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. 2015 – Dec. 2016

CERFACS
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Foreword

Welcome to the 2015-2016 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 also takes care more directly if necessary, of the prospective needs of its shareholders in fields which are insufficiently explored.

This report reflects its activity over the last two years.

During this period, we developped our Strategic Research Plan, written in 2014 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).

Our organization was based in 2015 on 4 scientific teams:

- CFD - Computational Fluid Dynamics (leader: Thierry Poinsot)
- GLOBC - Climate Modelling & Global Change (leader: Olivier Thual)
- ALGO - Parallel algorithms (leader: Serge Gratton)
- AE - Aviation and Environment (leader: Daniel Cariolle)

and a transverse team named CSG devoted to Computer Support (leader: Nicolas Monnier).

During 2016, we decided to reinforce the ALGO team and initiate new dynamics: a new team leader, Ulrich Rüde, joined CERFACS while Serge Gratton kept the leadership of the common Irit/CERFACS laboratory.

In September 2016, we also decided to reinforce transverse actions devoted to technological watch and codes optimization/ industrialization by creating a new activity called COOP [1] within the CSG team.

This activity report is written in independent parts so that readers interested mainly in a particular field will easily find both a detailed description of the work that has been achieved, and a complete list of references, including papers in the reviewed literature and internal reports (which can be made available upon request).

I sincerely hope that you will enjoy reading through the detailed reports of the teams and that you will find there enough interest to continue our collaboration or to initiate new ones.

Enjoy your reading.

Dr Catherine LAMBERT - CERFACS Director

[1] sCientific sOftware & Operational Performance

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.

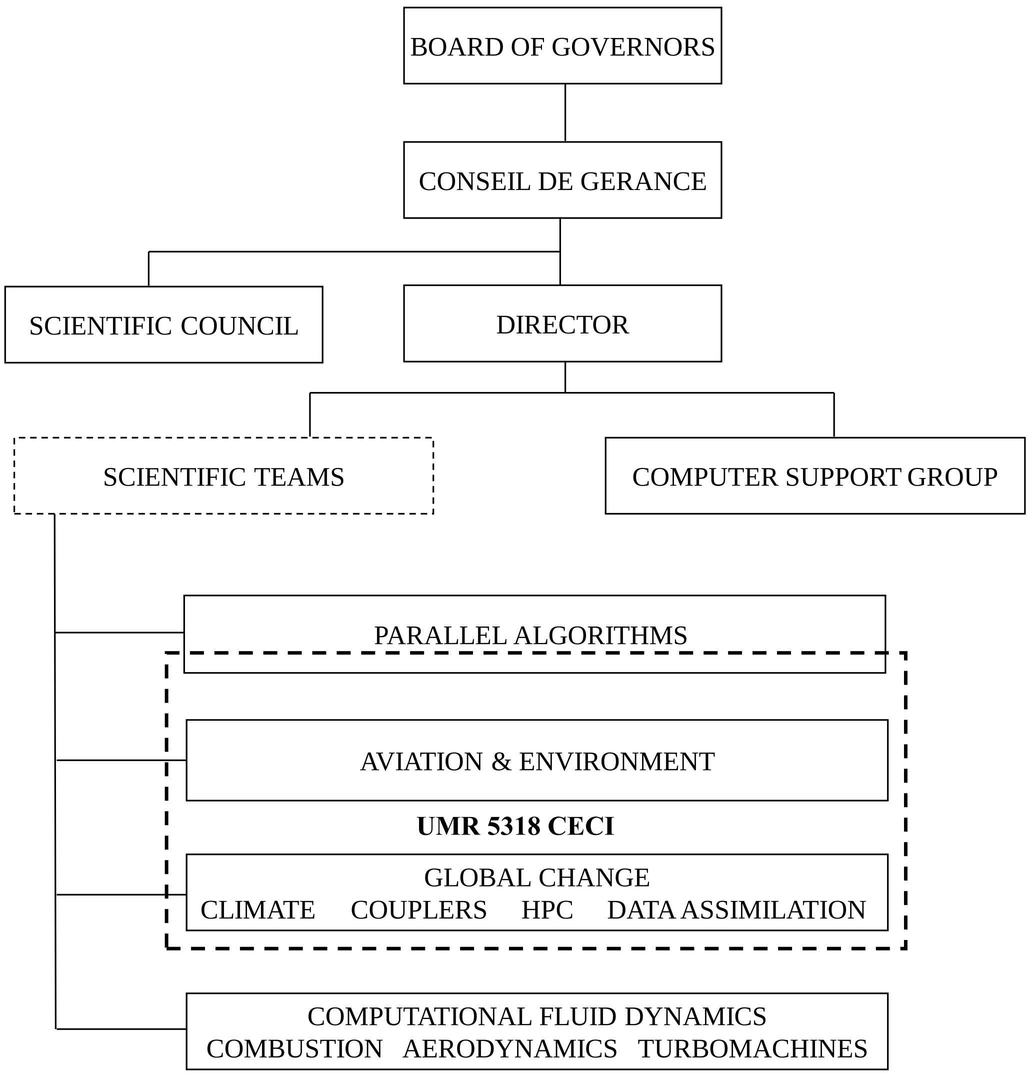
CERFACS Scientific Council met 2 times during this period 2015-2016 first under the chairmanship of Prof. Sébastien CANDEL then under the chairmanship of Prof. Jean-François Minster.

