoustic Scattering, Tech. Rep. TR/EMC/07/141, C.E.R.F.A.C.S, *42,av. G. Coriolis,31057 Toulouse Cedex France*.

[EMA12] Y. BOUBENDIR, A. BENDALI, and M. FARES, (2007), Coupling of a non-overlapping domain decomposition method for a nodal Finite Element Method with a Boundary Element Method, Tech. Rep. TR/EMC/07/17, C.E.R.F.A.C.S, *42,av. G. Coriolis,31057 Toulouse Cedex France*.

[EMA13] F. COLLINO and F. MILLOT, (2006), Implémetation d'une méthode itérative pour les problèmes de diffraction d'ondes avec condition d'impédance, Tech. Rep. CR/EMC/06/55, C.E.R.F.A.C.S, *42,av. G. Coriolis,31057 Toulouse Cedex France*.

[EMA14] F. COLLINO and F. MILLOT, (2006), Mise en oeuvre d'un calcul multipôle pour obstacle impédant, Tech. Rep. CR/EMC/06/5, C.E.R.F.A.C.S, *42,av. G. Coriolis,31057 Toulouse Cedex France*.

[EMA15] F. COLLINO, F. MILLOT, and S. PERNET, (2007), Boundary-Integral Methods for iterative solution of scattering problems with variable impedance surface condition, Tech. Rep. TR/EMC/07/18, C.E.R.F.A.C.S, *42,av. G. Coriolis,31057 Toulouse Cedex France*.

[EMA16] V. LEBRIS, (2007), Rayonnement pour l'aéroacoustique, Tech. Rep. WK/EMC/07/138, C.E.R.F.A.C.S, *42,av. G. Coriolis,31057 Toulouse Cedex France*.

[EMA17] F. MILLOT and S. PERNET, (2007), Rapport de synthèse sur la résolution des problèmes de diffraction d'ondes électromagnétiques avec condition d'impédance , Tech. Rep. TR/EMC/07/77, C.E.R.F.A.C.S, *42,av. G. Coriolis,31057 Toulouse Cedex France*.

[EMA18] S. PERNET, F. COLLINO, M. FARES, and F. MILLOT, (2006), Comparaison de formulations intégrales adaptées à la résolution des problèmes de diffraction d'ondes électromagnétiques avec condition d'impédance, Tech. Rep. CR/EMC/06/6, C.E.R.F.A.C.S, *42,av. G. Coriolis,31057 Toulouse Cedex France*.

[EMA19] N. ZERBIB, (2006), Méthodes de sous-structuration et de décomposition de décomposition de domaine pour la résolution des équations de Maxwell Application au rayonnement d'antenne dans un environnement complexe, Tech. Rep. TH/EMC/06/115, C.E.R.F.A.C.S, *42,av. G. Coriolis,31057 Toulouse Cedex France*.

6.3 Proceedings

[EMA20] A.-S. Bonnet-BenDhia, E.-M. Duclairoir, and J.-F. Mercier, (2007), Acoustic propagation in a flow : numerical simulation of the time-harmonic regime., *ESAIM Proceedings, Volume 22*.

10

ENScube Group

1 Introduction

Pierre-Henri Cros

N'S^3 Group is aiming at making use of CERFACS results and/or competencies to explore new application domains.

Currently, two activities are hosted.

The first one is managed by the project Heating, Ventilating and Air Conditioning flow modelling (HVAC) and is leaded by Gabriel Jonville. This activity is more oriented in CFD results and competencies exploitation to model and simulate airflows inside or around buildings and to supply support to traditional design and experimental methods for the management of comfort conditions. This activity is fully granted by consultancy contracts.

The second one is managed by the project development of Collaborative Solution and is leaded by Sébastien Milhac. This activity is more oriented in applied Information Technology R&D to set up prototypes of a platform proposing a large set of tools for distant collaboration in Computer Assisted Engineering (CAE) by using workstation. The objective is to deliver a prototype being completed and qualified through tests and demonstrations (level 8 of the Technology Readiness Level table) and to hold support to Airbus Cimpa and EADS ITS in its proof through successful (reliable and maintained) operation in services. This activity is mainly granted by European contracts.

2 Heating, Ventilation and Air Conditioning Flow Modelling

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

Air quality and thermal comfort are determining factors for optimal indoor conditions to enhance human comfort while optimizing energetic and economic resources.
The group has carried out thermo-airflow simulations for various applications using predictive computational fluid dynamics software to analyze and diagnose heating, ventilating and air conditioning systems.

