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. 2012 – Dec. 2014

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Foreword

Welcome to the 2012-2014 Cerfacs Scientific Activity Report.

CERFACS transfers knowledge and expertise between the world of basic research, where it is recognized and regarded as a full participant, and the world of applications, where it finds both its key objectives for the benefit of its shareholders and its other partners. CERFACS takes also care more directly if necessary, of the prospective needs of its shareholders in areas which are insufficiently explored.

This report reflects its activity over the last three years. During this period, a new director was appointed in october 2013 and in 2014 a Strategic Research Plan was developped for 2014-2017 with 5 core themes and 5 challenges as defined hereafter :

- Core Themes :
  - Coupling and interfaces,
  - Data Assimilation and optimization,
  - Uncertainties,
  - Numerical methods and linear algebra,
  - HPC and Prospects
- Challenges :
  - COUGAR (complete simulation of a gaz turbine),
  - PUMA (simulation of a complete aircraft),
  - CLIMATE (decadal cimate prediction),
  - DECOLA (simulation of spatial propulsion),
  - MODEST (modelisation for environment and safety).

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

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.

Catherine LAMBERT
CERFACS Director

CERFACS Structure

As a "Société Civile" CERFACS is governed by two bodies.
Firstly, the "Conseil de Gérance", composed of only 7 managers (in French, "Gérants") nominated by the 7 shareholders (see table i), follows quite closely the CERFACS activities and the financial aspects. It meets four times per year.
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 meets twice a year.

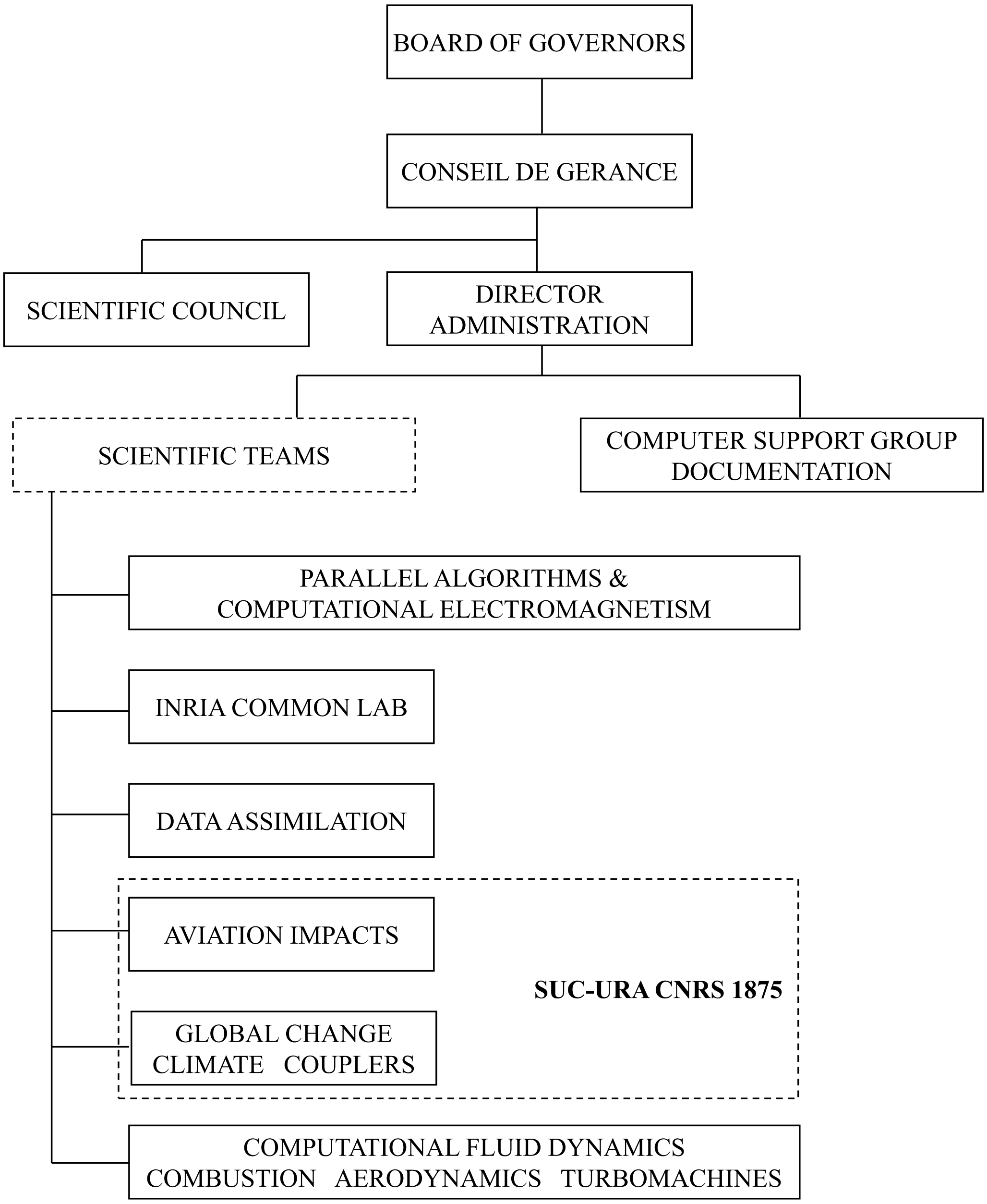
CERFACS Scientific Council met 3 times during this period 2012-2014 under the chairmanship of Prof. Sébastien CANDEL.

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

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

Table i : Société Civile Shareholders

CERFACS chart as of Dec. 31, 2014



CERFACS Staff

NAME	POSITION	PERIOD
GRATTON	Project Leader	2011/01
DUFF	Scientific Advisor	2011/01
FARES	Senior	1992/06
GUROL	Senior Ph.D student	2014/03 2010/02
MILLOT	Senior	1995/11
PERNET	Senior	2007/03-2012/05
TITLEY-PELOQUIN	Senior	2013/01-2014/12
VASSEUR	Senior	2007/05
WEAVER	Senior	1999/11
BEEZLEY	Post Doc	2012/09-2013/02
BYCKLING	Post Doc	2010/11-2012/02
DIOUANE	Post Doc Ph.D student	2014/10 2011/10-2014/09
JIRANEK	Post Doc	2008/11-2014/04
PICHENY	Post Doc	2011/09-2013/04
TROELTZCH	Post Doc	2011/11-2012/05
TSHIMANGA	Post Doc	2014/03
AHIDAR	Ph.D student	2011/10-2014/09
BERGOU	Ph.D student	2011/10-2014/12
CASSIER	Ph.D student Student	2014/11 2014/03-2014/09
FERREIRA LAGO	Ph.D student	2010/032013/06
PEYNAUD	Ph.D student	2009/10-2012/09
MERCIER	Ph.D student	2012/11
MURPHY	Ph.D student	2011/10-2013/09
SOUALMI	Ph.D student	2014/02
STEIF	Ph.D student	2008/10-2011/09
VANDAMME	Ph.D student	2014/10

TAB. ii: List of members of the PARALLEL ALGORITHMS project (1/2).

NAME	POSITION	PERIOD
JOSLIN	Engineer	2011/10-2012/12
LATRE	Engineer Student	2013/10 2013/03-2013/09
LAURENS	Engineer	2012/11-2014/04
MIETKA	Engineer	2013/10-2014/02
RINCON	Engineer Post Doc	2013/10 2011/10-2013/09
ARNAULT	Student	2013/02-2013/06
CLAYER	Student	2012/03-2012/07
HUME	Student	2014/06-2014/08
LAMHAF	Student	2012/07-2012/09
LECERF	Student	2014/03-2014/09
MASMOUDI	Student	2012/10-2013/07
BENDALI	Consultant	1996/01
COLLINO	Consultant	1994/04
TOINT	Consultant	2006/11
LENTO	Visitor	2014/02-2014/06
ROYER	Visitor	2013/06-2013/07
THIAM	Visitor	2013/05-2013/07

List of members of the PARALLEL ALGORITHMS project (2/2).

NAME	POSITION	PERIOD
GIRAUD	INRIA	2009/11
DUDOUIT	Ph.D student	2010/10-2014/07
SALAS MEDINAS	Ph.D student	2010/03-2013/08

TAB. iii: List of members of the CERFACS-INRIA common laboratory

NAME	POSITION	PERIOD
MONNIER	Project Leader	1996/12
D'AST	Engineer	1996/10
JONVILLE	Engineer	2010/10
LAPORTE	Engineer	1988/04
CONTRERAS	Technician	2011/09-2012/09
DEJEAN	Technician	1990/11
FLEURY	Technician	1999/10
VIDAL	Technician	2013/10
BOYE	Student	2012/03-2012/11
CASSSAGNE	Student	2013/04-2013/08
SANTINA	Student	2014/06-2014/08

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

NAME	POSITION	PERIOD
POINSOT	Project Leader	1992/09
CUENOT	Senior	1996/10
DAUPTAIN	Senior	2010/04
DENIAU	Senior	2006/11-2012/08
GICQUEL	Senior	2004/02
GOURDAIN	Senior	2008/02-2013/09
JOUHAUD	Senior	2001/10
MONTAGNAC	Senior	2000/11
PUIGT	Senior	2005/12
RIBER	Senior	2010/05
SICOT	Senior	2011/09-2014/08
STAFFELBACH	Senior	2008/11
VERMOREL	Senior	2007/11
BOUSSUGE	Engineer Research	2002/02
DOMBARD	Engineer Research	2013/01
BARRE	Post Doc Ph.D student	2014/02 2010/06-2013/10
BONHOMME	Post Doc	2014/02
DAVILLER	Post Doc	2013/02
DE LABROUHE	Post Doc	2014/02
DUROCHAT	Post Doc	2013/04-2014/03
FRANSEN	Post Doc Ph.D student	2013/05-2014/04 2010/01-2013/03
HANNEBIQUE	Post Doc Ph.D student	2013/01-2014/12 2009/10
HERMETH	Post Doc Ph.D student	2012/06-2014/05 2009/03-2012/04
KOLOMENSKIY	Post Doc	2011/05-2012/11
KRAUSHAAR	Post Doc	2011/12-2012/12
NEOPHYTOU	Post Doc	2010/12-2012/11
PECHEREAU	Post Doc	2014/10
PINEL	Post Doc	2010/05-2012/05
SHIN	Post Doc	2013/04-2014/03
VASS	Post Doc	2011/10-2013/10
VILLEDIEU	Post Doc	2012/11-2014-11
WANG	Post Doc	2011/07-2012/12
AILLAUD	Ph.D student	2014/10
BAUERHEIM	Ph.D student	2011/10
BECERRIL	Ph.D student Student	2013/10 2013/03-2013/08
BERGER	Ph.D student	2012/11
BIOLCHINI	Ph.D student	2014/06
BOCQUET	Ph.D student	2010/01-2013/03
BRIDEL-BERTOMEU	Ph.D student	2014/01
CAYOT	Ph.D student	2011/10
CHAUSSONNET	Ph.D student	2010/06-2013/09
COLLADO	Ph.D student	2009/09-2012/09

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

COREIXAS	Ph.D student Student	2014/09 2014/03-2014/08
CREVEL	Ph.D student	2010/09-2013/08
DAROUKH	Ph.D student	2014/01
DOUNIA	Ph.D student	2014/10
DURAN	Ph.D student	2011/01-2014/01
ESCLAPEZ	Ph.D student	2011/10
FALESE	Ph.D student	2010/05-2013/04
FELDEN	Ph.D student Student	2014/01 2013/04-2013/09
FERAND	Ph.D student	2014/03
FRANCOIS	Ph.D student	2010/05-2013/09
GHANI	Ph.D student	2012/02
GIRET	Ph.D student	2011/03-2014/02
GOMAR	Ph.D student	2010/09-2013/09
GROSNICKEL	Ph.D student Student	2014/10 2014/03-2014/08
JARAVEL	Ph.D student	2012/11
KOUPPER	Ph.D student	2012/01
LABARRERE	Ph.D student	2012/10
LACASSAGNE	Ph.D student	2013/10
LAPEYRE	Ph.D student	2011/10
LAHBIB	Ph.D student Student	2012/10 2012/03-2012/09
LE BRAS	Ph.D student Student	2012/10 2012/03-2012/09
LEONARD	Ph.D student	2010/06-2013/12
LIVEBARDON	Ph.D student	2011/11
MAESTRO	Ph.D student Engineer	2014/08 2014/03-2014/06
MARI	Ph.D student	2011/12
MISDARIIS	Ph.D student	2011/11-2014/12
MOTHEAU	Ph.D student	2010/11-2013/11
MOURET	Ph.D student Student	2012/10 2012/03-2012/09
NDIAYE	Ph.D student	2013/10
NI	Ph.D student Student	2013/11 2012/06-2012/08
PAPADOGIANNIS	Ph.D student	2012/01
PAULHIAC	Ph.D student	2011/12-2014/12
PEREZ ARROYO	Ph.D student	2013/10
QUILLATRE	Ph.D student	2010/10-2013/09
RICHARD	Ph.D student	2009/10-2012/09
ROCCHI	Ph.D student	2009/11-2013/01
RUIZ	Ph.D student	2008/10-2012/01
SADOUDI	Ph.D student	2011/11
SEGUI TROTH	Ph.D student Student	2013/10 2013/02-2013/07
SHUM-KIVAN	Ph.D student Student	2013/10 2013/02-2013/07

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

SIERRA SANCHEZ	Ph.D student	2008/10-2012/01
VANHAREN	Ph.D student Student	2014/01 2013/04-2013/10
WLASSOW	Ph.D student	2009/03-2012/03
ZHU	Ph.D student	2012/02
BERTHOUMIEUX	Engineer	2014/02-2014/08
BOUVY	Engineer	2013/01-2014/06
CAYOT	Engineer	2011/10
FOURNIER	Engineer Student	2013/10-2014/03 2013/03-2013/08
FRICHET	Engineer	2011/10-2013/02
GALLARD	Engineer Ph.D student	2014/04-2014/07 2011/01-2013/12
GUEDENEY	Engineer Ph.D student	2014/11 2008/11-2012/09
JACOB	Engineer	2012/01-2013/07
JAURE	Engineer Ph.D student	2012/06-2013/06 2009/04-2012/03
MOGE	Engineer	2014/01-2014/09
ABOU MANSOUR	Student	2012/03-2012/09
AMOUYAL	Student	2013/02-2013/06
ARROYO CALLEJO	Student	2012/03-2012/09
BOURGEOIS	Student	2013/02-2013/08
CASSAGNE	Student	2013/09-2014/01
DE OLIVEIRA	Student	2014-10-2014/12
DEWIDEHEM	Student	2014/06-2014/09
ERUDEL	Student	2013/04-2013/09
GENOT	Student	2013/06-2013/08
JAROSSAY	Student	2014/06-2014/08
KRAFT	Student	2012/06-2012/11
KUZMIN	Student	2012/04-2012/10
LEMESLE	Student	2014/04-2014/09
MAGNET	Student	2014/06-2014/08
MARTER	Student	2013/03-2013/08
MONTANELLI	Student	2013/04-2013/10
PARMENTIER	Student	2012/04-2012/09
PICHERIT	Student	2013/04-2013/09
SONNET	Student	2012/03-2012/08
TABEKO TAGNE	Student	2014/04-2014/10
VERDIN	Student	2013/07-2013/08
WU	Student	2012/07-2012/09
MOREAU	Consultant	2009/04
MULLER	Consultant	1997/11
NICOUD	Consultant	2001/10
RIZZI	Consultant	1987/10
SAGAUT	Consultant	2011/02
SCHONFELD	Consultant	2001/01
JIMENEZ SANCHEZ	Visitor	2013/04-2013/07
SCHOLL	Visitor	2013/05-2013/08

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

NAME	POSITION	PERIOD
THUAL	Project Leader	1991/09
DUCHAINE	Senior	2010/10
RICCI	Senior	2008/11
ROGEL	Senior	1998/10
TERRAY	Senior	1992/10
BOURIQUET	Research Engineer	2006/08-2012/08
MAISONNAVE	Research Engineer	2000/12
MOREL	Research Engineer	2000/03
PAGE	Research Engineer	2009/07
SANCHEZ	Research Engineer	2010/11
THEVENIN	Research Engineer	2008/09
VALCKE	Research Engineer	1997/02
BORCHI	Post Doc	2012/01-2013/02
CLARK	Post Doc	2014/01
CORTESI	Post Doc	2014/02
HAMON	Post Doc	2012/07-2013/06
MOUFFE	Post Doc	2011/09-2012/06
TITAUD	Post Doc	2010/06-2012/08
BADOR	Ph.D Student	2012/11
BARTHELEMY	Ph.D Student	2011/12
DAYON	Ph.D Student	2012/11
EL MOCAYD	Ph.D Student Student	2013/11 2013/04-2013/09
HABERT	Ph.D Student	2011/10-2014/09
HARADER	Ph.D Student	2011/10-2014/09
OUDAR	Ph.D Student Student	2013/10 2013/02-2013/09
PIAZZA	Ph.D Student	2010/10-2014/09
RUPRICH-ROBERT	Ph.D Student	2010/10-2014/03
BERTHON	Engineer	2013/04-2014/03
BESSIERES	Engineer	2014/01
BOUMEDIENE	Engineer Student	2014/10 2014/03-2014/09
BRETONNIERE	Engineer	2011/02-2012/07
CORRE	Engineer Ph.D Student	2012/10-2013/04 2008/10-2012/09
KIRSME	Engineer	2012/11-2014/05
MINVIELLE	Engineer	2012/01-2014/06
MONERIE	Engineer	2014/03
RADOJEVIC	Engineer	2014/08
ROCHOUX	Engineer Ph.D Student	2014/01-2014-01 2010/10-2013/11
TATARINOVA	Engineer	2013/09
TRESPEUCH	Engineer	2011/10-2012/06
YAN	Engineer	2011/02-2012/02

TAB. vi: List of members of the CLIMATE MODELLING & GLOBAL CHANGE project (1/2).

NAME	POSITION	PERIOD
ALBERTUS	Student	2013/05-2013/08
BART	Student	2012/02-2012/05
BUVRY	Student	2012/06-2012/09
EDWELL	Student	2012/02-2012/07
EMERY	Student	2013/02-2013/05
FRUCTUS	Student	2014/07-2014/07
LEAUTE	Student	2014/01-2014/06
NAKOULMA	Student	2012/02-2012/06
PINEL	Student	2014/01-2014/06
BOE	CNRS	2010/10
CASSOU	CNRS	2002/11
COQUART	CNRS	2006/12
FERNANDEZ	CNRS	2011/11-2013/05
MOINE	CNRS	2013/07-2014/12
PIACENTINI	Consultant	2007/06
MARCHAND	Visitor	2013/07-2013/07
MOORE	Visitor	2012/08-2012/08
LOPEZ	Visitor	2012/02-2012/05

List of members of the CLIMATE MODELLING & GLOBAL CHANGE project (2/2).

NAME	POSITION	PERIOD
CARIOLLE	Project Leader	2003/08
EMILI	Senior Post Doc	2014/02 2012/02-2014/01
MASSART	Senior	2004/12-2012/05
PAOLI	Senior	2004/07
THOURON	Senior Post Doc	2012/10 2010/10-2012/09
JAUMOUILLE	Engineer Post Doc	2013/02-2014/07 2010/02-2012/01
PICOT	Engineer Ph.D Student	2012/11-2014/04 2009/10-2012/09
PEIRO	Ph.D Student	2014/11
POUBEAU	Ph.D Student	2011/10
PRAGA	Ph.D Student	2011/09-2014/12
ZYRYANOV	Engineer	2012/02-2013/01
OUAALAYA	Student	2013/05-2013/09
PADRE	Student	2013/02-2013/06
MOINAT	Consultant	2013/01
PIACENTINI	Consultant	2007/10

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

CERFACS Wide-Interest Seminars

Philippe Pébay (Kitware SAS) : *Introduction à Paraview : Une application parallèle de visualisation et d'analyse de données issues du calcul scientifique.* (2012, January 19th)

Marc Bocquet (CEREA, joint laboratory Ecole des Ponts ParisTech and EdF R&D, Paris) : *Reconstruction of the Fukushima accident atmospheric source term using inverse modelling & Inverse modeling of regional carbon monoxide emissions using ground observations* (2012, January 25th)

Francisco-Javier Doblas-Reyes (ICREA, IC3) : *Prévision saisonnière et décennale : quelques réflexions sur le présent* . (2012, March 15th)

Marc Baboulin (INRIA, Université de Paris-Sud) : *Accelerating linear solutions on new parallel architectures.* (2012, March 20th)

Erik Hagersten (Chief Scientist, Rogue Wave Software, Professor Uppsala University) : *Optimizing for Multi/Many Cores Made Easy.* (2012, March 23th)

Boris Epstein and Sergey Peigin (OPTIMENGA Ltd & Academic college of Tel-Aviv-Jaffa) : *Industry-Strength Numerical Optimization : Application to Aerodynamic Shape Design.* (2012, March 28th)

Jean-Michel Muller and Florent de Dinechin (Ecole Normale Supérieure de Lyon) : *Contrôle des Erreurs de Roundoff.* (2012, April 17th)

James R. Dawson (University of Cambridge) : *Experimental studies of circumferential instabilities in an annular model gas turbine combustor.* (2012, April 26th)

Laurent Hascoet (INRIA) : *Automatic Differentiation of programs and its applications to scientific computing* . (2012, May 24th)

Jan Mandel (University of Colorado, Denver) : *Coupled atmosphere - wildland fire numerical simulation with WRF and SFIRE.* (2012, June 13th)

Frédéric Hecht (Laboratoire Jacques-Louis Lions, Université P&M Curie) : *Scalable Domain Decomposition Preconditioners in FreeFem++.* (2013, May 23rd)

Eric Darve (Stanford University) : *Fast linear algebra for matrices with low-rank hierarchical structures.* (2013, July 1st)

Olivier Talagrand (Laboratoire de Météorologie Dynamique, Ecole Normale Supérieure, Paris) : *Ensemble Variational Assimilation and Bayesian Estimation.* (2013, December 12th)

Anthony Weaver (CERFACS) : *Aspects of covariance modelling in variational ocean data assimilation.* (2013, December 13th)

Professor Ahmed Sameh (Department of Computer Science, Purdue University) : *Scalable Parallel Sparse Matrix Computations.* (2013, December 17th)

Mélanie Rochoux (CERFACS, Toulouse et Ecole Centrale Paris - CNRS - Laboratoire EM2C) : *Vers une meilleure prévision de la propagation d'incendies de forêt : Evaluation de modèles et Assimilation de données.* (2014, January 23rd)

Romain Desplats (CNES, Toulouse) : *Brevets et publications, protection des logiciels et opensource : que dois-je faire quand je pense avoir innové ?* (2014, April 29th)

Françoise Chatelin (CERFACS, Université Toulouse 1) : *Qualitative computing : alternative paths in computation.* (2014, May 22th)

Jean-Claude André (Académie des Sciences) : *Changement climatique : que penser de la géoingénierie ?* (2014, June 25th)

Venkata Ratnam (JAMSTEC) : *The importance of inclusion of air-sea interactions in a regional model.* (2014, December 9th)

Yushi Morioka (JAMSTEC) : *Remote and local impacts on the generation of the Indian Ocean Subtropical Dipole.* (2014, December 9th)

Takeshi Doi (JAMSTEC) : *SINTEX-F1/F2 seasonal prediction system past, present, and future.* (2014, December 9th)

1

Parallel Algorithms Project

Introduction

1.1 Introduction

The Parallel Algorithms Project conducts a dedicated research to address the solution of problems in applied mathematics by proposing advanced numerical algorithms to be used on massively parallel computing platforms. The Parallel Algorithms Project is especially considering problems known to be out of reach of standard current numerical methods due to, e.g., the large-scale nature or the nonlinearity of the problem, the stochastic nature of the data, or the practical constraint to obtain reliable numerical results in a limited amount of computing time. This research is mostly performed in collaboration with other teams at CERFACS and the shareholders of CERFACS as outlined in this report.

This research roadmap is known to be quite ambitious and we note that the major research topics have evolved over the past years. The main current focus concerns both the design of algorithms for the solution of sparse linear systems coming from the discretization of partial differential equations and the analysis of algorithms in numerical optimization in connection with several applications including data assimilation. These research topics are often interconnected as it is the case for e.g. large-scale inverse problems (so called big data inverse problems) or the solution of nonlinear systems that require approximate solutions of linearized systems. These research developments rely on a past research expertise in numerical analysis exploiting the structure of the problem in scientific computing, especially in qualitative computing.

A strong focus is given on mathematical aspects. Indeed efficient parallel algorithms are proposed together with their mathematical analysis. Main properties such as convergence of iterative methods, scalability properties, convergence to local or global minima are theoretically investigated.

Solution methods of sparse linear systems are considered in a broad sense by tackling both sparse direct methods and projection based iterative methods. These methods can also be combined to derive hybrid algebraic methods close to domain decomposition or multiscale methods. In addition to graph theory, these activities rely on a strong expertise in software development in linear algebra and on an up-to-date knowledge of the parallel computing platforms.

Optimization methods do occur in several applications at CERFACS. Most often the main goal is to improve the performance of a given system. The Parallel Algorithms Project is mainly focussing on both differentiable optimization and derivative-free optimization. The main research topics concern the convergence to local or global minima and the efficiency of the algorithms in practice.

The Parallel Algorithms Project is also deeply involved in the design and analysis of algorithms for data assimilation. Algorithms related to differentiable optimization or derivative-free optimization are considered together with filtering techniques. All these algorithms must be adapted and improved before tackling potential applications in seismic, oceanography, atmospheric chemistry or meteorology. The Parallel Algorithms Project has notably developed a specific expertise in the field of correlation error modelling based on the iterative solution of an implicitly formulated diffusion equation.

Finally the Parallel Algorithms Project takes an active part in the Training programme at CERFACS and is also regularly organizing seminars, workshops and international conferences in numerical optimization, numerical linear algebra and data assimilation.

S. Gratton.

Dense and Sparse Matrix Computations

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

P.R. Amestoy : Université de Toulouse, INPT (ENSEEIHT)-IRIT, *France* ; **I.S. Duff** : CERFACS, 42 Avenue Gaspard Coriolis, 31057, Toulouse, France and Building R 18, RAL, Oxon, OX11 0QX, England ; **J.-Y. L'Excellent** : INRIA and Laboratoire de l'Informatique du Parallélisme (UMR CNRS-ENS Lyon-INRIA-UCBL), Université de Lyon, 46, allée d'Italie, ENS Lyon, F-69364, Lyon Cedex, *France* ; **Y. Robert** : Laboratoire de l'Informatique du Parallélisme (UMR CNRS -ENS Lyon-INRIA-UCBL), Université de Lyon, 46, allée d'Italie, ENS Lyon, F-69364, Lyon Cedex 7, *France* ; **F.-H. Rouet** : Université de Toulouse, INPT(ENSEEIHT)-IRIT, *France* ; **B. Uçar** : Centre National de la Recherche Scientifique and Laboratoire de l'Informatique du Parallélisme (UMR CNRS-ENS Lyon-INRIA-UCBC), Université de Lyon, 46, allée d'Italie, ENS Lyon, F-69364, Lyon Cedex 7, *France*

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

2.2 Design, implementation, and analysis of maximum transversal algorithms.

I.S. Duff : CERFACS, 42 Avenue Gaspard Coriolis, 31057, Toulouse, France and Building R 18, RAL, Oxon, OX11 0QX11, *England* ; **K. Kaya** : CERFACS, 42 Avenue Gaspard Coriolis, 31057, Toulouse, *France* ; **B. Uçar** : Centre National de la Recherche Scientifique and Laboratoire de l'Informatique du Parallélisme (UMR CNRS-ENS Lyon-INRIA-UCBC), Université de Lyon, 46, allée d'Italie, ENS Lyon, F-69364, Lyon Cedex 7, *France*

We report on careful implementations of seven algorithms for solving the problem of finding a maximum transversal of a sparse matrix. We analyse the algorithms and discuss the design choices. To the best of our knowledge, this is the most comprehensive comparison of maximum transversal algorithms based on augmenting paths. Previous papers with the same objective either do not have all the algorithms discussed

in this paper or they used non-uniform implementations from different researchers. We use a common base to implement all of the algorithms and compare their relative performance on a wide range of graphs and matrices. We systematize, develop and use several ideas for enhancing performance. One of these ideas improves the performance of one of the existing algorithms in most cases, sometimes significantly. So much so that we use this as the eighth algorithm in comparisons.

2.3 Preconditioners based on strong subgraphs.

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This paper proposes an approach for obtaining block diagonal and block triangular preconditioners that can be used for solving a linear system $Ax = b$, where A is a large, nonsingular, real, $n \times n$ sparse matrix. The proposed approach uses Tarjan's algorithm for hierarchically decomposing a digraph into its strong subgraphs. To the best of our knowledge, this is the first work that uses this algorithm for preconditioning purposes. We describe the method, analyse its performance, and compare it with preconditioners from the literature such as ILUT and XPABLO and show that it is highly competitive with them in terms of both memory and iteration count. In addition, our approach shares with XPABLO the benefit of being able to exploit parallelism through a version that uses a block diagonal preconditioner.

2.4 Partitioning strategies for the block Cimmino algorithm.

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In the context of the block Cimmino algorithm, we study preprocessing strategies to obtain block partitionings that can be applied to general linear systems of equations $Ax = b$. We study strategies that transform the matrix AA^T into a matrix with a block tridiagonal structure. This provides a partitioning of the linear system for row projection methods because block Cimmino is essentially equivalent to block Jacobi on the normal equations, and the resulting partition will yield a two-block partition of the original matrix. Therefore, the resulting block partitioning should improve the rate of convergence of block row projection methods such as block Cimmino. We discuss a method for obtaining a partitioning using a dropping strategy that gives more blocks at the cost of relaxing the two-block partitioning. We then use a hypergraph partitioning that works directly on the matrix A to reduce directly the connections between blocks. We give numerical results showing the performance of these techniques both in their effect on the convergence of the block Cimmino algorithm and in their ability to exploit parallelism.

2.5 The augmented block Cimmino distributed method.

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We introduce and study a novel way of accelerating the convergence of the block Cimmino method by augmenting the matrix so that the subspaces corresponding to the partitions are orthogonal. This results in a requirement to solve a relatively smaller symmetric positive definite system. We consider ways to reduce the size of this system using a controlled departure from orthogonality. We illustrate the performance of our method on some realistic test problems.

Iterative Methods and Preconditioning

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

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In a wide number of applications in computational science and engineering the solution of large linear systems of equations with several right-hand sides given at once is required. Direct methods based on Gaussian elimination are known to be especially appealing in that setting. Nevertheless, when the dimension of the problem is very large, preconditioned block Krylov space solvers are often considered as the method of choice. The purpose of this paper is thus to present iterative methods based on block restarted GMRES that allow variable preconditioning for the solution of linear systems with multiple right-hand sides. The use of flexible methods is especially of interest when approximate possibly iterative solvers are considered in the preconditioning phase. First we introduce a new variant of block flexible restarted GMRES that includes a strategy for detecting when a linear combination of the systems has approximately converged. This explicit block size reduction is often called deflation. We analyze the main properties of this flexible method based on deflation and notably prove that the Frobenius norm of the block residual is always nonincreasing. We also present a flexible variant based on both deflation and truncation to especially be used in case of limited memory. Finally we illustrate the numerical behavior of these flexible block methods for large industrial simulations arising in geophysics, where indefinite linear systems of size up to 1 billion unknowns with multiple right-hand sides have been successfully solved in a parallel distributed memory environment.

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

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

3.3 A modified block flexible GMRES method with deflation at each iteration for the solution of non-hermitian linear systems with multiple right-hand sides.

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We propose a variant of the block GMRES method for the solution of linear systems of equations with multiple right-hand sides. We investigate a deflation strategy to detect when a linear combination of approximate solutions is already known that avoids performing expensive computational operations with the system matrix. This is especially useful when the cost of the preconditioner is supposed to be larger than the cost of orthogonalization in the block Arnoldi procedure. We specifically focus on the block GMRES method incorporating deflation at the end of each iteration proposed by Robbé and Sadkane (M. Robbé and M. Sadkane, Linear Algebra Appl., 419 (2006), pp. 265–285). We extend their contribution by proposing that deflation be performed also at the beginning of each cycle. This change leads to a modified least-squares problem to be solved at each iteration and gives rise to a different behavior especially when multiple restarts are required to reach convergence. Additionally we investigate truncation techniques, aiming at reducing the computational cost of the iteration. This is particularly useful when the number of right-hand sides is large. Finally, we address the case of variable preconditioning, an important feature when iterative methods are used as preconditioners, as investigated here. The numerical experiments performed in a parallel environment show the relevance of the proposed variant on a challenging application related to geophysics. A savings of up to 35% in terms of computational time—at the same memory cost—is obtained with respect to the original method on this application.

3.4 An improved two-grid preconditioner for the solution of three-dimensional Helmholtz problems in heterogeneous media.

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In this paper, we address the solution of three-dimensional heterogeneous Helmholtz problems discretized with second-order finite difference methods with application to acoustic waveform inversion in geophysics. In this setting, the numerical simulation of wave propagation phenomena requires the approximate solution of possibly very large indefinite linear systems of equations. For that purpose, we propose and analyse an iterative two-grid method acting on the Helmholtz operator where the coarse grid problem is solved inaccurately. A cycle of a multigrid method applied to a complex shifted Laplacian operator is used as a preconditioner for the approximate solution of this coarse problem. A single cycle of the new method is then used as a variable preconditioner of a flexible Krylov subspace method. We analyse the properties of the resulting preconditioned operator by Fourier analysis. Numerical results demonstrate the effectiveness of the algorithm on three-dimensional applications. The proposed numerical method allows us to solve three-dimensional wave propagation problems even at high frequencies on a reasonable number of cores of a distributed memory computer.

3.5 Energy backward error : interpretation in numerical solution of elliptic partial differential equations and convergence of the conjugate gradient method.

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Backward error analysis is of great importance in the analysis of the numerical stability of algorithms in finite precision arithmetic, and backward errors are also often employed in stopping criteria of iterative methods for solving systems of linear algebraic equations. The backward error measures how far we must perturb the data of the linear system so that the computed approximation solves it exactly. We assume that the linear systems are algebraic representations of partial differential equations discretised using the Galerkin finite element method. In this context, we try to find reasonable interpretations of the perturbations of the linear systems which are consistent with the problem they represent and consider the optimal backward perturbations with respect to the energy norm, which is naturally present in the underlying variational formulation. We also investigate its behaviour in the conjugate gradient method by constructing approximations in the underlying Krylov subspaces which actually minimise such a backward error.

3.6 GMRES convergence bounds that depend on the right-hand side vector.

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We consider the convergence of the algorithm GMRES of Saad and Schultz for solving linear equations $Bx = b$, where $B \in \mathbb{C}^{n\times n}$ is nonsingular and diagonalizable, and $b \in \mathbb{C}^n$. Our analysis explicitly includes the initial residual vector r_0. We show that the GMRES residual norm satisfies a weighted polynomial least-squares problem on the spectrum of B, and that GMRES convergence reduces to an ideal GMRES problem on a rank-1 modification of the diagonal matrix of eigenvalues of B. Numerical experiments show that the new bounds can accurately describe GMRES convergence.

Nonlinear Systems and Optimization

4.1 Linear regression models, least-squares problems, normal equations, and stopping criteria for the conjugate gradient method.

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Minimum-variance unbiased estimates for linear regression models can be obtained by solving least-squares problems. The conjugate gradient method can be successfully used in solving the symmetric and positive definite normal equations obtained from these least-squares problems. Taking into account the results of Golub and Meurant (1997, 2009), Hestenes and Stiefel (1952), and Strakos and Tichy (2002), which make it possible to approximate the energy norm of the error during the conjugate gradient iterative process, we adapt the stopping criterion introduced by Arioli (2005) to the normal equations taking into account the statistical properties of the underpinning linear regression problem. Moreover, we show how the energy norm of the error is linked to the χ^2 distribution and to the Fisher-Snedecor distribution. Finally, we present the results of several numerical tests that experimentally validate the effectiveness of our stopping criteria.

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

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The main result of this paper is the formulation of an explicit expression for the condition number of the truncated least squares solution of $Ax = b$. This expression is given in terms of the singular values of A and the Fourier coefficients of b. The result is derived using the notion of the Fréchet derivative together with the product norm on the data $[A, b]$ and the 2-norm on the solution. Numerical experiments are given to confirm our results by comparing them to those obtained by means of a finite difference approach.

4.3 The optimization test environment.

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The Optimization Test Environment is an interface to efficiently test different optimization solvers. It is designed as a tool for both developers of solver software and practitioners who just look for the best solver for their specific problem class. It enables users to (i) Choose and compare diverse solver routines ; (ii) Organize and solve large test problem sets ; (iii) Select interactively subsets of test problem sets ; (iv) Perform a statistical analysis of the results, automatically produced as, PDF, and JPG output. The Optimization Test Environment is free to use for research purposes.

4.4 Globally convergent evolution strategies.

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In this paper we show how to modify a large class of evolution strategies (ES's) for unconstrained optimization to rigorously achieve a form of global convergence, meaning convergence to stationary points independently of the starting point. The type of ES under consideration recombines the parent points by means of a weighted sum, around which the offspring points are computed by random generation. One relevant instance of such an ES is covariance matrix adaptation ES (CMA-ES). The modifications consist essentially of the reduction of the size of the steps whenever a sufficient decrease condition on the function values is not verified. When such a condition is satisfied, the step size can be reset to the step size maintained by the ES's themselves, as long as this latter one is sufficiently large. We suggest a number of ways of imposing sufficient decrease for which global convergence holds under reasonable assumptions (in particular density of certain limit directions in the unit sphere). Given a limited budget of function evaluations, our numerical experiments have shown that the modified CMA-ES is capable of further progress in function values. Moreover, we have observed that such an improvement in efficiency comes without weakening significantly the performance of the underlying method in the presence of several local minimizers.