The general organization of CERFACS is depicted in the CERFACS chart, where the computing support group is shown 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, 2016



CERFACS Staff

NAME	POSITION	PERIOD
RUDE	Team Leader	2016/06
DUFF	Scientific Advisor	2011/01
FARES	Senior	1992/06
GUROL	Senior	2014/03
MILLOT	Senior	1995/11-2015/07
VASSEUR	Senior	2007/05-2016/08
WEAVER	Senior	1999/11
DIOUANE	Post Doc	2014/10-2015/04
DE LOZZO	Post Doc	2016/10
MYCEK	Post Doc	2016/12
TSHIMANGA	Post Doc	2014/03-2016/02
CASSIER	Ph.D student	2014/11-2014/06
FILLION	Ph.D student Student	2015/10 2015/03-2015/09
GUILLET	Ph.D student	2015/08
LATRE	Ph.D student Engineer	2015/10 2013/10-2015/03
LUNET	Ph.D student	2015/01
MERCIER	Ph.D student	2012/11-2015/11
MURPHY	Ph.D student	2011/10-2015/09
SOUALMI	Ph.D student	2014/02
VANDAMME	Ph.D student	2014/10
LELEUX	Engineer	2016/10
MENETRIER	Engineer	2015/10-2016/03
RINCON	Engineer	2013/10-2015/09
BENDALI	Consultant	1996/01-2015/12
CHATELIN	Consultant	1992/01
COLLINO	Consultant	1994/04
GRATTON	Team Leader	2011/01-2015/09
VICENTE	Consultant	2016/01

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

NAME	POSITION	PERIOD
AMESTOY	IRIT	2015/01
BUTTARI	IRIT	2015/01
GRATTON	IRIT	2015/01
RUIZ	IRIT	2015/01
SIMON	IRIT	2015/01
LENTI	IRIT	2015/01-2016/07
YANG	IRIT	2016/10
ZHANG	IRIT	2014/10-2015/12

Table iii: List of members of the CERFACS-IRIT common lab.

NAME	POSITION	PERIOD
GIRAUD	INRIA	2009/11
FOURNIER	Ph.D student	2015/03

Table iv: List of members of the CERFACS-INRIA collaboration.

NAME	POSITION	PERIOD
POINSOT	Team Leader	1992/09
CUENOT	Senior	1996/10
DAUPTAIN	Senior	2010/04-2016/09
DAVILLER	Senior Post Doc	2016/02 2013/02-2015/01
GICQUEL	Senior	2004/02
JOUHAUD	Senior	2001/10
MONTAGNAC	Senior	2000/11
PUIGT	Senior	2005/12
RIBER	Senior	2010/05
STAFFELBACH	Senior	2008/11-2016/09
VERMOREL	Senior	2007/11
BOUSSUGE	Research Engineer	2002/02
DOMBARD	Research Engineer	2013/01
BALAN	Post Doc	2015/10
BAUERHEIM	Post Doc	2016/10
BARRE	Post Doc	2014/02-2015/04
BIDADI	Post Doc	2015/07-2016/09
BONHOMME	Post Doc	2014/02-2016/02
DE LABROUHE	Post Doc	2014/02
ESCLAPEZ	Post Doc Ph.D student	2016/10 2011/10-2015/05
GUEDOT	Post Doc	2015/09-2016/11

Table v: List of members of the COMPUTATIONAL FLUID DYNAMICS team (1/3).