2.1 Thermo-airflow simulations of aircraft painting hall ventilation

In the frame of the second phase of the Paintsim project (cf. Activity Report 2004-2005 for the first phase), numerical airflow simulations of the ventilation in aircraft painting hall have been performed during years 2006 and 2007.
The overall objective of this project was to obtain numerical tools for the design and the optimization of ventilation systems in aircraft painting halls. These tools were identified and implemented during the first phase of the project.
The second phase of this project aimed at validating the numerical simulation process and the numerical results, with a finer model implementation for geometrical and physical parameters.
Numerical validation on test cases has been realized to evaluate the mesh refinement level necessary for the blowing vents simulation and to identify the most suited physical models for density and turbulence. Further, the geometric representations of the blowing vents and the associated boundary condition types have been studied. Steady and unsteady formulations have been used for the modelling of the Navier-Stokes equations.
The computations have been performed on a quadri-processor computer of 16Gb main memory capacity. The run times range between 12 and 72 CPU hours for one computational case depending on simulation parameters such as mesh resolution, turbulence model or thermal conditions.
The simulation process was applied to a painting hall with several operation cases of the ventilation system. Numerical simulation results showed good correlations with both observations and on-site measurements. They allowed studying the ventilating airflow and the trajectories of pollutants (Fig. 2.1).
Several tools for quantifying the simulation results have been developed. In particular, they allow computing the direct extraction rate of the flow path lines, the angular deviation of the flow in relation to the blowing direction and the extraction efficiency of a weighted particles cloud. These tools permit to analyze the indoor airflow for a given configuration and to quantify the efficiency of ventilation, especially for pollutant extraction.
The second phase of this project brought confidence in numerical airflow simulation for painting hall and proved that simulation results are useful and pertinent.
As a consequence, the simulation process is now used to design new painting hall and will be used to optimize existing halls.

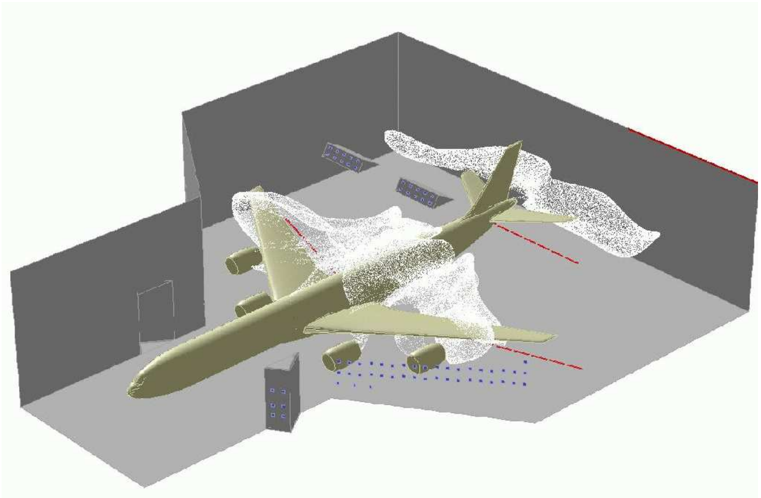


FIG. 2.1 – Particles tracking in the ventilating flow during the wing painting phase.

2.2 Airflow simulations of a blowing plenum in a computer room

For the construction of a new computer data center, a numerical simulation study has been realized to help the design of the blowing plenum beneath the floor of the computer room.
Simulation of data center cooling has become a useful means for the design and management of data centers. The aim of this study was to verify the adequate sizing of the plenum and its ventilation system in order to optimize the airflow.
Geometrical modelling of the plenum considered several positions of the blowing armoire, the paddle form and several heights of the plenum. At the ground level of the room, two types of perforated slab have been modelled with several ground distributions. The volume of the plenum has been meshed with a hexahedral structured mesh of 1.1 million cells.
A velocity enforced boundary condition has been applied to plenum inlet surfaces upstream the paddles. For the plenum outlet zones, the air flows through the perforated slabs with specified permeability and pressure loss factor.