4.5 Simulated polyhedral clouds in robust optimization.

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Past studies of uncertainty handling with polyhedral clouds have already shown strength in dealing with higher dimensional uncertainties in robust optimization, even in case of partial ignorance of statistical information. However, in thousands or more dimensions current implementations would still be computationally too expensive to be useful in real-life applications. In this paper we propose a simulation based approach for optimization over a polyhedron, inspired by the Cauchy deviates method. Thus we achieve a computationally efficient method to use polyhedral clouds also in very high dimensions.

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

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

4.7 Conjugate-gradients versus multigrid solvers for diffusion-based correlation models in data assimilation.

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This article provides a theoretical and experimental comparison between conjugate gradients and multigrid, two iterative schemes for solving linear systems, in the context of applying diffusion-based correlation models in data assimilation. In this context, a large number of such systems has to be (approximately) solved if the implicit mode is chosen for integrating the involved diffusion equation over pseudo-time, thereby making their efficient handling crucial for practical performance. It is shown that the multigrid approach has a significant advantage, especially for larger correlation lengths and/or large problem sizes.

4.8 Simple backward error bounds for linear least-squares problems.

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We consider two upper bounds on the normwise backward error (BE) for linear least-squares problems. The advantage of these bounds is their simplicity. Their behaviour in commonly-used iterative methods can be analyzed more easily than that of the BE itself, and the bounds can also be estimated very cheaply in such methods. It is known that each of these upper bounds can be orders of magnitude larger than the BE. Then one may ask : under which conditions is each of the bounds a good estimate of the BE ? We partially answer this question by giving sufficient conditions for each bound to be a good estimate of the BE. We illustrate these results with some numerical examples.

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

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

4.10 Derivative-free optimization for large-scale nonlinear data assimilation problems.

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The computation of derivatives and the development of tangent and adjoint codes represent a challenging issue and a major human time-consuming task when solving operational data assimilation problems. The ensemble Kalman filter provides a suitable derivative-free adaptation for the sequential approach by using an ensemble-based implementation of the Kalman filter equations. This article proposes a derivative-free variant for the variational approach, based on an iterative subspace minimization (ISM) technique. At each iteration, a subspace of low dimension is built from the relevant information contained in the empirical orthogonal functions (EOFs), allowing us to define a reduced 4D-Var subproblem which is then solved using a derivative-free optimization (DFO) algorithm. Strategies to improve the quality of the selected subspaces are presented, together with two numerical illustrations. The ISM technique is first compared with a basic stochastic ensemble Kalman filter on an academic shallow-water problem. The DFO algorithm embedded in the ISM technique is then validated in the NEMO framework, using its GYRE configuration.

4.11 Using approximate secant equations in limited memory methods for multilevel unconstrained optimization.

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The properties of multilevel optimization problems defined on a hierarchy of discretization grids can be used to define approximate secant equations, which describe the second-order behavior of the objective function. Following earlier work by Gratton and Toint (2009) we introduce a quasi-Newton method (with a linesearch) and a nonlinear conjugate gradient method that both take advantage of this new second-order information. We then present numerical experiments with these methods and formulate recommendations for their practical use.

4.12 Quasi-Newton updates with weighted secant equations.

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We provide a formula for variational quasi-Newton updates with multiple weighted secant equations. The derivation of the formula leads to a Sylvester equation in the correction matrix. Examples are given.

4.13 Observations thinning in data assimilation.

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We propose to use an observation-thinning method for the efficient numerical solution of large-scale incremental four- dimensional (4D-Var) data assimilation problems. This decomposition is based on exploiting an adaptive hierarchy of the observations. Starting with a low-cardinality set and the solution of its corresponding optimization problem, observations are successively added based on a posteriori error estimates. The particular structure of the sequence of associated linear systems allows the use of a variant of the conjugate gradient algorithm which effectively exploits the fact that the number of observations is smaller than the size of the vector state in the 4D-Var model. The new algorithm is tested on a one-dimensional-wave equation and on the Lorenz 96 system, the latter one being of special interest because of its similarity with numerical weather prediction systems.

4.14 Stochastic conditioning of matrix functions.

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We investigate the sensitivity of matrix functions to random noise in their input. We propose the notion of a stochastic condition number, which determines, to first order, the sensitivity of a matrix function to random noise. We derive an upper bound on the stochastic condition number that can be estimated efficiently by using "small-sample" estimation techniques. The bound can be used to estimate the median, or any other quantile, of the error in a function's output when its input is subjected to random noise. We give numerical experiments illustrating the effectiveness of our stochastic error estimate.

4.15 A surrogate management framework using rigorous trust-region steps.

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Surrogate models are frequently used in the optimization engineering community as convenient approaches to deal with functions for which evaluations are expensive or noisy, or lack convexity. These methodologies do not typically guarantee any type of convergence under reasonable assumptions. In this article, we will show how to incorporate the use of surrogate models, heuristics, or any other process of attempting a function value decrease in trust-region algorithms for unconstrained derivative-free optimization, in a way that global convergence of the latter algorithms to stationary points is retained. Our approach follows the lines of search/poll direct-search methods and corresponding surrogate management frameworks, both in algorithmic design and in the form of organizing the convergence theory.

4.16 A merit function approach for direct search

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In this paper it is proposed to equip direct-search methods with a general procedure to minimize an objective function, possibly nonsmooth, without using derivatives and subject to constraints on the variables. One aims at considering constraints, most likely nonlinear or nonsmooth, for which the derivatives of the corresponding functions are also unavailable. The novelty of this contribution relies mostly on how relaxable constraints are handled. Such constraints, which can be relaxed during the course of the optimization, are taken care of by a merit function and, if necessary, by a restoration procedure. Constraints that are unrelaxable, when present, are treated by an extreme barrier approach. One is able to show that the resulting merit function direct-search algorithm exhibits global convergence properties for first-order stationary constraints. As in the progressive barrier method (C. Audet and J. E. Dennis Jr., SIAM J. Optim., 20 (2009),

pp. 445–472), we provide a mechanism to indicate the transfer of constraints from the relaxable set to the unrelaxable one.

4.17 Sensitivity and conditioning of the truncated total least squares solution.

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We present an explicit expression for the condition number of the truncated total least squares (TLS) solution of $Ax \approx b$. This expression is obtained using the notion of the Fréchet derivative. We also give upper bounds on the condition number, which are simple to compute and interpret. These results generalize those in the literature for the untruncated TLS problem. Numerical experiments demonstrate that our bounds are often a very good estimate of the condition number, and provide a significant improvement to known bounds.

4.18 Differentiating the method of conjugate gradients.

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The method of conjugate gradients (CG) is widely used for the iterative solution of large sparse systems of equations $Ax = b$, where $A \in \mathbb{R}^{n\times n}$ is symmetric positive definite. Let x_k denote the kth iterate of CG. This is a nonlinear differentiable function of b. In this paper we obtain expressions for J_k, the Jacobian matrix of x_k with respect to b. We use these expressions to obtain bounds on $\|J_k\|_2$, the spectral norm condition number of x_k, and discuss algorithms to compute or estimate $J_k v$ and $J_k^T v$ for a given vector v.

4.19 B-preconditioned minimization algorithms for variational data assimilation with the dual formulation.

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Variational data assimilation problems in meteorology and oceanography require the solution of a regularized nonlinear least-squares problem. Practical solution algorithms are based on the incremental (truncated Gauss-Newton) approach, which involves the iterative solution of a sequence of linear least-squares (quadratic minimization) sub-problems. Each sub-problem can be solved using a primal approach, where the minimization is performed in a space spanned by vectors of the size of the model control vector,

or a dual approach, where the minimization is performed in a space spanned by vectors of the size of the observation vector. The dual formulation can be advantageous for two reasons. First, the dimension of the minimization problem with the dual formulation does not increase when additional control variables are considered, such as those accounting for model error in a weak-constraint formulation. Second, whenever the dimension of observation space is significantly smaller than that of the model control space, the dual formulation can reduce both memory usage and computational cost.
In this article, a new dual-based algorithm called Restricted B-preconditioned Lanczos (RBLanczos) is introduced, where B denotes the background-error covariance matrix. RBLanczos is the Lanczos formulation of the Restricted B-preconditioned Conjugate Gradient (RBCG) method. RBLanczos generates mathematically equivalent iterates to those of RBCG and the corresponding B-preconditioned Conjugate Gradient and Lanczos algorithms used in the primal approach. All these algorithms can be implemented without the need for a square-root factorization of B. RBCG and RBLanczos, as well as the corresponding primal algorithms, are implemented in two operational ocean data assimilation systems and numerical results are presented. Practical diagnostic formulae for monitoring the convergence properties of the minimization are also presented

4.20 The discretizable molecular distance geometry problem.

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Given a simple weighted undirected graph $G = (V, E, d)$ with $d : E \rightarrow \mathbb{R}^+$, the Molecular Distance Geometry Problem (MDGP) consists in finding an embedding $x : V \rightarrow \mathbb{R}^3$ such that $\|x_u - x_v\| = d_{uv} \quad \forall u, v \in V$. We show that under a few assumptions usually satisfied in proteins, the MDGP can be formulated as a search in a discrete space. We call this MDGP subclass the Discretizable MDGP (DMDGP). We show that the DMDGP is NP-hard and we propose a solution algorithm called Branch-and-Prune (BP). The BP algorithm performs remarkably well in practice in terms of speed and solution accuracy, and can be easily modified to find all incongruent solutions to a given DMDGP instance. We show computational results on several artificial and real-life instances.

4.21 Discretization orders for distance geometry problems.

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Given a weighted, undirected simple graph $G = (V, E, d)$ (where $d : E \rightarrow \mathbb{R}^+$), the distance geometry problem (DGP) is to determine an embedding $x : V \rightarrow \mathbb{R}^k$ such that $\forall i, j \in E \|x_i - x_j\| = d_{ij}$. Although, in general, the DGP is solved using continuous methods, under certain conditions the search is reduced to a discrete set of points. We give one such condition as a particular order on V. We formalize the decision problem of determining whether such an order exists for a given graph and show that this problem is NP-complete in general and polynomial for fixed dimension k. We present results of computational experiments on a set of protein backbones whose natural atomic order does not satisfy the order requirements and compare our approach with some available continuous space searches.

4.22 A non-stationary space-time Gaussian process model for partially converged simulations.

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In the context of expensive numerical experiments, a promising solution for alleviating the computational costs consists of using partially converged simulations instead of exact solutions. The gain in computational time is at the price of precision in the response. This work addresses the issue of fitting a Gaussian process model to partially converged simulation data for further use in prediction. The main challenge consists of the adequate approximation of the error due to partial convergence, which is correlated in both design variables and time directions. Here, we propose fitting a Gaussian process in the joint space of design parameters and computational time. The model is constructed by building a nonstationary covariance kernel that reflects accurately the actual structure of the error. Practical solutions are proposed for solving parameter estimation issues associated with the proposed model. The method is applied to a computational fluid dynamics test case and shows significant improvement in prediction compared to a classical kriging model.

4.23 Quantile-based optimization of noisy computer experiments with tunable precision.

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This article addresses the issue of kriging-based optimization of stochastic simulators. Many of these simulators depend on factors that tune the level of precision of the response, the gain in accuracy being at a price of computational time. The contribution of this work is two-fold : first, we propose a quantile-based criterion for the sequential design of experiments, in the fashion of the classical expected improvement criterion, which allows an elegant treatment of heterogeneous response precisions. Second, we present a procedure for the allocation of the computational time given to each measurement, allowing a better distribution of the computational effort and increased efficiency. Finally, the optimization method is applied to an original application in nuclear criticality safety. This article has supplementary material available online. The proposed criterion is available in the R package DiceOptim.

4.24 Constrained regional recovery of continental water mass time-variations from GRACE-based geopotential anomalies

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We propose a "constrained" least-squares approach to estimate regional maps of equivalent-water heights by inverting GRACE-based potential anomalies at satellite altitude. According to the energy integral method, the anomalies of difference of geopotential between the two GRACE vehicles are derived from along-track K-Band Range-Rate (KBRR) residuals that correspond mainly to the continental water storage changes, once a priori known accelerations (i.e. static field, polar movements, atmosphere and ocean masses including tides) are removed during the orbit adjustment process. Newton's first law merely enables the Difference of Potential Anomalies from accurate KBRR data and the equivalent-water heights to be recovered. Spatial constraints versus spherical distance between elementary surface tiles are introduced to stabilize the linear system to cancel the effects of the north-south striping. Unlike the "mascons" approach, no basis of orthogonal functions (e.g., spherical harmonics) is used, so that the proposed regional method does not suffer from drawbacks related to any spectrum truncation. Time series of 10-day regional maps over South America for 2006-2009 also prove to be consistent with independent data sets, namely the outputs of hydrological models, "mascons" and global GRACE solutions.

4.25 Sequential estimation of surface water mass changes from daily satellite gravimetry data.

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We propose a recursive Kalman filtering approach to map regional spatio-temporal variations of terrestrial water mass over large continental areas, such as South America. Instead of correcting hydrology model outputs by the GRACE observations using a Kalman filter estimation strategy, regional 2-by-2 degree water mass solutions are constructed by integration of daily potential differences deduced from GRACE

K-band range rate (KBRR) measurements. Recovery of regional water mass anomaly averages obtained by accumulation of information of daily noise-free simulated GRACE data shows that convergence is relatively fast and yields accurate solutions. In the case of cumulating real GRACE KBRR data contaminated by observational noise, the sequential method of step-by-step integration provides estimates of water mass variation for the period 2004-2011 by considering a set of suitable a priori error uncertainty parameters to stabilize the inversion. Spatial and temporal averages of the Kalman filter solutions over river basin surfaces are consistent with the ones computed using global monthly/10-day GRACE solutions from official providers CSR, GFZ and JPL. They are also highly correlated to in situ records of river discharges (70-95 %), especially for the Obidos station where the total outflow of the Amazon River is measured. The sparse daily coverage of the GRACE satellite tracks limits the time resolution of the regional Kalman filter solutions, and thus the detection of short-term hydrological events.

Propagation

5.1 Source point discovery through high frequency asymptotic time reversal.

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Given local frequency domain wave data, the Numerical Micro-Local Analysis (NMLA) method (Benamou et al., 2004) and its recent improved version (Benamou et al., 2011) gives a pointwise numerical approximation of the number of rays, their slowness vectors and corresponding wavefront curvatures. With time domain wave data and assuming the source wavelet is given, the method also estimates the travel-time. The paper provides a non technical presentation of the improved NMLA algorithm and presents a numerical application which can be interpreted as a high frequency asymptotic version of the classical time reversal method (Borcea et al., 2003). A detailed technical presentation of the algorithm is available in Benamou et al. (2011) and more numerical experiments can be found in Collino and Marmorat (2011).

5.2 Localized adaptive radiation condition for coupling boundary and finite element methods applied to wave propagation problems.

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The wave propagation problems addressed in this paper involve a relatively large and impenetrable surface on which a comparatively small penetrable heterogeneous material is positioned. Typically the numerical solution of such problems is by coupling boundary and finite element methods. However, a straightforward application of this technique gives rise to some difficulties that are mainly related to the solution of a large linear system whose matrix consists of sparse and dense blocks. To face such difficulties, the adaptive radiation condition technique is modified by localizing the truncation interface only around the heterogeneous material. Stability and error estimates are established for the underlying approximation scheme. Some alternative methods are recalled or designed making it possible to compare the numerical efficiency of the proposed approach.

5.3 Scattering of a scalar time-harmonic wave by n small spheres by the method of matched asymptotic expansions.

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In this paper, we construct an asymptotic expansion of a time-harmonic wave scattered by N small spheres. This construction is based on the method of matched asymptotic expansions. Error estimates give a theoretical background to the approach.

5.4 Scattering by a highly oscillating surface.

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The boundary function method (A. B. Vasiléva, V. F. Butuzov, and L. V. Kalachev, 1995) is used to build an asymptotic expansion at any order of accuracy of a scalar time-harmonic wave scattered by a perfectly reflecting doubly periodic surface with oscillations at small and large scales. Error bounds are rigorously established, in particular in an optimal way on the relevant part of the field. It is also shown how the maximum principle can be used to design a homogenized surface whose reflected wave yields a first-order approximation of the actual one. The theoretical derivations are illustrated by some numerical experiments, which in particular show that using the homogenized surface outperforms the usual approach consisting in setting an effective boundary condition on a flat boundary.

5.5 Extension to non-conforming meshes of the Current and charge Combined Integral Equation.

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We bring out some mathematical properties of the current and charge boundary integral equation when it is posed on a surface without geometrical singularities. This enables us to show that it is then possible to solve this equation by a boundary element method that requires no interelement continuity. In particular, this property allows the use of meshes on various parts of the surface obtained independently of each other. The extension to surfaces with geometrical singularities showed that acute dihedral angles can lead to inaccuracies in the results. We built a two-dimensional version of this equation which brought out that the wrong results are due to spurious oscillations concentrating around the singular points of the geometry. Noticing that the system linking the current and the charge is a saddle-point problem, we have tried augmenting the approximation of the charge to stabilize the numerical scheme. We show that this stabilization procedure, when coupled with a refinement of the mesh in the proximity of the geometrical singularities, obtained by a simple subdivision of the triangles, greatly reduces the effect of these instabilities.

5.6 Mathematical justification of the Rayleigh conductivity model for perforated plates in acoustics.

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This paper is devoted to the mathematical justification of the usual models predicting the effective reflection and transmission of an acoustic wave by a low porosity multiperforated plate. Some previous intuitive approximations require that the wavelength be large compared with the spacing separating two neighboring apertures. In particular, we show that this basic assumption is not mandatory. Actually, it is enough to assume that this distance is less than a half-wavelength. The main tools used are the method of matched asymptotic expansions and lattice sums for the Helmholtz equations. Some numerical experiments illustrate the theoretical derivations.

5.7 Numerical study of acoustic multiperforated plates.

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It is rather classical to model multiperforated plates by approximate impedance boundary conditions. In this article we would like to compare an instance of such boundary conditions obtained through a matched asymptotic expansions technique to direct numerical computations based on a boundary element formulation in the case of linear acoustic.

5.8 Matched asymptotic expansions of the eigenvalues of a 3-D boundary-value problem relative to two cavities linked by a hole of small size.

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In this article, we consider a domain consisting of two cavities linked by a hole of small size. We derive a numerical method to compute an approximation of the eigenvalues of an elliptic operator without refining in the neighborhood of the hole. Several convergence rates are obtained and illustrated by numerical simulations.

5.9 Time-harmonic acoustic scattering in a complex flow : a full coupling between acoustics and hydrodynamics.

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For the numerical simulation of time harmonic acoustic scattering in a complex geometry, in presence of an arbitrary mean flow, the main difficulty is the coexistence and the coupling of two very different phenomena : acoustic propagation and convection of vortices. We consider a linearized formulation coupling an augmented Galbrun equation (for the perturbation of displacement) with a time harmonic convection equation (for the vortices). We first establish the well-posedness of this time harmonic convection equation in the appropriate mathematical framework. Then the complete problem, with Perfectly Matched Layers at the artificial boundaries, is proved to be coercive and compact, and a hybrid numerical method for the solution is proposed, coupling finite elements for the Galbrun equation and a Discontinuous Galerkin scheme for the convection equation. Finally a 2D numerical result shows the efficiency of the method.

5.10 Transmission eigenvalues for inhomogeneous media containing obstacles.

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We consider the interior transmission problem corresponding to the inverse scattering by an inhomogeneous (possibly anisotropic) media in which an impenetrable obstacle with Dirichlet boundary conditions is

embedded. Our main focus is to understand the associated eigenvalue problem, more specifically to prove that the transmission eigenvalues form a discrete set and show that they exist. The presence of Dirichlet obstacle brings new difficulties to already complicated situation dealing with a non-selfadjoint eigenvalue problem. In this paper, we employ a variety of variational techniques under various assumptions on the index of refraction as well as the size of the Dirichlet obstacle.

5.11 Effective conditions for the reflection of an acoustic wave by low-porosity perforated plates.

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This paper describes an investigation of the acoustic properties of a rigid plate with a periodic pattern of holes, in a compressible, ideal, inviscid fluid in the absence of mean flow. Leppington and Levine (J. Fluid Mech., vol. 61, 1973, pp. 109-127) obtained an approximation of the reflection and transmission coefficients of a plane wave incident on an infinitely thin plate with a rectangular array of perforations, assuming that a characteristic size of the perforations is negligible relative to that of the unit cell of the grating, itself assumed to be negligible relative to the wavelength. One part of the present study is of methodological interest. It establishes that it is possible to extend their approach to thick plates with a skew grating of perforations, thus confirming recent results of Bendali et al. (SIAM J. Appl. Math., vol. 73 (1), 2013, pp. 438-459), but in a much simpler way without using complex matched asymptotic expansions of the full wave or to a grating of multipoles. As is well-known, effective compliances for the plate can then be derived from the corresponding approximations of the reflection and transmission coefficients. These compliances are expressed in terms of the Rayleigh conductivity of an isolated perforation. Consequently, in one other part of the present study, the methodology recently introduced by Laurens et al. (ESAIM, Math. Model. Numer. Anal., vol. 47 (6), 2013, pp. 1691-1712) to obtain sharp bounds for the Rayleigh conductivity has been extended to include the case for which the openings of the perforations on the upper and lower sides of the plate are elliptical in shape. This not only enables the determination of these bounds and of the associated reflection and transmission coefficients for actual plates with tilted perforations but also yields single expressions covering all usual cases of perforations : straight or tilted with a circular or an elliptical cross-section.

5.12 Explicit computation of the electrostatic energy for an elliptical charged disc.

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This letter describes a method for obtaining an explicit expression for the electrostatic energy of a charged elliptical infinitely thin disc. The charge distribution is assumed to be polynomial. Such explicit values for this energy are fundamental for assessing the accuracy of boundary element codes. The main tools used are an extension of Copson's method and a diagonalization, given by Leppington and Levine, of the single-layer potential operator associated with the electrostatic potential created by a distribution of charges on the elliptical disc.

5.13 Lower and upper bounds for the Rayleigh conductivity of a perforated plate.

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Lower and upper bounds for the Rayleigh conductivity of a perforation in a thick plate are usually derived from intuitive approximations and by physical reasoning. This paper addresses a mathematical justification of these approaches. As a byproduct of the rigorous handling of these issues, some improvements to previous bounds for axisymmetric holes are given as well as new estimates for tilted perforations. The main techniques are a proper use of the Dirichlet and Kelvin variational principlesin the context of Beppo-Levi spaces. The derivations are validated by numerical experiments in 2D for the axisymmetric case as well as for the full three-dimensional problem.

Qualitative Computing

Even the most striking principles can fade when they become habits. Behind obviousness, lies an intact and powerful information potential. Computation relies on algebraic laws and structures which depend on the context of any given problem. This algebraic framework is often taken for granted as an implicit basis for further calculations, that will depend on this initial step. There is no ultimate or best tool, no magic wand for Computation. Among the large variety of algebraic possibilities, the aim is to realise a comparative survey of standard methods and to determine the potential of alternative solutions to the classical matrix approach. This review revisits the most basic properties of multiplication within algebras over real numbers. It forms the core of our understanding of nonlinearity.

However in nature, phenomena are most always analysed as a coupling of two or more simpler phenomena : coupling is an ubiquitous way to express non linear diversity. These more analytic aspects are approached by spectral coupling of hermitian matrices and by the concept of composition of continuous functions. A concept which represents a multiplication which is itself a nonlinear map, rather than being linear by distributivity with respect to addition, as this is classically assumed for any algebra.

The reader is referred to the reports “Beyond and behind linear algebra”, TR /PA/14/80 and “Project description : Algebraic structures for information processing associated with Dickson algebras” TR/PA/13/106, which detail the activity of QC during the past three years.

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2

CERFACS-Inria joint laboratory

CERFACS-Inria joint laboratory

The objectives of the joint lab on High Performance Computing between CERFACS and Inria are to go beyond what each partner can go alone ; in particular, jointly study, design and implement parallel scalable algorithms and numerical schemes for large scale simulations. We give below a short overview of the various actions undertaken during the 2011-2014 period.

Among the challenges to face for extreme computing comes first code coupling to address multi-physics simulations. In collaboration with the CERFACS Open-PALM team and in the context of the PhD thesis of C. Vuchener [10] (Inria, funded by the French ministry of research) and M. Predari (Inria, funded by the Conseil Régional Aquitaine), new partitioning strategies have been investigated and implemented to not only balance the work of the individual codes but also the complete coupled simulation. Cases study were provided by CERFACS for the coupling of the AVBP and the AVTP codes. A side effect of this collaboration has been the work of G. Wang (post-doc CERFACS) who implemented an implicit solver in AVTP thanks to the support of HiePACS on parallel sparse linear systems solutions.

Fruitful joint research activities have developed in the framework of the FP7 Marie-Curie ITN MYPLANET where CERFACS was PI and Inria one of the partners. In that framework, the CFD team and Inria HiePACS project have co-advised the PhD thesis of P. Salas (Inria, funded by MYPLANET) who studied, designed and implemented strategies to recycle spectral information between successive eigensolutions involved in the nonlinear eigenvalue problem arising from the thermo-acoustic instability study [2, 3]. The prototype of the new numerical schemes have been implemented in the AVSP simulation code. Thanks to a better coupling of the eigensolvers and the new recycling strategies a speed-up close to one hundred was observed between the beginning and the end of the PhD work. Furthermore much larger problems can nowadays be solved [9, 8]. P. Salas has also collaborated with M. Zounon (Inria, funded by ANR RESCUE) to address the emerging critical question at extreme scale related to the resilience [1]. Within this collaboration, robust numerical techniques have been designed and validated on a small test example from AVSP. In addition to this work on the parallel eigensolvers for thermo-acoustic instability studies, M. Falese [5] (CERFACS, funded by MYPLANET) visited Inria Bordeaux for a few months to work on mesh adaptation with the BACCHUS project. His aims was to apply the metric adaptation concept to unsteady LES simulations. Indeed, Large Eddies Simulation has it's own rules and it is challenging to see how to use mesh adaptation in this contest. M. Falese tested several criterion to drive the mesh modification and developed an interface between the AVBP simulation code and the remesher MMG3D. Thanks to the mesh adaptivity techniques, some combustion phenonema were well captured by the parallel simulations while using much smaller meshes. We refer to section 2.2.2 of Computation Fluid Dynamics chapter.

Inria HiePACS and Algo-EMA jointly co-advised the PhD thesis of Y. Dudouit [4] (CERFACS, funded by a Total contract managed by CERFACS for the joint lab) who worked on space and time refinements for elastodynamic simulations. This thesis benefited from the CERFACS experience in Discontinuous Galerkin methods for wave propagation phenonema and Inria expertise in parallel computing. The parallel mixed MPI-Thread prototype code successfully implemented local time stepping for mesh refinement on Cartesian grids with PLM.

Inria HiePACS and PAE jointly co-advised the PhD thesis of A. Praga [7, 6] (funded by CERFACS) who worked on a parallel conservative advection model on the sphere, which is intended to form the basic framework for a future global three-dimensional chemistry transport model. Thanks to one hand to the use of a fully analycally defined grid that preserves approximatively cell area at mid and high latitudes and on a second hand to a finite volume discretization technique, a parallel scalable solver with very low memory footprint has been implemented. We refer to section 3.2 of Aviation & Environment chapter.

Algo-CERFACS was involved in the first training session organized in Bordeaux on parallel linear algebra in the framework of the PATC programme. Related to training, a few internships from ENSEIRB were hosted at CERFACS in the CSG group working mainly on watching technology activities on emerging computing platforms. Those students followed an ENSEIRB specialty where many Inria researchers are given lectures on various HPC topics related to computational sciences.

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3

Data Assimilation

Introduction

The Data Assimilation activity at Cerfacs concerns the theoretical and practical development of data assimilation algorithms in the fields of oceanography, atmospheric chemistry, hydraulics/hydrology and wildland fire propagation. The common methodological issues regarding optimization, covariance modeling, and ensemble data assimilation are at the core of the activity. This activty has resulted in promoting data assimilation to new fields in geosciences.
This work is carried out in close collaboration with CERFACS's shareholders (Météo-France, EDF, CNES) as well as with operational centres (ECMWF, Met Office, SCHAPI) and academic institutes (Université Pierre et Marie Curie, INRIA).

Atmospheric Chemistry

2.1 Free-troposphere ozone re-analyses with satellite data

Accurate and temporally resolved fields of free-troposphere ozone are of major importance to quantify the intercontinental transport of pollution and the ozone radiative forcing. Since the vertical transport of ozone at the tropopause can be significant, a precise characterization of both low-stratosphere and upper-troposphere is required to determine free-troposphere ozone. We used a global chemical transport model (Modèle de Chimie Atmosphérique à Grande Echelle, MOCAGE) in combination with a linear ozone chemistry scheme to examine the impact of assimilating observations from the Microwave Limb Sounder (MLS) and the Infrared Atmospheric Sounding Interferometer (IASI).
The MLS instrument has been flying onboard the Aura satellite in a sun-synchronous polar orbit since August 2004. It measures millimeter and sub-millimeter thermal emission at the atmospheric limb, providing vertical profiles of several atmospheric parameters with high precision. It allows the retrieval of about 3500 stratospheric profiles per day with a nearly global latitude coverage between 82 S and 82 N. IASI thermal infrared interferometer was launched in 2006 onboard the Metop-A platform. It is a meteorological sensor dedicated to the measurement of tropospheric temperature, water vapor and of the tropospheric content of a number of trace gases. Thanks to its large swath of 2200 km, IASI enables an over-pass over each location on Earth's surface twice daily. The assimilation of the two instruments was performed by means of a variational algorithm (4D-Var) and allowed to constrain stratospheric and tropospheric ozone simultaneously.
The analysis was first computed for the months of August and November 2008 and validated against ozonesonde measurements to verify the presence of observations and model biases. Furthermore, a longer analysis of 6 months (July-December 2008) showed (Fig. 2.1) that the combined assimilation of MLS and IASI is able to globally reduce the uncertainty (root mean square error, RMSE) of the modeled ozone columns from 30 to 15% in the upper troposphere/lower stratosphere (UTLS, 70-225 hPa). The assimilation of IASI tropospheric ozone observations (1000-225 hPa columns) decreased the RMSE of the model from 40 to 20% in the tropics (30S-30N), whereas was not effective at higher latitudes. Results were confirmed by a comparison with additional ozone data sets like the Measurements of OZone and wAter vapour by aIrbus in-service airCraft (MOZAIC) data, the Ozone Monitoring Instrument (OMI) total ozone columns and several high-altitude surface measurements.
Finally, the analysis has little sensitivity to the assimilation parameters. We concluded that the combination of a simplified ozone chemistry scheme with frequent satellite observations is a valuable tool for the long- term analysis of stratospheric and free-tropospheric ozone. This study provides a basis for further computation of global ozone re-analyses for the last decade.

2.2 Assimilation of surface data for air quality

The VALENTINA-MOCAGE system allows for the assimilation of both satellite measurements and surface observations (ground-based stations from Airbase) in the European GEMS domain (with a 0.2 x 0.2 degrees resolution) and can be easily extended to other domains and resolutions.
Based on this assimilation system, the AE team has developed the Météo-France operational surface ozone near real time analysis. Since the summer 2010, the system produces daily surface ozone analysis of the

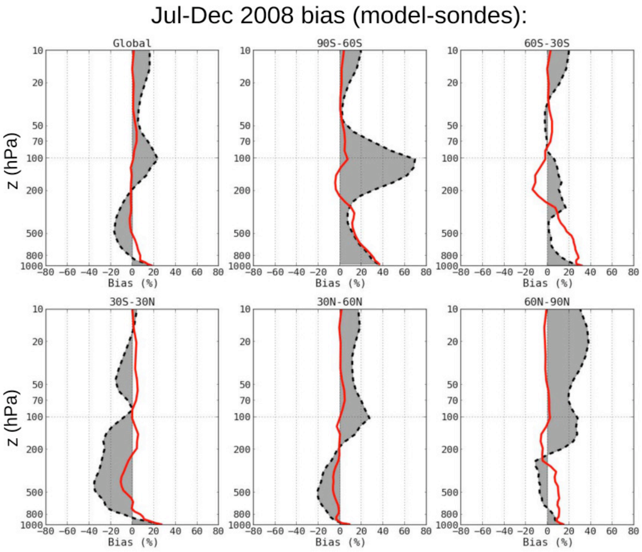

FIG. 2.1: Global and zonal (90S-60S, 60S-30S, 30S-30N, 30N-60N, 60N-90N) validation of MLS+IASI analysis versus ozonesonde profiles (July-December 2008). Bias (model minus sondes) normalized with the climatology (control run in black, analysis in red).

previous day according to the ground based stations. The evaluation of this analysis with independent data shows very good performances. A daily surface NO2 analysis of the previous day will be produced in the near future.

Since 2010, we also have participated with Météo-France to the ozone and NO2 reanalyses of several past years in the context of the MACC and MACC-II projects. The performance of VALENTINA-MOCAGE is good compared to the performance of the other models that participate to the project. The NO2 and O3 ground based stations have been assimilated separately with VALENTINA in the European GEMS domain in the context of the MACC and MACC-II projects. Two opposite seasons are studied, a summer period (July 2010) and a winter period (January 2012). Results show a very good performance in the ozone analysis (Fig. 2.2. The quality of the NO2 analysis depends on the typical regions (urban, rural, ...). The validation with independent stations shows that it is difficult to reduce the NO2 analysis bias, specially for urban sites. A work is done to characterize the appropriate observations/representativity error to apply for each sites and species.

The VALENTINA system still needs some improvements. In particular, we continue to focus our work on the background error covariance matrix (BECM). Results show that having flow-dependant BECM from an ensemble of assimilations can improve the analysis and the forecast. We have studied the impact of flow-dependant BECM (Jaumouillé et al., 2012) of a summer and a winter periods of 2010.

We developed a parameterization for the BECM that would be cheaper than running an ensemble of assimilations. Preliminary results have been obtained during the last summer period, they concern the transport of the background error covariances with the flow. In particular, we have shown possible to describe the transport of the length-scale tensor, leading to anisotropic correlation functions. We use filtering techniques to extract the main characteristics (variances, length-scales). As a consequence, we have been able to explore the question of isotropization of correlation, a technique that corresponds to a change of

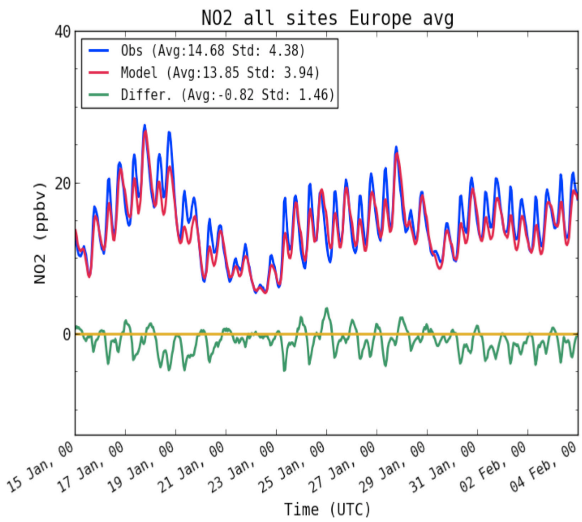

FIG. 2.2: Time series of the average concentration over Europe of the surface ozone for the period 4 to 22 July 2010 (top) and of the average concentrations of the surface NO2 for the period 15 January to 4 February 2012 (bottom). Blue line : surface observations, Red line : VALENTINA analysis, Green line : difference between analysis and observations.

coordinate so that the resulting correlations are nearly locally isotropic. This aspect is of particular interest since this offers an opportunity to improve the modelisation of the BECM and its numerical cost.

2.3 References

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Hydraulics/hydrology

Water resource and natural hazards management is a crucial societal and financial stake that requires a solid capacity of anticipating systems changes. This capacity relies on the understanding and the prediction of hydrodynamic flows. The anticipation need is also exacerbated by the impact of climate change. In spite of the significant advances in numerical modelling, hydrodynamics are described with a non-negligible uncertainty range that is linked to the approximate description of hydraulic parameters, meteorological, hydrological and geographical data. These uncertainties translate inevitably into errors in the hydraulic variables that are of interest for the model users and thus limit the predictive capacity of hydraulic models. While observing means are also improving, especially the space assets, observation of rivers can only provide an incomplete and uncertain description of the hydrodynamics in the present. DA offers a convenient framework for quantifying and reducing uncertainties in hydraulics models, making the most of various available observations. The benefits of DA have been greatly demonstrated in meteorology. Still its use remains limited in hydraulics, especially in the framework of operational applications for which community modelling software are used.

Scientific studies in the fields of hydraulics at Cerfacs consist of applying DA methods and analyzing their benefits in an operational framework for applicative cases. This work strongly relies on the collaboration with hydraulic modelling or observation experts as the expertise at Cerfacs is mostly in DA techniques. As of today, these projects rely mostly on the collaboration between Cerfacs and 3 of Cerfacs's shareholders : the Laboratoire National d'Hydraulique et Environnement (LNHE) at EDF R&D, Cnes and Météo-France. Other collaborations exist with governmental, academic or private institutes such as Schapi, Cerema, Irstea, HSM, Legos and Nasa. It also strongly relates to and benefits from the DA axis at Cerfacs for oceanography and atmospheric chemistry. It benefits from Cerfacs's expertise in the use of coupling software, such as OpenPALM, to build an integrated platform where the hydraulic models are coupled with the DA algorithms. It should finally be noted that this axis strongly relates to the uncertainty quantification part of the HPC theme and the MODEST Cerfacs challenge (see Cerfacs SRP).

The main achievements for the "Modelling and data assimilation for lake and river hydraulics" project at Cerfacs over the last 4 years are described in the followings.