IAFRATE	Post Doc	2016/01
JARAVEL	Post Doc Ph.D student	2016/02-2016/12 2012/11-2016/01
LAPEYRE	Post Doc Ph.D student	2016/11 2011/10-2015/04
LE BRAS	Post Doc Ph.D student	2016/05 2012/10-2016/03
LIVEBARDON	Post Doc Ph.D student	2015/07-2016/03 2011/11-2015/04
MISDARIIS	Post Doc	2015/01
PAULHIAC	Post Doc	2015/10-2015/08
AILLAUD	Ph.D student	2014/10
BECERRIL	Ph.D student	2013/10-2016/11
BERGER	Ph.D student	2012/11-2016/02
BIOLCHINI	Ph.D student	2014/06
BIZZARI	Ph.D student Student	2015/10 2015/03-2015/09
BRIDEL-BERTOMEU	Ph.D student	2014/01-2016/12
CAMPET	Ph.D student Student	2015/10 2015/03-2015/08
CATCHIRAYER	Ph.D student	2015/03
CAYOT	Ph.D student	2011/10-2015/12
COLLIN	Ph.D student	2015/05
COREIXAS	Ph.D student	2015/01
DAROUKH	Ph.D student	2014/01
DOUNIA	Ph.D student	2014/10
DUPUIS	Ph.D student	2015/10
FELDEN	Ph.D student	2014/01
FERAND	Ph.D student	2014/03
FIORE	Ph.D student	2016/02
GALLEN	Ph.D student Student	2016/10 2016/02-2016/07
GHANI	Ph.D student	2012/02-2015/05
GROSNICKEL	Ph.D student	2014/10
HARNIEH	Ph.D student Student	2015/10 2015/03-2015/08
JONCQUIERES	Ph.D student Student	2015/11 2015/03-2015/09
KOUPPER	Ph.D student	2012/01-2015/01
LABARRERE	Ph.D student	2012/10-2015/09
LACASSAGNE	Ph.D student	2013/10
LAHBIB	Ph.D student	2012/10-2015/12
LAURENT	Ph.D student	2016/10
MAESTRO	Ph.D student	2014/08
MOURET	Ph.D student	2012/10-2016/02
MUSCAT	Ph.D student Student	2015/10 2015/03-2015/09
NDIAYE	Ph.D student	2013/10
NI	Ph.D student	2013/11

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

PACAUD	Ph.D student	2016/11
PAPADOGIANNIS	Ph.D student	2012/01-2015/03
PEREZ ARROYO	Ph.D student	2013/10-2016/09
POTIER	Ph.D student	2014/11
ROCHETTE	Ph.D student Student	2015/10 2015/02-2015/08
ROY	Ph.D student Student	2016/11 2016/03-2016/10
SADOUDI	Ph.D student	2011/11-2015/05
SEGUI TROTH	Ph.D student	2013/10
SHUM-KIVAN	Ph.D student	2013/10-2016/12
THOMAS	Ph.D student	2016/02
VANHAREN	Ph.D student	2014/01
WISSOCQ	Ph.D student	2015/03
ZHU	Ph.D student	2012/02-2015/01
ASTOUL	Engineer	2016/12
DUPUY	Engineer	2016/10
GUILBAUD	Engineer Student	2016/10 2016/04-2016/09
GUEDENEY	Engineer	2014/11-2016/04
MARAIT	Engineer	2015/08-2016/07
ODIER	Engineer	2015/07-2016/12
PECHEREAU	Engineer Post Doc	2016/10 2014/10-2016/09
QUEGUINEUR	Engineer	2016/11
BAROUILLET	Student	2015/02-2015/08
CUNHA CALDEIRA	Student	2015/03-2015/09
HAMRI	Student	2015/06-2015/09
MENDEZ ROJANO	Student	2015/03-2015/08
PINEAU	Student	2015/03-2015/09
CHU	Student	2016/04-2016/09
DEDIEU	Student	2016/06-2016/09
DRAY	Student	2016/06-2016/08
GAURIER	Student	2016/07-2016/12
JETTOU	Student	2016/03-2016/09
LAMRANI	Student	2016/06-2016/08
QUESTIAUX	Student	2016/07-2016/09
SILVA TERZAN	Student	2016/06-2016/07
SIMIRIOTIS	Student	2016/04-2016/09
STACHURA	Student	2016/04-2016/09
TALEUAN	Student	2016/06-2016/09
WANG	Student	2016/04-2016/09
MOREAU	Consultant	2009/04
MULLER	Consultant	1997/11
NICOUD	Consultant	2001/10
SAGAUT	Consultant	2011/02
SCHONFELD	Consultant	2001/01
BUSCHMANN	Visitor	2016/09-2016/02