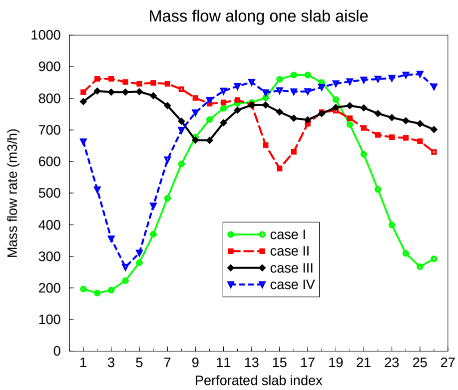


FIG. 2.2 – Mass flow profiles through the perforated slab for different plenum configurations.

Airflow computational fluid dynamics simulations have been performed solving the steady Navier-Stokes equations. The numerical results allowed identifying the optimum plenum height and the best position of the blowing armoires to obtain homogeneous mass flow rate through the perforated slabs (Fig. 2.2, case III). This optimization improved the efficiency of ventilation and the use of air conditioning resources.

2.3 Air conditioning simulation of an office with a double-skin front

In the frame of an office building project with a double-skin front subjected to solar radiation, numerical simulation studies have been realized to design the air conditioning system.
Buildings with a transparent double-skin front in the north of Europe are common but in the south this is not the case and the behavior of the front is not well-known.
This type of building is composed of a front with internal and external glasses separated by a canal of 20 to 80 cm thickness. This canal is ventilated with solar protection between both glasses. This allows controlling overheating inside the office due to solar radiation. An important number of parameters influence the thermo-aeraulic behavior of the double-skin front :

- the weather conditions, the front orientation and geometry define the received global solar radiation,
- the type of solar protection and its position influence the local behavior and the transmitted solar radiation into the office,
- the ventilation strategy and the mass flow rate in the canal act towards the heat transfer coefficients.

The geometry of a single person office has been modeled containing a person, a desk, a chair, a computer, some lights, a cooled ceiling, an air inlet vent, the internal glass, a blind, an air outlet vent and the external glass. An unstructured tetrahedral mesh of 3.6 million of cells has been generated.
In order to examine the impact of these parameters several computational fluid dynamics simulations have been realized coupled with a radiation model. The temperature (Fig. 2.3) and the velocity obtained at each point inside the office allowed specifying the blown air temperature, the cooled ceiling temperature, the internal glass characteristics and the blind solar characteristics.

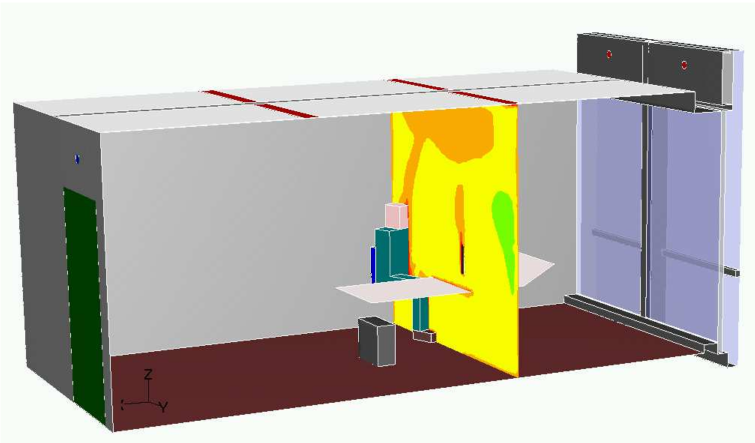


FIG. 2.3 – Temperature field in a vertical plane inside the office.

2.4 Wind simulation on a future district

In the frame of a new public district construction development, wind simulations around the urban environment have been performed. For the considered site, the wind rose from Meteo-France indicates that two wind directions are dominant and thus potentially uncomfortable for both people but also for the commercial fitting out.
The objective of this study was to show the impact of dominant winds near the ground according to the shape and the establishment of buildings, the type and the size of the vegetation.
The geometry of the district has been built from Autocad data files. Buildings, roads, parks and pedestrian ways have been modeled. A volume mesh with 8 million tetrahedral cells has been generated around the district, on a ground surface of 100 ha.
The ground was divided into several zones and the boundary conditions applied on ground used a roughness coefficient depending on the class for each zone. Two wind directions have been considered, one blowing from west and one from south-east direction, with a wind speed of 22 km/h corresponding to the more frequent mean velocity.
Computational fluid dynamics simulations allowed characterizing those zones that are exposed to the wind and those zones that are protected from wind (Fig. 2.4). While the district development project is globally well designed regarding wind concern some spots were identified as wind corridors. To treat these places several development propositions have been formulated. In summary, these numerical results helped the urbanism department to conceive and verify the correct development of this district.