3.1 Improved flood forecasting and water resources management capacity using DA with the 1D hydraulic model MASCARET

The illustration of this work is presented with the development of the DAMP (Data Assimilation with Mascaret) prototype that assimilates in-situ data. This prototype issued for real-time flood forecasting at SCHAPI, is also being improved with 3 on going PhDs (J. Habert, S. Barthélémy and N. El Mocayd) and this method has been implemented at EDF for water resources applications. This work was presented in Habert et al. (2014, OT), Ricci et al. (2011, RA).

3.2 Investigating and developing the use of variational DA techniques to improve the modelling of the 2D and 3D hydrodynamics for rivers and lakes with the TELEMAC software developed at EDF

As of today, the illustration of this work is presented in Ricci et al. (2014, OT) for the 3D modelling of the hydrodynamics of the Berre lagoon where the protection of the ecosystem and the operation of a hydroelectricity power plant are at stake and strongly relate to the representation of the salinity stratification. A 3D-Var FGAT DA algorithm is used to sequentially correct the initial salinity state assimilating in-situ salinity observations. The minimization is performed in a space spanned by vectors of the size of the observation vector to reduce memory usage and computational cost. The background error covariance matrix for salinity is modelled using a diffusion operator. It was shown that the sequential correction of the salinity state improves the representation of the strongly stratified salinity field over the assimilation window as well as in the short-term forecast.

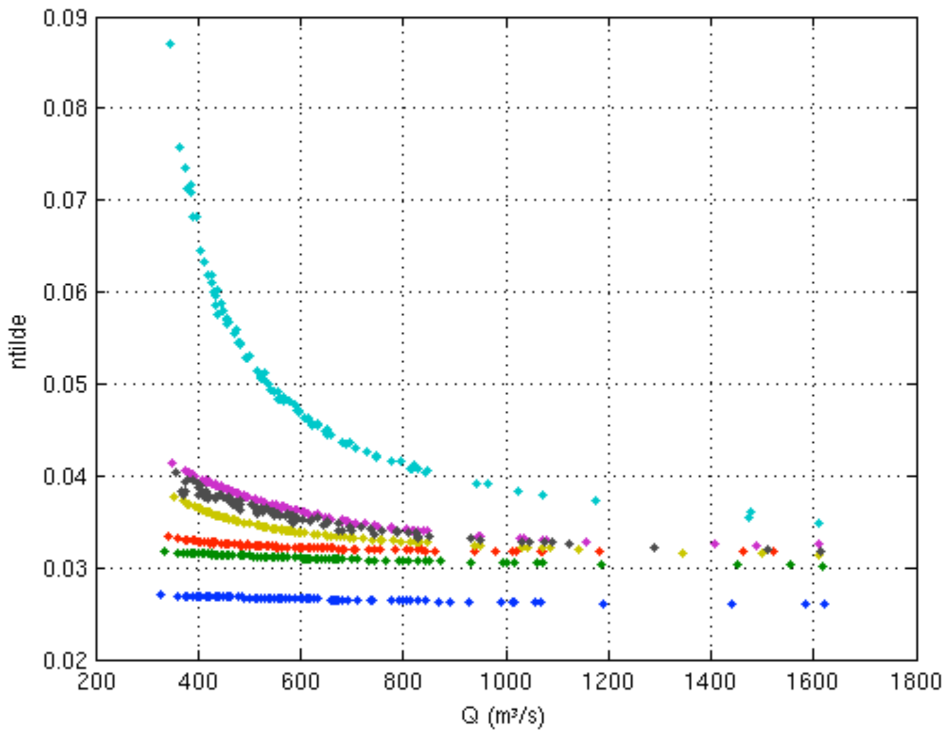

FIG. 3.1: Corrected friction coefficient for a uniform geometry equivalent to a 7 km reach-averaged section (one color per reach) of the Garonne River accounting for the variability of the wetted area and the slope over the reach. (L. Berthon 2013, TOSCA funding).

3.3 Investigating the use of remote sensing data for hydraulic and hydrology modelling

This axis aims at demonstrating the benefits of up-coming remote sensing missions such as the SWOT mission (CNES, NASA) that will allow for unprecedented high resolution and global coverage observation of continental waters. Small, medium and large scales are investigated as this question is raised in the framework of hydraulics modeling, medium and large scale hydrology modeling in hydrology, in collaboration with the appropriate experts for these different studies (see Figure 3.1). N. El Mocayd PhD co-funded by CNES and EDF started in 2013 on this subject, especially on the benefits of the use of SWOT like data for the correction of hydraulic parameters (friction, bathymetry) (Andreadis et al., 2014, OT). The Cerfacs is also involved in regional to large scale modelling studies in hydrology that relates to the use of SWOT data : V. Halfinger's PhD at CNRM (co-funded by Météo-France and CNES) on the use of SWOT data for regional hydrology modelling on the Garonne catchment area and C. Emery's PhD at LEGOS (co-funded by CNES and Météo-France) on the use of SWOT data for the modelling of the Niger river. It should be noted that a Workshop dedicated to the assimilation of SWOT data in hydrology and hydraulic was organized at Cerfacs in 2013 in collaboration with CNES, LEGOS and JPL (NASA).

Oceanography

A summary of the main achievements in ocean DA during the last period is given below. The work has been conducted within the framework of several projects : COMBINE (FP7) - an integrated project contributing to the development of climate prediction systems ; ADTAO (RTRA STAE) - a project aimed at developing mathematical methods for variational assimilation ; and VODA (ANR) and LEFE - projects focused specifically on the development of NEMOVAR. This work has contributed to international research programmes CLIVAR (GSOP) and GODAE-OceanView (GOV).

4.1 Development and operational implementation of NEMOVAR

NEMOVAR is a variational DA system for the community ocean model NEMO. NEMOVAR originates from the OPAVAR system developed at Cerfacs. It has been in development since 2006, initially as a collaborative project between CERFACS and ECMWF, and later extended to include the Met Office and INRIA/LJK (Mogensen et al., 2009, OT). This partnership is formalized through a Memorandum of Understanding. During the last period, NEMOVAR became operational at both ECMWF (Balmaseda et al., 2013, RA ; Mogensen et al., 2012, TR) and Met Office (Waters et al., 2014, RA). Cerfacs has played a major role in the scientific design, technical development and performance evaluation of NEMOVAR. NEMOVAR has been developed for both climate and ocean-forecasting applications (Balmaseda et al., 2013, RA ; Cummings et al., 2009, RA ; Waters et al., 2014, RA).
Key algorithmic features of NEMOVAR (covariance models, minimization algorithms) that have been developed by Cerfacs have been incorporated into variational DA systems for other widely used models : ROMS (Moore et al., 2011, RA ; Moore et al., 2013, OT), which is a US-based community model specializing in coastal ocean forecasting, and the hydrological model TELEMAC (Ricci et al., 2014, TR ; see previous section).

4.2 Application of NEMOVAR to global ocean reanalysis

Cerfacs has contributed to the production and evaluation of global ocean reanalyses in collaboration with ECMWF (Balmaseda et al., 2010, RA ; Balmaseda et al., 2013, RA). These analyses have been used for climate studies, initializing coupled models for seasonal and decadal forecasts (e.g., by various groups in COMBINE), and inter-comparison projects sponsored by GSOP and GOV (Corre et al., 2012, RA ; Heimback et al., 2009, OT ; Lee et al., 2009, OT ; Lee et al., 2010, RA, Stammer et al., 2009, OT).

4.3 Advances in theoretical and algorithmic aspects of DA

Mirouze and Weaver (2010, RA) describe a method for modelling correlation functions based on an implicitly formulated diffusion equation. They characterize the class of correlation functions implied by implicit diffusion, and analyze various aspects of the method including the specification of boundary conditions (especially important in oceanography where land geometry is complex), normalization procedures to obtain the correct (unit) amplitude of the correlation function, and numerical implementation. A parallel version of the method was developed for modelling background error correlations in NEMOVAR

as part of the PhD work of Mirouze (2010, RA). Examples of the spatial correlation structures generated by the method at selected points in a global configuration of NEMO are illustrated in Figure 3, left panel. The correlation length scales used for the left panel are geographically and directionally dependent, and have been estimated using an ensemble method ; the zonal length scales are illustrated in the right panel.
Weaver and Mirouze (2013, RA) present a unifying theoretical framework for characterizing correlation functions generated by explicit and implicit diffusion schemes in n-dimensional Euclidean space and on the sphere. The paper also describes and illustrates a method for accounting for inhomogeneous and anisotropic correlations estimated from an ensemble of perturbations. The implicit diffusion method has also been applied to the problem of modelling error correlations and inverse error correlations of gridded data products (mean dynamic topography, SST) commonly used in ocean DA (Weaver and Piacentini, 2012, OT).
Gürol et al. (2014, RA) present an observation-space (dual) minimization algorithm (RPCG) that was applied in two operational ocean DA systems (NEMOVAR and ROMS). They illustrated the significant benefits of the algorithm, compared to conventional model-space (primal) algorithms, in terms of reducing computational cost and memory. This work was done in collaboration with researchers from the ROMS community and CERFACS ALGO team.

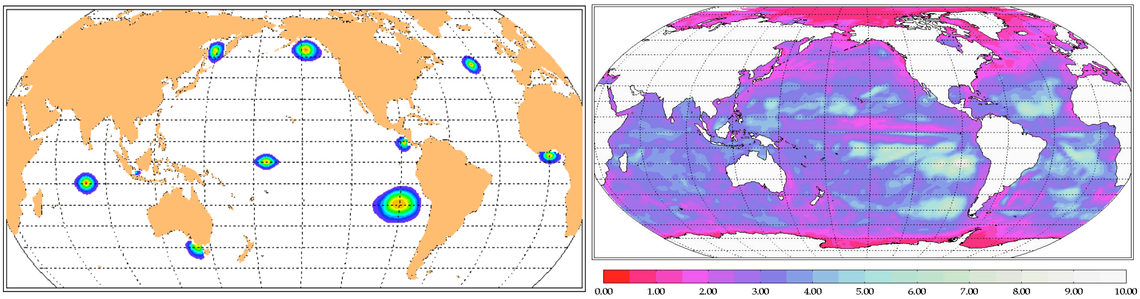

FIG. 4.1: Left panel : univariate correlation functions at selected points, generated using an implicitly formulated diffusion operator. The correlation length scales are spatially and directionally dependent and have been estimated using an ensemble method. Right panel : the zonal correlation length scales used in the left panel. (From Mirouze 2010).

4.4 Ensemble-variational DA : preparing the next-generation version of NEMOVAR

Forecast ensembles provide uncertainty information that can be used for defining flow-dependent background error covariances in DA. Daget et al. (2009, RA) explored the use an ensemble method for defining flow-dependent variances in a global version of the OPAVAR system. Operational versions of NEMOVAR at ECMWF and Met Office currently do not have the capacity to use ensembles for defining the background error covariance matrix ($\mathbf{B}$) (as in Daget et al., 2009, RA). ECMWF does produce an ensemble of ocean analyses (ORAS4) with NEMOVAR but these are currently decoupled from $\mathbf{B}$. Weaver et al. (2014, CO) applied observation-space assimilation diagnostics to evaluate the spread in ORAS4. These diagnostics can be used to guide the specification of an inflation factor in future ensemble-formulated versions of $\mathbf{B}$. Recent developments at Cerfacs have laid the groundwork to introduce ensembles in NEMOVAR through hybrid formulations of $\mathbf{B}$. A major redesign of the $\mathbf{B}$ code was required to allow for this capability.

Wildfire Modelling

Real-time prediction of the direction and speed of a propagating wildfire has direct applications in fire risk management and fire emergency response. The future perspective of climate change tends to favour extreme drought events and to alter precipitations ; these conditions dramatically increase the risk for the development of large highly destructive wildfires. In this context, accurate predictions of the resulting change in fire regime and intensity cannot only rely on the analysis of past observed wildfire events ; the use of a data-driven wildfire spread simulator that takes full advantage of the recent technological advances for geo-referenced front-tracking becomes essential. The dynamics of wildfires feature complex multi-physics processes (interactions between pyrolysis, combustion and flow dynamics, radiation and convection heat transfer, as well as atmospheric dynamics and chemistry) occurring at multiple scales (vegetation, topographical and meteorological micro/meso-scales). Relevant insight into wildfire dynamics has been obtained in recent years via detailed numerical simulations performed at flame scales but because of the high computational cost, flame-scale CFD is currently restricted to research projects and is not compatible with operational applications. In contrast, a regional-scale viewpoint is adopted in current operational wildfire spread simulators and the fire is described as a two-dimensional front that self-propagates normal to itself into unburned vegetation ; the local propagation speed is called the rate of spread (ROS). Still, this approach is limited in scope because of the large uncertainties associated with the ROS model that should be reduced combining fire sensor observations (airborne or spatial remote sensing provides new ways to monitor real-time fire front) into the propagation model via Data Assimilation (DA) algorithms.

A data driven prototype simulator was developed at SUC : the Firefly model is constrained by the assimilation of airborne observations of the fire front position with a Kalman Filter DA algorithm as illustrated in Figure 4. This work was achieved in the framework of M. Rochoux's PhD funded by the ANR-IDEA project in close collaboration between SUC and CFD team at CERFACS as well as with University of Maryland, SPE at University of Corte and EM2C at Ecole Centrale de Paris. The data assimilation algorithm features either a parameter estimation approach (in which the control variables are the ROS input parameters such as e.g., wind conditions, vegetation properties), or a state estimation approach (in which the control variables are the two-dimensional coordinates of the discretized fire front). These two approaches are implemented based on the OpenPALM dynamic coupler combined with the Parasol functionality for generating ensembles of Firefly fire front trajectories. The prototype data-driven simulator was evaluated in a series of synthetic cases, including configurations with spatially varying vegetation properties and temporally varying wind conditions, and in a validation test corresponding to a controlled grassland burning experiment. In all test cases, data-driven simulations were successful at significantly decreasing the distance between observed and simulated fire fronts and at providing an optimized forecast of the wildfire behaviour. While used as a preliminary approach to wildfire spread forecast in Rochoux et al. (2013, RA, a) and Rochoux et al. (2013, RA, b), the choice of the extended Kalman filter (EKF) algorithm was considered questionable because it assumes a linear relationship between control space and observation space ; this linear assumption is believed to be of limited value in general wildfire problems in which the wind conditions may vary and the vegetation properties are potentially strongly heterogenous. The modification to an EnKF approach was explored in Rochoux et al. (2012, OT, a) in which some of the observation model non-linearities were accounted for. Despite its linear combination of ensemble members as well as of its Gaussian assumption on the modelling and observation error statistics, the optimality of the EnKF was demonstrated based on comparative studies to particle filters that are more general Bayesian filters and that still produced equivalent results to the EnKF (daSilva et al., 2014, RA). A reduced-cost EnKF strategy based on polynomial chaos (PC-EnKF) was designed (paper submitted to NHESS, Rochoux et al. 2014, Part I), the polynomial-based surrogate model being used in place of the forward model Firefly during the EnKF prediction step to generate a large number of model simulation members at no cost and without loss of accuracy. In order to allow for a spatially varying correction of the front position, a spatially distributed correction along the fireline was implemented with a state estimation approach. For a proper representation of the error statistics, the generation of the forecast estimates must represent the anisotropy in fire propagation that results from spatial variations in vegetation properties and from temporally-fluctuating wind conditions (paper submitted to NHESS, Rochoux et al. 2014, Part II). The resulting data-driven simulator can in turn be used to provide a near-future forecast of the wildfire location. Results indicate that the forecast performance of a parameter estimation or state estimation approach may be limited to near-term predictions (i.e., at short lead-times). The forecast performance highly depends on the consistency between the assimilation frequency and the spatial/temporal variability of all the errors that are corrected in the data assimilation procedure (either the ROS model parameters or the locations of the fire front markers). In particular, the variability of these errors is determined by the persistence of the initial condition of the wildfire-spread model (i.e., the time period over which memory effects induced by the dependence on the initial condition affect the simulation) as well as by the temporal and spatial variability of the environmental conditions (e.g., wind conditions, vegetation properties).

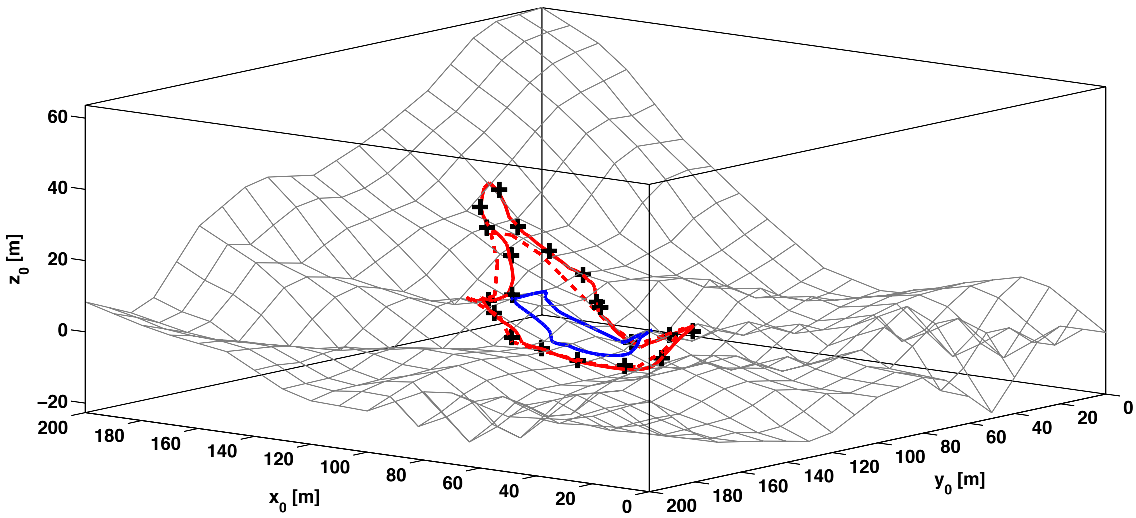

FIG. 5.1: Assimilation of fire front positions (black crosses) for correction of wildfire propagation model parameter and state over a complex topography terrain (Rochoux 2014, VII International Conference on Forest Fire Research)

Publications

6.1 Journal Publications

[DA1] M. A. Balmaseda, K. Mogensen, and A. T. Weaver, (2013), Evaluation of the ECMWF ocean reanalysis system ORAS4, *Quarterly Journal of the Royal Meteorological Society*, **139**, 1132–1161.

[DA2] M. Coustau, S. Ricci, V. Borrell-Estupina, C. Bouvier, and O. Thual, (2013), Benefits and limitations of data assimilation for discharge forecasting using an event-based rainfall runoff model, *Natural Hazards and Earth System Science*, **13**, 583–596.

[DA3] W. da Silva, M. Rochoux, H. Orlande, M. Colaço, O. Fudym, M. El Hafi, B. Cuenot, and S. Ricci, (2014), Application of particle filters to regional-scale wildfire spread, *High Temperatures–High Pressures*, **43**.

[DA4] E. Emili, B. Barret, S. Massart, E. Le Flochmoen, A. Piacentini, L. El Amraoui, O. Pannekoucke, and D. Cariolle, (2014), Combined assimilation of IASI and MLS observations to constrain tropospheric and stratospheric ozone in a global chemical transport model, *Atmospheric Chemistry and Physics*, **14**, 177–198.

[DA5] S. Gürol, A. T. Weaver, A. M. Moore, A. Piacentini, H. G. Arango, and S. Gratton, (2014), B-preconditioned minimization algorithms for variational data assimilation with the dual formulation, *Quarterly Journal of the Royal Meteorological Society*, **140**, 539–556.

[DA6] E. Harader, V. Borrell Estupina, S. Ricci, M. Coustau, O. Thual, A. Piacentini, and C. Bouvier, (2012), Correcting the radar rainfall forcing of a hydrological model with data assimilation : application to flood forecasting in the Lez Catchment in Southern France, *Hydrology and Earth System Sciences Discussions*, **9**, 3527–3579.

[DA7] E. Jaumouillé, S. Massart, A. Piacentini, D. Cariolle, and V.-H. Peuch, (2012), Impact of a time-dependent background error covariance matrix on air quality analysis, *Geoscientific Model Development*, **5**, 1075–1090.

[DA8] M. Martin, M. Balmaseda, L. Bertino, P. Brasseur, G. Brassington, J. Cummings, Y. Fujii, D. Lea, J. Lellouche, K. Mogensen, P. Oke, G. C. Smith, C. E. Testut, G. A. Waagbo, J. Waters, and A. T. Weaver, (2014), Status and future of data assimilation in operational oceanography, *Journal of Operational Oceanography*, **in press**.

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[DA10] O. Pannekoucke, E. Emili, and O. Thual, (2014), Modelling of local length-scale dynamics and isotropizing deformations, *Quarterly Journal of the Royal Meteorological Society*, **140**, 1387–1398.

[DA11] V. Pedinotti, A. Boone, S. Ricci, S. Biancamaria, and N. Mognard, (2014), Assimilation of satellite data to optimize large-scale hydrological model parameters : a case study for the SWOT mission, *Hydrology and Earth System Sciences*, **18**, 4485–4507.

[DA12] M. C. Rochoux, B. Cuenot, S. Ricci, A. Trouvé, B. Delmotte, S. Massart, R. Paoli, and R. Paugam, (2013), Data assimilation applied to combustion, *Comptes Rendus Mécanique*, **341**, 266 – 276. Combustion, spray and flow dynamics for aerospace propulsion Combustion, spray and flow dynamics for aerospace propulsion.

[DA13] M. Rochoux, B. Delmotte, B. Cuenot, S. Ricci, and A. Trouvé, (2013), Regional-scale simulations of wildland fire spread informed by real-time flame front observations, *Proceedings of the Combustion Institute*, **34**, 2641 – 2647.

[DA14] M. C. Rochoux, C. Emery, S. Ricci, B. Cuenot, and A. Trouvé, (2014), Towards predictive data-driven simulations of wildfire spread &ndash ; Part 2 : Ensemble Kalman Filter for the state estimation of a front-tracking simulator of wildfire spread, *Natural Hazards and Earth System Sciences Discussions*, **2**, 3769–3820.

[DA15] M. C. Rochoux, S. Ricci, D. Lucor, B. Cuenot, and A. Trouvé, (2014), Towards predictive data-driven simulations of wildfire spread &ndash ; Part I : Reduced-cost Ensemble Kalman Filter based on a Polynomial Chaos surrogate model for parameter estimation, *Natural Hazards and Earth System Sciences Discussions*, **2**, 3289–3349.

[DA16] J. Waters, D. J. Lea, M. J. Martin, I. Mirouze, A. Weaver, and J. While, (2015), Implementing a variational data assimilation system in an operational 1/4 degree global ocean model, *Quarterly Journal of the Royal Meteorological Society*, **141**, 333–349.

[DA17] A. T. Weaver and I. Mirouze, (2013), On the diffusion equation and its application to isotropic and anisotropic correlation modelling in variational assimilation, *Quarterly Journal of the Royal Meteorological Society*, **139**, 242–260.

6.2 Conferences Proceedings

[DA18] S. Barthélémy, S. Ricci, N. Goutal, O. Thual, and O. Le Pape, (2013), Data Assimilation with the Ensemble Kalman Filter on the 1D hydraulic code Mascaret. XXth TELEMAC-MASCARET User Conference, Karlsruhe (Germany), BAW, 16-18 octobre 2013.

[DA19] S. Barthélémy, S. Ricci, N. Goutal, O. Thual, and E. Le Pape, (2014), Data Assimilation with MASCARET and multi-dimensional coupling between Telemac and Mascaret, HIC, Aoű̂t 2014, New-York, USA.

[DA20] S. Barthélémy, S. Ricci, N. Goutal, O. Thual, and E. Le Pape, (2014), Data Assimilation with MASCARET and multi-dimensional coupling between Telemac and Mascaret, SimHydro, Juin 2014, Nice, France.

[DA21] S. Barthélémy, S. Ricci, O. Panneckoucke, O. Thual, and P.-O. Malaterre, (2012), Data Assimilation on a flood wave propagation model : emulation of an ensemble Kalman filter algorithm, Conference on ensemble methods in gesciences, Novembre 2012, Toulouse, France.

[DA22] S. Barthélémy, S. Ricci, O. Panneckoucke, O. Thual, and P.-O. Malaterre, (2012), Data Assimilation on a flood wave propagation model : emulation of an ensemble Kalman filter algorithm, HIC (Hydro Informatics Conference). Juillet 2012, Hambourg, Allemagne.

[DA23] S. Barthélémy, S. Ricci, O. Panneckoucke, O. Thual, and P.-O. Malaterre, (2012), Data Assimilation on a flood wave propagation model : emulation of an ensemble Kalman filter algorithm, Simhydro, Septembre 2012, Nice.

[DA24] L. Berthon, L. Biancamaria, N. Goutal, S. Ricci, and M. Durand, (2014), Towards the estimation of reach-averaged discharge from SWOT data using a Manning's equation derived algorithm. Application to the Garonne River between Tonneins-La Réole. EHGU, 27 April-2 May, Vienna, Austria.

[DA25] S. Biancamaria, E. Rodriguez, N. Goutal, S. Ricci, N. Mognard, P. Rogel, and E. Le Pape, (2012), Satellite (SWOT) and airborne wide-swath altimeters to study the Garonne River. "20 years of progress in radar altimetry symposium ", Venise-Italie, 24-29 septembre 2012.

[DA26] M. Coustau, E. Harader, V. Borrell Estupina, C. Bouvier, O. Thual, and A. Piacentini, (2013), Benefits and drawbacks of using data assimilation for hydrological modelling in karstic regions : recent work on the Lez basin. Assemblée de l'IAHS, Goteborg, Sweden.

[DA27] W. da Silva, M. Rochoux, H. Orlande, M. Cola¸co, O. Fudym, M. El Hafi, B. Cuenot, and S. Ricci, (2013), Application of particule ffilter in moving frontier problems, 4th Inverse Problems. Design and Optimization Symposium (IPDO), Albi, France, 26-28 June.

[DA28] S. Gürol, A. T. Weaver, S. Gratton, A. M. Moore, A. Piacentini, and H. G. Arango, (2012), B-preconditionned minimization aalgorithm for variational assimilation with the dual formulation. 4eme colloque National sur l'Assimilation de données, 17-19 December, Nice, France.

[DA29] S. Gürol, A. T. Weaver, S. Gratton, M. Moore, A. Piacentini, and H. G. Arango, (2013), B-preconditioned minimization aalgorithm for variational assimilation with the dual formulation. 6th WMO International Symposium on Data Assimilation, NCEP, 7-11 October, Washington, USA.

[DA30] J. Habert, S. Ricci, A. Piacentini, G. Jonville, E. Le Pape, O. Thual, and N. Goutal, (2012), Estimation of lateral inflows using data assimilation in the context of real-time flood forecasting for the Marne catchment in France Simhydro, 12-14 Septembre, Nice, France.

[DA31] J. Habert, S. Ricci, A. Piacentini, G. Jonville, T. Morel, F. Duchaine, A. Thevenin, E. Le Pape, O. Thual, N. Goutal, F. Zaoui, and R. Ata, (2012), Estimation of lateral inflows using data assimilation in the context of real-time flood forecasting for the Marne catchment in France. In XIXth TELEMAC-MASCARET User Conference : Oxford, UK, October 18-19, 2012.

[DA32] V. Häfliger, E. Martin, A. Boone, F. Habets, C. David, P.-A. Garambois, H. Roux, and S. Ricci, (2013), Evaluation of a regional hydrometeorological model for the simulation of river water levels in the framework of the SWOT mission, EGU - 7-12 April, Viena, Austria.

[DA33] E. Harader, V. Borrell-Estupina, S. Ricci, M. Coustau, O. Thual, A. Piacentini, and C. Bouvier, (2012), HydrolFrance data assimilation using a non-sequential Extended Kalman Fileter for the correction of rainfall forcing : case study of the Lez catchment in Southern France. Syim-Hydro, New Frontiers in simulation, 12-14 Septembre, Nice, France.

[DA34] E. Harader, S. Ricci, V. Borrell Estupina, J. Boé, L. Terray, and S. Somot, (2013), Precipitation externes and hydrological iimpact in Southern France using the ALADIN Med-CORDEX ssimulation. 7th Workshop HyMeX, 7-10 October, Cassis, France.

[DA35] E. Harader, S. Ricci, V. Borrell Estupina, J. Boé, L. Terray, and S. Somot, (2013), Understanding iimpact of future climate conditions upon floflood in the Lez catchment using the ALADIN Med-CORDEX ssimulation. Assemblée de l'IAHS, l'IAPSO, l'IAPSEI et l'IUGG, Knowledge for the future, 22-26 June, GŽteborg, Sweden.

[DA36] E. Harader, S. Ricci, V. Borrell Estupina, J. Boé, L. Terray, and S. Somot, (2014), The added value of high resolution regional modelling with ALADIN-Climate for the reporduction of extreme precipitation over France. 3rd International MedCORDEX workshop, 26-28 mai, Palaiseau, France.

[DA37] E. Mouffe, A. Getirana, S. Ricci, C. Lion, S. Biancamaria, Boone, A., N. Mognard, and P. Rogel, (2012), Automatic calibration of global flow routing model pparameter in the amazon basin using virtual SWOT data : GFall Meeing, American Geophysical Union (AGU), San Francisco (USA) 5-9 December.

[DA38] E. Mouffe, A. Getirana, S. Ricci, C. Lion, S. Biancamaria, A. Boone, N. Mognard, and P. Rogel, (2012), Towards SWOT data assimilation for hydrology : Automatic calibration for global flow routing model pparameter in the amazon basin, SimHydro 2012, 2-4 June, Sophia-Antipolis, France.

[DA39] E. Mouffe, A. Getirana, S. Ricci, C. Lion, S. Biancamaria, M. Boone, A., N., and P. Rogel, (2012), Automatic calibration of global flow routing model pparameter in the amazon basin using virtual SWOT data : GFall Meeing, American Geophysical Union (AGU), San Francisco (USA) 5-9 December. POSTER.

[DA40] V. Pedinotti, A. Boone, N. Mognard, S. Ricci, S. Biancamaria, C. VLion, J. Crétaux, and F. Papa, (2012), The impact of the assimialtIon of SWOT satellite data into a large scale hydrological model parametrization over the Niger basin, 20 Years of Progress in Radar Altimetry, Symposium, 24-29 September, Venise, Italy.

[DA41] V. Pedinotti, A. Boone, N. Mognard, S. Ricci, S. Biancamaria, and C. Lion, (2013), Assimilation des données virtuelles du satellite (SWOT) : impact sur les paramètres d'un modèle hydrologique à grande échelle. AMA, Paris, France.

[DA42] V. Pedinotti, A. Boone, N. Mognard, S. Ricci, S. Biancamaria, and C. Lion, (2013), The impact of the assimilation of SWOT satellite data into a large scale hydrological model parametrization over the Niger basin. EGU, 7-12 April, Viena, Austria.

[DA43] A. Piacentini, S. Ricci, E. Le Pape, J. Habert, G. Jonville, N. Goutal, S. Barthélémy, T. Morel, F. Duchaine, and O. Thual, (2012), Towards operational flood forecasting using Data Assimilation. H23C-1367 in 2012 AGU Fall Meeting, 3-7 December 2012, San Francisco, USA/.

[DA44] S. Ricci, O. Pannekoucke, O. Thual, S. Barthélémy, and F. Ninove, (2012), Emulation of a Kalman Filter algorithm on a diffusive flood wave propagation model. SymHydro, New Frontiers in simulation, 12-14 Septembre, Nice, France.

[DA45] S. Ricci, A. Piacentini, S. Barthélémy, E. Le Pape, O. Thual, N. Goutal, F. Zaoui, and A. Riadh, (2013), Data assimilation with Mascaret : Towards operational flood forecasting and model pparameter correction XIXth TELEMAC-MASCARET User Conference, 16-19 October, Oxford, U.K.

[DA46] S. Ricci, A. Piacentini, G. Jonvielle, J. Habert, S. Barthélémy, E. Le Pape, O. Thual, N. Goutal, F. Zaoui, and A. Riadh, (2012), Data assimilation for hydraulics : application to flood forecasting Uncertainty Modelling in Hydraulics Symposium, 28-29 June, Stressa, Italy.

[DA47] S. Ricci, A. Piacentini, E. Le Pape, J. Habert, G. Jonville, N. Goutal, S. Barthélémy, T. Morel, F. Duchaine, and O. Thual, (2012), Towards operational flood forecasting using Data Assimilation. Fall Meeting American Geophysical Union (AGU), San Francisco (USA), 5-9 December.

[DA48] S. Ricci, A. Piacentini, A. Riadh, N. Goutal, E. Razafindrakoto, F. Zaoui, M. Gant, T. Morel, F. Duchaine, and O. Thual, (2012), A variational Data Assimilation algorithm to better estimate the salinity for the Berre Lagoon with TeTelemac Fall Meeting, American Geophysical Union (AGU) San Francicsco (USA) 5-9 December.

[DA49] S. Ricci, A. Piacentini, A. Riadh, N. Goutal, A. T. Weaver, and R. Ata, (2012), A variational Data Assimilation algorithm to better estimate the salinity for the Berre Lagoon with TeTelemac. Sixth Symposium on Data Assimilation, 7-11 October, College Park, MD, USA.

[DA50] S. Ricci, A. Piacentini, O. Thual, N. Goutal, R. Ata, E. Razafindrakoto, and M. Gant, (2013), Data assimilation for the modmodel of the Berre Basin with T3D. XIXth TELEMAC-MASCARET User Conference, 16-19 October, Oxford, U.K.

[DA51] S. Ricci, A. Piacentini, A. T. Weaver, R. Ata, and N. Goutal, (2013), A variational Data Assimilation algorithm to estimate the salinity for the Berre Lagoon with TeTelemac3D. XXth TELEMAC-MASCARET User conference, 16-18 October, Karlsruhe, Germany.

[DA52] S. Ricci, A. Piacentini, A. T. Weaver, R. Ata, and N. Goutal, (2014), A Variational data assimilation Algorithm to Estimate Salinity in the Berre Lagoon with TeTelemac, IAEG, 15-19 September, Turin, Italy.

[DA53] S. Ricci, A. Piacentini, A. T. Weaver, R. Ata, and N. Goutal, (2014), Variational data assimilation with telemac. Proof of concept for model state correction on the Berre lagoon 3d-model ?. 11th International Conference on Hydroinformatics, HIC, Ne York City, 2014.

[DA54] S. Ricci, (2012), Reducing uncertainties in hydrodynamics modemodel using Data Assimilation 4th French National Symposium on Data Assimilation (LEFE), Nice, France, 17-19 december.

[DA55] M. Rochoux, J.-M. Bart, S. Ricci, B. Cuenot, and A. Trouvé, (2012), Towards data-driven ssimulation of wildfire spread using ensemble-based data assimilation, 4th French National Symposium on Data Assimilation (LEFE) Nice, France, 17-19 December.

[DA56] M. Rochoux, J.-M. Bart, S. Ricci, B. Cuenot, and A. Trouvé, (2012), Towards data-driven ssimulation of wildfire spread using ensemble-based data assimilation, Fall Meeting American Geophysical Union (AGU), San Francisco (USA), 5-9 December.

[DA57] M. Rochoux, J.-M. Bart, S. Ricci, B. Cuenot, and A. Trouvé, (2012), Towards data-driven ssimulation of wildfire spread using ensemble-based data assimilation. international Conference on Ensemble Methods in Geophysical SScience, 12-16 November, Toulouse, France.

[DA58] M. Rochoux, C. Emerey, S. Ricci, B. Cuenot, J. B. Filippi, T. Morel, and A. Trouvé, (2013), Regional-scale simulation of wiidland fire spread using ensemble-based data assimilation, in Eastern States Section of the Combustion Institute Fall Technical Meeting, 13-16 October.

[DA59] M. Rochoux, C. Emerey, S. Ricci, B. Cuenot, J. B. Filippi, T. Morel, A. Trouvé, C. Allouache, M. Durand, and M. Taillardat, (2013), Data-driven ssimulation of regional-scale wildfire spread using ensemble-based data assimilation. Numerical Simulation of Forest FFire, from combustion to emissions, Cargèse (France), 13-17 May.

[DA60] M. Rochoux, C. Emery, S. Ricci, B. Cuenot, and A. Trouvé, (2014), Comparative study of parameter estimation and state estimation approaches in data-driven wildfire spread modmodel. VII International Conference on Forest Fire Research, Coimbra, Portugal, 14-20 November.

[DA61] M. Rochoux, C. Emery, S. Ricci, B. Cuenot, and A. Trouvé, (2014), Ensemble Data Assimilation for fire spread modmodel. 35th International Symposium for Combustion, San Francisco, USA, 3-8 August.

[DA62] M. Rochoux, C. Emery, S. Ricci, B. Cuenot, and A. Trouvé, (2014), Towards predictivie simulation of wildfire spread at regional scale using ensemble-based data assimilation to correct the fire position, in Fire Safety Science - Proceedings of the Eleventh International Symposium, International Association for Fire Safety Science. url :www.iafss.org/publications :.

[DA63] A. T. Weaver and A. Piacentini, (2012), Representing ensemble covariances with a diffsuion operator International Conference on Ensemble Methods in Geophysical SScience, 12-16 November, Toulouse, France.

[DA64] A. T. Weaver, L. Corre, and M. Balmaseda, (2013), Evaluation of the ECMWF ensemble of ocean reanalyses using assimilation diagnostics. 6th WMO International Symposium on Data Assimilation, 7-11 October 2013, Washington, USA.

[DA65] A. T. Weaver, L. Corre, and M. A. Balmaseda, (2013), Evaluation of the ECMWF ensemble of ocean reanalyses using assimilation diagnostics. Journées Groupe Mission Mercator Coriolis, 23-24 April, 2013, Toulouse, France.