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

NAME	POSITION	PERIOD
THUAL	Team Leader	1991/09
DUCHAINE	Senior	2010/10
RICCI	Senior	2008/11
ROCHOUX	Senior	2015/15
ROGEL	Senior	1998/10
TERRAY	Senior	1992/10
MAISONNAVE	Research Engineer	2000/12
MOINE	Research Engineer	2015/01
MOREL	Research Engineer	2000/03
PAGE	Research Engineer	2009/07
SANCHEZ	Research Engineer	2009/05
THEVENIN	Research Engineer	2008/09-2015/05
VALCKE	Research Engineer	1997/02
BARTHELEMY	Post Doc Ph.D Student	2015/10 2011/12-2015/04
CORTESI	Post Doc	2014/02-2015/04
GOUBANOVA	Post Doc	2015/01-2016/09
LLOVEL	Post Doc	2015/02
MONERIE	Post Doc Engineer	2015/07-2016/07 2014/03-2015/07
BADOR	Ph.D Student	2012/11-2016/02
BONNET	Ph.D Student	2015/10
COLMET DAAGE	Ph.D Student	2015/05
EL MOCAYD	Ph.D Student	2013/11-2016/12
HABERT	Ph.D Student	2011/10-2015/09
OUDAR	Ph.D Student	2013/10-2016/12
QASMI	Ph.D Student	2015/11
BESSIERES	Engineer	2014/01-2016/12
BOUMEDIENE	Engineer	2014/10-2015/04
DAYON	Engineer Ph.D Student	2016/01 2012/11-2015/12
DROUARD	Engineer	2015/01-2016/12
MOUSSU	Engineer	2016/12
PIVAN	Engineer	2016/10
RADOJEVIC	Engineer	2016/09-2016/12
SERAZIN	Engineer	2012/11-2015/12
TATARINOVA	Engineer	2013/09-2015/02
AYOUB	Student	2015/04-2015/05
BRENIERE	Student	2015/07-2015/08
AMINI	Student	2016/02-2016/07
LE CHENADEC	Student	2016/04-2016/09
VIALARET	Student	2016/05-2016/07
BOE	CNRS	2010/10
CASSOU	CNRS	2002/11
COQUART	CNRS	2006/12
MSADEK	CNRS	2015/10

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

PIACENTINI	Consultant	2007/06
GARCIA SERRANO	Visitor	2016/06-2016/08
NIANG	Visitor	2016/07-2016/07
VARGEL	Visitor	2016/02-2016/07

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

NAME	POSITION	PERIOD
CARIOLLE	Team Leader	2003/08
EMILI	Senior	2014/02
JONVILLE	Research Engineer	2000/03
PAOLI	Senior	2004/07
THOURON	Senior	2012/10
CLARK	Post Doc	2014/01-2015/12
REA	Post Doc	2016/03
SIC	Post Doc	2015/01-2016/12
PEIRO	Ph.D Student	2014/11
POUBEAU	Ph.D Student	2011/10-2015/04
AUGUSTE	Engineer Post Doc	2016/11 2014/11-2016/11
AUDOUIN	Student	2016/01-2016/02
HARTMANN	Student	2016/01-2016/02
KAYANAKIS	Student	2016/01-2016/02
PEYRAT	Student	2016/01-2016/02
MOINAT	Consultant	2013/01
PIACENTINI	Consultant	2007/10

Table vii: List of members of the AVIATION & ENVIRONMENT team.