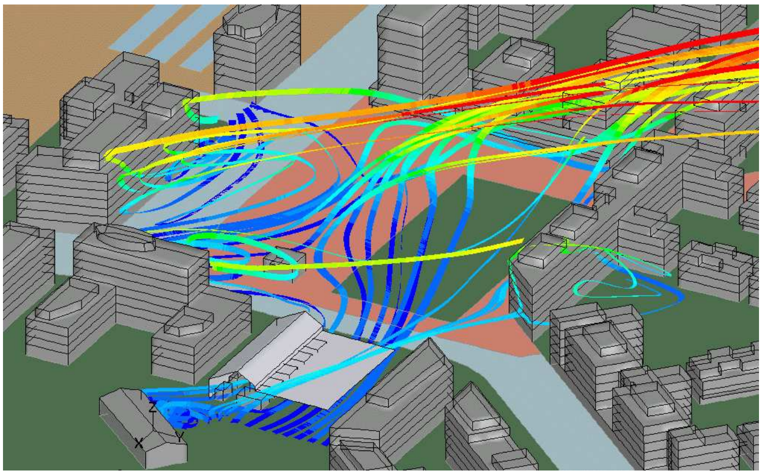


FIG. 2.4 – Path lines at the entrance of the square for western wind.

3 Development of collaborative working solutions

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

3.1 Introduction

The first version of the N'S^3 solution is a Computer Supported Collaborative Working tool designed to ease the co-operation between remote partners in the context of numerical simulation projects.
Being a hardware/software package, it is allowing creating a virtual meeting room with distant partners where users can co-visualize and co-manipulate office document and 3D data.
Relying on Linux and Windows for the collaborative functionalities, on three screens to have an intuitive GUI and on ISDN lines to secure the exchanges of information, this version of the N'S^3 solution is requiring the users to move to a dedicated place.

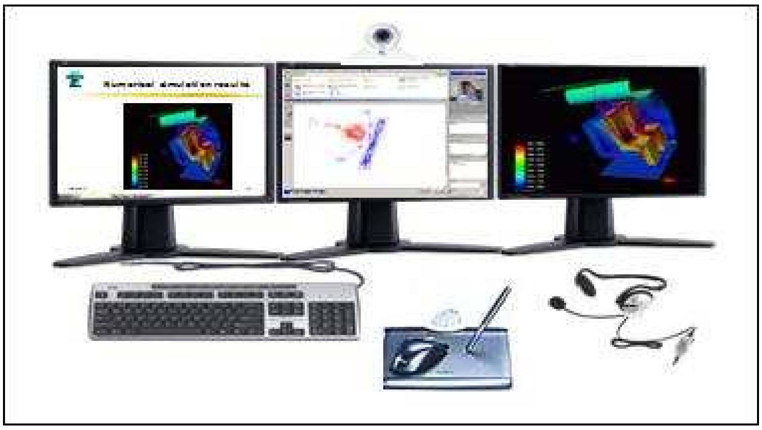


FIG. 3.1 – N'S^3 solution, first version.

This N'S^3 solution is still installed at Turbomeca to follow remotely and collaboratively the results of CFD numerical simulations realized by L. Gicquel's project (CFD team).
The definition and the design of the new version rely on Turbomeca returns of experience and on N'S^3 team involvement in the VIVACE European project which was intending to achieve in the context of the Extended Enterprise a cost reduction of the aircraft design and development phases combined with a reduction in the lead time.
In both cases it has been highlighted the need for accessing from any workstation a web based collaborative workspace offering at least the same possibilities as the first N'S^3 solution version.
Thanks to the progress of the security on Internet and web technology, N'S^3 team has worked on the N'S^3 solution to propose it as a secure collaborative workspace accessible from the user's workstation :

FIG. 3.2 – N’S^3 solution, collaborative workspace.

3.2 Work achieved

3.2.1 Project management

To develop this new version of the N’S^3 solution, the team leaded by Sébastien Milhac, who is in charge of the project management and java developments, and Sven Kufer, who is in charge of NS3D developments, has been reinforced in 2007 by the arrival of Fabrice Oliveira, a web developer.
A close cooperation has been set up with AIRBUS-CIMPA to industrialize and to deploy this new version of the N’S^3 solution and with EADS-ITS to welcome the web server in a secure environment.
The project management of these three partners team is based on the CMMI approach which provides guidance for quality processes.
In this context, different tools are used to manage the project :
– Progress document : to identify, evaluate and follow each task with his responsible.
– Planning : to know the delivery of each component.
– Reporting document : to communicate on the advancement of the project and follow the risks or problems identified.