[DA66] A. T. Weaver, (2012), Representing covariances in variational data assimilation using a diffusion operator. MATHIAS 2012, 25-26 October, Paris, France.

[DA67] A. T. Weaver, (2013), Assimilation Diagnostics : Examples from ORAS4, CLIVAR GSO/GODAE Ocean Reanalyses Intercomparison Workshop, ECMXF, 1-3 July 2013, Reading, UK.

[DA68] A. T. Weaver, (2013), Covariance modmodel and minimization for variational ocean data assimilation. Recent advances in Optimization, 24-26 July, Toulouse, France.

[DA69] A. T. Weaver, (2014), Examples of representing observation error correlations in variational ocean data assimilation. ESA International Workshop on Correlated Observation Errors in Data Assimilation, University of Reading, 23-24 April 2014, Reading, UK.

6.3 Technical Reports

[DA70] C. Allouache, M. Durand, M. Taillardat, M. Rochoux, and S. Ricci, (2013), Assimilation de données pour la propagation des feux de forêt. Rapport de projet de modélisation ENM. 14 février 2013 Technical Report, TR-CMGC-13-114, tech. rep., CERFACS/CNRS SUC URA 1875, TOULOUSE, FRANCE.

[DA71] C. Doche, M. Ricci, and M. Rochoux, (2013), Vers l'assimilation de données pour la simulation des feux de forêts Ĺ l'échelle régionale.Technical Report TR-13-5, tech. rep., CERFACS/CNRS SUC URA 1875, TOULOUSE, FRANCE.

[DA72] C. Emery, M. Rochoux, and S. Ricci, (2013), Regional-Scale Wildfire Spread Simulations with a Complex Topography : Data Assimilation for Model State Estimation. Technical Report TR-CMGC-13-55, tech. rep., CERFACS/CNRS SUC URA 1875, TOULOUSE, FRANCE.

[DA73] C. Emery, M. Rochoux, S. Ricci, and A. Trouvé, (2013), State estimation using data assimilation for simulation of regional scale wildfire spread with complex topography. Technical Report, TR-CMGC-13-63, tech. rep., CERFACS/CNRS SUC URA 1875, TOULOUSE, FRANCE.

[DA74] S. Gürol, A. T. Weaver, A. M. Moore, A. Piacentini, H. Arango, and S. Gratton, (2012), B-preconditioned minimization algorithms for variationnal data assimilation using the dual-space formulation. Technical Report TR-PA-12-118, tech. rep., CERFACS.

[DA75] J. Habert, S. Ricci, E. Lepape, A. Piacentini, G. Jonville, O. Thual, N. Goutal, F. Zaoui, and R. Ata, (2013), Estimation of lateral inflows using data assimilation in the context of real-time flood forecasting for the Marne catchment in France. Technical Report, TR-CMGC-13-76, tech. rep., Cerfacs, Toulouse, France.

[DA76] K. Mogensen, M. A. Balmaseda, and A. T. Weaver, (2012), The NEMOVAR ocean data assimilation system as implemented in the ECMWF ocean analysis for System 4. ECMWF Tech. Memo., 668, 60 pp.Also registered as a CERFACS Technical Report TR-CMGC-12-30, tech. rep., CERFACS.

[DA77] S. Ricci, A. Piacentini, A. T. Weaver, R. Ata, and N. Goutal, (2013), A Vairational Data Assimilation Algorithm to Estimate Salinity in the Berre Lagoon with Telemac3D. Technical Report, TR-CMGC-13-55, tech. rep., CERFACS/CNRS SUC URA 1875, TOULOUSE, FRANCE.

[DA78] M. Rochoux, C. Emery, S. Ricci, and B. Cuenot, (2013), Towards predictive simulation of wildfire spread at regional scale using ensemble-based data assimilation to correct the fire front position. Technical Report, TR 13-57, tech. rep., CERFACS/CNRS SUC URA 1875, TOULOUSE, FRANCE.

[DA79] M. Rochoux, S. Ricci, D. Lucor, B. Cuenot, A. Trouvé, and J.-M. Bart, (2012), Towards predictive simulation of wildfire spread using a reduced-cost ensemble Kalman filter based on polynomial chaos approximation. in Proceedings of the Summer Program, Center for Turbulence Research, NASA-AMES Stanford University, June/july 2012, tech. rep.

[DA80] A. Thevenin and A. Piacentini, (2012), Rapport d'étape intermédiaire du projet OPTIMAL (Optimisation et parallélisation de MOCAGE opérationnel, tech. rep., CERFACS/CNRS SUC URA 1875.

[DA81] A. Thevenin, A. Piacentini, and B. Josse, (2012), Rapport final de la convention de collaboration de recherche 3.2.28/11 (Optimisation et parallélisapara de MOCAGE opérationnel, tech. rep., CERFACS/CNRS SUC URA 1875.

[DA82] A. Thevenin, A. Piacentini, and B. Josse, (2013), Rapport final de la convention de collaboration de cherche 3.2.01/13 (Optimisation et paralléisation de la chaîne opérationnelle MOCAGE), tech. rep., CERFACS/CNRS SUC URA 1875.

6.4 Thesis

[DA83] M. Rochoux, (2014), *Vers une meilleure prévision de la propagation d'incendies de forêt : Evaluation de modèles et Assimilation de données.*, PhD thesis, Ecole Centrale de Paris.

4

Coupling tools and HPC Climate Modeling

Introduction

Code coupling is an important research and applicative topic into which the Cerfacs is a major player for many years. Indeed, from the applicative point of view, coupling models or codes is an efficient way to develop, test and deploy many types of applications such as : data assimilation platforms, multi-physic and multi-component simulations, online post-processing or design optimization. In this specific field, the Cerfacs carries on researches in order to improve the methodologies and the performance of its open source couplers OASIS3-MCT (interfaced with the MCT library developed by the Argonne National Laboratory) and OpenPALM (co-developed with ONERA). A coupler is a library that facilitates the sequential or concurrent execution of existing components as well as the exchange of data between these components. This is achieved in part via a collection of primitives that are called in the codes as well as via more complex mechanisms for application scheduling. The Cerfacs also plays a key role of networking at the international level : the Cerfacs organized in 2010 the first workshop of the series "Coupling Technologies for Earth System Modelling", actively participated in the 2nd workshop help in Boulder in 2013 and is now in the organizing committee of the 3rd workshop planned in Manchester in April 2015.
As climate model spatial resolution is getting finer, in line with increasing available computing power on High Performance Computing (HPC) systems, the amount of data generated by climate simulations is getting very large. On the road to exascale, volumes of data generated will continue to increase, even if techniques of data output reduction (e.g. storing the data on coarser output grids) are applied. In this field, Cerfacs carries research on strategies for high-resolution climate modeling as well as contrail simulations on highly parallel HPC systems. To support these simulations, innovative solutions must be developed to handle large data volumes generated as well as on uncertainties quantification of model outputs.

OASIS

The OASIS coupler is an open source software developed at Cerfacs to couple numerical codes modelling the different components of the Earth System (oceanic and atmospheric general circulation, sea-ice, land, atmospheric chemistry, etc.) developed independently by different research groups. Today, the OASIS coupler is used by about 35 climate modelling groups in France and in Europe but also in many other countries around the world. Five of the seven European climate Earth System Models participating to the 5th Coupled Model Intercomparison Project use the OASIS3 coupler (Valcke, 2013).
In particular, OASIS is used by our team and at the Centre National de Recherches Météorologiques (CNRM) of Météo-France to assemble different Coupled GCMs (CGCMs) in the framework of various national, European or international projects ; for example, CNRM-CM5 developed jointly by CNRM and Cerfacs for CMIP5, based on ARPEGE-Climat V5 T127 atmosphere model, SURFEX surface module, OPA9/NEMO V3 ocean model in the ORCA1 configuration (1 degree) and GELATO sea-ice model, or the high-resolution prototype Cerfacs-HR into which ARPEGE-Climat V5.3 T359 (50 km) is coupled to NEMO V3.4 in the ORCA025 configuration (0.25 degree).

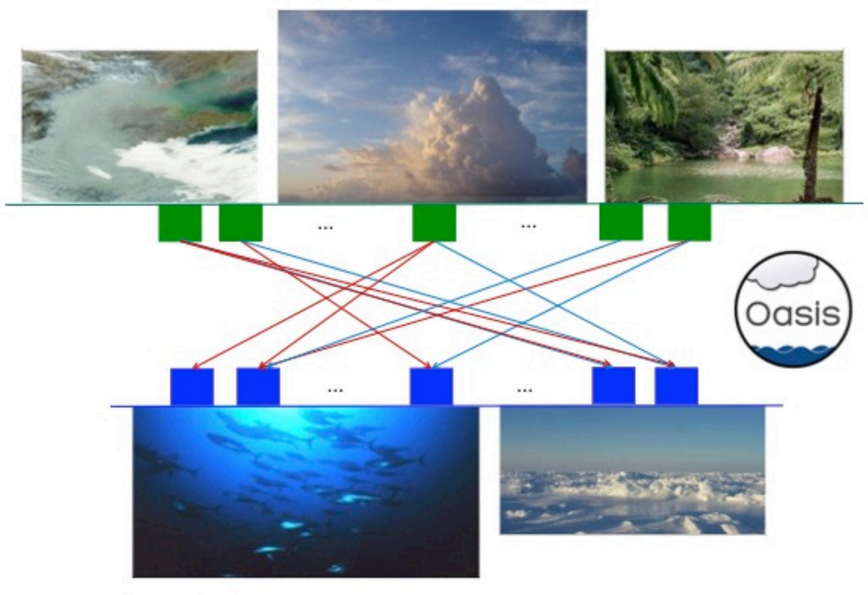

FIG. 2.1: Figurative representation of a coupling managed by OASIS between an atmospheric code including a land scheme and an ocean code including a sea-ice model

The latest fully parallel version of the coupler, OASIS3-MCT, was significantly refactored with respect to the previous OASIS3 version as it is now interfaced with the Model Coupling Toolkit (MCT) developed

by the Argonne National Laboratory in the USA. After compilation OASIS3-MCT forms a library to link to the component model codes, which main function is to interpolate and exchange the coupling fields. OASIS3-MCT supports coupling of 2D logically-rectangular fields but 3D fields and 1D fields expressed on unstructured grids are also supported using a one dimension degeneration of the structures. In OASIS3-MCT, MCT implements fully parallel regridding, as a parallel matrix vector multiplication based on pre-computed weights and addresses, and distributed exchanges of the coupling fields. Even if the underlying implementation has evolved significantly, usage of OASIS3-MCT in the codes has largely remained unchanged, keeping the same Application Programming Interface (API) than in the previous OASIS3 version, based on flexibility and minimal invasiveness (Valcke et al., 2012).
Tests done with a "toy" model reproducing real coupling exchanges between two codes (without any physics or dynamics) have shown the good behaviour of OASIS3-MCT at high number of cores. This is illustrated on Figure 2.2. The codes use respectively the NEMO ORCA025 grid (1021x1442 grid points) and the Gaussian Reduced T799 grid (843 000 grid points). Figure 2.2 shows the time of a ping-pong (back and forth) exchange between the two codes as a function of the number of cores used to run each code, for up to 4000 cores on the TGCC Bullx Curie thin nodes and 8000 cores on BSC IBM MareNostrum III.

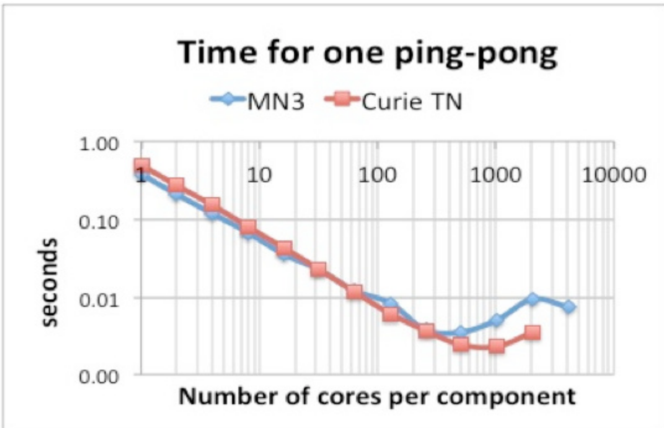

FIG. 2.2: Time of a back and forth exchange between two codes using respectively the ORCA025 grid and the Gaussian Reduced T799 grid, as a function of the number of cores used to run each code on the TGCC Bullx Curie thin nodes and on BSC IBM MareNostrum III.

Since its first release in July 2012, more than 350 OASIS3-MCT downloads were registered from groups in Europe but also in Canada, USA, Colombia, India, Japan, China, Saudi Arabia, etc. Among these groups, many have effectively migrated to OASIS3-MCT, in general for relatively high-resolution version of their coupled model, for example all IPSL labs, ETHZ in Switzerland, SMHI in Sweden, MPI-M and the regional climate modelling community COSMO in Germany, the UK Met Office, or the BoM in Australia. The latest official releases of the ocean NEMO model and the atmospheric WRF model now include the OASIS3-MCT API. Three-day sessions of general training on OASIS3-MCT are offered twice a year, generally in May and November. In addition, the OASIS web site has been completely redesigned within the IS-ENES European project (see http ://verc.enes.org/oasis).This web site is continuously maintained and standard OASIS user support is provided through its forum but also by mail and phone exchanges, as required.
Besides the permanent manpower ensured by Cerfacs and CNRS, the IS-ENES2 project is the main source of external funding for the development and maintenance of the OASIS3-MCT coupler. IS-ENES2 is the InfraStructure for the European Network for Earth System Modelling 2, funded for 8 MEuros over 2013-2017 under the EC-FP7. In IS-ENES2, 28 pm is devoted to maintain a strong community network around OASIS3-MCT and to further optimise it for massively parallel platforms.

OpenPALM

The OpenPALM coupler has proven to be a flexible and powerful parallel dynamic coupler. Originally designed for data assimilation, its application domains now extend far beyond and its user community is constantly increasing (Piacentini et al., 2011). The remarkable feature of OpenPALM is that it supports dynamic coupling, which means that codes to be coupled can be launched at any time during the simulation, in a loop or under a specific condition. Thanks to PrePALM, its evolved Graphical User Interface, the user can easily describe such complex coupling algorithms, which are then realized by the OpenPALM driver. The more recent interfacing of CWIPI developed by ONERA in OpenPALM has extended its use to many additional domains (see below). In the context of this collaboration, the OpenPALM web site has been completely revised (www.cerfacs.fr/globc/PALM_WEB) and the coupler has become open source since January 2011.

The main developments realised in the coupler during the last three years are :

- Interfacing of CWIPI, a library developed by ONERA for parallel remapping of coupling fields expressed on 1D, 2D or 3D non-structured meshes. Its efficiency has been shown for coupled systems running on up to 30000 cores. It has allowed the development of the TurboAVBP system coupling many AVBP (a parallel CFD code for reactive unsteady flow simulations on hybrid grids) instances used at Cerfacs, IMFT and Sherbrooke University (see Figure 3.1)

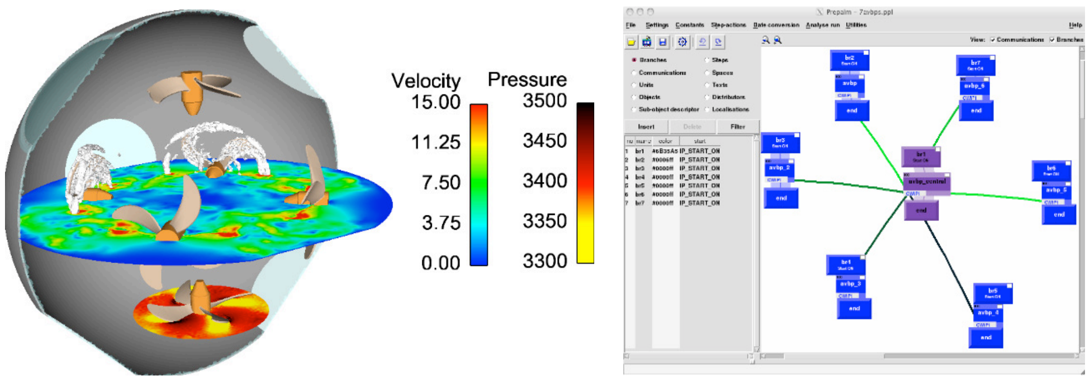

FIG. 3.1: TurboAVBP, coupling of many AVBP instances

- The development of PARASOL an additional running enviroment allowing the concurrent launching of n instances of the same parallel code on pools of m processes. PARASOL allows to easily manage this type of applications via communications of vectors of input parameters and vectors of solutions for these n instances. PARASOL has allowed the development of ensemble Kalman filters for data assimilation in hydrology and in forest fire modelling.
- Development of a TCP/IP client-server environment allowing the coupling of applications for which the source code is not available. Thanks to this development, coupling of codes like Fluent, Abaqus or Samcef via OpenPALM is now possible.

As a data assimilation framework, the OpenPALM coupler is used in the operational suite of the MERCATOR ocean forecasting system and for research purposes by the “Research and development”

team selected by the GMMC (Groupe Mission MERCATOR CORIOLIS). It is also used in the French project ADOMOCA for atmospheric chemistry data assimilation and by Cerfacs together with EDF/LNHE and SCHAPI for the design and implementation of specific data assimilation methods for hydrology and hydraulics. Furthermore, the MOCAGE-Valentina 3D-VAR Suite for Real Time Air Quality forecasting, based on a prototype of OpenPALM is routinely used by Météo-France and it is part the FP7 EU project MACC. In the MACC II follow-on, it is evolving into an OpenPALM-based application for the multi-variate assimilation of chemical components of the atmosphere to be used for Air Quality forecasting of reanalyses.
As a code coupler OpenPALM is also intensively used for many mutli-physic and multi-component studies in the Computational Fluid Dynamic team of Cerfacs. Firstly, an important axis deals with aerothermal for aeronautic (combustion chambers, turbine blades, ...) and automotive applications. In this context, a coupled model based on three codes (AVBP for the convection, AVTP for the conduction in solids and PRISSMA for the radiation) was developed with OpenPALM. Another multi-physic problem involving mechanical fluid-structure interaction is addressed by coupling the fluid solver AVBP and the commercial structure code MARC. This coupled model is installed and used by engineers at Herakles (SAFRAN group). Another important coupled problem is the multi-component simulation of a whole engine, ie. compressor-combustion chamber-turbine.This is a crucial step in engine simulation as it allows to take into account dynamic, thermal and acoustic interactions between these three components. Such simulations imply the coupling of different flow solvers to treat the fixed and rotating parts. The first part of the informatic tool have been developed and tested.
Having proved its efficiency, OpenPALM is now spreading in the scientific and engineering community. Among its users, we find 6 of the 7 Cerfacs shareholders : SAFRAN (SNECMA Vernon and Villaroche, HERACLES, TURBOMECA), Airbus-Group, ONERA, CNES, CNRM (Météo France), EDF and about 70 other institutions. An important part of industrial use is supported via the FUI project COSMOS+ (2012-2015), which aims to develop and implement a multiphysics coupling tool to meet the needs of industry and research in the aerospace field. This project provides resources to develop the OpenPALM Cerfacs-ONERA coupling environment, to define coupling strategy in a multidisciplinary environment and to address great challenges of industrial simulations not achievable today. Among other tasks, Cerfacs has the responsability of leading a work package on code instrumentation for coupling.
Over 2009-2014, 16 3-day training sessions on OpenPALM coupler were held for a total of about 140 trainees. These trainings were held at Cerfacs in Toulouse, and also at ONERA Châtillon and at CINES Monpellier under PRACE.

High Performance Computing

A global strategy was deployed to gradually adapt our climate model to High Performance Computing (HPC), targeting higher parallelism and, as such, higher resolution (25-50Km). Taking part to MF-ECMWF and NEMO community effort, scalability of our ESM has been improved (Maisonnave, 2010a) and its capability to face Exascale related issues like resilience (Maisonnave, 2012a, TR) has been analysed. Scalability of a composite system is bounded by the less scalable component. Our global strategy takes into account not only the scalability of FORTRAN model codes but also the performances of the whole climate simulation work-flow. Figure 1 describes how computations are traditionally performed (red basis) : on a few CPUs, GCMs computations, interrupted by coupling interpolations and output writing on disk, are followed by a post-processing phase. In a global scalable mode (blue basis), parallel model computations are performed in parallel (task parallelism), at the same time as output and first post-processing operations (co-processing).

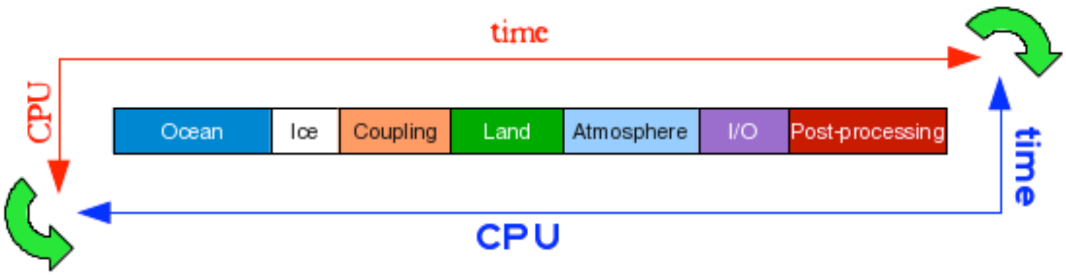

FIG. 4.1: From sequential to parallel climate model work-flow

We took benefit of major improvements on coupling techniques described above in the OASIS section to remove from our ESM any bottleneck related to coupling. Thanks to the IS-ENES I & II FP7 project, coupler functionality at high resolution were intensively tested and adapted to various configurations that will help to increase model accuracy and complexity in the future without performance losses : global/regional coupling (Maisonnave, 2013a, Masson et al., 2012a), coupling with icosahedral grids (Maisonnave, 2014a), high frequency coupling (Maisonnave, 2011a). In order to precisely estimate performances of each coupled model component, a specific performance measurement tool was developed in collaboration with the OASIS user community (Maisonnave et al., 2013a). The IPSL XIOS I/O server was successfully tested at high end resolution (Masson et al., 2012b) and included in our ESM on a PRACE platform. Finally, treating the outputs of our ESM as a coupling between the main simulation codes and a small additional program allowing interpolation on a coarser grid allowed to drastically reduce the atmospheric post-processing duration and volume of produced diagnostics (Maisonnave, 2013a). Remaining analysis operations have been parallelized (Bretonnière, 2012). Such improvements did facilitate granting and realization of 3 PRACE Regular Access Projects for multi scale coupling : PULSATION, in collaboration with IPSL, BULL, Mercator-Ocean and OMP (Maisonnave et al., 2012b), SPRUCE providing 27 Mhrs on Bullx Curie at TGCC for high resolution seasonal forecast in collaboration with Meteo-France and Mercator ocean (Maisonnave et al., 2012c, TR) and HiResCLIM with 10 Mhrs on the IBM MareNostrum3 at BSC for high resolution decadal predictions in collaboration with SMHI and IC3. Solving issues related to high resolution requires expertise from both computational and geophysical research staff, and in our laboratory we started studying mesoscale impact on large scale circulation (Déqué et al., 2013, TR and Piazza et al., 2014, OT). Accelerating the performances of our biggest configurations, our work ensures that results are delivered at a reasonnable paste (5 simulated years per day), which is essential for the scientific production of our team. Another strong activity in HPC concerned the aviation and environment theme. Over the last 5 years, this activity was awarded two prestigious grants in computational science : the 2011 PRACE award and the 2012 and 2013 INCITE awards managed by the US Department of Energy. In the PRACE project, which was a collaboration with the Laboratoire d'Aérologie and Météo France, we carried out large-eddy simulations of atmospheric turbulence in the UTLS using the mesoscale atmospheric model Méso-NH on computational grids of up to 8 billions grid points.. This study allowed for a detailed analysis of turbulence in strongly stratified flows at sub-kilometer scales that are of interest for the dispersion of aircraft emissions and that were never studied before (Paoli et al., 2014, RA). In the INCITE projects, we carried out large-eddy simulations of contrail-to-cirrus transition on time scales of 1 hour after emission, using again Meso-NH on computational meshes of up to 1 billion grid points with all the microphysical and radiative modules activated. The simulations were typically run on 32,000 computing cores of the IBM BG/P and IBM BG/Q at Argonne National Lab. This study was extremely useful to understand the relative role of atmospheric turbulence and radiative transfer in setting the microphysical and optical properties of ice crystals as a function of contrail age. It also provided practical guidelines for the contrail parameterization in global models. A paper describing the results of the study is in preparation.

Big Data

To support the users of climate data simulations output, a two-fold interlinked strategy is being used. The first one is to provide the climate change impacts community tools to access climate data, tailored to their needs. For this objective we designed, prototyped, and made operational the climate4impact.eu web portal dedicated for the impacts community within the EC FP7 IS-ENES and IS-ENES2 projects (Plieger et al., 2013b, TR). This portal enables the users to access data and to perform data processing and downscaling without the need for the users to download all required input data into their local systems, taking advantage of the high-speed network bandwidth between ESGF servers and the climate4impact servers. This work is done in close collaboration with CNRS-IPSL, MétéoFrance CNRS-GAME, KNMI, SMHI, University of Cantabria, Wageningen University Research and CMCC. Within this strategy, a very efficient climate indices data processing calculation code has been developed (named icclim), which has been integrated with the US NCAR NCPP CoG group Open Climate GIS (ocgis) open-source software library. The portal climate4impact and its data processing services will also be used within the FP7 CLIPC project (Figure 5.1) into which Cerfacs is a partner. CLIPC is building a climate toolbox for the future GMES Copernicus platform.

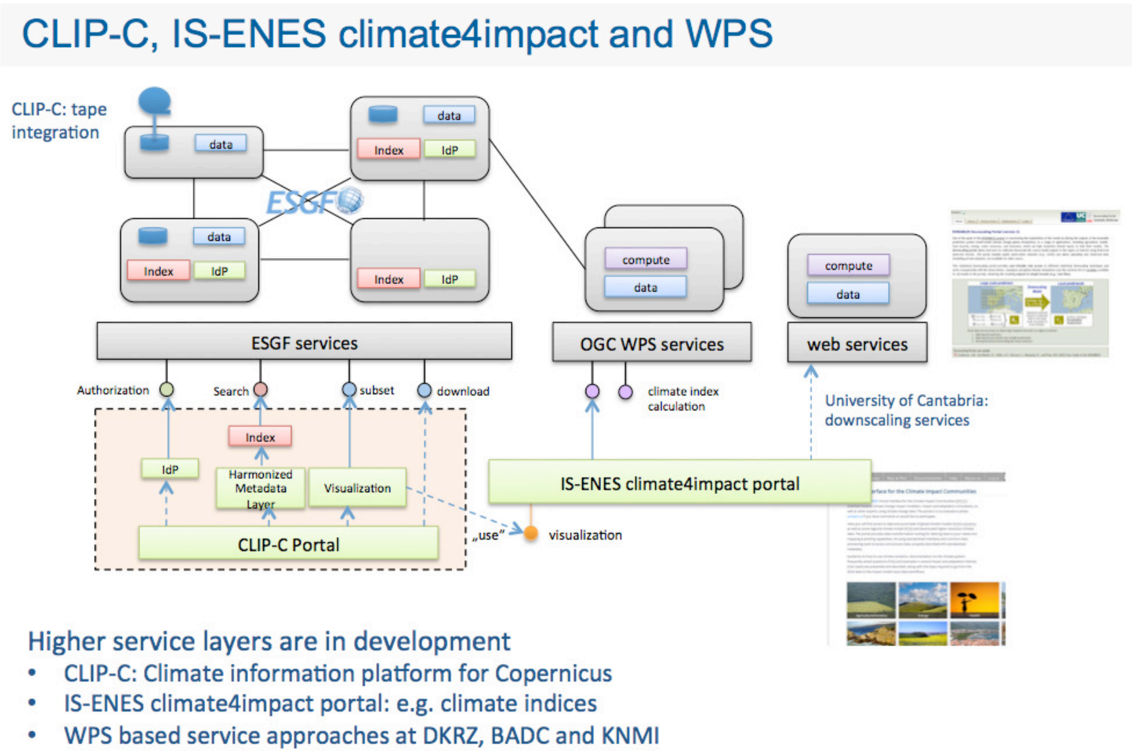

FIG. 5.1: Integration of IS-ENES climate4impact within ESGF and CLIPC (Climate Toolbox of the future Copernicus GMES Platform)

The second strategy is to perform data reduction near the data storage, using common approaches with other scientific fields within the EC FP7 EUDAT project, which includes as partners scientific communities and data centres throughout Europe. The objective is to perform execution of workflows near the data storage, through an interface called the Generic Execution Framework (GEF, Dima et al., 2013) (Figure 5.2). Strong collaboration is taking place with MPI-M, DKRZ and CINES. The first prototype for the ENES climate community was first implemented at CINES in France.
Further integration of these two strategies into the climate community ESGF infrastructure is beginning to take place within the newly created ESGF Compute Working Team, lead by PCMDI, into which Cerfacs, Météo-France CNRM-GAME and CNRS-IPSL are actively participating.

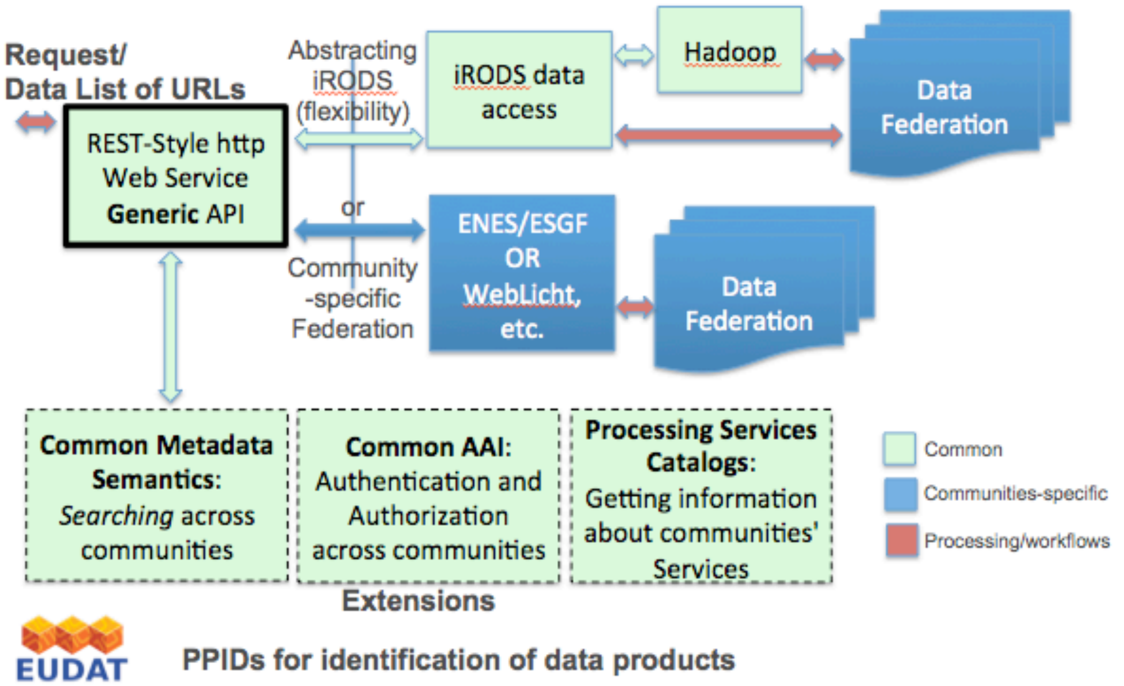

FIG. 5.2: Schematic of Common Services within EUDAT scientific communities, along with a generic interface to data reduction and workflows execution near the data storage (Generic Execution Framework (GEF))

Uncertainty Quantification

Uncertainties Quantification (UQ) has become a mandatory step for application oriented numerical modeling, strengthened with the development of High Performance Computing. The main idea in UQ is to quantify the uncertainty in model outputs (the quantities of interest QOI) that is due to errors of various natures (aleatory, epistemic) in the model. In the context of geophysics, epistemic uncertainties relate to model parameters, input data geometry, simplification of the model physics or numerical discretization. Random errors are typically due to initial conditions and boundary conditions as well as calibration and validation data sets. Classical UQ methods are based on a Monte-Carlo approach to estimate the density probability functions (PDF) of the QOI with respect to the PDF of the uncertainty sources. However, it usually implies a large number of integrations of the model associated with a significant computational cost. In order to reduce the computational cost, building a surrogate model is often necessary using intrusive or non-intrusive approaches. UQ relates to Data Assimilation (DA) domain, especially ensemble based methods, as it allows identifying which variables should be included in the control vector and offers a way to efficiently compute errors statistics using the surrogate model in place of the direct model in the ensemble integrations. UQ also relates to climate study where advanced statistical methods are developed to differentiate variability coming from intrinsic or anthropogenic sources. In a complementary approach, one objective is to benefit from the recent developments of high resolution coupled climate models to assess the low frequency variability (1-10 years) induced by meso-scale oceanic eddies. Taking into account these scales is mandatory to separate the deterministic (atmospherically-forced) and chaotic (intrinsic) parts of the low-frequency ocean variability.

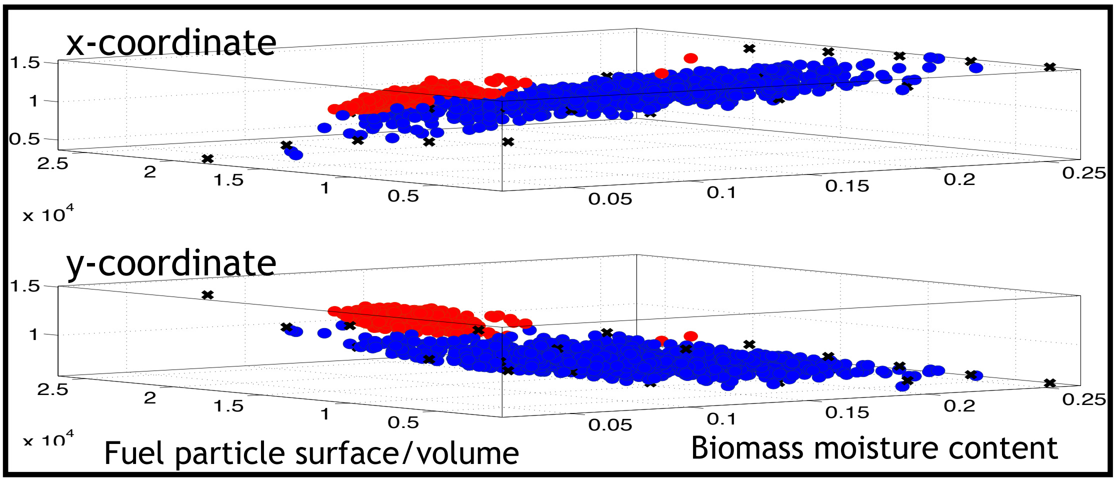

FIG. 6.1: Surrogate model surface response of the x- and y-coordinates of one fire front marker with respect to humidity and fuel particle surface/volume ratio. Black crosses correspond to quadrature roots, EnKF forecast estimates are in blue and EnKF analysis estimates are in red (from Rochoux PhD thesis 2014).

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5

Climate Variability and Global Change

Introduction

Cerfacs has traditionally carried out theoretical and applied research on climate variations, on a broad range of spatial and temporal scales, with a special focus during the last few years on decadal to centennial time scales. Both internal and external variations, including that due to anthropogenic forcing, have been studied, with a specific interest in trying to disentangle their respective influence on 20th century climate evolution. The 2012-2014 period has also seen the emergence at the Cerfacs of an important research effort on decadal climate predictions. It has culminated in the development and application of a decadal prediction system within the Coupled Model Intercomparison Project Phase 5 exercise. This effort has required basic upstream research, necessary to interpret and improve decadal predictions, including modeling studies on decadal predictability and on the mechanisms responsible for decadal climate variations, from global to local scales. In parallel, the work on projections of future anthropogenic climate change has been pursued, focusing on impacts particularly relevant for the society, and with the overall objective to better characterize and, if possible, reduce the different sources of uncertainty involved.

Climate variability at seasonal to decadal time scales

Delineating the relative role of anthropogenic forcing, natural forcing, and long-term internal variability in the climate evolution presents a significant scientific challenge. During the period 2009-2014, the Cerfacs has undertaken a number of works aimed at : 1) characterising the observed 20th century climate variability by understanding the different contributions of internal and external factors 2) investigating air-sea interaction processes on a broad range of spatial and time scales.

2.1 Characterization of observed climate variability

The observed climate variability has been studied at regional as well at a global scale by using the instrumental records and reanalyses for both the atmosphere and the ocean. At regional scale, our regions of interest are Europe and France. Cattiaux et al. (2011 RA) have studied the temporal evolution of cold winters in Europe and they show that the extreme cold winters (in particular the winter of 2009/2010) are mitigated by long-term climate warming induced by anthropogenic forcing, even if the associated large-scale circulation remains unchanged. Boé and Habets (2014 RA) have shown that large multi-decadal variations in French river flows exist on the instrumental period, especially in spring. These multi-decadal variations are found to be associated with the atmospheric circulation response to the low-frequency fluctuations of the North Atlantic Ocean named Atlantic Multidecadal Variability (AMV). The amplitudes of these decadal variations are comparable to those projected in the next decades in response to increasing carbon dioxide emissions, implying that they need to be accounted for in any rigorous forecast exercise.
From a more global perspective, the recent long-term changes and decadal variability in the upper ocean heat content as represented by model based ocean reanalyses and an data objective analysis has been investigated (Corre et al. 2012 RA). The mean temperature above the 14 ˚C isotherm has been used as a convenient, albeit simple, way to isolate thermodynamical changes by filtering out dynamical changes related to thermocline vertical displacements. The global upper ocean observations and reanalyses exhibit very similar warming trends (0.045 ˚C per decade) over the period 1965-2005, superimposed with marked decadal variability in the 1970s and 1980s. Our work shows that the spatial signature of anthropogenic changes is qualitatively different from those of the internal decadal variability associated to the Pacific Interdecadal Oscillation and the Atlantic Multidecadal Oscillation. Results also show that even if the global upper ocean observations and reanalyses exhibit very similar global warming trends over the period 1965-2005, large discrepancies between the different products still exist at regional scales, particularly in the Atlantic.