NAME	POSITION	PERIOD
MONNIER	Team Leader	1996/12
DAUPTAIN	Senior	2016/10
STAFFELBACH	Senior	2016/10
D'AST	Engineer	1996/10
LAPORTE	Engineer	1988/04
DEJEAN	Engineer	1990/11
FARCY	Engineer	2016/11
HANNEBIQUE	Engineer	2016/09
LEGAUX	Engineer	2016/07
BLAIN	Technician	2016/03
FLEURY	Technician	1999/10
VIDAL	Technician	2013/10-2015/08
MARAIT	Student	2015/02-2015/07
NASRI	Student	2015/06-2015/06
GRASSET	Student	2016/04-2016/09
SARRAUTE	Student	2016/06-2016/09

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

CERFACS Wide-Interest Seminars

Christophe Genolini (Université Paris 10) : *Statistique et Big data, vers une nouvelle synergie.* (2015, February 26th)

Pierre Sagaut (CERFACS) : *Résultats récents sur l'emploi des méthodes de Boltzmann sur réseau pour l'aérodynamique et l'aéroacoustique.* (2015, March 10th)

Philippe Escudier & Michel Avignon (CNES), **Cathy Dubois** (CNAM) : *Observer la Terre depuis l'espace, Enjeux des données spatiales pour la société.* (2015, March 24th)

Jacqueline Chen (Sandia National Laboratories, Livermore, CA 94550) : *Towards Exascale Combustion Simulations: Combustion Modified Flow in Turbulent Wall-Bounded and Free Shear Flows.* (2015, April 24th)

Juan Carlos DOLADO-PEREZ (CNES) : *Modelling the long term evolution of the space debris population.* (2015, June 11st)

V. Balaji(NOAA/GFDL and Princeton University) : *Climate computing: the state of play.* (2015, September 3rd)

Prof. Carlo SCALO (University of Purdue) : *Modeling of Thermoacoustic Energy Generation and Extraction.* (2015, September 17th)

Michael Prather (University of California, Irvine) : *Uncertainties in the causal chain from human activities to climate change: A brief history of emissions scenarios and the uncertainties in using them.* (2015, October 8th)

Michael Prather (University of California, Irvine) : *Evaluation of Surface Ozone over Europe and USA: Present-day observations & hindcasts, future projections from chemistry-climate models.* (2015, November 12nd)

Paul Clavin (Aix-Marseille Université, CNRS, Centrale Marseille, IRPHE UMR7342) : *Nonlinear waves and fronts in flows: From flames, shocks and detonations to the explosion of stars.* (2015, November 18th)

Jean-Michel Tanguy (Commissariat Général au Développement Durable) : *Les drones au service du développement durable.* (2016, January 6th)

Joaquim R. R. A. Martins (University of Michigan) : *Optimisation numérique de la conception d'une aile d'avion: Rêve ou réalité?* (2016, March 8th)

Romain Desplats (Responsable Propriété Intellectuelle, CNES) : *Innovations, Inventions, logiciels et opensource, Que dois-je faire dans cette dynamique ?* (2016, March 23rd)

Roland Martin, Etienne Gondet & Pascal Dayre (Observatoire Midi-Pyrénées) : *Présentation de 2 Axes transverses à l'OMP et 2 projets en cours au sein des réseaux du CNRS .* (2015, May 10th)

Eric Blayo (Professeur de l'Université Joseph Fourier de Grenoble, Laboratoire Jean Kuntzmann) : *Aspects mathématiques et numériques du couplage de modèles.* (2016, July 1st)

Ulrich Rüde (Cerfacs, Universität Erlangen-Nuernberg) : *Towards Extreme Scale Simulation.* (2016, September 15th)

Eric Pardyjak (University of Utah) : *High-Resolution Modeling of Environmental Transport Processes for Sustainable Cities.* (2016, October 6th)

Tapan K. Sengupta (High Performance Computing Laboratory, Dept. of Aerospace Engineering, IIT Kanpur, INDIA) : *DNS of Turbulence from Receptivity Stage: Case of Zero-Pressure Gradient Boundary Layer.* (2016, October 12nd)

Vincent Baudoui (CENAERO FRANCE) : *Optimisation robuste d'une chambre de combustion.* (2016, November 4th)