3.2.2 Architecture

The main improvement was to develop a web version of the first version of the N'S^3 solution which main results was to make specific hardware no more requested and to replace the ISDN lines with a VPN SSL built on the company network and able to cross the firewall in a secure way.

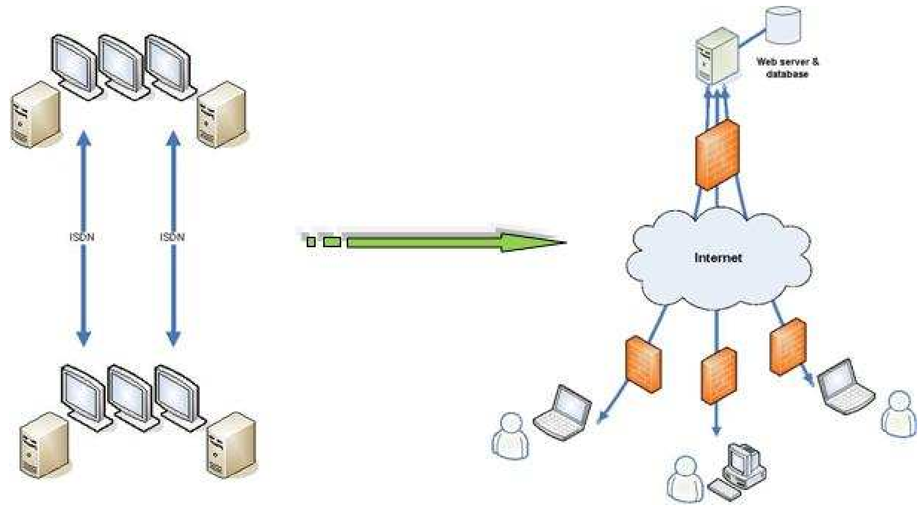


FIG. 3.3 – N'S^3 solution, architecture.

To achieve the N'S^3 solution web version, the following tasks have been undertaken :
- Install and configure an Apache server, a Tomcat server and a MySQL Database
- Develop and set up the portal in html, php and javascript,
- Install a VPN SSL equipment to secure the access to the server.

3.2.3 Collaborative and management functionalities

Once the portal of the application developed, the next step was to develop a web version of the functionalities presented by the first version of the N'S^3 solution :
- Audio/ video was redeveloped with the red5 technology.
- Whiteboard, chat and application sharing with remote control were redeveloped in java using the JSDT API.
- NS3D, the 3D data synchronized viewer, was redeveloped in java using the java web start technology.

Then another main improvement was made by developing new functionalities around the meeting management :
- File Sharing : gives the possibility to the users to exchange data through the server.
- Notes : gives the possibility to take some notes during the meeting.
- Snapshot manager : allows users to create, comment, store and reuse screen captures.
- Data manager : users can link data with a meeting and list the participants to the meeting who have access to it.
- Appendices manager : each one can link appendices (private data) to the meeting allowing a quick access during the meeting.
- Contacts and participants manager : allows users to manage their contacts, list and invite easily the participants.

– Meeting and archived meeting manager. An added value which is presented in the next chapter.
Each functionality was linked to the portal in order to have an intuitive GUI.