2.2 Understanding the role of internal variability versus external forcings

The effect of external influences on climate can be estimated by comparing observations with idealized experiments performed by changing in the model the external forcing contributions, and by analysing the physical processes involved. The effort has focused on changes observed during the instrumental period, particularly on the last 50 years, when human activity has grown fastest and observations are more reliable.

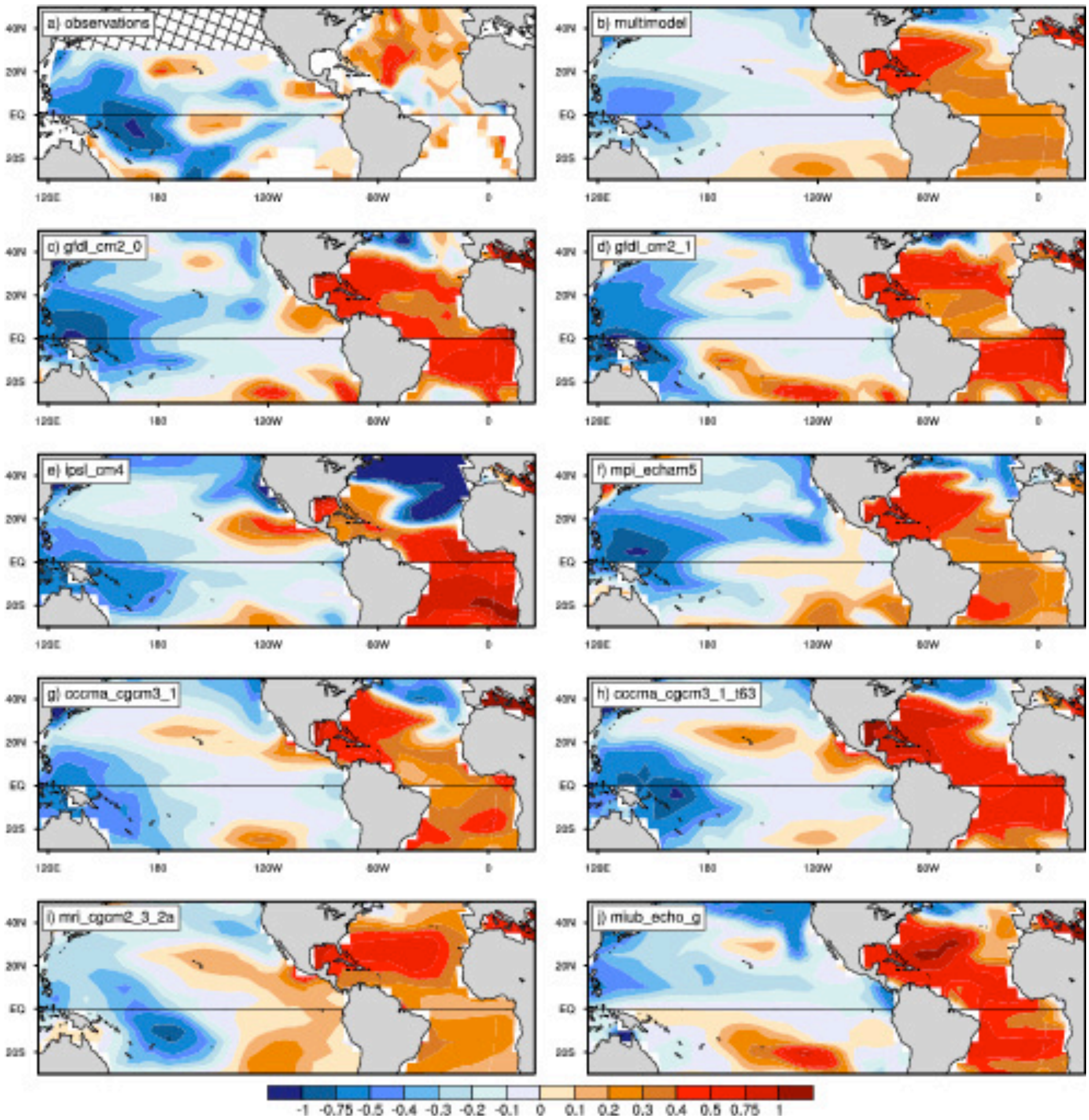

FIG. 2.1: Rate of observed and modeled future SSS changes : a) Recent (1970-2002) observed SSS trend (per century) and b) Multimodel average SSS changes (per century) between the end of the 21st and 20th centuries (2070-2099 - 1970-1999). Simulated changes for individual models : c), d), e), f) without fresh water flux adjustments and g), h), i), j) with fresh water flux adjustments. From Terray et al. 2012 RA.

In collaboration with CNRM/GAME researchers, the Cerfacs has made some significant contributions to the detection and attribution (D&A) field. First, we have conducted the first D&A study on near-surface tropical ocean salinity changes. Recent (1970-2010) in-situ salinity observations show an enhanced hydrological cycle leading to an accentuation of salinity contrasts within and in between tropical ocean basins. The causes of these near-surface salinity changes have been investigated by using in-situ data (with a sustained collaboration with the ORE SSS scientists based at LEGOS) and the CMIP3 (Coupled Model Intercomparison Project phase 3) multi-model database, including both long control pre-industrial as well as historical simulations (Terray et al. 2012 RA). Results show that the anthropogenic-induced effect acts to freshening the western tropical Pacific, while the tropical Atlantic becomes saltier. This anthropogenically-induced amplification of the mean inter-basin tropical surface salinity gradient (and thereby of the mean tropical hydrological cycle) is already detectable in recent observations, meaning that its amplitude and pattern significantly differs from changes due to internal variability alone. In contrast, changes for the North Atlantic are within the range of the internal variability and then non detectable (Figure 2.1).

Our second contribution, still through a strong and sustained collaboration with CNRM/GAME, concerned the improvement of the traditional optimal fingerprint methodology that has been commonly and widely used for the last twenty years in all D&A studies. The latter often involves a projection onto a reduced order basis to improve the estimation of internal variability covariance matrix, a key ingredient of D&A methods. It is thus necessary to arbitrarily select a truncation level in the eigenvector basis and D&A results can be very sensitive to the chosen level. By using a regularized estimate of the internal variability covariance matrix, we showed that a much more objective and accurate method can be achieved leaving all other aspects of the optimal fingerprinting approach unchanged (Ribes et al., 2013 RA). We have then applied this new method to detect and attribute anthropogenic changes in the evolution of global near-surface temperature (Ribes and Terray, 2013 RA), confirming the major influence of anthropogenic forcing on the recent global temperature warming. However, the results also showed that it is still problematic to clearly separate the effects of greenhouse gases versus those of aerosols with the current model estimates of the fprced response. These results have been extensively used in the D&A chapter of the last assessment report (AR5) of the International Panel for Climate Change (IPCC).

Based on the new generation of improved coupled models used in the Coupled Model Intercomparison Project phase 5 (CMIP5), we have also undertaken studies to understand the 20th century variability and trends in some climate signals such as North Atlantic sea surface temperatures (Terray 2012 RA) and on the atmospheric Southern Annular Mode - SAM - (T. Oudar Ph.D, TR). With regard to the North Atlantic SSTs, we have assessed the relative roles of greenhouses gases, anthropogenic aerosols, natural forcings and internal variability in their decadal fluctuations using multi-model climate simulations driven by estimates of observed external forcings. While the latter are the main source of decadal variability in the tropics and subtropics, there is a large contribution from the unforced component to subpolar Atlantic variations. Reconstruction of forced response patterns suggests that anthropogenic forcing is the main cause of the North Atlantic accelerated warming of the last three decades while internal variability has a dominant contribution to the early 20th-century temperature multi-decadal swings and recent abrupt changes in the subpolar Atlantic. Regarding the SAM, analysis of the CERFACS/CNRM climate model has shown that its recent evolution is driven by combined forcings including ozone depletion, greenhouse gases as well as aerosols. A complete and robust attribution statement is still lacking due to the likely rejection of forcing response additivity hypothesis and the absence of multi-member simulations with only one forcing at the time (not existing for ozone and aerosols).

2.3 Links between atmospheric circulation regimes and the North Atlantic ocean variability

The Cerfacs has pioneered the use of weather regimes in climate studies related to continental variables such as land temperature and precipitation. We have worked on the possible extension of this approach to the problem of finding the daily atmospheric regimes imprint on both tropical and extratropical North Atlantic Ocean. Based on reanalyses products, the response of the surface ocean to the large-scale atmospheric forcing has first been investigated by a weather-typing approach (Cassou et al. 2011, RA). Results are indicative of strong relationships between daily large-scale atmospheric circulation and ocean surface over the entire Atlantic basin. These findings have then motivated the development of a statistical downscaling methodology to reconstruct the sea surface atmospheric variables necessary to force an ocean model (Minvielle et al. 2011 RA, Minvielle PhD TR). Along this direction, the interannual variability of subtropical sea-surface-height (SSH) anomalies, estimated by satellite and tide-gauge data, has been investigated in relation to wintertime daily North Atlantic weather regimes (Barrier et al., 2013 RA). Further modelling-based studies have confirmed the specific physical links between each of the classical North Atlantic weather regimes and the North Atlantic Ocean circulation (Barrier et al. 2014 RA). The results suggest that the Atlantic Ridge (AR), negative NAO (NAO-), and positive NAO (NAO+) regimes induce a fast (at monthly-to-interannual time scales) adjustment of the gyres via topographic Sverdrup dynamics and of the meridional overturning circulation via anomalous Ekman transport. In contrast, the wind anomalies associated with the Scandinavian blocking regime (SBL) are ineffective in driving a fast wind-driven oceanic adjustment.

2.4 Influence of sea surface temperature fronts on the atmosphere

There is now a large body of work suggesting that ocean-atmosphere interaction in frontal regions is very different from the traditional picture coming from basin-scale studies at seasonal to interannual time scales. While the latter shows that the ocean is mostly passive (its variability essentially reflects the atmospheric forcing), recent observations and modelling experiments have demonstrated that small-scale sea surface temperature (SST) patterns can indeed influence a large range of atmospheric parameters, both locally and remotely. The boreal winter atmospheric response to the Gulf Stream sea surface temperature gradients has thus been studied by using a high-resolution global atmospheric model in the framework of the ANR-ASIV project. A first experiment has been performed with a high spatial (0.25 $^{\circ}$) and temporal (daily) SST forcing. A twin-experiment has also been performed by spatially smoothing the SST patterns only along the North Atlantic frontal zone. The impact of small-scale SST patterns, obtained by looking at the difference between the two experiments, indicates, not only a strong meso-scale local atmospheric response (in terms of winds, heat fluxes and precipitation) due to hydrostatic surface pressure adjustment, but also some remote large-scale effects, affecting the weather regimes spatial patterns and the North Atlantic storm track characteristics (Figure 2.2) (From M. Piazza PhD 2014).

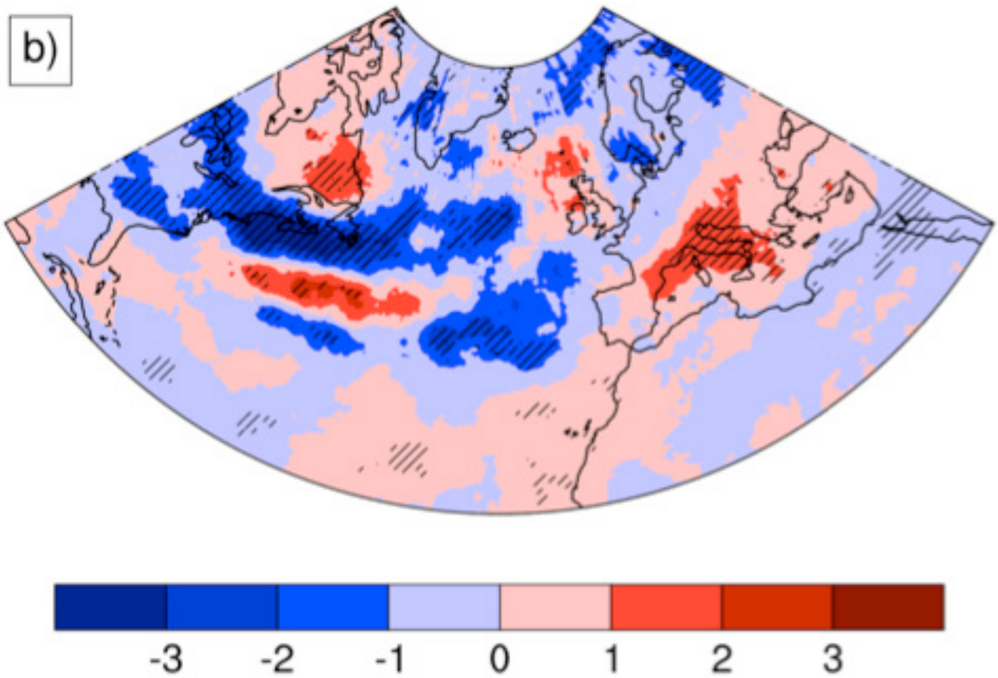

FIG. 2.2: Differences between the storm tracks density over North Atlantic during winter for an experiment forced by SSTs at high spatial resolution minus a second experiment forced by SST at low resolution in the Gulf Stream region (regions where differences are statistically significant at the 5% level are hatched). Units : number of trajectories per season. From Piazza et al. 2014 RA submitted

Decadal predictability and prediction

The 2009-2014 period corresponds for the Cerfacs to the emergence and full development of a new research theme centered on decadal predictability and prediction. This theme is at the core of the 2020 DECLIPP CERFACS project whose main objective is to achieve the development and scientific evaluation of an interannual to decadal prediction system using very high-resolution (horizontal resolution 25 km globally, with a well resolved stratosphere) climate models. This builds up on the early (early 2000's) Cerfacs effort dedicated to decadal variability and potential predictability studies based on the perfect model framework (the FP6 PREDICATE and DYNAMITE projects).

The first 2 years (2009-2011) have been almost entirely devoted to the setup, realization and basic evaluation of the decadal hindcasts or "near term" coupled experiments, performed within the WCRP/CMIP5 exercise. Cerfacs actively participated to the development of the new version of the CNRM-CM general circulation model (named CNRM-CM5) led by Météo-France (CNRM/GAME/GMGEC). The exact same model (same binaries, same resolution and same input files, Voldoire et al. 2013 RA) has been used in both CMIP5 centennial (carried out by CNRM/GAME) and decadal exercises (carried out by the Cerfacs) ; the latter only differs from historical simulations forced by observed natural and anthropogenic forcings by the initialization step. An original initialization technique based on nudging the ocean model towards the oceanic reanalysis in fully coupled mode was used to generate observed initial conditions. The use of the exact same code in the two centers is the concrete result of a long-lasting collaboration that was needed to pool the limited resources devoted to the development and evaluation of the CNRM-CM5 model. This task was very demanding and absorbed a large part of the Cerfacs human resources over the 2009-2012 period. It required a full investment from all the team members. In 2011-2012, the CORE hindcasts of CMIP5 considered as the "entry ticket" for model intercomparison studies, have been successfully completed. Figure 3.1 shows the predicted evolution of the anomalous global temperature predicted by the CNRM-CERFACS system materialized by the curves of different color together with the observations.

Model results have been rapidly conformed to CMIP5 compliance and published very early on the local CNRM-CERFACS Earth System Grid (ESG) node. It appeared that we were "first in time" among the 12 participating groups to the decadal initiative, to provide the data to the community through ESG. Additional experiments have been subsequently carried out and also published on ESG so that all together, the full-packaged CNRM-CERFACS hindcasts have been extensively used in model intercomparison studies from the beginning. In total, more than 5000 years of simulated climate have been performed requiring 200 000 CPU hours on the Météo-France NEC supercomputer and generating 120 Terabytes of data. The CNRM-CERFACS decadal forecasts have been included in Chapter 11 of the 5th IPCC assessment report dedicated to decadal predictability and prediction. The decadal forecast activity in Cerfacs has been supported by the EC-FP7 COMBINE project coordinated by MPI, the GICC- EPIDOM project and the PRECLIDE project sponsored by the BNP-Paribas foundation, both coordinated by Cerfacs researchers.

Besides fundamental science, the Cerfacs has also been very active to build capacity and knowledge on the theme of decadal forecasts. A vulgarization article has been published (Cassou and Mignot 2013 OT) and numerous invited talks in front of very diverse public (Forum ALLENVI, GICC seminars etc., general public) gave us the opportunity to better convey the messages inherent to decadal prediction and predictability, its successes but also its limits. In addition, the Cerfacs expertise in climate forecast is well recognized as materialized by a current membership in the WCRP/WGSIP/Decadal Climate Prediction Panel (DCPP) since early 2013.

Within this general context, four main axes of research have been followed over 2009-2014 as documented below.

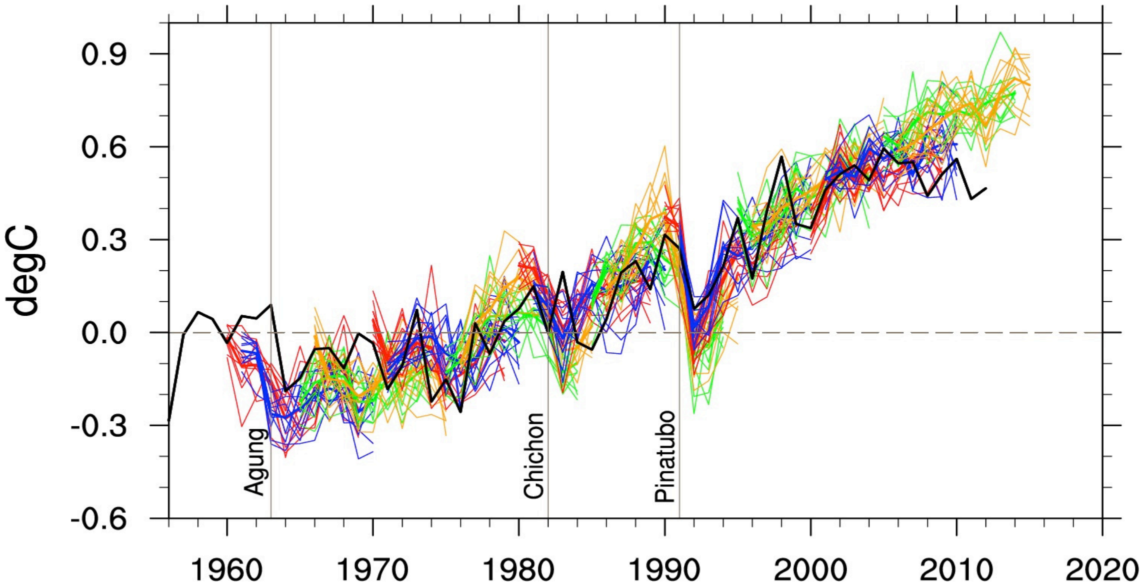

FIG. 3.1: Observed (black) and predicted (color) global temperature anomalies by the CNRM-Cerfacs system. Each color represents a given starting date and corresponds to a 10-member ensemble of 10-yr forecasts.

3.1 Understanding of the physical mechanisms involved in the drift of the model when integrated in forecast mode.

In Sanchez-Gomez et al. (2014 RA, submitted), a special attention has been devoted to the tropical Pacific characterized by a strong initial shock leading to a systematic excitation of an El Niño event during the first year of the forecasts. Such a shock is associated with the imbalance between the model wind and the tropical ocean initial conditions in the subsurface that are taken from a preliminary coupled simulation where the ocean component is restored towards the NEMOVAR (Daget et al 2009 RA) reanalysis. The emergence of a systematic strong El Niño at the earliest lead times perturbs the model adjustment of the entire climate system through teleconnections, especially over the North Atlantic basin. A hybrid method, in which the subsurface ocean restoring is only applied outside the 15oN-15oS tropical to ensure tropical subsurface/wind compatibility, has been implemented to reduce the ENSO shock ; the latter configuration is the one retained for CMIP5 decadal forecasts. The drift in the North Atlantic is also documented in Sanchez-Gomez et al. (2014 RA, submitted). Multitude processes characterized by very different timescales (rapid drift due to the atmosphere leading to a rapid slackening of the ocean circulation, water masses reorganization etc.) are presented over the 10-yr forecast range. Such an approach devoted to drift dynamics could be very useful to pinpoint the main mechanisms leading to systematic biases of the coupled systems and can provide some clues and pathways to reduce the latter. In addition to the understanding of the biases development per se, a special study has been also devoted to the bias correction method recommended in climate prediction. In collaboration with Météo-France, we have applied the Model Output Statistics (MOS) technique traditionally used in operational weather forecast, to the CNRM-CM5 decadal hindcasts. The potential added value of such a method has been thoroughly documented through the use of classical skill scores and confidence intervals (Y. Leauté, Master's thesis OT).

3.2 Understanding of the physical mechanisms involved in the decadal-to-centennial variability/previsibility of the CNRM-CM5 model in the North Atlantic.

Within the GICC-EPIDOM project and as a pre-requisite to better understand the sources and the levels of the predictability of the model in real hindcasts, the processes at the origin of the low-frequency fluctuations of the North Atlantic basin have been investigated in the model (Ruprich-Robert and Cassou 2014 RA). Their role in the predictability of the model Atlantic Multidecadal Variability (AMV) has then be estimated in a perfect model framework. Results highlight the importance of the salinity field in controlling both the persistence and decay of the AMV events in CNRM-CM5. The onset of the latter appears to be though unpredictable in the model since they correspond to the ocean integration of the low frequency portion of the white noise spectrum of the North Atlantic atmospheric variability. Potential predictability diagnostics reveal that the range and nature of predictability of the AMV is conditional to the initial states of the forecast. Predictability is found for marked phases of the AMV up to 30 years while it is lost for weak-to-moderate phases of the AMV after 10-15 years. In all cases though, the North Atlantic predictability is tightly linked to the water density of the subpolar gyre and in particular to the evolution of the integrated salinity whose fluctuations are mainly driven by anomalous transport either from the south through the North Atlantic Drift or from the North through the East Greenland Current connecting the Arctic to the mid-latitude Atlantic ocean.

3.3 Skill evaluation of the decadal forecasts.

Within the EC-FP7 COMBINE project and also thanks to tight collaborations within the decadal prediction community, the Cerfacs has participated to the multi-model evaluation and understanding of the forecast skill as a function of lead-time (Meehl et al 2014 RA). The results support the growing evidence that the current generation of climate models, adequately initialized, have significant skill in predicting years ahead not only the anthropogenic warming but also part of the internal variability of the climate system. An important finding is that the multi-model ensemble mean does generally outperform the individual forecasts, a well-documented result for seasonal forecasting, supporting the need to extend the multi-model framework to real-time decadal predictions in order to maximize the predictive capabilities of currently available decadal forecast systems. In Bellucci et al (2014 RA), the performance for all the European models is presented and the CNRM-CERFACS decadal prediction system appears as one of the most skillful for several climate indices except for the tropical North Atlantic/Sahel precipitation where the model is clearly deficient. The model biases over these regions are being tackled within the ongoing EC-FP7 PREFACE project.

3.4 Improving climate prediction systems.

There is now a large body of evidence suggesting that one need to increase model resolution in order to adequately represent some air-sea interaction key processes (such as the influence of oceanic fronts on the atmospheric boundary layer and the storm-tracks). Needless to say, progress in improving the model physics and parameterizations will also be required. The latest year of the 2009-2014 period has been devoted to the development and setup of a high resolution configuration of a new coupled system, hereafter CERFACS-HR prototype, whose atmospheric (ARPEGE) and oceanic (NEMO) components are the same as in CNRM-CM5 while LIM and ISBA are respectively the sea-ice and land surface components instead of GELATO and SURFEX. The atmospheric resolution is 50km x 50km with 31 levels over the vertical while the ocean resolution is $\frac{1}{4}$ of degree on average and 75 vertical levels (with a 1-meter resolution in the upper 20 meters). Such a development takes place within the ongoing EC-FP7 SPECS project and yearly forecasts covering the 1993-2012 period are currently being performed. GLORYS reanalyses from Mercator-Ocean that assimilate in situ temperature and salinity as well as satellite sea-level data are used in SPECS to generate initial conditions in a full initialization mode instead of NEMOVAR in CMIP5. The computational cost of the decadal forecast exercise as a whole using the CERFACS-HR configuration is such that only PRACE computers can provide the needed resources. Several projects with Cerfacs leadership or participation have been selected since 2012 : SPRUCE in collaboration with CNRM about high-resolution seasonal forecasts, HighResClim for decadal forecasts in support to SPECS.

Anthropogenic perturbations and impacts

The 2009-2014 period has seen the completion and publication of different studies of the impacts of climate change over France. Those studies were based on the statistical downscaling of climate models from the CMIP3 exercise with a weather typing method developed during the previous period by the Cerfacs. Different areas have been tackled in collaboration with specialists of the subject : continental hydrology (Boé et al. 2009 RA, Quintana Segui et al. 2010 RA, Joigneaux et al. 2011 RA, Habets et al. 2013 RA), ecosystems (Delpierre et al. 2009 RA, Cheaib et al. 2012 RA for forests, Armandine Les Landes, 2014 RA for wetlands), and agriculture (Gouache et al. 2012 RA, 2013 RA).

Concurrently, some works have been undertaken to pave the way for new estimations of the impacts of climate change over Europe and France, more accurate and more relevant for the society, building on the availability of new multi-model ensembles of climate projections (CMIP5 for global models, CORDEX for regional climate models.) To improve upon previous generations impact studies, works in three directions have been conducted, in the overall objective to estimate more accurately different important uncertainties involved in this kind of study (mainly from climate scenarios, climate models, downscaling methods and internal variability) and to reduce these uncertainties and/or errors when possible.

4.1 Better characterization of climate change signals and of the impacts of internal variability

Some analyses have been conducted in order to characterize the climate change signals directly in CMIP5 projections on weather phenomena especially relevant for the society but not necessarily much studied in that context : record-breaking temperatures over Europe within the ANR-SEEN project (Bador et al., 2014 submitted RA) and storms in the North-Atlantic/Europe sector (T. Oudar, Master's thesis). In these studies, a special interest has been given to the emergence of the climate change signals from the noise due to internal variability. More classically, future temperature and precipitation changes in Europe have also been studied (Terray and Boé 2013 RA) but thanks to the availability of several members differing only by the initials conditions for many CMIP5 models, it has also been possible to characterize the relative importance of uncertainties due to internal variability compared to the one due to climate models and scenarios (Terray and Boé 2013 RA). The impact of internal variability on the uncertainties in precipitation change over France in the 4 or 5 coming decades is very large. Without a potential reduction of those uncertainties thanks to the work on decadal predictions (see previous section), it imposes a stringent limit to the possible accuracy of climate and impact projections for the coming decades, which is useful to be known by policy-makers for adaptation strategies. This approach is therefore being extended to impacts variables (e.g. river flows) thanks to a statistical downscaling method that has been developed to allow a large number of climate simulations and members to be downscaled (see below).

4.2 Reduction of the uncertainties and/or errors in statistical downscaling methods

The main theoretical weakness of statistical downscaling is that a statistical relation between large-scale predictors and the high resolution local variables of interest (e.g. precipitation) is derived and evaluated using present-day observations and then applied to the future climate. The implicit hypothesis of the temporal transferability of the statistical downscaling method to the future climate is not necessarily justified and has received little attention to date. The transferability to the future climate of a statistical downscaling method lies on the choice of the predictors, that must capture all the physical processes involved with climate change. Our work has therefore been oriented towards an improved selection of predictors compared to previous studies, for a statistical downscaling method oriented towards hydrological applications over France, and a much better evaluation of the temporal transferability hypothesis with the development of a specific methodological framework (ANR ECHO project).

One of the most prominent signals in climate projections over France is a large decrease in summer precipitation, which is difficult to be taken into account by statistical downscaling methods, as it involves local processes. An observational study has been conducted to better understand how local processes such as soil-atmosphere interactions impact summer precipitation (Boé 2013 RA). This work has allowed some potentially interesting predictors to be identified. These predictors and others have been assessed for the statistical downscaling of precipitation within a specific methodological framework, based on the concept of perfect model, to test effectively and thoroughly in a multi-model framework the transferability hypothesis (Dayon et al., 2014 submitted RA). Instead of observations, the statistical downscaling relation is built using present-day predictors and precipitation simulated by a regional climate model. The entire projections are then downscaled, and future downscaled and simulated precipitation changes can be compared. This approach has shown that statistical downscaling methods that seem correct based on classical present-day evaluation are in fact not well transferable to the future climate. It strongly suggests that what are often identified, as uncertainties due to downscaling methods in impact studies, might often be, to a large extent, errors. The downscaling method is being applied to the downscaling of a large ensemble of CMIP5 projections to correctly estimate the uncertainties due to climate scenarios, climate models and internal variability after hydrological modelling.

Other approaches have also been investigated. To study extreme flooding events in southeastern France, a strategy based on high-resolution regional climate simulations with adapted bias correction methods from the CORDEX project has been developed (Ph.D thesis of E. Harader).

4.3 Reduction of the uncertainties due to climate models.

Current multi-model climate projections and hence impact projections suffer from large uncertainties. In our previous impact studies based on CMIP3 models and mentioned above, a special care has been given to the correct estimation of the uncertainties due to climate models. The logical way forward is to try to reduce those uncertainties. As a first step, it is necessary to understand the main physical processes responsible for them. Some studies have been conducted towards this objective. A study has been dedicated to the understanding of the opposite response to anthropogenic forcing of the Northern Annular Mode in winter between CMIP3 and CMIP5 multi-models (Cattiaux and Cassou 2013 RA). Another study has focused on the role of land-atmosphere interactions and cloud feedback in summer climate change in France (Boé and Terray 2014 RA).

In a long-term perspective, understanding the processes that are responsible of the uncertainties of a given variable is a mandatory step to select the aspects of climate models that need to be improved in priority. In a near term perspective, it is also necessary, in order to define useful metrics, to assess the relative credibility of different models, give more weight to the more realistic ones in the ensemble estimate and therefore reduce the associated uncertainties and/or errors. For example, we have shown that models with a strong negative interannual-correlation in summer between cloud cover and temperature tend to simulate larger decreases in cloud cover in the future climate and larger surface warming (Figure 4.1 and Terray and Boé 2013 RA, Boé and Terray 2014 RA). To assess the usefulness of this metric and devise the best way to use it, we have developed a methodological framework based on the concept of perfect model. It basically consists to try to predict the climate change signal of a given model, based only on its simulation of present-day climate and on present-day and future climate simulations from an ensemble of other models. It has been applied to summer temperature change in France to test different methodological issues. Metric-based methods using the metric related to cloud temperature interactions generally lead to large reductions of errors compared to the ensemble mean, but the sensitivity to several methodological choices is important (Boé and Terray, 2014 submitted RA).

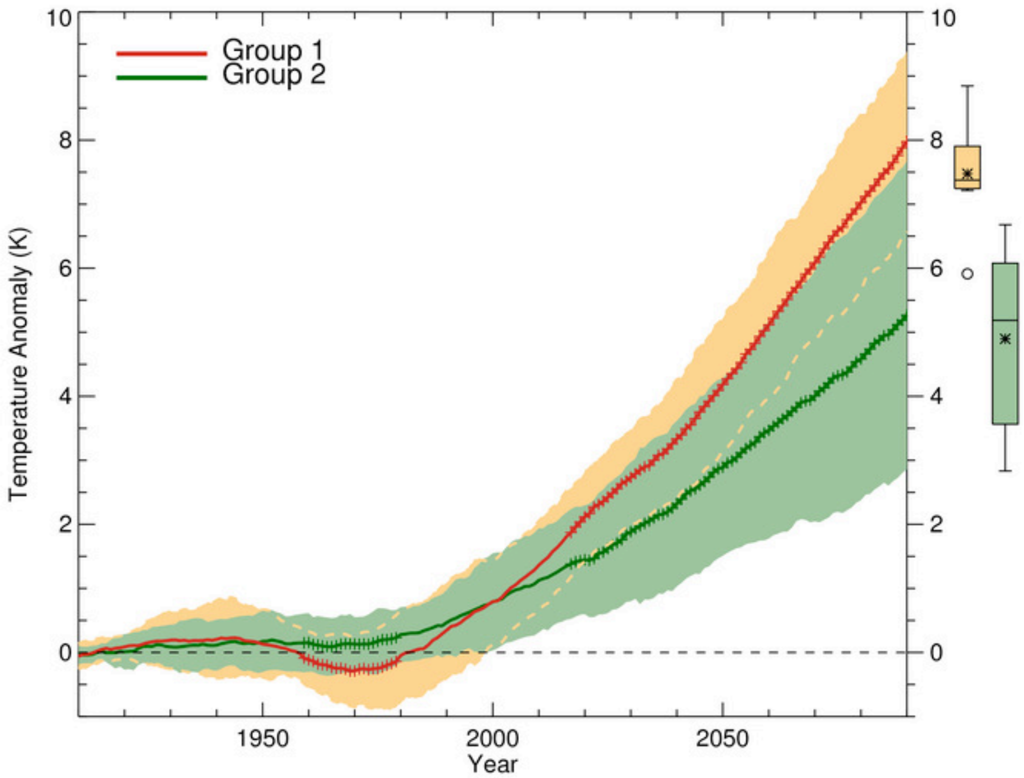

FIG. 4.1: Time evolution of France summer mean surface air temperature anomalies (K) relatively to the 1900-1929 climatology for the means of two groups of models (historical merged with RCP8.5 simulations). Group 1 : models with strongly negative present-day summer surface air temperature-cloud cover correlations (red line). Group 2 : models with weakly negative ones (green line). Surface air temperature time series have been low-pass filtered with a simple 21-year running mean. Shading and dashed lines give the envelope defined by the [5-95%] model range for each group of models. From Terray and Boé 2013 RA.

Publications

5.1 Journal Publications

[CM1] N. Barrier, C. Cassou, J. Deshayes, and A.-M. Treguier, (2013), Response of North Atlantic Ocean Circulation to Atmospheric Weather Regimes, *Journal of Physical Oceanography*, **44**, 179–201.

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6

Computational Fluid Dynamics

Introduction

CFD is one of the main activities at CERFACS. It is also the field which probably has the most direct contacts with industry because the tools developed in the CFD team are used more and more for the design of real systems, especially in the aeronautics field. This explains why the activities of the team evolve fast. Since 2010, the CFD field has been undergoing major evolutions. One of them is the introduction of unsteady methods (LES in most cases) not only in research but also in almost all applications. Another one is the generalization of multiphysics tools.

The CFD report is split in two main parts :

– Combustion (leader : B. Cuenot)
– Aerodynamics (leader : J.F. Boussuge)

The interaction between these two parts of the team has kept growing because the fields they work on are now intersecting : for example turbomachinery combines both aerodynamic studies and combustion. The development of high-order methods for LES or the treatment of walls in LES formulations are also common research themes. Aircraft noise, which combines aerodynamic and combustion noise, is studied jointly. Pre and post processing techniques are developed in collaboration.

The following sections provide a summary of the most remarkable results obtained by the CFD team since 2011. A few salient points are pointed out here :

Academic excellence

The CFD team continues to publish in the best journals and to produce PhDs at a high rate. Table 1.1 provides the number of papers published per year in A journals as well as the number of PhD defended. With an average of 13 permanent researchers present in the team over this period, the number of papers

Year	Papers in A journals	PhD defended
2011	25	9
2012	27	10
2013	24	9
2014	30	11

TAB. 1.1: Number of papers in A journals and PhD defended in the CFD team

published per year and permanent researcher is 2 which is in the typical range of CNRS laboratories in similar fields. Many PhDs work in the team, confirming the importance of formation : more than 35 PhD students are present in the team in 2014. Many of these PhDs have received prizes (I. Duran, E. Collado and B. Franzelli : L. Escande prize, F. Crevel : EDF P. Caseau prize, E. Collado : Novela prize, B. Franzelli and P. Sierra : A. Earhart prize) and all have found positions in industry or academia rapidly. B. Franzelli is now a CNRS full time researcher at EM2C Paris. The team has also won an ERC grant (see below) and its leader was awarded the 2014 aeronautic prize by the 3AF association (Association d'Aeronautique et d'Astronautique de France).

The ERC advanced grant INTECOCIS on combustion instabilities

In 2013, IMF Toulouse and CERFACS have won an ERC (European Research Council) INTECOCIS advanced grant in the field of thermoacoustics (intecocis.inp-toulouse.fr). This 2.5 Meuros grant allows the development of a joint thermoacoustics team in Toulouse where IMFT and CERFACS team collaborate to study combustion instabilities in multiple systems from small laboratory burners to full rocket engines. Considering that combustion instabilities were already strong topics at both IMFT and CERFACS, this means that this group is probably the largest thermoacoustics team worldwide today (10 researchers at IMFT and 12 at CERFACS). This topic also extends to combustion noise which is becoming another active field of research because its relative contribution increases rapidly in aircraft and helicopter noise.

The development of LES for turbomachinery
While LES for combustion has been highly successful over the last ten years and CERFACS with its partners (IMFT, EM2C, CORIA, STANFORD) has played a major role in the field, LES for turbomachinery is still an open topic, mainly because of the complexity of the geometries and of the wall treatments. The CFD team has been exploring multiple solutions to build high-fidelity methods for turbo machinery flows. In the CN2020 program supported by SAFRAN, CERFACS has contributed with three solvers (AVBP, YALES2 and JAGUAR, a spectral difference code) to test which methods were showing the best potential to perform multistage LES on massively parallel machines (billions of points on hundreds of thousand processors). The strategy elaborated by CERFACS has been to explore a first solution based on the solvers used for LES of reacting flow (AVBP and YALES2, order of accuracy 3 to 4) while developing a new class of higher-order codes (more than 4) in a spectral difference tool called JAGUAR.