Michael Prather (University of California, Irvine) : *How do pollution episodes and heatwaves interact? The co-occurrence of extremes in ozone, particulate matter, and temperature .* (2016, November 7th)

Ulrich Rüde (Cerfacs, Universität Erlangen-Nuernberg) : *Lattice Boltzmann Methods on the way to exascale.* (2016, December 8th)

1

Parallel Algorithms

Introduction

1.1 Introduction

The Parallel Algorithms team conducts research on advanced numerical algorithms to address the solution of problems in Computational Science and Engineering on massively parallel computing platforms. The Parallel Algorithms team studies the design, the analysis and the implementation of innovative algorithms for problems that are out of reach of current standard numerical methods. Such limitations can be due to the computational cost when extremely fine resolutions are required, or innovative new methods may be needed for special nonlinear problems or when the stochastic nature of the data must be considered. This kind of research is mostly performed in collaboration with other teams at CERFACS and the shareholders of CERFACS. In particular, many linear-algebra and optimization-related research activities are done in collaboration with colleagues at IRIT in the context of the joint CERFACS-IRIT Common Laboratory. Examples of this are found in Sections 2.1, 2.3, 2.4, 2.6, 4.5, and 4.7.

The Parallel Algorithms team builds on three decades of successful work on parallel numerical methods at the forefront of computational mathematics and is now striving to open its scope into new areas. The field is currently characterized by the continued progress in computer technology to ever higher degree of parallelism that leads to an unprecedented need for scalable algorithms, and the recent drive towards using the abundance of data available from sensors and measurements. Finally, the rapid entry of computational methods into nontraditional application fields opens avenues of opportunity and at the same time creates new challenges for the use of numerical algorithms.

In many applications of computational science and engineering, classical forward simulations are now used as building blocks for more complex and challenging computational goals. These include optimizaton problems, inverse problems, model reduction techniques, and data driven computing. In the past few years, the Parallel Algorithms team has successfully developed new research directions in these fields. This includes especially research in the context of optimization and data assimilation. Additionally, the systematic quantification of uncertainties has become a field of research that is expected to become even more important in the future as the basis of decision support systems in fields of scientific or societal relevance.

Naturally these research topics are interconnected, since e.g. large-scale inverse problems (as they arise in big data applications) or the solution of nonlinear systems eventually all require approximate solutions of linearized systems. These developments rely on the strong research expertise in mathematical modelling, numerical analysis, partial differential equations, integral equations, scientific computing, and computational science that is present within the Parallel Algorithms team. For the research of the Parallel Algorithms team it is essential to identify the abstract mathematical structure of a given problem and to exploit it in the design of the algorithms. We point here especially to the unique research performed in qualitative computing where the suitability of nontraditional algebraic structures for problems in scientific computing is being analysed (Section 6).

Generally, the role of the Parallel Algorithms team within CERFACS is to bridge from the fundamental mathematical aspects to research for real-life applications. To this end, novel parallel algorithms and methods are proposed, designed, and analysed in terms of their accuracy and their computational cost. This research includes the quantification of convergence properties, the study of the accuracy achieved, and especially also the efficiency and scalability of the methods on advanced parallel computer architectures.

The solution of sparse linear systems is considered by tackling both sparse direct methods as well as projection based iterative methods. These methods can also be combined to derive hybrid algebraic methods close to domain decomposition or multiscale and multigrid methods. In addition to graph theory, linear algebra, and functional analysis, these activities rest upon the strong expertise in scientific software development and on an up-to-date knowledge of the current parallel computing platforms.
Optimization methods occur in several applications at CERFACS. Most often the main goal is to improve the performance of a given system. The Parallel Algorithms team works in 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 team 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 seismology, oceanography, atmospheric chemistry or meteorology. The Parallel Algorithms team 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 team 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, high performance computing, computational science and engineering, and data assimilation.

Ulrich Rüde

Dense and Sparse Matrix Computations

2.1 Parallel computation of entries of A^{-1}.

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*; **F.-H. Rouet**: UNIVERSITÉ DE TOULOUSE, INPT(ENSEEIHT)-IRIT, *France*

We consider the computation in parallel of several entries of the inverse of a large sparse matrix. We assume that the matrix has already been factorized by a direct method and that the factors are distributed. Entries are efficiently computed by exploiting sparsity of the right-hand sides and the solution vectors in the triangular solution phase. We demonstrate that in this setting, parallelism and computational efficiency are two contrasting objectives. We develop an efficient approach and show its efficiency on a general purpose parallel multifrontal solver.