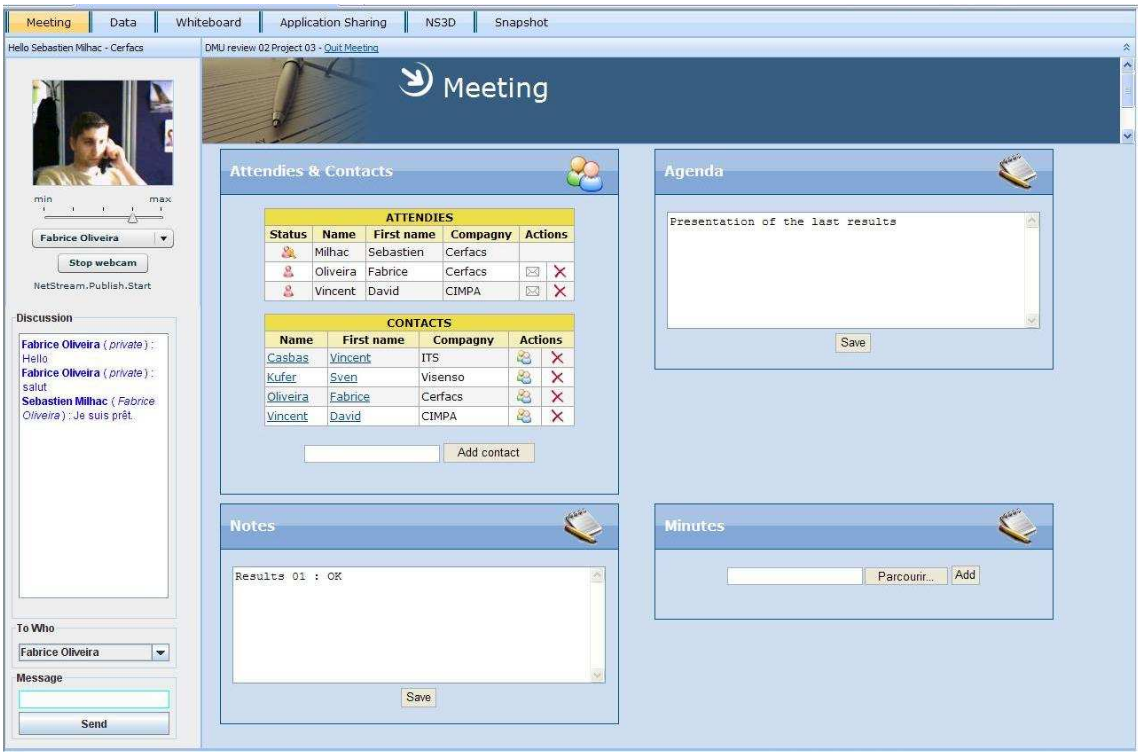


FIG. 3.4 – N'S^3 solution, GUI.

3.2.4 Meeting and archived meeting manager

The new functionality meeting manager eases the preparation, the holding and the exploitation of meetings. It helps the user to manage the meetings during the different phases.

FIG. 3.5 – N'S^3 solution, meeting manager.

The main progress which is one of the added value of the new version of the N'S^3 solution is the archived meeting manager. It gives the possibility to come back to an old meeting and all the information linked to it : list of participants, used or exchanged data, notes, snapshots and minutes.
It's a very useful functionality to prepare a meeting based on the previous one.

The following figure presents the different states of a meeting :

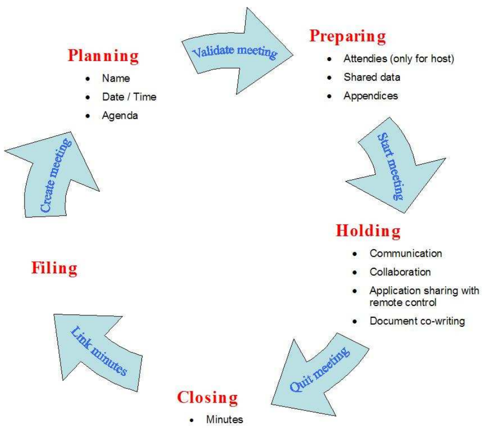


FIG. 3.6 – N'S^3 solution, meeting states.

3.3 Next steps

Two objectives for next phase :

– Install the web version between Turbomeca and CERFACS and deploy it within AIRBUS CIMPA which is composed of different sites in France, Germany and England to test it in operation.
– Develop new functionalities to manage EDM (Engineering Data Management) and PLM (Product Life Management) processes and introduce IAM (Identity and Access Management) in the access management.