Coupling
Stand-alone CFD methods are slowly losing ground, compared to coupling techniques which allow multi physics to be taken into account. The following pages show how the CFD team collaborates with the GlobC team and ONERA to develop the OpenPalm coupling software and to incorporate coupling in most of our simulations. This is necessary for dual heat transfer problems, for radiation of for multi domain problems such as chamber / turbine coupling. Coupling is not only a field of research in terms of physics : it rapidly becomes a computer science question where CERFACS has chosen to couple individual solvers using OpenPalm rather than merge all in a single solver because industry applications will clearly go into this direction.

The introduction of new topics
The arrival of Total as a shareholder of CERFACS has allowed to open new fields of research : the simulation of explosions in buildings has been quite successful, leading to an INCITE project in 2013 and 2014 (18 and 80 million CPU hours on the BG/Q of Argonne). Petrochemistry also provided exciting new topics where CERFACS studied the reacting flow inside a ribbed duct in collaboration with Von Karman Institute, Stanford and ISAE Toulouse.

High-order methods
Most present solvers used at CERFACS are high-order codes, using typically third-order accurate methods. The idea of extending these methods to higher-order techniques while still being able to handle unstructured meshes is growing fast and the development of the JAGUAR solver at CERFACS (spectral difference) as well as the collaboration with CENAERO on DG (Discontinuous Galerkin) techniques are very dynamic fields of activity at CERFACS. This report presents examples of the astonishing accuracy of such techniques in multiple test cases.

Elearning and training
The Elearning web site of CERFACS contains a large section dedicated to CFD and works quite well (elearning.cerfacs.fr). It is now associated to a very intense training program (www.cerfacs.fr/19-25708-Home.php) which provides formations on LES, combustion, mesh generation, acoustics, etc.

Combustion

Combustion science and technology cover a large variety of different physics, which are often coupled. They include chemistry, thermodynamics, acoustics, heat transfer, multiphase flow and turbulence. Being able to take into account all important physics and their coupling in simulations is a key point to obtain accurate predictions of a burner efficiency, thermal behavior, ignition performance, pollutant emissions, etc. All these aspects are addressed by the CFD team and presented below (turbulent combustion, noise and combustion instabilities, multi-physics).
Another key aspect of simulation at CERFACS is High Performance Computing, as CERFACS is deeply convinced that it is an essential contribution to the progress in simulation and modeling. To always maintain a high scalability, CERFACS codes are constantly adapted to the successive machine architectures.
Applications are mostly in the field of aeronautic propulsion, but also concern now explosions, petrochemistry, turbo-machinery and new burner concepts such as Constant Volume Combustion (CVC).

2.1 Turbulent Combustion Modelling

2.1.1 Chemistry and pollutant emissions (C. Becerril, A. Felden, T. Jaravel, G. Lecocq, B. Cuenot, E. Riber, O. Vermorel)

flame structure limit the prediction capabilities for complex non-adiabatic turbulent spray flames in real geometries. CERFACS has used both approaches for a long time in collaboration with its academic partners, but during the last three years, CERFACS has started to work on a new approach using analytically reduced chemical schemes, derived from detailed kinetics using mathematical methods based on graph theory or sensitivity analysis. Such schemes typically contain ten to fifteen species [4]. As they include all main physical chemical paths, they are able to predict with good accuracy complex flames in various conditions. The computational cost associated to the increased number of species to be solved, is affordable today in Large Eddy Simulation (LES) of complex flames in real geometries thanks to the increase in computational power. CERFACS collaborates on this topic with Dr P. Pepiot from Cornell University and uses the chemistry reduction tool called YARC to derived analytically reduced schemes adapted to LES (PhD of A. Felden, 2014-2017). First tests on methane combustion confirm the great capacities of such schemes. LES of the TNF Sandia D turbulent methane-air flame showed very good agreement with experimental results and a reasonable computing cost (PhD of T. Jaravel, 2013-2016). These schemes also reproduce the correct physics at very high temperature in the context of ignition.
In parallel to chemistry modeling, CERFACS develops models for pollutants. The analytically reduced schemes have been shown to accurately predict CO, as they contain the main physical chemical paths producing CO. For NOx, CERFACS has shown in the LES of the TNF Sandia D flame that an analytically reduced scheme can be enriched by three additional species to correctly reproduce NOx levels. Soot is the product of much more complex processes, starting by nucleation (formation of the first particles) that occurs through collisions of polycyclic aromatic hydrocarbons (PAHs). This step is followed by particle size increase due to mass addition on the surface, either C2H2 addition or condensation (PAHs addition). Simultaneous oxidation by both O2 and OH may counteract particle growth and even lead to particle size decrease. Finally, soot particles aggregate to form nano-size particles. Accounting for all these physical and chemical features is very challenging in terms of modeling and computing resources. As a first step,

CERFACS has proposed to use a phenomenological two-equations soot model [2] and to couple it with a hybrid chemical description (reduced chemistry for the flame and tabulated chemistry for the soot gaseous precursors, i.e. OH ad C2H2). The model has been evaluated in academic configurations of counterflow diffusion sooting flames [CFD49] and compared with a fully tabulated method as well as measurements in a lab-scale turbulent swirled flame, leading to encouraging results [CFD116].

2.1.2 Two-phase combustion (P. Sierra, G. Hannebique, G. Chaussonnet, D. Paulhiac, F. Shum-Kivan, E. Riber, B. Cuenot)

Two approaches are available in AVBP to compute the dispersed liquid phase found in all combustion systems using liquid fuels. The Eulerian approach considers the spray ensemble average and solves it as a continuous phase, while the Lagrangian approach tracks individual droplet trajectories. In the PhD of P. Sierra (defended in 2012), the Eulerian model implemented in AVBP has been improved to account for the uncorrelated motion of particles following the ideas of Masi et al [6, CFD84]. A new evaporation model has also been developed, to better fit experimental data by an improved evaluation of the diffusion coefficients of the mixture surrounding the droplet. G. Hannebique (PhD, 2010-2013) performed a systematic comparison of Eulerian (mono-disperse) and Lagrangian (both mono-disperse and poly-disperse) formulations on simple test cases and on lab-scale and real gas turbine configurations. Both approaches give very similar results for mono-disperse sprays. However the impact of polydispersity was found to be important on the local flame structure [CFD26]. This work was continued by D. Paulhiac (PhD 2011-2014) who extended the two-phase combustion model to the various possible regimes, in particular individual droplet burning. Comparisons with the experiment of Cambridge [5] showed the good behavior of the model and the capacity of AVBP to simulate complex two-phase flames (Fig 2.1), where droplets can burn both in classical gaseous mode but also as isolated droplets surrounded by burnt gas. Recently, F. Shum-Kivan (PhD, 2013-2016) has started to work on the computational efficiency of the Lagrangian solver, in particular the optimum domain partitioning under both flow and spray constraints.

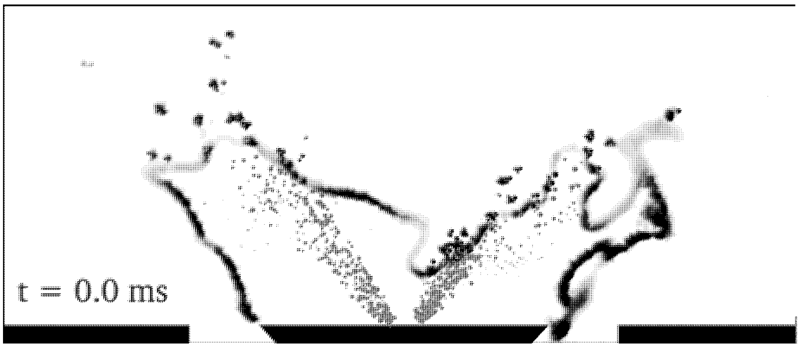

FIG. 2.1: LES of the Cambridge burner : view of the spray and the flameexhibiting purely gaseous combustion and single droplet burning.

Another important feature in liquid burners is the presence and impact of liquid films. These may appear first at injection, when the atomizer is placed in a diffuser and generates a spray that impacts the walls, or in piston engine with direct injection with spray impact on the piston bowl. Downstream in the combustion chambers, liquid films may also form when droplets impact the walls, in particular before ignition. Liquid films have important consequences on the combustor behavior in terms of wall heat exchange, turbulent flame structure, unburnt fuel and pollutants. The implementation of a model for spray-wall interaction (splash and rebound), liquid film motion and re-atomization, has been made by G. Chaussonnet (PhD 2010-2013, First European project), to compute airblast atomizer injection in gas turbines. The model was validated against the experimental data of [1] and applied to a real industrial configuration showing the strong impact of the liquid films.

2.1.3 Ignition (L. Esclapez, D. Barré, C. Becerril, B. Cuenot, L. Gicquel)

Very lean combustion has recently gained high interest especially to lower NOx emissions while keeping engine efficiency. However, the resulting weaker combustion leads to less favorable conditions for ignition. The ignition process of a combustion chamber can be decomposed into four steps. First, a spark plug or a laser beam deposits energy to create a plasma with very high pressure and temperature in a small volume around the igniter. Second if the energy deposit is sufficient and local conditions are favorable, a small flame kernel is formed. Then, the kernel expands and propagates upstream to ignite the first injector. Finally, the injector-to-injector flame propagation leads to the full relight of the combustion chamber. CERFACS works on all these steps to improve knowledge of the ignition process. The first step has been studied during the internship of C. Becerril (2013) within the ANR project FAMAC (2012-2016) performing Direct Numerical Simulation of the first instants after energy deposit to better account for the first chemical reactions. A strong collaboration with the experimental team of B. Renou at CORIA in the framework of the KIAI European project within the PhD of D. Barre (2011-2014) and L. Esclapez (2012-2015) has enabled considerable progress for the three other steps. Cross-comparisons between experiments and LES in a non-premixed methane-air single burner have shown the capacity of LES to predict ignition probability [CFD39]. Moreover, to improve the ICRIT-LES tool developed to generate an ignition probability map from non-reactive simulations, a large number of LES of ignition sequences are currently post-processed (PhD of L. Esclapez). Finally, LES of full transient ignition sequences in a multi-injector burner have been performed varying the inter-injector distance (Fig. 2.2). Comparisons with measurements show the capacity of LES to predict the ignition time and the propagation mode. The detailed analysis of LES results allowed to identify the driving mechanisms leading to the different propagation modes [CFD39]. The methodology developed in this academic configuration is currently being applied in a real prototype combustor from Safran Snecma within the LEMCOTEC European project (Fig. 2.6).

FIG. 2.2: LES ignition sequence in the KIAI multi-burner configuration of CORIA.

2.2 Combustion instabilities and combustion noise

2.2.1 Combustion noise (C. Silva, C. Becerril, M. Leyko, C. Lapeyre, T. Livebardon, M. Ferand, T. Poinsot, G. Staffelbach, F. Nicoud, S. Moreau)

Aircraft noise is one of the strongest noises generated by men and studying the interaction of flames and noise has become an important issue today : like NOx or soot, combustion noise is a 'pollutant' produced by engines and its control and prediction are now major topics at CERFACS with multiple PhDs, an ANR (DISCERN) and an EC (RECORD) project. In certain cases, combustion noise enters a resonant loop leading to combustion instabilities and engine damage : this topic has always been a strong field for CERFACS, and has grown even more recently with the beginning in 2013 of an ERC (European Advanced Council) advanced grant in collaboration with IMFT (intecocis.inp-toulouse.fr). The noise created inside the combustion chamber itself is now a significant part of the total noise created by aircraft of helicopters because other noise sources have been strongly reduced in the last twenty years. Combustion noise can be heard now and it must be understood to be controlled. The mechanisms leading to combustion noise in a cavity like an engine are subtle : part of the noise ("direct noise") is simply due to unsteady combustion acting like a monopole source ; another part ("indirect noise") is due to the interaction of the hot pockets generated in the chamber with the turbine flow : when pockets of hot and light gases are accelerated in a turbine stage, additional indirect noise is produced and this is a major contribution in most gas turbines. With the support of its shareholders, CERFACS has been studying these phenomena for five years in collaboration with Univ. Montpellier, Univ. Sherbrooke, EM2C in Paris and DLR Berlin. This work is also supported by the ANR DISCERN program (coord : EM2C, Dr Ducruix) and the EC RECORD project (coord : DLR, Dr Bake) which provide unique experimental data. M. Leyko (SNECMA) and C. Silva (SNECMA) initiated this study and showed that combining LES within a combustion chamber with analytical tools for noise generation through turbine stages (essentially based on Marble and Candel theory (J. Sound Vib. 1977, 55) for compact nozzles) was the proper approach to predict both direct and indirect noise in gas turbines. Their PhDs work were applied to helicopter engines by T. Livebardon (TURBOMECA) and aircraft engines by I. Duran (SNECMA) and M. Ferand (SNECMA). The method was tested in the choked combustion chamber of EM2C by C. Lapeyre (CERFACS). In parallel, a major theoretical breakthrough was achieved when the analytical approach of Marble and Candel was extended to non-zero frequencies and published in J. Fluid Mech. [CFD20]. CERFACS methods allow now to compute the impedances of compressors and turbines at all frequencies of interest (typically longitudinal modes). These impedances are crucial inputs for CONOCHAIN (Fig. 2.3), the complete simulation tool for combustion noise which CERFACS has set up to predict both direct and indirect noise in gas turbines. CONOCHAIN has been tested on a full helicopter engine (ECTEENI project coordinated by Dr Bouty, TURBOMECA) and is being tested on an aircraft engine in 2015.

Multiple publications have been produced in the last five years in this project, presenting the methods [CFD21, CFD20], the validations in elementary cases [CFD22, 3] and the application to complete engines [CFD37]. The next step in this field is the fully coupled computation of chamber and turbine flows : this is one of the applications of the COUGAR CERFACS challenge which aims at computing a full gas turbine. As the tools to do this become available, the analytical method used for noise production and propagation through the turbine can be verified, improved and ultimately replaced by a full simulation. This evolution will be mandatory to compute the noise of new engine concepts such CVC (Constant Volume Combustion) or RDE (Rotating Detonation Engines) where the chamber operates in a pulsated mode and the turbine is fed with an unsteady flow. Such systems can not be designed anymore on a modular basis (chamber on one side and turbine on the other one) like before. The conception must be based on a coupled simulation of chamber and turbine together and probably compressor too as envisioned with COUGAR.

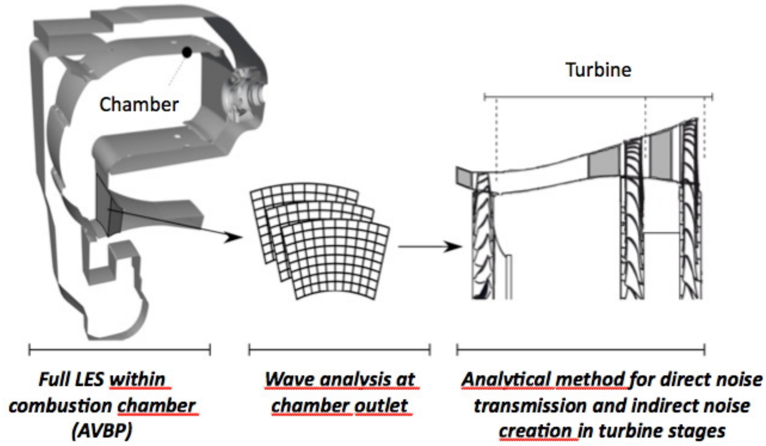

FIG. 2.3: The CONOCHAIN tool to predict combustion noise : an LES is performed in the chamber. All waves are measured in the outlet planes and propagated into the turbine stages using theory to obtain both direct and indirect noise in the outlet nozzle.

2.2.2 Combustion instabilities (P. Salas, M. Falese, E., P. Wolf, D. Shin, M. Bauerheim, A. Ghani, D. Maestro, S. Hermeth, F. Ni, A. Ndiaye, G. Staffelbach, T. Poinsot, L. Gicquel, J. Dombard, L. Giraud, F. Nicoud)

Combustion noise, as described in the previous section, is a one-way process : flames make noise and this noise is propagated. If this noise is reflected and can influence flames in a feedback loop, then the noise level can increase by 20 to 40 dB, leading to combustion instabilities. These instabilities are not 'noise' : they can destroy an engine in a few seconds and reach amplitudes of the order of the mean pressure. Combustion instabilities are often the main reason why LES methods are introduced in industry : no other method can capture these resonant mechanisms where combustion and acoustics couple, leading to excessive noise, vibration, quenching, flashback and in most cases, engine damages. CERFACS was the pioneer in this field and has developed now a full chain of simulation tools for combustion instabilities called QUIET (Fig. 2.4). This tool incorporates methods as expensive as LES of full unsteady combustion in complex chambers but also acoustic solvers where only the acoustic field is searched for or fully analytical techniques developed recently to complement numerical solvers and provide guidelines for control or UQ studies. The beginning of the ERC advanced grant INTECOCIS (intecocis.inp-toulouse.fr) has been a major thrust since 2013 : the collaboration of IMFT and CERFACS teams on thermoacoustics makes Toulouse the world largest group in this field. This collaboration reaches also far beyond Toulouse and CERFACS collaborates actively on thermoacoustics with EM2C, Cambridge, NTNU or Stanford, leading the research in this field as shown for example by the invited lecture on thermoacoustics given by Dr Poinsot at the 2014 APS DFD meeting in San Francisco.

Combustion instability studies cover first the identification of mechanisms in simple cases such as the gaseous combustor of Un. Twente [CFD29], studied within the LIMOUSINE EC Marie Curie project coordinated by CERFACS or the Mercato ONERA liquid-fuel combustor studied within the COPA GT Marie Curie project also coordinated by Dr. B. Cuenot at CERFACS. These studies are accompanied by applications to real engines for SNECMA, TURBOMECA, HKS or ANSALDO combustors [CFD32, CFD53, CFD27, CFD46]. In many cases, being able to compute the impedances of compressors and turbines is a major issue (like for combustion noise studies) and CERFACS has developed new techniques for this question [CFD9, CFD20]. What is called 'indirect noise' in the world of combustion noise has a counter part in thermoacoustics called 'mixed modes' : hot spots can create transmitted acoustic waves

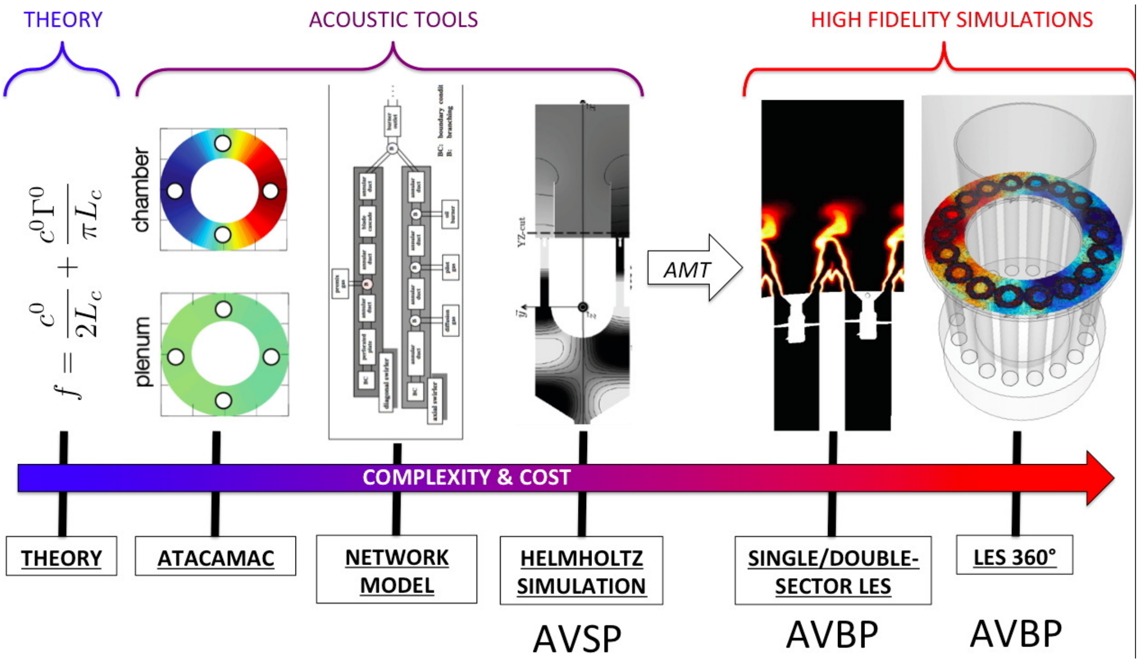

FIG. 2.4: QUIET : a summary of the methods developed at CERFACS to study combustion instabilities

in nozzles but can also induce reflections where acoustic waves come back to the chamber and lead to resonances. As an example, Fig. 2.5 shows a mixed mode where hot pockets travels at the convection speed from the chamber, create a reflected acoustic wave when they hit the outlet nozzle and trigger a new pocket formation in the primary zone. This work, published in JFM [CFD52], provides new insight into these instabilities which are not controlled by acoustic modes only and require new models.

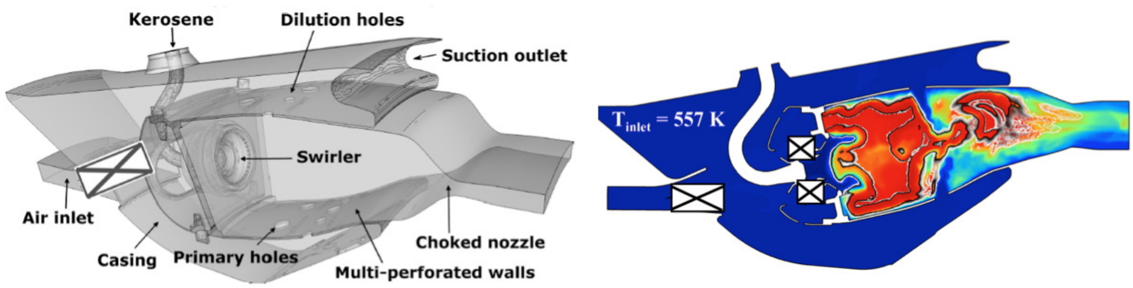

FIG. 2.5: LES of a mixed oscillation mode in an aircraft engine. Pockets of burnt gases separate from the primary zone and impinge the outlet nozzle where they create a reflected acoustic wave.

A significant evolution since 2012 is the development of theory and of a purely analytical method (called ATACAMAC) dedicated to the prediction of unstable azimuthal modes in annular chambers. This method (zero CPU cost) has become a complementary technique for LES and acoustic solvers which have significant CPU costs. ATACAMAC has received a strong interest in the academic community [CFD11, CFD40, CFD41] because it allows to investigate problems which are far beyond the capabilities of simulation tools such as the work published in J. Fluid Mech. on symmetry breaking in annular chambers [CFD42]. Analytical methods also allow to introduce UQ (Uncertainty Quantification) methods into thermoacoustics to give not only the growth rate of a given mode but also the possible dispersion of this growth rate taking into account uncertainties and therefore the stability probability of each mode (work in collaboration with Stanford and Univ. Montpellier in the UMRIDA EC project).

Among all possible combustion instability modes, oscillations associated with transverse modes (for example between lateral walls) are the most destructive. These high-frequency oscillations (sometimes called screech) can reach amplitudes where the unsteady pressure is of the order of the mean pressure, leading to a destruction of the engine in a few cycles. CERFACS is developing new LES and acoustic tools to study their development because LES reveals that transverse modes appear in many gas turbines studied at CERFACS even though experimentalists often do not see them as long as the engine resists.

Of course, the development of efficient massively parallel solvers for LES but also for three-dimensional acoustic solvers (Fig. 2.4) remains essential : CERFACS works with INRIA on AVSP solvers (the Helmholtz code of CERFACS) to improve its efficiency on massively parallel machines and the thesis of P. Salas (joint work between INRIA and CERFACS) allowed to introduce multiple recent methods for large linear systems which dominate the resolution in acoustic solvers in frequency domain such as AVSP. For LES, AVBP remains one of the only solvers able to compute full annular chambers today and its development on parallel architectures remains a major work in the team. These capacities allow to study very complicated chambers such as rocket engines for example in PRACE projects (collaboration with EM2C and IMFT).

Finally studies of combustion instabilities will also rely more and more on simulations including both chamber and turbine (at least the first stages of the turbine) because the first stages clearly interact with the combustion process. For example, during oscillations, the outlet High Pressure Stator might un-choke, drastically changing the boundary condition. This is a mechanism which will require full coupling. Such fully coupled computations have already started at CERFACS but not yet for unstable regimes.

2.3 Heat transfer and multi-physics

Aerothermal coupled simulations (R. Fransen, S. Berger, D. Lahbib, P. Aillaud, T. Grosnickel, L. Gicquel, L. M. Segui Troth, F. Duchaine, T. Poinsot)

Qualifying accurately the thermal state of any industrial device is at the root of the design phase of any aeronautical or thermal application. It is the key physical element that measures the thermal efficiency of any engine that is assembled to represent a reference and ideal thermodynamic cycle. Heat losses are a primary source of deviation from the ideal reference and therefore needs to be qualified not only to improve existing designs but also to ensure durability and reliability of the different components of the engine. To address such issues and improve state-of-the-art, code coupling of the three-heat transfers physical processes has been chosen : i.e. LES (AVBP) for flow turbulent convection, solid conduction (AVTP) and radiation (PRISSMA). Fully unsteady in nature this chain has first been applied to steady state problems of interest to CERFACS' partners and for validation. These demonstrations cover :
- Multiperforated plate heat transfer (PhD of D. Lahbib)
- Turbine blade applications involving external and internal cooling problems [CFD79, CFD102]
- Thermal state evaluation of a helicopter combustion chamber [CFD122, CFD126]

The use of the coupled chain results first in the generation of new design tools for CERFACS' partners. Such tools then aim at providing numerical databases on canonic configurations to enhance the comprehension of complex thermally coupled flow physics as well as the elaboration of new models.

2.4 Applications

2.4.1 Spatial propulsion (R. Mari, L. Lacassagne, T. Bridel, L. Potier, B. Cuenot, E. Riber, O. Vermorel, L. Gicquel, G. Staffelbach, L. Selle)

Spatial propulsion is a very specific topic, which requires the use of a dedicated version of AVBP to account for supercritical and transcritical thermodynamics. Since the pioneer work of T. Schmitt (PhD defended in 2010), important efforts have been devoted to further develop the modeling and simulation of cryogenic combustion in collaboration with EM2C Laboratory (Dr. T. Schmitt and Pr. S. Candel). One particularly critical issue in rocket engines is heat transfer : reactants injected at temperatures of the order of 100K, immediately burn after injection and reach temperatures above 3000K. This means that the solid parts of the injection system are exposed to extremely high temperature gradients, generating strong and fluctuating heat fluxes which eventually lead to thermal fatigue. In addition, the important heat flux to the solid raises the question of the possibility of flame detachment. The only way to address such problems is to perform CFD-heat transfer coupled simulations. This was the research project of R. Mari (PhD CNES-SNECMA, 2011-2014), who developed a methodology for such coupled simulations in the context of rocket engines, and studied the impact on flame stabilization in lab-scale and real configurations [CFD83]. The work is now continued by L. Potier, who started his PhD (CNES-SNECMA) in 2014, with the objective to investigate the behavior of the cooling systems in combustion chambers.
In the period of the present report, two additional activities linked to spatial propulsion have started.
The first one is still linked to the study of combustion, but in solid propellers. In such systems, aluminium particles are released together with the burnt gas produced by the combustion of the solid propellant, and in turn are consumed in an individual particle burning regime, adding locally important heat sources. Solid propellers are known for there tendency to generate various types of hydrodynamic instabilities, which are highly undesirable as they reduce the system efficiency and even increase the risk of damage to the rocket and the satellite. The impact of the burning aluminum particles on these instabilities is not very well understood and this is the topic of L. Lacassagne (PhD, CIFRE SAFRAN 2013-2016).
The second new activity is the study of flow stability in rotor/stator cavities of turbo-pumps, addressed through the funding by SAFRAN Vernon and CNES of the PhD research of T. Bridel. This research project is conducted in collaboration with the IRPHE laboratory who provides experimental data.

2.4.2 Aeronautical engines (G. Hannebique, L. Esclapez, T. Jaravel, M. Bauerheim, L. Labarrère, E. Riber, B. Cuenot, A. Dauptain, G. Staffelbach)

G. Hannebique (PhD, 20110-2013) applied the two-phase reacting flow solver to the configuration of the TLC European project to predict ignition in the presence of a spray in a gas turbine. The methodologies described above have also been used to help the design of a new burner in the European project LEMCOTEC (Fig 2.6), coordinated by Safran. AVBP simulations allowed to characterize the burner in terms of ignition capabilities (L. Esclapez, PhD 2012-2015), pollutant emissions (T. Jaravel, PhD 2013-2016) and combustion instabilities (M. Bauerheim, PhD 2011-2014).
The activity on multi-perforated liners Conjugate Heat Transfer (CHT) problems, supported by the PhD of D. Lahbib (2nd y., Cifre Turbomeca), led to two major outcomes : a reliable database of a coupled multi perforated plate at flight conditions was created, and the thermal model of Cottin developed at ONERA has been implemented and tested. This work showed the accuracy of Cottin's thermal flux modelling at injection sides but a strong inaccuracy (50% missing) at suction sides, and emphasized a systematic flaw in the current implementations. Next year, the activity will focus on the design of an improved thermal flux model, and on the creation of a second database at flight condition for azimuthal perforations. An article on the CHT phenomenology near a multi-perforated liner is in preparation.
Constant Volume Combustion (CVC) is still a pioneering field for CERFACS, which is supported by the PhD of L. Labarrere (2nd y., Cifre DGA-Comat). In 2014, large eddy simulations of an experimental

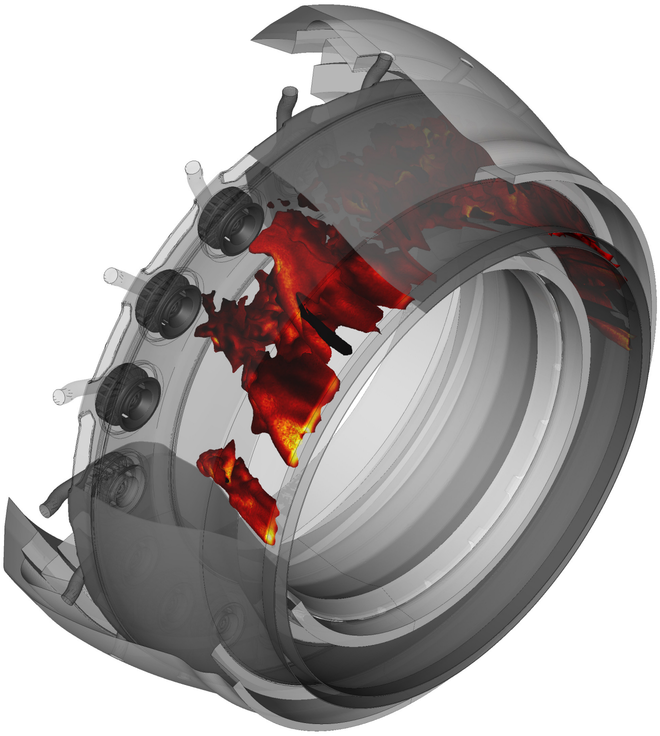

FIG. 2.6: LES ignition sequence in the LEMCOTEC prototype combustore.

CVC chamber (Thermoreacteur, Pprime, Poitiers) has been performed using two innovative moving mesh approaches to handle moving valves : Lagrangian Immersed Boundary, where the mesh is fixed, and MISCOG, where the mesh around the valves is rotating. Meanwhile, a 0D model has been built, using both inputs of the experiments and the simulations. An article comparing the pros and cons of LIB and MISCOGs approaches for CVC is in preparation.

2.4.3 LES of turbomachinery (J. Delaborderie, G. Wang, C. Koupper, D. Papadogiannis, L.M. Segui-Troth, L. Gicquel, F. Duchaine)

During the 2012-2014 period, a new tool (TurboAVBP) dedicated to Large Eddy Simulation of turbomachinery stages was developed based on the AVBP solver (G. Wang - RTRA). Large Eddy Simulations of turbomachinery stages is being investigated through multiple sides. First, LES numerically compliant solutions are required and must ensure proper treatment of the rotating interface in agreement with LES numerical constraints : i.e. high-order, low dispersion and dissipation schemes [CFD114, CFD128, CFD55]. Second, validations and assessment of the TurboAVBP tool for real applications have been obtained by D. Papadogiannis for the experimental MT1 configuration and a demonstration of a fully integrated combustor / high pressure turbine simulations has been obtained [CFD123]. To complement this demonstration, an application dedicated to the turbine-generated noise : i.e. direct versus indirect noise has been investigated by D. Papadogiannis (PhD, COPA-GT project 2012-2014). For combustor / turbine predictions, specific characterizations of exit temperature and turbulence profiles are studied by C. Koupper within the EU project FACTOR which addresses more specifically issues linked to the relative position of the high pressure distributor and fuel injector relative position as well as combustor turbine interactions

[CFD122, CFD47, CFD48]. All these actions are further supplemented by fundamental research in the field of LES modeling and its coupling with near wall turbulent flow approaches (L. Troth, PhD COPA-GT).

2.4.4 Piston engines (A. Misdariis, O. Vermorel, T. Poinsot)

Downsizing is a major pathway in order to improve engine efficiency and reduce CO2 emissions. Its principle is to increase the specific load at which the engine is operated. The resulting higher fresh gases pressures and temperatures inside the cylinder however tend to favour the appearance of abnormal combustion (i.e. unwanted and uncontrolled auto-ignition of fresh gases) that can damage the engine. This kind of abnormal combustion, still misunderstood, is thus a clear limit to further use downsizing. Within the Ph.D work of A. Misdariis [CFD51], an innovative methodology combining a new model to reproduce auto-ignition and code coupling to better predict heat transfer phenomena (combustion in the cylinder-AVBP, heat conduction in the cylinder head-AVTP) has been developed. Validations against experimental data in the framework of the ANR project ICAMDAC led by IFP Energies Nouvelles, have shown the potential of this methodology to reproduce abnormal combustions such as knocking or rumble and their sensitivity to various critical parameters (spark advance, fresh gas temperature, wall temperature, ...).

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

The consequences of gas explosions can be devastating causing numerous fatalities and destruction of large parts of industrial facilities. In the explosion of a gas cloud, the main issue is the pressure increase (the so-called over-pressure) which controls the severity of the explosion and is determined by a complex unsteady interaction between combustion, turbulence and geometry. Predicting, controlling and reducing this over-pressure in case of industrial accidents are thus key points in any safety related procedure.

The PhD work of P. Quillatre [CFD34, CFD147] has shown that Large Eddy simulation is a promising solution to improve numerical prediction capabilities in realistic explosion configurations if massively parallel machines are available. Fig. 2.7 is an example of an explosion simulation performed thanks to two INCITE allocations of a total of 100 million CPU hours awarded in 2013 and 2014.

This work is now continued with the PhD thesis of O. Dounia started in 2014 in collaboration with Total. Its objective is to study recent and novel methods used to mitigate the devastating consequences of vapour cloud explosions. These methods use solid particle inhibitors injected in the flammable cloud to prevent flame acceleration and thus reduce the associated over-pressure.

2.4.6 Chemical processes (M. Zhu, E. Riber, B. Cuenot)

Based on its expertise in reacting flow simulations, the team has started a research activity on the modeling and computing of problems of chemical processes, ie., reacting flows in heated / cooled pipes, in collaboration with Total, the University of Ghent, the Von Karman Institute and the University of Stanford. In comparison with combustion, such problems involve slower and usually endothermic chemistries and require more detailed chemical description. As a consequence there is no reacting front and the combustion regime corresponds to low Dahmkohler numbers, ie., does not need turbulence / chemistry interaction modeling. One particular issue is however linked to the heat transfer at the pipe walls, which controls the chemical behavior of the whole system. The prediction of wall flows and turbulent heat transfer is still a challenge for LES and was the first objective of M. Zhu (PhD funded by Total, 2012-2015) for her research project on steam-cracking of ethane and butane [CFD129]. The second objective of M. Zhu was to develop a methodology to compute the behavior of the full system, which is typically few tens of meters long, in a reasonable time. Results turned to be very encouraging and demonstrated the feasibility and accuracy of LES applied to petrochemistry.

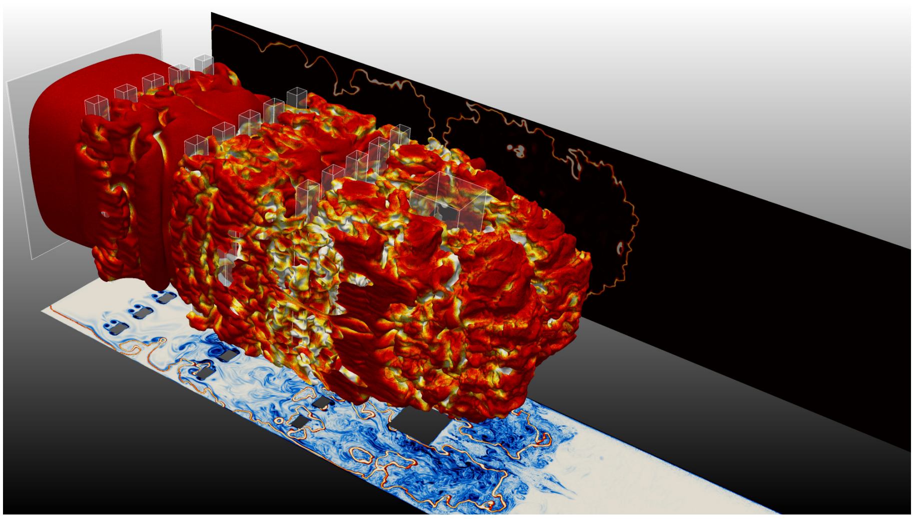

FIG. 2.7: LES of transition to explosion in a square duct (INCITE Grant 2014).