2.2 Preconditioning linear least-squares problems by identifying a basis matrix.

M. Arioli: TU-BERLIN AND UNIVERSITÉ DE TOULOUSE, CIMI, INPT (ENSEEIHT)-IRIT, *France*; **I.S. Duff**: CERFACS, 42 AVENUE GASPARD CORIOLIS, 31057, TOULOUSE, FRANCE AND BUILDING R 18, RAL, OXON, OX11 0QX, ENGLAND

We study the solution of the linear least-squares problem $\min_x \|b - Ax\|_2^2$ where the matrix $A \in \mathbb{R}^{m\times n}$ ($m \geq n$) has rank n and is large and sparse. We assume that A is available as a matrix, not an operator. The preconditioning of this problem is difficult because the matrix A does not have the properties of differential problems that make standard preconditioners effective. Incomplete Cholesky techniques applied to the normal equations do not produce a well conditioned problem. We attempt to bypass the ill-conditioning by finding an n by n nonsingular submatrix B of A that reduces the Euclidean norm of AB^{-1}. We use B to precondition a symmetric quasi-definite linear system whose condition number is then independent of the condition number of A and has the same solution as the original least-squares problem. We illustrate the performance of our approach on some standard test problems and show it is competitive with other approaches.

2.3 The block Cimmino method.

I. S. Duff: CERFACS, 42 AVENUE GASPARD CORIOLIS, 31057, TOULOUSE, FRANCE AND BUILDING R 18, RAL, OXON, OX11 0QX, *England*; **R. Guivarch**: UNIVERSITÉ DE TOULOUSE, INPT(ENSEEIHT)-IRIT, *France*; **D. Ruiz**: UNIVERSITÉ DE TOULOUSE, INPT(ENSEEIHT)-IRIT, *France*; **M. Zenadi**: UNIVERSITÉ DE TOULOUSE, INPT(ENSEEIHT)-IRIT, *France*

The block Cimmino method is a block projection algorithm that is effectively the same as using a block Jacobi algorithm on the normal equations. Since the algorithm is inherently very parallel and can use a parallel solver like MUMPS on the individual blocks, it is a good potential approach for solving sparse systems on upcoming extreme scale computers. We have had two papers on this method published in high quality journals: one concerning the partitioning to obtain the block form and the other on a method of accelerating convergence by augmenting the original system. A code for this has been written in C++ and is available through github. It is one of the codes being used in the EoCoE Project discussed in Section 2.6.

2.4 Uncovering Hidden Block Structure.

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We develop a multistep procedure for discovering the structure in a matrix. In this work we combine standard combinatorial techniques with a novel clustering technique that combines numerical and structural analysis. We discuss the use of partitioning schemes based on this cluster decomposition in preconditioning and block iterative methods.

2.5 Direct Methods for Sparse Matrices.

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The first edition of the book "Direct Methods for Sparse Matrices" by Duff, Erisman, and Reid was published in 1986 so one can easily see that much new research and many advances have been made since that time including far more research on methods that exploit parallelism. It is with great pleasure that we can report that the Second Edition will be published by OUP in December of 2016. In addition to consideration of the influence of new computer architectures there is significantly more description of partitioning and ordering algorithms and tree-based factorization methods including both supernodal and multifrontal.

2.6 Testing solvers on applications in the energy sector.

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In the context of the CoE Project EoCoE (Centre of Excellence in Energy), we are examining the performance of a range of codes from CERFACS and IRIT on a raft of applications from the energy sector, including oil, water, and fusion. The codes in question are:

- MUMPS
- qr_mumps
- GMRES and other Krylov solvers

- Block Cimmino and ABCD

with two recent additions: a multigrid code HHG from Ulrich Ruede at Erlangen and a domain-decomposition code HPDDM from Pierre Jolivet. The project received a big boost towards the end of 2016 by the recruitment of a full-time engineer to work on the project.