The following table summarizes N'S^3 solution progress :

Functions	2004	2007	2009
Audio - video	X	X	X
Whiteboard	X	X	X
Chat	X	X	X
Application sharing with remote control	X	X	X
3D viewer for CAE Data	X	X	X
3D viewer for CAD Data			X
File sharing		X	X
Notes		X	X
Snapshot manager		X	X
Data manager		X	X
Appendices manager		X	X
Meeting manager		X	X
Contacts and participants manager		X	X
Archived meeting manager		X	X
EDM functionality			X
PLM functionality			X
Activities customization			X
Identify and Access Management			X

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Computer Support Group

1 Introduction

Nicolas Monnier

1.1 Key responsibilities

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

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

1.2 General strategy

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

2 Architecture and Actions

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

2.1 CERFACS' computing resources (As of Dec 07).

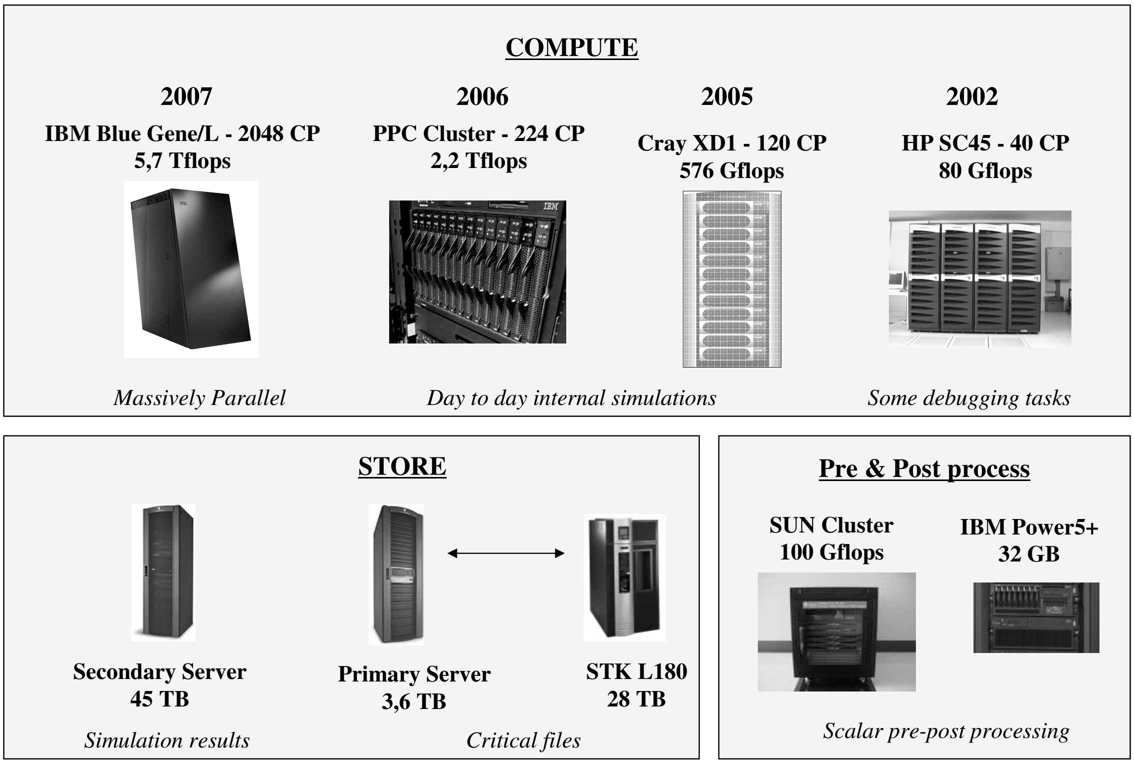

FIG. 2.1 – Internal Facilities - Dec. 2007

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

- Computing power : More than 10 times faster with two new configurations.
  - An IBM JS21 cluster, installed in september 2006, offers a peak performance of 2.2 Tflop/s with 224 PowerPC cores. This new cluster increase significatively our day-to-day simulation power.
  - One of major issue to prepare codes to petaflop resources needs to adapt them on massively parallel servers. An IBM Blue Gene/L, installed in july 2007, offers a peak performance of 5.7 Tflop/s with 2 048 PowerPC cores to help researchers to adapt their codes on this kind of supercomputer and deliver an efficient power to large simulation problems.

These two servers shares a 9 TB parallel filesystem based on a GPFS solution.

- Storage : The capacity of our fileserver dedicated to the storage of large simulations has been upgraded from 16 TB to 45 TB. This new storage capacity is mainly dedicated to climate results generated on Meteo-France's Supercomputers.
- Pre and Post processing : The increase of our computing power asked us to set up more powerfull solutions to visualize bigger data sets and generate bigger meshes. An 8 nodes AMD cluster and an IBM Power5 server with 32 GB memory have been installed during the period to prepare and exploit some of the Blue Gene/L bigger data sets.

2.2 Software environment and Support.

CERFACS' software environment covers three domains :

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