2.4.7 PERICLES (J. Dombard)

The PERICLES project (Partenariat d'Etude et de Recherche entre Industriels et le CERFACS en LES) aims at applying the most advanced simulation tools of CERFACS to address complex problems (so-called ńfrontierż problems) encountered by the "Bureaux d'Etude (BE)" of Safran. It acts as a bridge between CERFACS and Safran, allowing to :
- speed-up the integration and use of the models and tools developed by the PhD students at CERFACS,
- develop efficient methods in direct link with the BE to answer often urgent questions in a short delay,

The scientist in charge of PERICLES benefits fully from the expertise of the whole research team (seniors, PhD students, post -docs). All results are confidential, their publication is in general not allowed by Safran, but the questions brought by PERICLES are usually fed back to the rest of the team, leading to new studies and open academic activities.
PERICLES started with the recruitment of Dr. J. Dombard in january 2013. Today it is used by all BE of Safran. Applications cover a wide range of systems and physics : aircraft, helicopter, and rocket engines. Most computations for Turbomeca and Snecma are based on Large Eddy Simulation, extended to reacting two-phase flows, with AVBP. More complex simulations, as for example coupled CFD - heat transfer in solids (code AVTP) or flows with real gas thermodynamics are also realized.
The reliability and maturity of the research numerical tools developed at CERFACS for TRL (Technology Readiness Level) 4 to 6 are demonstrated by the quality, diversity and rapidity of PERICLES studies. Figure 2.8 shows the flow in a shocked nozzle calculated with LES and illustrates the feasibility of unsteady simulations with shock capturing methods.

2.5 Numerical Tools

2.5.1 Code development and HPC (F. Duchaine, S. Jauré, C. Fournier, O. Vermorel, G. Staffelbach)

Following the global and natural trend to ever more large and complex simulations, CERFACS has continued developing and optimizing its main CFD solver, the LES code AVBP. Originally written in Fortran 77, the code has been completely rewritten in Fortran 90 during the last 3 years. The code is now

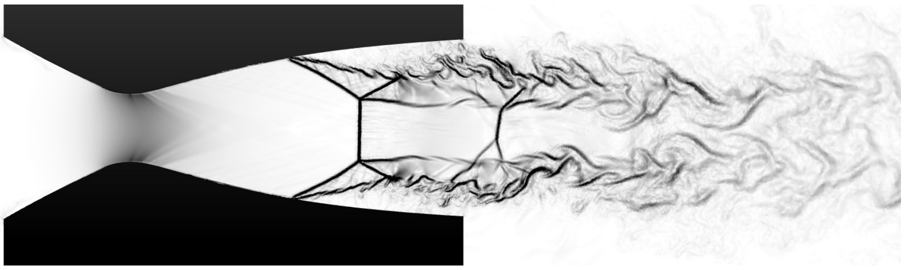

FIG. 2.8: LES of flow detachment in an exhaust nozzle of a rocket engine.

fully parallel, contrary to previous versions where the partitioning of the initial mesh and the IOs were treated sequentially. Partitioning is now ensured by the PT-SCOTCH or ParMETIS libraries and IOs use the parallel library PHDF5. With this new version, the first simulations with more than one billion elements have been performed on more than 100 000 processors thanks to INCITE and PRACE allocations. In the frame of the "Coeur Numérique 2020" project, new functionalities have been added to the solver to allow computing turbomachinery applications, i.e. multi-stages compressors or turbines.

High performance computing is carried out via bilateral collaborations with National (CINES, TGCC, IDRIS, CALMIP), European (Juelich Supercomputing Center JSC, Barcelona Supercomputing Center BSC) and American (Argonne National Labs, Oakridge National labs) computing centers. HPC optimization and application is part of each scientific excellence participation to the INCITE and PRACE programs with application ranging from gas turbine ignition, to transcritical flame interaction and confined domain explosions. Additionally optimization of CERFACS tools and solvers for future architectures and access to new systems are guaranteed via the participation of CERFACS and AVBP to European project on exascale computing (DEEP) as well as to the Intel Parallel Computing Centers program. The visibility of CERFACS on these themes is also confirmed by direct contracts between CERFACS and Intel ou IBM who fund CERFACS researchers to develop codes on new architectures.

2.5.2 Graphical User Interfaces (A. Bonhomme, A. Dauptain, E. Riber)

CERFACS experience in the last five years has shown that the major bottleneck to disseminate HPC to industry was not the codes themselves but the way industrial users could have access to these codes and run them efficiently. In practice, developing user interfaces has become as important as developing solvers. Therefore in the last five years CERFACS has developed an innovative Graphical User Interfaces (GUI), dedicated to very large codes running on massively parallel architectures. The C3Sm project is a software suite enabling the control of various tools related to combustion : AVBP (CFD, Reactive Large Eddy Simulation), YALES2 (Corias Large Eddy Simulation solver), AVTP (Thermal solver), PRISSMA (Radiation solver), AVSP(Helmholtz solver), CHORUS (Indirect noise computation), ATACAMAC (Combustion Instabilities prevision), AAP (Conjugate Heat Transfer coupled Solvers). Updates of the C3Sm suite are constantly transferred to Industry (Snecma Villaroche, Snecma Vernon, Turbomeca Bordes) and Academia (Ecole Centrale, CORIA, ONERA). Major achievements of 2014 are the first release of AVBP 7.0 under C3Sm, and the first Conjugate Heat Transfer setup at Safran thanks to C3Sm.

This original expertise about GUIs is also applied on other CERFACS topics outside the CFD team : since october 2014, the ocean-atmosphere coupler OASIS-3 MCT is released with a GUI based on the same graphical engine, OpenTEA. This GUI is now used during the OASIS Training sessions. In 2015, CERFACS will work on a GUI for the data assimilation components of EDF’s MASCARET(1-D Saint Venant equation solver).

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Aerodynamics

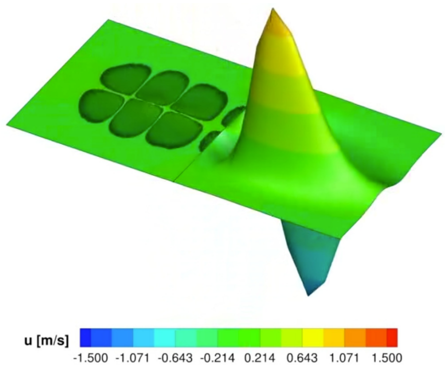
Aerodynamics activities cover a wide range of topics ranging from developing new numerics methods, testing new approaches and making advanced CFD simulations, all this in a high performance computing environment. Several CFD solvers with different approaches are used (RANS/URANS/LES for turbulence modeling, structured or unstructured mesh, Navier-Stokes or Boltzmann governing equations). All these activities allow Cerfacs to have a global vision of the CFD world which is very beneficial to our partners. Recent work has focused on Large Eddy Simulations, the goal being to bring this approach to our industrial partners either for aircraft or turbomachinery applications. In addition to standard CFD approach, Cerfacs invests in new paradigms which are very promising for the near future. Those approaches concern very high-order methods (based on spectral difference approach) and Lattice Boltzmann Method.

3.1 Numerical methods

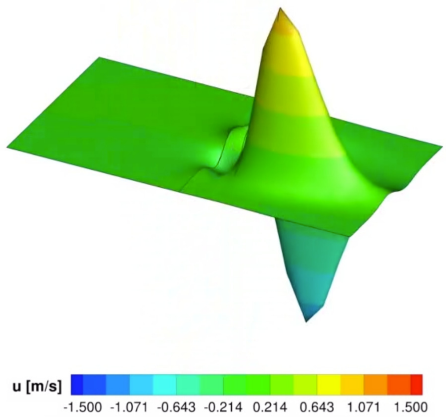
3.1.1 Extension of *elsA* high-order schemes to realistic configurations (P. Cayot, S. Le Bras, J. Vanharen, G. Daviller, G. Puigt, M. Montagnac)

With respect to aeroacoustic applications, using high-order numerical methods for Large Eddy Simulations (LES) and dedicated boundary conditions [CFD63] is necessary to correctly resolve noise source mechanisms in turbulent flows. However, performing LES for complex geometrical configurations, such as installed dual stream jets, involving wall bounded flows at high Reynolds numbers, leads to prohibitive LES computational costs due to the resolution of the flow boundary layers. In addition, the study of complex geometries becomes problematic in terms of mesh generation for multiblock structured grids solvers. In this sense, to address the challenge of LES of industrial configurations at high Reynolds numbers, new numerical methods have been implemented in the *elsA* software. The idea it to keep a structured framework when the geometry is simple, and to switch to an unstructured paradigm in complex shape zones. The work performed during the period concerns three main activities : nonconforming grid interface, high-order schemes for unstructured grids and wall-modeled LES.

Non-conforming grid interface for unsteady flow : Non-conforming Grid Interfaces (NGI) help to generate a structured mesh for complex geometry. The principle of NGI is to split the interface between blocks into several facets on which a unique flux is computed. Following the decomposition of any mesh interface into facets, the flux on any cell interface is obtained as the sum of fluxes on several facets. This treatment is fully conservative for plane interface. Even if they are used routinely for steady computations, their analysis for unsteady flows was not fully characterized. Before using NGI with high-order schemes for LES, Cerfacs studied their behavior in detail. A theoretical framework has been proposed for a spectral analysis of the numerical scheme applied on the NGI between two structured blocks. Then the effect of grid refinement or coarsening on the stability of the numerical scheme has been considered. Eventually, the new theoretical results were compared to numerical results showing that the mesh refinement/coarsening are the cause of instabilities, poor accuracy and reflection of high-frequency waves (Figs. 3.1). A new approach to compute partial fluxes, which is based both on a high-order extrapolation that accounts for the local metric and on a Riemann solver, improved the results and reduced spurious modes.



(a) Without metric correction. High-frequency waves are reflected by the nonconforming grid interface.

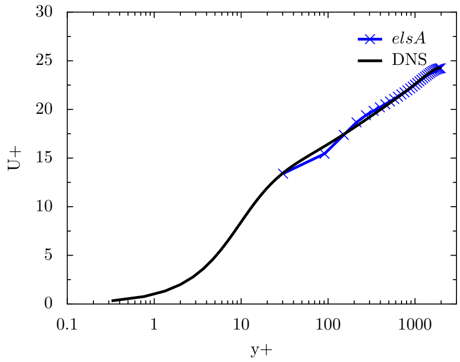


(b) With metric correction. High-frequency waves are filtered.

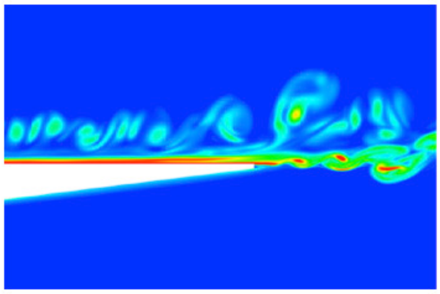
FIG. 3.1: Vortex convection through a nonconforming grid interface.

High-Order Finite Volume Unstructured schemes for LES in *elsA* software : Complex geometries require structured and unstructured zones. Therefore, in order to have the same level of accuracy throughout the computational domain, it is necessary to have numerical methods which are consistent with such a mesh. Cerfacs worked to add to the *elsA* solver the ability to use unstructured mesh with higher-order schemes. The first constraint is to deal with a cell-centered finite volume approach as used for the structured grid solver. The second constraint is to develop a scheme with the most compact formulation possible (for High Performance Computing constraints). A new diffusion scheme based on a Green-Gauss formula has been developed. Its formulation is compact and only needs data easily available in a cell centered framework. The gradient effective order was analyzed on several test cases and proved to be of second order which is sufficient for the simulation of convected dominated flows. For convection, a new family of schemes was built using a directional stencil. The idea is to construct a high-order scheme by the use of extrapolations using conservative values and their gradients. The combination of gradients depends on four real parameters and choosing wisely these parameters permits to create a family of schemes with an order between three and six. These schemes are currently tested on academic test cases.

Wall-Modeled LES (WMLES) : A major obstacle to the use of LES in industry is related to the computation cost when the configuration contains walls and the Reynolds number is high. One solution to compute physics at the wall with a reasonable computational cost is to perform LES using wall models. The introduction of a wall model removes the need for a fine mesh near the wall, making high Reynolds number computations feasible. The expertise of Cerfacs in the field of wall modeling is already well recognized. Wall treatment is strongly related to the solver, to the numerical methods used and to the target application. In that context, Cerfacs studied the use of wall modeling with high-order schemes for aeroacoustic simulation. An analytic wall law (for high-order scheme) has been implemented and first validated on the standard channel flow configuration (Fig. 3.2a). Then this new wall law was tested on an isolated cold jet [9]. The aerodynamic results show a good interaction between the wall model and the jet development inside the nozzle (Fig. 3.2b). This approach allows a better physics representation inside the jet nozzle which is compulsory to obtain accurate acoustic results [7, 8].



(a) Mean streamwise velocity profile in wall unit for a turbulent channel flow with adiabatic walls at $Re_\tau = 2003$. WMLES results are compared to the Direct Numerical Simulation (DNS) of Hoyas and Jiménez [10].



(b) Vorticity field in the vicinity of the nozzle of an isolated isothermal subsonic jet flow at $M = 0.6$ and $Re_D = 5.7 \times 10^5$.

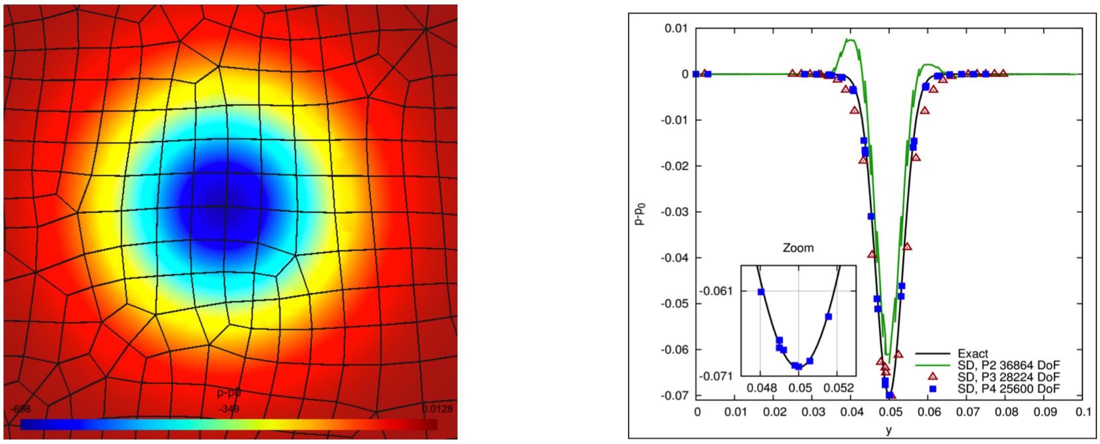
FIG. 3.2: Wall-Modeled LES (WMLES) results.

3.1.2 A new kind of high-order scheme for LES : Spectral Difference (N. Villedieu, G. Puigt, J-F. Boussuge, M. Lemesle, I. Marter, J. Vanharen, M. Kuzmin)

Developing accurate schemes (for LES) depends highly on the mesh strategy. Even if standard approaches (implicit compact, Finite Difference, WENO... schemes) are easy to implement in a structured framework, the situation is much more complex for unstructured grids which are mandatory for complex industrial applications.

Recently, several interesting paradigms were published in the literature : they are all members of spectral discontinuous methods family. The principle is to define a high-order polynomial representation of the quantities inside all mesh cells by interpolation from several degrees of freedom. These approaches do not assume that the reconstructed quantities are continuous at the interface and in many aspects, spectral discontinuous methods reuse many results from the finite volume approximation. Among these methods which can be considered for unstructured grids, Cerfacs focuses attention on the Spectral Difference approach. The principle is to solve the strong form of the equations, as in Finite Difference, but the discontinuity in reconstructed quantities at mesh interfaces is explicitly taken into account via a Riemann solver. The work began in 2012 by a mathematical analysis of the approach and by the development of a prototype. A year later, Cerfacs initiated the development of a new solver called JAGUAR and participated in May 2013 to the Second International Workshop on High Order Methods. The results showed three interesting features. First, the use of high-order discontinuous spectral approaches is (CPU time) competitive, compared with standard approaches. Second, such an approach is weakly sensitive to mesh quality (Fig. 3.3a). This is a key point when considering highly complex geometry. Finally, very accurate results can be obtained, for example : a difference of pressure of $0.07Pa$ can be convected over large distances in a flow at atmospheric conditions - $100000Pa$-).

In addition, Navier-Stokes governing equations were implemented and validated on several test cases (Taylor Green Vortex and channel flow). Then, in order to optimize the mesh used, the hp-refinement technique was considered : the goal is to refine in space (h) when the solution is not regular and to increase the accuracy (p) when the flow is smooth. Finally, Cerfacs has started to study the treatment of discontinuity. In fact, it is well-known that polynomial reconstruction leads to oscillations near a discontinuity. But industrial applications are transonic. Thus, several approaches to handle shocks have been tested and



(a) Solution of a vortex convection on twisted mesh after 50 passages

(b) Solution sensibility to the polynomial order

FIG. 3.3: JAGUAR features on the vortex convection test case

validated on academic test cases. In the near future it will be necessary to validate these approaches on industrial configurations.

3.1.3 Convergence acceleration by multi-frequency harmonic balance technique (F. Sicot, T. Guedeney, A. Gomar, F. Gallard, G. Puigt)

Three-dimensional steady turbulent flow simulations are handled routinely in the industry, but unsteady turbulent flow simulations still require large computational times and an acceleration of the calculations is mandatory to reduce design cycles. In fact, many industrial applications involve flows periodic in time and a transient regime responsible of a large CPU time must be bypassed.

During the last years, CERFACS was involved in the development of the Harmonic Balance Technique (HBT) for periodic flows : this technique consists in transforming a periodic unsteady computation into several steady computations coupled by a source term. All steady computations can be seen as a snapshot of the flow at some time instants uniformly distributed over the period. Such an approach enables to save CPU time using a dedicated time integration procedure, but it main interest is the monitoring of convergence.

A turbomachinery flow (URANS approach) contains by nature several frequencies, following the theory of Tyler and Sofrin. The technique valid for one frequency and its harmonics was extended to several frequencies in the literature, using transformations equivalent to the Discrete (direct and inverse) Fourier transforms. However, applying this approach directly leads in general to non-physical solutions and the computation stops. Cerfacs performed an analysis on a simplified configuration and highlighted the fact that the stability issue was related to the conditioning of the matrix that defines the source term. This point had never been explained in the literature before. Cerfacs analyzed two ways to control the stiffness of the source term : one approach comes from the electronics field and the second one is based on solving an optimization problem. The latest technique was able to solve the stability issue problem [CFD69]. Moreover, the HBT approach was validated on turbomachinery aeroelastic problems.

3.1.4 New Large-Eddy Simulation approach for a turbomachinery stage (N. Gourdain, F. Sicot, G. Mouret, J-F. Boussuge)

A better understanding of turbulent unsteady flow is a necessary step towards a breakthrough in the design of modern compressors. With the increase in computing power, Large-Eddy Simulation (LES) emerges as a promising technique to improve both knowledge of complex physics and reliability of flow solver predictions. However these simulations are very expensive for industrial applications, especially when a 360° configuration should be considered. There are some paths to explore in order to reduce the computational cost of LES, with acceptable physical restrictions. In that regard, the use of the well-known phase-lagged boundary conditions allows a reduction of a 360° configuration to a single passage per row configuration. The main difficulty with such conditions is the need to store the flow over one period at the phase-lagged interfaces. The most popular method to reduce the memory cost is to store only the coefficients of the Fourier Series Decomposition (FSD) of the temporal signal. The FSD is truncated to a limited number of harmonics and the coefficients are updated at each time step. This method assumes that the flow is perfectly periodic in time, which is a fair assumption in unsteady RANS for operating points dominated by periodic rotor/stator interactions (wakes and potential effects). Unfortunately, such a periodic assumption is no longer true for LES. Thus, Cerfacs developed a new method adapted to LES in which a Proper Orthogonal Decomposition replaces the FSD. This decomposition does not make any assumption on the spectrum of the flow. The compression is done by removing the smallest singular values which are the ones that contain the least energy. This method has been validated with respect to URANS simulation on a single stage compressor and will be applied to the LES of this same compressor next year.

3.1.5 Shape Optimization (X. Pinel, M. Montagnac)

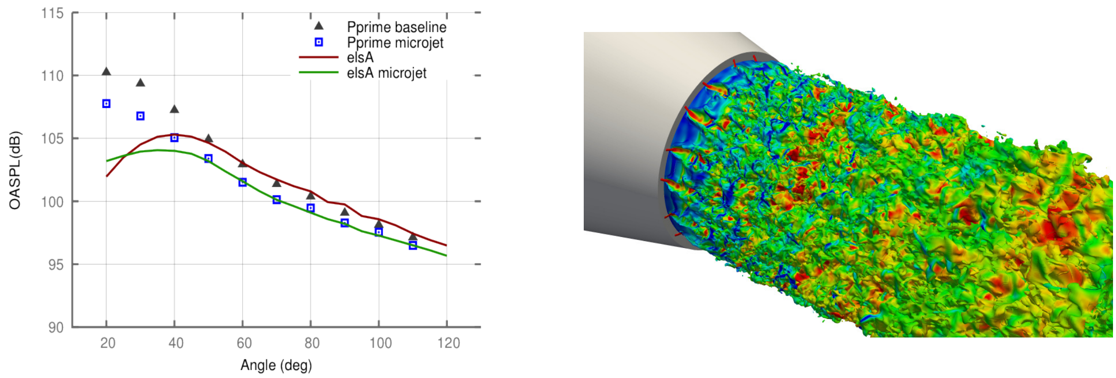
Cerfacs is involved in shape optimization field via the use of adjoint techniques (see Sec. 3.2.3) and a high-fidelity solver to compute the objective function. The choice of the optimization algorithm is heavily constrained by the computational cost implied by one function evaluation. Thus, gradient-based optimization algorithms are particularly valued for their speed of convergence although they only give a local optimum. Therefore, the gradient of the objective function with respect to the design variables is computed through the discrete adjoint method that only requires a linear system resolution for each function and constraint.
A new block Krylov method, named block flexible GMRES with deflated restarting (BFGMRES-DR), has been developed in the *elsA* software to solve simultaneously the discrete adjoint equations of RANS equations for multiple right-hand sides (objective and constraint functions) [CFD72]. This method enables to solve the adjoint linear systems faster than traditional standard Krylov methods, e.g. FGMRES, or approximate Newton methods.

3.2 Applications

3.2.1 Aeroacoustic simulations (G. Daviller, C. Pérez Arroyo, R. Biolchini, H. Deniau, G. Puigt, J-F. Boussuge, M. Montagnac)

Jet-noise reduction by fluidic active control : Developing solutions to control and reduce jet noise generated by aircrafts is a major concern as underlined in ACARE recommendations. The Large-Eddy Simulation of a high Reynolds isothermal single jet ($Re = 10^6$, $M = 0.9$) controlled by fluidic crossed actuators has been realized following two complementary paths : a simplified approach and a full simulation.

- Simplified approach : The LES simulation of such configuration including the geometry and the microjets (see Fig. 3.4b) can be very CPU demanding due to large scale separation between the main jet and the microjets. In order to reduce the CPU cost, a study based on some approximations has been conducted : the microjets are modeled by the mean of source term, the nozzle geometry is not taken into account and the transition to turbulence is performed by mean of a forcing term. Even with such approximations, the results (see Fig 3.4) captured the jet noise reduction. The aerodynamic and acoustic results are in good agreement with the experimental data and show that the local modification of the jet flow using microjets lead to a reduction in the overall noise of 1 dB for observation angles between $40°$ and $120°$. An increase of the microjets speed blowing would certainly increase this trend.



(a) OASPL comparison

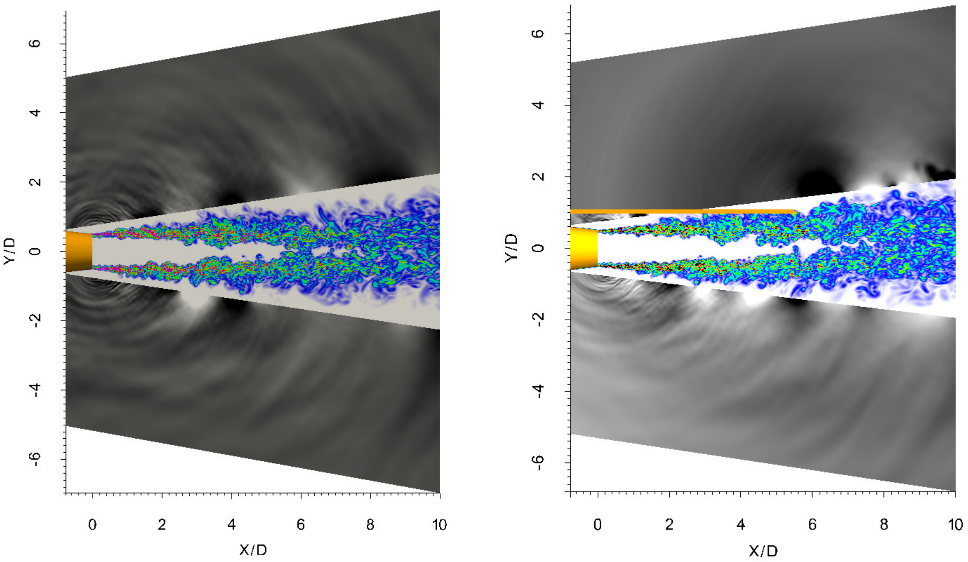
(b) Isosurface of streamwise velocity $U = 0.5U_j$, colored with density

FIG. 3.4: Jet noise reduction

- Full simulation : The brute force LES simulation has been done with the *elsA* software on a 2 billion point mesh. The microjets are fully discretized in the nozzle lip in order to match the experimental conditions.
A direct noise computation of the controlled jet is performed using 8 pairs of crossed microjets imposed via a non reflecting (NSCBC) boundary condition inside the nozzle leap. The resulting near-field velocity of the main jet and the microjets action is depicted on Fig. 3.4b. The microjets influence on the main jet is local and does not induce significant modifications on the mean flow field downstream the jet potential core. However, a decrease of the sound pressure level in the low-frequency range is observed. In agreement with experimental results from Institut Pprime, the local increase of the turbulence level in the impact zone is correlated to a significant reduction of the radiated overall sound pressure level.

Installation effect on jet noise : This activity tackles the issue of the jet noise interaction of an ultra-high bypass ratio engine in the vicinity of the aircraft wing. Our first activity focused on academic configurations in order to better understand the physical mechanisms driving the jet installation effect. In this context, high-order Large Eddy Simulations were performed on a single-stream jet interacting with a flat plate. In this framework, CERFACS and Pprime Institute (Poitiers) work in close collaboration in order to realize, validate and analyze numerical simulation of the most relevant small-scale experimental configurations (Fig.3.5). In the near future, the flat plate will be replaced by a wing profile.

Supersonic underexpanded jets : For an aircraft in cruise conditions, the major part of the noise perceived in the aft-cabin comes from the turbofan, which consists of both shock-cell and turbulent mixing noise. In fact, the secondary stream is cold, supersonic and under-expanded. The pressure mismatch leads to the formation of (diamond-shaped) shock-cells which strongly interact with the turbulent structures



(a) Isolated jet

(b) Jet interacting with a flat plate

FIG. 3.5: Installation effect on a single-stream jet.

developing in the mixing layer around the potential core, as illustrated on Figure 3.6. This interaction process produces intense noise components on top of the turbulent mixing noise, which makes supersonic jets noisier than their subsonic counterpart. The result is a broadband shock-cell noise, radiated in the forward direction, that impinges the aircraft fuselage and then it is transmitted inside. In order to simulate such configuration, Cerfacs extended the *elsA* subsonic high-order scheme to be able to take shocks into account. On a single jet, our simulations achieved good agreement against experimental results in terms of flow behavior (shock-cell patterns, turbulence levels, ...) and in also in terms of the acoustics in the near and far-field. This work is done in collaboration with Leicester, VKI and IMFT.

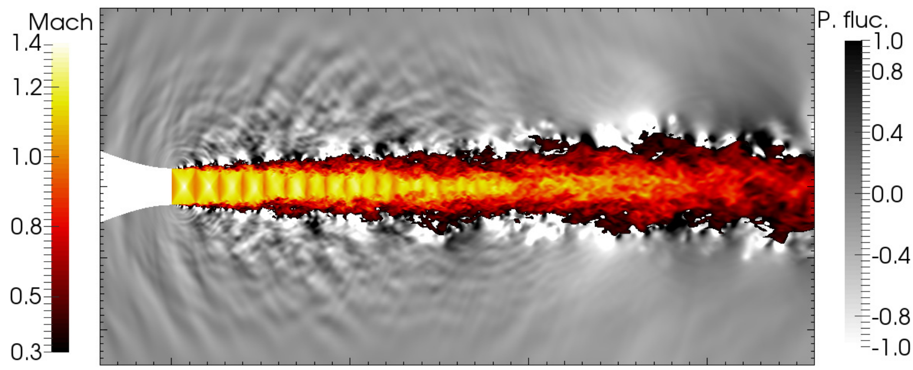
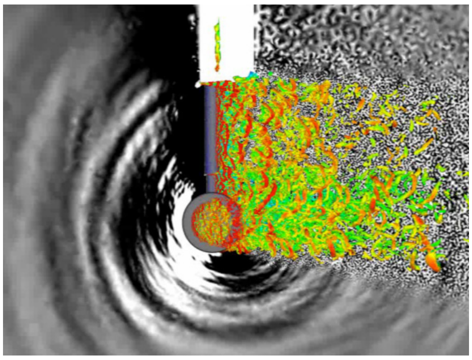
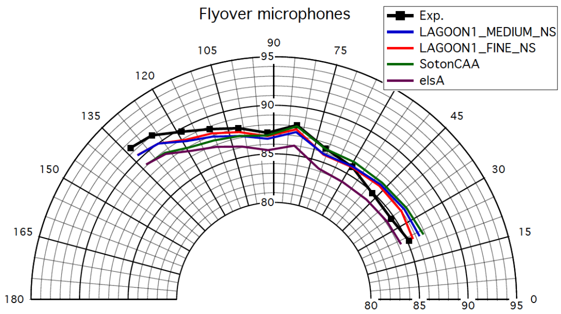


FIG. 3.6: Visualization of a shock-cell pattern for a jet at $M_j = 1.15$.

LES of unsteady turbulent flows around landing gears for aerodynamic noise prediction : For an aircraft in landing conditions, the major part of noise comes from the airframe (landing gear and high lift devices). Such configurations imply very complex geometries that are difficult to handle with a structured mesh even if it is normally desirable for aeroacoustic simulations. Thus, Cerfacs evaluated the use of the unstructured approach with our in-house AVBP solver. The selected configuration was a Airbus landing-gear model called LAGOON (Fig. 3.7a). Studies on mesh influence and wall treatment have been conducted. The final results (Fig. 3.7b) show a good agreement between experimental and numerical data and are in line with other state-of-art results from others solver (*elsA* and SotonCAA).



(a) LAGOON/Dilatation field (Grayscale) with iso-Q criterion surface (done with AVBP).



(b) OASPL comparison of solver for the flyover configuration.

FIG. 3.7: Lagoon configuration

3.2.2 Lattice Boltzmann Method (J-C. Jouhaud, J-F. Boussuge, C. Coreixas, G. Puigt)

Lattice Boltzmann Methods (LBM) are becoming a serious alternative to traditional methods for unsteady flows around very complex geometries. The mesh generation process which is time consuming with standard CFD approaches is fully automatic with LBM : Cartesian grids with different levels of refinement are used and the complex geometry is accounted for by means of « immersed boundary ». Moreover, this approach is accurate and efficient on massively parallel platforms.
LBM is a new class of mesoscopic particle based approach to simulate fluid flows : this method find its origin in a molecular description of a fluid and can directly incorporate physical terms stemming from knowledge of the interaction between molecules.
Cerfacs is involved in the analysis of LBM solutions since 2012, firstly using the commercial software PowerFlow (developed by EXA). During one year, Cerfacs in collaboration with Airbus and EXA has evaluated the capacity of LBM to simulate aeronautical complex flows (high-lift system, landing gear and open-rotors). More recently, Cerfacs joined the initiative around the French LBM solver called LaBS (Lattice Boltzmann Solver). This software is owned by a consortium composed of three industrial companies (AIRBUS Group, Renault, C-S) and two scientific laboratories (ENS Lyon, LM2P2 Aix-Marseille University). After an initial period of test (simulations of flows around cavities and landing-gear), Cerfacs will be involved in the development process. In the framework of the "FSN Intensive Computations" called CLIMB, Cerfacs will develop the possibility to simulate high Mach numbers flows.

3.2.3 Shape Optimisation (F. Gallard, H. Montanelli, M. Montagnac)

Cerfacs conducts activities in numerical optimisation for aircraft preliminary design since 2005. The general framework consists in an optimisation problem with several hundreds of design variables and a few constraints for typical industrial configurations. The software environment is provided by Airbus Group, and it can accept the Onera CFD solver as a plug-in.

Multidisciplinary Design Optimisation : Cerfacs took part in the OSYCAF (Optimisation d'un système couplé fluide-structure représentant une aile flexible) project funded by the STAE foundation from April 2010 to June 2013. The objective was to setup a MDO methodology for an aero-structural optimisation process in collaboration with three other organisms from Toulouse (Onera, ISAE, UPS). The OSYCAF project (http ://www.cerfacs.fr/osycaf) promoted a session in Optimisation in the second colloquium MUSAF that was held in Toulouse in September 2013.

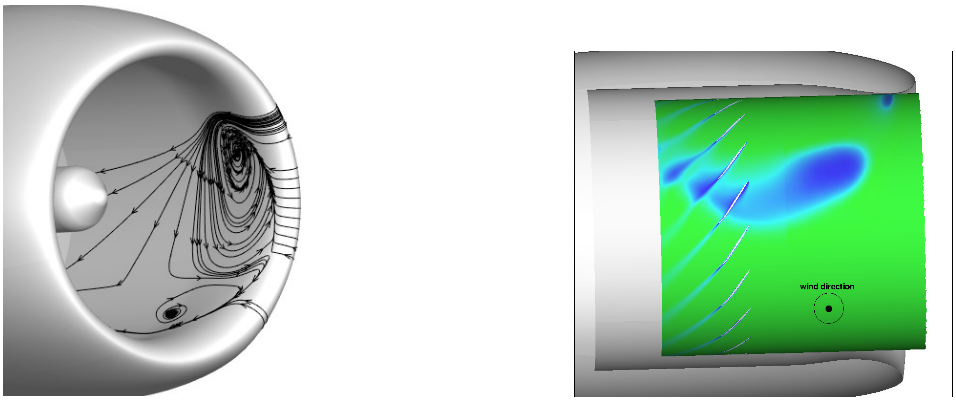
Multipoint Aerodynamic Shape Optimisation : The single-point optimisation, e.g. at the cruise condition, often leads to a shape that has a sharp performance increase around the given condition, but that behaves badly at other conditions.
During his PhD, F. Gallard investigated the formulation of the optimisation problem to improve the efficiency of an aerodynamic shape over multiple missions, or multiple conditions [CFD153]. He introduced a new method, named Gradient Span Analysis method, that gives a minimal set of operating conditions to insert into the weighted sum model to solve the multipoint optimisation problem. The weights associated to these conditions are computed with the utopia point, or unattainable aspiration, method. He performed first the optimisation of the rigid shape and then took into account the aeroelastic effects.

3.2.4 Turbomachine (N. Gourdain, F. Sicot, J-F. Boussuge, F. Crevel, Y. Sadoudi, M. Daroukh, P. Vass)

Cerfacs is involved in the simulation of many turbomachinery configurations such as compressors, turbines or open-rotors. One of the most challenging computation done recently, is a full surge cycle with a 360^0 configuration (PhD awarded by the P. Caseau prize). Recent studies focus on air intake configurations : to reduce fuel consumption, the current trend is to reduce the length of the nacelle by reducing the space between the nacelle tip and the fan or by integrating the structural pylons into the Outlet Guide Vanes (OGV) row. These evolutions have a strong influence on the physics around the fan which can be the source of aerodynamic or aeroacoustic problems.

Fan operability The air inlet of a jet engine plays a key role on engine operability : it channels the flow to the fan in such a way that it should be as smooth and uniform as possible. One of the most critical operating points is at take-off in the presence of cross-wind which can generate a detached flow at the nacelle tip (Fig. 3.8a) and lead to high distortions on the fan. Cerfacs studied such configurations with RANS and URANS approaches for isolated inlet and also coupled inlet/fan/OGV assembly. It results that the presence of the fan enlarged its operating range by sucking the separation occurring between the inlet tip and the fan as shown in Fig. 3.8b. The computations showed that accounting for the presence of the fan is compulsory for a properly inlet design.

Fan noise On classical engines (long nacelle and homogeneous OGV), it is considered that the fan / OGV interaction mechanisms are the main contributor to the fan tonal noise. In order to have a deep understanding of this noise source in the future engines where the pylon is integrated into the OGV row, 360° URANS computations of the fan / OGV / IGV module have been performed (Fig. 3.9). It has been shown that the presence of the pylon into the OGV row has a strong influence on the modal composition of the radiated tones and that it could even explain the radiation of a tone which would have been cut-off in a homogeneous configuration.
The inclusion of a short nacelle in the simulation has been done recently. This implies high distortions of the flow in front of the fan, especially when the inlet is non-axisymmetric. These distortions are responsible



(a) Streamlines in the isolated inlet : boundary layer separation

(b) Entropy levels in the inlet sucked by the fan's effect

FIG. 3.8: Air intake under crosswind conditions

of new tonal noises. Analytical methods based on the Amiet theory have shown a strong influence of the engine rotation speed. 360° URANS computations of the air inlet / fan / OGV / IGV module are also currently performed to quantify the importance of both sources (distorsion / fan interaction and fan / OGV interaction).

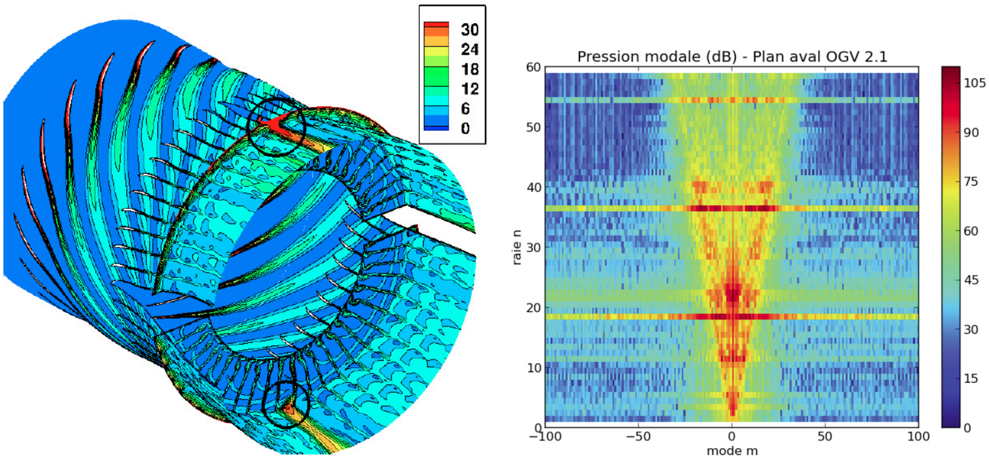
3.3 HPC

3.3.1 CPU efficiency (M. Montagnac)

During the year 2014, works were carried out to optimize CPU performance of the *elsA* software in collaboration with the Onera working group 'Performances elsA' which established a list of potentially interesting actions related on improving spatial and temporal localities of data. Temporal locality indicates that elements that were accessed recently will probably be used in the near future. Spatial locality indicates that close items in memory tend to be referenced at the same time. These techniques are crucial to achieve good CPU performance on machines with hierarchies of cache memories.
Concretely, to obtain this data locality, CERFACS has mainly modified the *elsA* kernel in order to work with primitive values and not conservative ones, subroutines were merged and some array indexes have been swapped. With these modifications, gains up to 50 % of the original CPU time were obtained on specific test cases.

3.3.2 CPU efficiency on hybrid solver (M. Montagnac, G. Puigt)

A hybrid grid approach was implemented recently inside the *elsA* kernel (Sec. 3.1.1). The principle is to consider structured blocks and multi element-shape unstructured zones inside a single hybrid mesh. Our definition of hybrid grid is not the same as in the literature, where hybrid grids represent a multi element unstructured grid.
In *elsA*, both structured and unstructured approaches follow a face-based paradigm, leading to the computation of one flux per mesh interface and then transferring the flux over the left and right volume increments.
Cerfacs was involved in the development and implementation of parallel features for unstructured grids and also in the establishment of a computational chain based on METIS library. The efficiency of the



(a) Instantaneous entropy field (b) Modal composition in a downstream plane

FIG. 3.9: 360° URANS computation of a fan with heterogenous OGV.

computational loops was increased by data ordering to avoid cache misses. If the connectivity graph between cells is represented by the symmetric matrix M ($M_{i,j} = 1$ if cells i and j share a face, else, $M_{i,j} = 0$), an optimization of data placement in memory consists in changing the matrix M in order to have a shape as close to a diagonal as possible.

3.3.3 Antares (A. Gomar, T. Léonard, J-F. Boussuge, M. Montagnac)

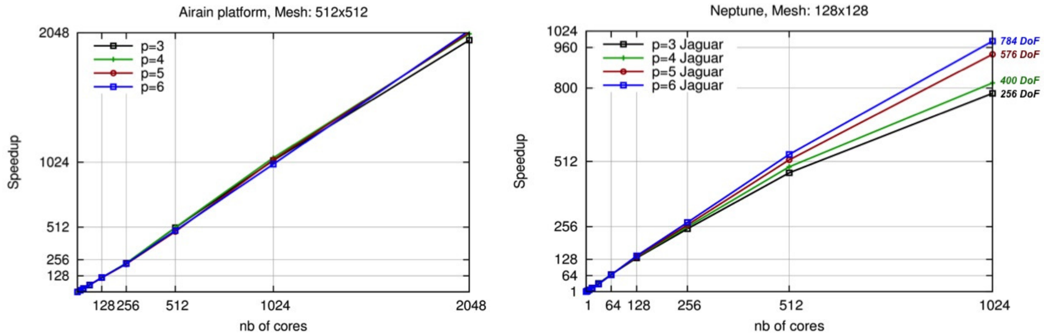
Cerfacs develops a generic data-processing library called ANTARES (www.cerfacs.fr/antares) both to post-process data generated during simulations and to co-process data (in situ) during massively parallel simulations to reduce the amount of generated data. The co-processing mode has been tested up to 8000 cores with the *elsA* Onera software, and allows to manipulate large amount of data (tested up to two billion of mesh points).

This Python library of Antares is developed in an open source philosophy that gives a clear view of the algorithms used to process data to users, enabling its use for research purposes. The large choice of features available within the Python community enables to write complex data analysis procedures. It is currently provided to many research labs and industries (ISAE, PPRIME, University of Sherbrooke, DynFluid, Airbus, Snecma, TurboMéca, CEA)

3.3.4 JAGUAR Performance (A. Cassagne, N. Villedieu, G. Puigt, J-F. Boussuge, A. Genot)

From the beginning of the development of the JAGUAR solver (Sec. 3.1.2 for details), efforts were dedicated to the implementation of a flexible and efficient data structure. Several approaches were tested which means the code has been rewritten several times before obtaining the best performance. The key points found are :

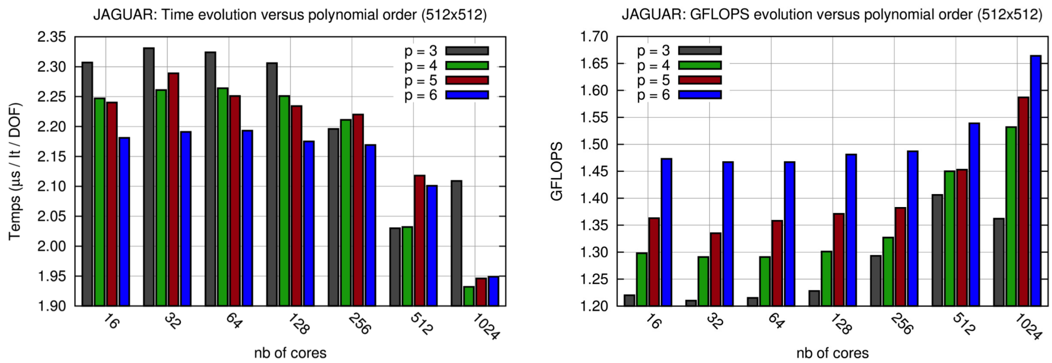
– algorithms using matrix vector products : Matrix vector products are the basic linear algebra operations and all computational cores are optimized for these operations.
– cache optimisation : In order to minimize the CPU time lost due to cache misses, the computational loops in JAGUAR are designed to take care of the cache size.
– local treatment : This is intrinsically due to the Spectral Difference method where many operations are performed on the degrees of freedom of the cell, without needing information from the surrounding elements.



(a) Strong scalability on a medium mesh

(b) Strong scalability on a small mesh

FIG. 3.10: Analysis of the strong scalability of JAGUAR.



(a) Time per iteration and per degree of freedom depending on the polynomial order p

(b) GFlops depending on the polynomial order p

FIG. 3.11: Analysis of the serial performance of JAGUAR

Once the data structure was optimized, CERFACS worked on the efficiency of the MPI implementation. A linear speed-up from 1 to 2048 cores (Fig. 3.10a) was obtained. Even with a small number of degrees of freedom (400) per CPU core, the parallel efficiency (80%) is still very good (Fig. 3.10b). Indeed, the perfect parallel efficiency is obtained from 1000 degrees of freedom per core.

Cerfacs and CINES used a PRACE preparatory access to enhance the JAGUAR platform using a hybrid OpenMP/MPI paradigm. The goal was to consider OpenMP for the treatment inside a node, and MPI to perform communications between nodes. Such an approach is a key point for massively parallel simulations (O(100 000) cores) for which it is necessary to minimize the MPI data exchange.

To fully determine the performance of the JAGUAR solver, an analysis of the CPU cost has been done (Fig. 3.11). A restitution time of $2.2\mu s$ per iteration and per degree of freedom (Fig. 3.11a) is obtained, what is quite good considering the high-order of the solution. This can be explained by the high level of use of the computational core : the GFLOPS obtained are almost twice as big as standard CFD solvers (Fig. 3.11b).

JAGUAR was also extended to GPGPU platforms via CUDA language. After an optimization on a single GPU card, a multi-card version using the MPI paradigm has been developed. The efficiency obtained is similar to what is seen in recently published literature (Fig. 3.12). A GPGPU platform is only efficient if a large amount of work is associated to each GPU card (only compatible with big meshes). This use limits the interest of GPGPU architectures compared to regular supercomputers.

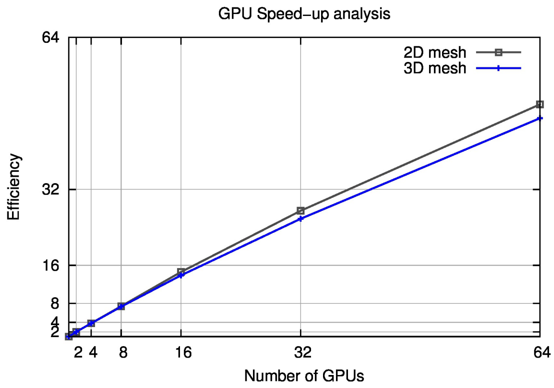


FIG. 3.12: Strong scalability analysis on a cluster of 64 GPGPU

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[CFD126] F. ShumKivan, F. Duchaine, and L. Gicquel, (2014), LARGE-EDDY SIMULATION AND CONJUGATE HEAT TRANSFER IN A ROUND IMPINGING JET, In *Proceedings of ASME Turbo Expo 2014 : Turbine Technical Conference and Exposition*, Dusseldorf, Germany, GT2014–25152.

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[CFD131] A. Eyssartier, (2012), *LES of two-phase reacting flows : Stationary and transient operating conditions - TH/CFD/12/122*, PhD thesis, Université de Toulouse - INPT, Megep.

[CFD132] S. Hermeth, (2012), *Mechanisms affecting the dynamic response of swirled flames in gas turbines - TH/CFD/12/84*, PhD thesis, Université de Toulouse - INPT, Megep.

[CFD133] S. Jauré, (2012), *Méthodologies pour le couplage Simulation aux Grandes Echelles/Thermique en environnement massivement parallèle - TH/CFD/12/114*, PhD thesis, Université de Toulouse - Ecole doctorale : Mécanique, Energétique, Génie civil, Procédés - Dynamique des Fluides - December, 13.

[CFD134] T. Pedot, (2012), *Modélisation du couplage thermique entre la combustion et l'encrassement des tubes dans un four de raffinerie - TH/CFD/12/19*, PhD thesis, Institut National Polytechnique, Université de Toulouse - MeGeP énergétique et transferts.

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[CFD139] M. Falese, (2013), *A study of the effects of bifurcations in swirling flows using large eddy simulation and mesh adaptation - TH/CFD/13/82*, PhD thesis, Université de Toulouse - Ecole Doctorale MEGEP.

[CFD140] R. Fransen, (2013), *Simulation aux Grandes Echelles pour la modélisation aérothermique des aubages de turbines refroidies - TH/CFD/13/35*, PhD thesis, Université de Toulouse - MeGeP - Dynamique des Fluides.

[CFD141] G. Hannebique, (2013), *Etude de la structure des flammes diphasiques dans les brûleurs aéronautiques - TH/CFD/13/21*, PhD thesis, Université de Toulouse - MeGeP - Dynamique des Fluides.

[CFD142] E. Motheau, (2013), *Accounting for mean flow effects in a zero-Mach number thermo-acoustic solver : Application to entropy induced combustion instabilities - TH/CFD/13/84*, PhD thesis, Université de Toulouse - MeGeP - Dynamique des Fluides.

[CFD143] P. Salas, (2013), *Numerical and physical aspects of thermoacoustic instabilities in annular combustion chambers - TH/CFD/13/85*, PhD thesis, Université Bordeaux 1 - INRIA.

[CFD144] D. Barré, (2014), *Numerical simulation of ignition in aeronautical combustion chambers - TH/CFD/14/7*, PhD thesis, Université de Toulouse - MeGeP - Dynamique des Fluides.

[CFD145] M. Bauerheim, (2014), *ETUDE THEORIQUE ET NUMERIQUE DES EFFETS DE BRISURE DE SYMETRIE SUR LES MODES THERMO-ACOUSTIQUES AZIMUTAUX DANS LES CHAMBRES ANNULAIRES.*, PhD thesis, Université de Toulouse, France - MeGeP.

[CFD146] G. Chaussonnet, (2014), *Modeling of liquid film and breakup phenomena in Large-Eddy Simulations of aeroengines fueled by airblast atomizers - TH/CFD/14/15*, PhD thesis, Université de Toulouse - MeGeP - Dyphasique.

[CFD147] P. Quillatre, (2014), *Simulation aux grandes échelles d'explosions en domaine semi-confiné - TH/CFD/14/14*, PhD thesis, Institut National Polytechnique de Toulouse - MeGeP - Energétique et Transferts.

[CFD148] J.-P. Rocchi, (2014), *Large Eddy Simulations of the ignition phase in a cryogenic rocket engine*, PhD thesis, Université de Toulouse - Ecole doctorale MEGeP Dynamique des Fluides.

[CFD149] M. Rochoux, (2014), *Vers une meilleure prévision de la propagation d Õ incendies de forêt : évaluation de modèles et assimilation de données*, PhD thesis, Ecole Centrale Paris - Sciences Pour lÕIngénieur.

[CFD150] S. Bocquet, (2013), *Modélisation de paroi et injection de turbulence pariétale pour la simulation des grandes échelles des écoulements aérothermiques - TH/CFD/13/91*, PhD thesis, Université de Toulouse, Institut National Polytechnique de Toulouse - Ecole Doctorale MEGEP.

[CFD151] F. Crevel, (2013), *Simulation numérique de l' écoulement en régime de pompage dans un compresseur axial multi-étage - TH/CFD/13/54*, PhD thesis, Ecole Centrale de Lyon - LMFA.

[CFD152] B. Francois, (2013), *Simulations aérodynamiques instationnaires de doublet d'hélices rapides contra-rotatives : Evaluation de méthodes numériques efficaces, Prévision et analyse des efforts 1P - TH/CFD/13/96*, PhD thesis, Université Pierre et Marie Curie - SMAER.

[CFD153] F. Gallard, (2014), *Optimisation de forme d' un avion pour sa performance sur une mission - TH/CFD/14/16*, PhD thesis, Université de Toulouse - ISAE - Aeronautique et Astronautique.

[CFD154] J.-C. Giret, (2014), *Simulations aux grandes échelles des éecoulements instationnaires turbulents autour des trains dŠ atterrissage pour la prédiction du bruit aérodynamique - TH/CFD/14/13*, PhD thesis, Université de Toulouse - MeGeP - Mécanique des Fluides.

[CFD155] A. Gomar, (2014), *Multi-Frequential Harmonic Balance Approach for the Simulation of Contra-Rotating Open Rotors : Application to Aeroelasticity*, PhD thesis, Arts et Métiers ParisTech, Paris (Mécanique-matériaux) - CERFACS - Dynfluid.

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7

Aviation and Environment

Climate Impact of aviation

1.1 Introduction

The aircraft emissions have an impact on atmospheric chemistry and on the radiative balance of the atmosphere. Contrails formed by condensation of water vapour onto exhaust aerosols and soot particles trigger the formation of cirrus clouds. Emissions of nitrogen oxides perturb the natural chemical cycles and lead to ozone production or destruction depending on local air mass composition and insolation. These ozone perturbations along with the emissions of CO_2, water vapour and ice particles formation, soot particles, sulphuric aerosols from the burning kerosene give an additional contribution to the green house forcing. 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. The objective of the AE team is to obtain a better quantification of the impacts of aviation on climate. The following sections describe the main activities on that theme conducted at AE under the period under review.

Those researches are supported at CERFACS by the CORAC (Comité d' Orientation sur la Recherche Aéronautique Civile) group through the TC2 and IMPACT projects, which are now funded by the DGAC. They are conducted in cooperation with CNRM, LA, LaMP, LIVE, LMD, LSCE laboratories, and with Météo-France, ONERA and Dassault.

1.2 Contrail formation

Large-eddy simulations of sub kilometer-scale turbulence in the UTLS were carried out with the mesoscale atmospheric model Méso-NH using the computational resources provided by a PRACE allocation on the Bull-X supercomputer at CRCT-CEA. Different levels of turbulence were generated using a large-scale stochastic forcing technique that was especially devised to treat atmospheric stratified flows. Flow topology, turbulence statistics and energy spectra were analyzed in detail by increasing the grid resolution to 2 m resulting in computational meshes of up to 8 billion gridpoints. Because of atmospheric stratification, turbulence is substantially anisotropic, and large elongated structures form in the horizontal directions, in accordance with theoretical analysis and spectral simulations of stably stratified flows (see Fig. 1.1). It was also found that the inertial range of horizontal kinetic energy spectrum, generally observed at scales larger than a few kilometers, is prolonged into the sub-kilometric range, down to the Ozmidov scales that obey isotropic Kolmogorov turbulence.

This work served as a basis for the study of formation and early development of contrails where the generated atmospheric turbulence fields were used as background fields to initiate the (Crow) vortex instability. It was shown that turbulence has a first order effect on the dynamical features of the wake in the vortex regime and has to be taken into account for a correct a description of the contrail (see Fig.1.2). On the other, the global ice characteristics such as ice mass and optical depth are found to be less affected by turbulence, with the background humidity and temperature exhibiting a larger impact on the number of surviving ice particles and size distribution.

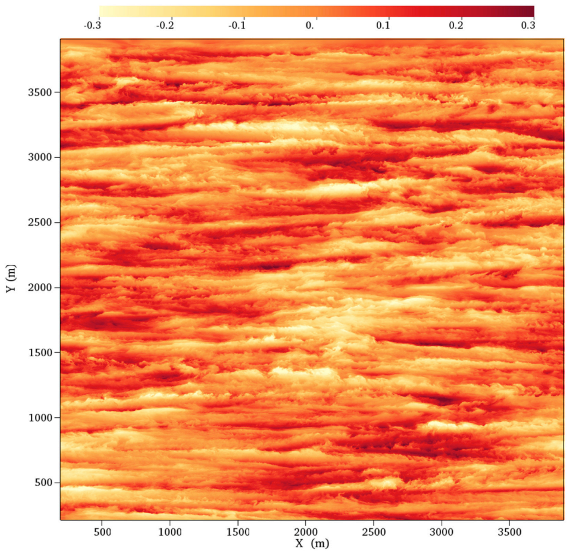


FIG. 1.1: Snapshot of potential temperature fluctuations in a vertical cross-section of the computational domain.

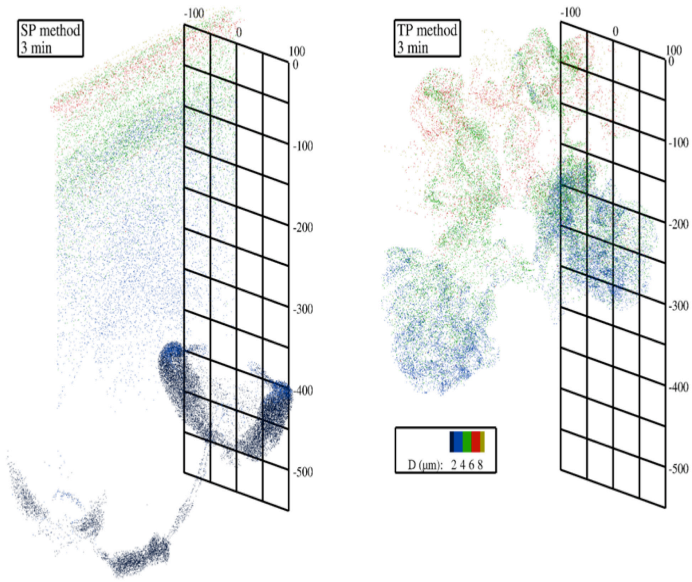


FIG. 1.2: Spatial distribution of ice particles in a 5 minutes old contrail colored with the ice diameter without (left) and with (right) atmospheric turbulence.

1.3 From contrail to cirrus clouds

Our main goals were
- to develop a model for the simulation of the contrail evolution from its formation up to its interaction with the atmosphere ;
- to quantify coefficients of the parameterizations that are needed to include the aircraft emissions into large scale models ; and
- to predict the distribution of ice particles inside a contrail for the evaluation of its radiative impact.

The contrail was simulated using Méso-NH atmospheric model (jointly developed at CNRM and Laboratoire d'Aerologie) coupled to microphysical scheme specifically developed for this study. 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 later regime. In this study, we simulated the contrail behaviour between 5 minutes and 60 minutes after emission. Although previous works in the literature focused on the impact of wind shear on the development of the contrail, less emphasis has bee 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 (see above). To our knowledge, our study constitutes the first simulation of the diffusion regime with an early transition of a contrail into young cirrus that takes into account the impact of background atmospheric turbulence and with radiative transfert. One important result of our work is that the radiation transfer is the key mechanism controlling the global ice characteristics and the vertical extension of the contrail, and is predominant on the atmospheric turbulence on time scale beyond 20 minutes (see figure 1.3). This effect is magnified during the day by the direct heating at the top of the contrail in the visible band that adds to the heating at the bottom in the infrared band from the Earth surface. This work, based on LES simulations, gives very useful results to develop parameterizations of contrails radiative forcing for climate models.

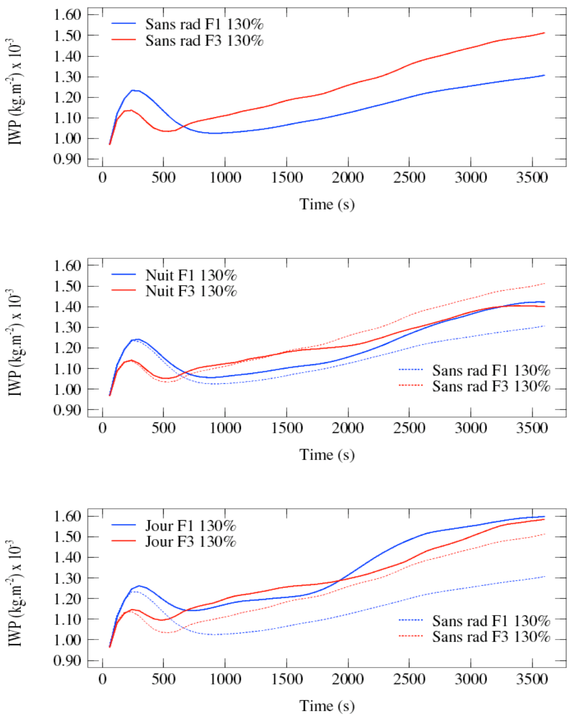


FIG. 1.3: temporal evolution of the Ice water Path for mild (blue) and high (red) turbulence without radiative transfer (top panel) ; with radiative transfer and night conditions (center panel) ; with radiative transfer and day conditions (bottom panel). The dashed lines in the center and bottom panels reproduce the case without radiative transfer and are reported for the sake of comparison.

Impact of launchers

Due to its expertise on the impact of emissions on the atmosphere, the AE team has been contacted by the CNES to conduct evaluations of the impact on the stratospheric composition of rockets launched from the Kourou facility. To this end a chemical transport model has been developed and adapted for the Ariane, Vega and Soyouz rockets. In addition a large-eddy simulation (LES) of booster jet has been carried out for the first time using the turbo-AVBP code. The most significant results are given below. This work has been supported by CNES, and by ESA through the ATILA project coordinated by the Imperial College (UK).

2.1 Simulation of the evolution of booster exhausts

Solid Rocket Boosters (SRB) eject high quantities of gas and particles as they cross the atmosphere. These emissions are known for interacting with atmospheric ozone. The main source of ozone depletion comes from the emissions of hydrogen chloride (HCl) that is largely converted to radical chlorine during a process called afterburning, as it occurs in the zones of high temperature of the jet just after the gas leaves the nozzle. The radical chlorine resulting from this phenomenon reacts with ozone in a very destructive catalytic cycle that can last for several hours and ends when the chlorine is converted back to HCl by reactions with hydrogen-containing molecules, like methane. The simulation of the plume and its chemistry is particularly complex (the jet is highly supersonic, multi-species, reactive, and is several kilometers long). The model should accurately predict the jet dynamics and the afterburning process, and capture the mixing between the exhaust gas and the atmosphere, which are essential ingredients to get a reliable distribution of the chemical species in the plume and to initialize larger-scale atmospheric models. The approach of Large-eddy simulations (LES) was chosen as it offers a good prediction of the turbulence, which has a crucial effect on combustion. The calculations made are representative of a generic SRB jet at 20 km of altitude.

Firstly, three-dimensional LES of a non-reactive SRB jet (including the nozzle) were performed using the AVBP code. To achieve the simulation on a long computational domain while keeping the computational cost relatively low, the MISCOG (Multi Instances Solvers Coupled via Overlapping Grids) method, developed at CERFACS (Wang, 2013), was applied to couple two sub-domains. The application of this coupling made it possible to extend the computational domain up to 400 nozzle exit diameters downstream of the nozzle, while dividing the computational cost by 5. The resulting jet is supersonic coflowing under-expanded. Four regions were identified in the flow, which are characteristic of this kind of jets : a pressure adaptation region, a potential core, a transition zone and a self-similar region. These zones are shown in Fig. 2.1. The results of this work were detailed in a journal article (Poubeau et al., 2014 (a)).

In a second step, the chemical mechanism responsible for the creation of active chlorine (Cl, Cl_2) in the hot plume has been studied. The afterburning process consists in the oxidation of hydrogen molecules and carbon monoxide emitted by the booster, forming free radicals O, H and OH, water H_2O and carbon dioxide CO_2. The free radicals produced during hydrogen combustion are involved into a partial conversion of HCl, also present in the exhaust gas, into active chlorine Cl and Cl_2. In order to obtain a first evaluation of the effect of this chemistry, a 1D model was developed. It consists in applying the afterburning chemistry on streamlines obtained from the single-species LES described in the previous section.

This simple and cost-free calculation, conducted with the open-source solver Cantera, managed to capture the expected chemical steps. A diffusion flame clearly appears in the mixing, where concentrations of radicals are high, and HCl is partially converted in Cl. Downstream from the flame, the chlorine Cl is

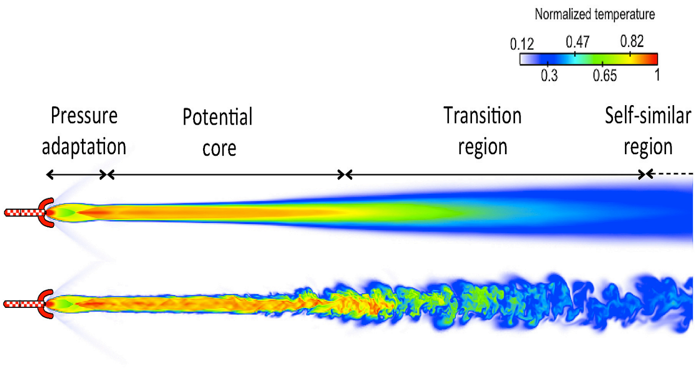


FIG. 2.1: Cut of the jet showing averaged (top) and instantaneous (bottom) temperature up to 160 nozzle exit diameters downstream from the nozzle.

totally converted into Cl_2. At the center of the jet, 24$\%$ of HCl is converted to active chlorine Cl or Cl_2. This percentage is of the same order of magnitude as previous simulations or direct measurements. The results of this study are detailed in the proceedings of an ASME conference (Poubeau et al., 2014 (b)).
The final step of this study is to perform reactive LES of the SRB jet. The chemical mechanism was reduced in order not to penalize the time step of the LES and maintain an affordable computational cost. The first results of this simulation are shown in Fig. 2.2. Qualitatively, they agree very well with the results of the 1D model previously described. A precise distribution of the chlorine species will be obtained, and the impact of turbulence on this distribution will be assessed.

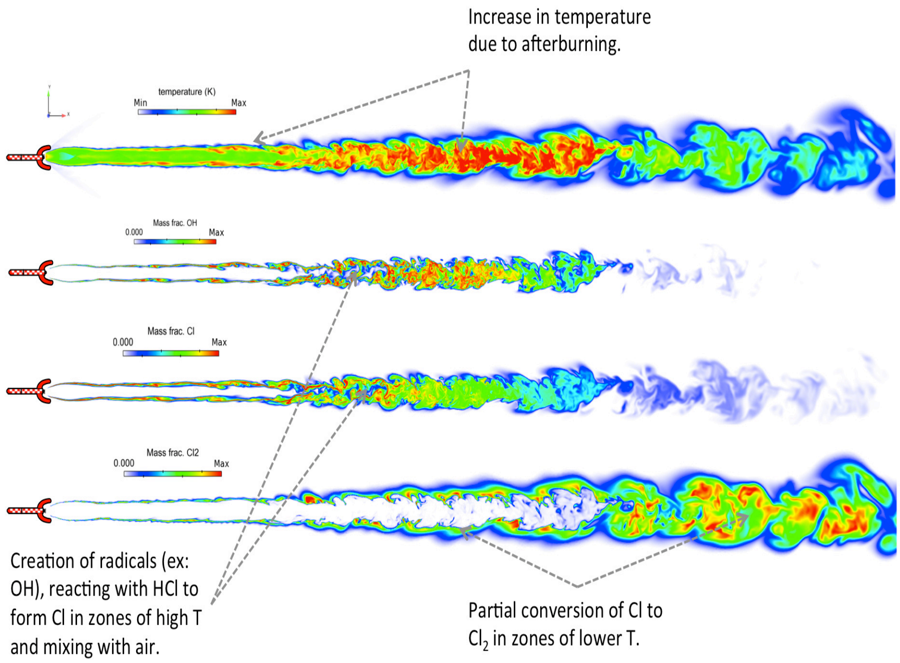


FIG. 2.2: Cut of the jet showing the temperature and the mass fractions of species OH, Cl and Cl_2, up to 200 nozzle exit diameters downstream from the nozzle exit.

Model developments

3.1 ASIS : a chemical solver for atmospheric chemistry models

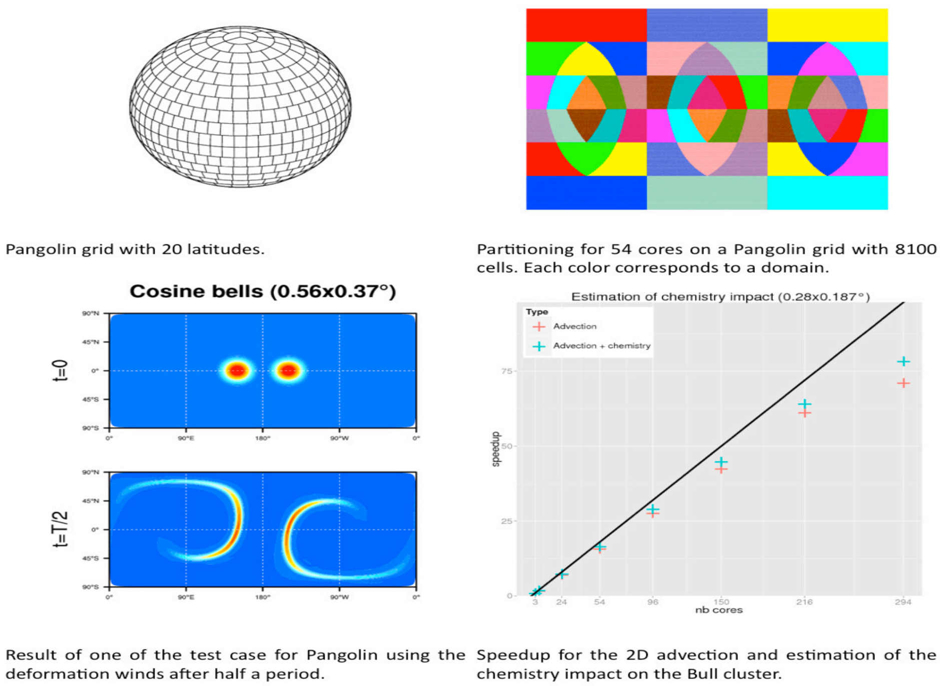
Chemical Transport Models (CTMs) combine the solution of a set of PDEs that accounts for the transport and the chemical transformation of minor trace species. In most of the CTMs the various processes are decomposed in successive time integrations of the equation representative of various processes : transport, surface emissions, washout, dry deposition, and chemistry in gas phase or heterogeneous at the surface of atmospheric particles. We have developed in cooperation with INRIA a versatile solver that treats the couple set of stiff differential equations arising from the gas phase chemistry. The new solver, named Adaptative Semi-Implicit Scheme (ASIS), has the main following characteristics :

1. Perfect mass conservation (at the computer precision)
2. Easy to implement and maintain (no pre-processor is needed)
3. Adaptation of the time stepping according to the state of the system
4. Usage of standard algebra libraries for the solution of linear equations (LU decomposition, Gauss-Siedel algorithm, GMRES)

This solver, which is computational efficient compared to other reference approaches (i.e. KPP based on Rosenbrock scheme) has been implemented within the model of Mars of the IPSL (cooperation with F. Lefevre), and within the MOCAGE model of Météo-France that uses a comprehensive chemistry scheme (with more than 90 species and 300 reactions). A 0D version of the model is available to the scientific community.

3.2 PANGOLIN : a 2D transport model on the sphere for parallel computation

Global three-dimensional chemistry-transport models (CTMs) play an important role in monitoring and predicting the composition of the atmosphere. Those models include large-scale transport, emissions and chemical transformations of trace species and sub-scale grid processes like convection and deposition. In CTMs, advection by large-scale winds is a key process that must be handled by numerical transport algorithms. For these algorithms, mass conservation for the considered species, monotonicity and numerical accuracy are especially important for long simulations where accumulation of errors and bias must be avoided. The PhD thesis of A. Praga consists of developing a conservative advection model on the sphere for parallel architectures, which is intended to form the basic framework for a future CTM. The adopted scheme is based on a flux-form (Eulerian) tracer transport algorithm on a reduced latitude-longitude grid. A finite-volume approach was chosen as it provides an easy way to ensure mass preservation. Furthermore, parallelizing the model is then reduced to a domain decomposition problem. The specificity of the model, named Pangolin (for PArallel implementatioN of a larGe scale multi-dimensiOnaL chemIstry-traNsport scheme), lies in the grid definition where the number of cells on a latitude circle is progressively decreased towards the pole in order to obtain a grid which preserves approximately the cell areas at mid- and high-latitudes. This results in a custom reduced Gaussian grid (see Fig.3.1), which avoids the so-called pole problem which arises from the convergence of the meridians that severely limits the size of the time-steps



Pangolin grid with 20 latitudes.

Partitioning for 54 cores on a Pangolin grid with 8100 cells. Each color corresponds to a domain.

Result of one of the test case for Pangolin using the deformation winds after half a period.

Speedup for the 2D advection and estimation of the chemistry impact on the Bull cluster.

FIG. 3.1: Mains characteristics of the PANGOLIN model.

for Eulerian models. To construct the reduced grid, one difficulty is to define a structure that avoids treating the poles as special cases, as that can impact the precision and properties of the advection algorithm. Thus we have chosen to adopt a semi-structured approach. The grid is not regular as the number of cells varies with the latitude, but the coordinates of cell interfaces can be computed analytically.

The current version of Pangolin has been validated for the bidimensional advection using a new testing suite and results of state-of-the-art schemes in Lauritzen et al. (2014). The test cases use deformational and non-divergent winds such as the analytical solution is known after a full period (see figure 3.1). It was found that Pangolin performs in the same range as other models, with a slower numerical convergence speed however. As our goal is to match the performance of these models, this loss in accuracy can be compensated using finer grids.

Therefore, we aim for an adequate algorithm exploiting the grid features to achieve efficiency and scalability on massively parallel architectures. Fine control over parallelization was obtained using the Message Passing Interface (MPI) library. In that context, the advection scheme must be chosen as to balance its accuracy versus the size of parallel communications. Furthermore, grid properties were carefully studied to improve the parallel version. Especially, a custom domain decomposition consistent with our grid was designed. This results in an analytical decomposition optimal when the number of cores is on the form, where p is a divider of the number of latitudes on an hemisphere (see Fig. 3.1). To hide the communication time as much as possible, we used non-blocking communications. The parallel version was validated up to 294 cores on the Bull cluster at CERFACS for the 2D advection. The observed speed-ups of the model are rather good, but gradually depart from the ideal speed-up when the number of cores increases as shown in Fig. 3.1. The final version of Pangolin will be combined with chemistry modelling. As the chemistry computation is fully local, we can estimate the performances of the chemistry-transport model. The chemical time-step was obtained from the new ASIS solver developed within the AE team (see above). Adding the chemistry greatly increases the computational load in a subdomain and thus improves the scalability. On the other hand, communication volumes only increase linearly as a function of the number of tracers, as expected.

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