2.7 Methods for solving discontinuous-Galerkin finite element equations with application to neutron transport.

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Although the title of this article may not appear to be appropriate for this part of the activity report, the work done at CERFACS as part of this cotutelle concerned the solution of sparse structured equations. This work is described in Chapter 3 of the thesis by Steven Murphy. Standard sparse direct solvers are used in a novel way to solve the resulting equations and a novel exploitation of the blocking results in much faster solution and the ability to solve larger problems than was previously possible.

Methods for Numerical Linear Algebra with Applications

3.1 On a second-order expansion of the truncated singular subspace decomposition.

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We present a second-order expansion for singular subspace decomposition in the context of real matrices. Furthermore, we show that, when some particular assumptions are considered, the obtained results reduce to existing ones. Some numerical examples are provided to confirm the theoretical developments of this study.

3.2 Reducing complexity of algebraic multigrid by aggregation.

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A typical approach to decrease computational costs and memory requirements of classical algebraic multigrid methods is to replace a conservative coarsening algorithm and short-distance interpolation on a fixed number of fine levels by an aggressive coarsening with a long-distance interpolation. Although the quality of the resulting algebraic multigrid grid preconditioner often deteriorates in terms of convergence rates and iteration counts of the preconditioned iterative solver, the overall performance can improve substantially. We investigate here, as an alternative, a possibility to replace the classical aggressive coarsening by aggregation, which is motivated by the fact that the convergence of aggregation methods can be independent of the problem size provided that the number of levels is fixed. The relative simplicity of aggregation can lead to improved solution and setup costs. The numerical experiments show the relevance of the proposed combination on both academic and benchmark problems in reservoir simulation from oil industry.

3.3 Limited memory preconditioners for symmetric indefinite problems with application to structural mechanics.

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We present a class of limited memory preconditioners (LMP) for solving linear systems of equations with symmetric indefinite matrices and multiple right-hand sides. These preconditioners based on limited memory quasi-Newton formulas require a small number k of linearly independent vectors and may be used to improve an existing first-level preconditioner. The contributions of the paper are threefold. First, we derive a formula to characterize the spectrum of the preconditioned operator. A spectral analysis of the preconditioned matrix shows that the eigenvalues are all real and that the LMP class is able to cluster at least k eigenvalues at 1. Secondly, we show that the eigenvalues of the preconditioned matrix enjoy interlacing properties with respect to the eigenvalues of the original matrix provided that the k linearly independent vectors have been prior projected onto the invariant subspaces associated with the eigenvalues of the original matrix in the open right and left half-plane, respectively. Third, we focus on theoretical properties of the Ritz-LMP variant, where Ritz information is used to determine the k vectors. Finally, we illustrate the numerical behaviour of the Ritz limited memory preconditioners on realistic applications in structural mechanics that require the solution of sequences of large-scale symmetric saddle-point systems. Numerical experiments show the relevance of the proposed preconditioner leading to a significant decrease in terms of computational operations when solving such sequences of linear systems. A saving of up to 43% in terms of computational effort is obtained on one of these applications.

Nonlinear Optimization and Data Assimilation

4.1 A parallel evolution strategy for an earth imaging problem in geophysics.

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We propose a new way to compute a rough approximation solution, to be later used as a warm starting point in a more refined optimization process, for a challenging global optimization problem related to earth imaging in geophysics. The warm start consists of a velocity model that approximately solves a full-waveform inverse problem at low frequency. Our motivation arises from the availability of massively parallel computing platforms and the natural parallelization of evolution strategies as global optimization methods for continuous variables. Our first contribution consists of developing a new and efficient parametrization of the velocity models to significantly reduce the dimension of the original optimization space. Our second contribution is to adapt a class of evolution strategies to the specificity of the physical problem at hands where the objective function evaluation is known to be the most expensive computational part. A third contribution is the development of a parallel evolution strategy solver, taking advantage of a recently proposed modification of these class of evolutionary methods that ensures convergence and promotes better performance under moderate budgets. The numerical results presented demonstrate the effectiveness of the algorithm on a realistic 3D full-waveform inverse problem in geophysics. The developed numerical approach allows us to successfully solve an acoustic full-waveform inversion problem at low frequencies on a reasonable number of cores of a distributed memory computer.

4.2 Globally convergent evolution strategies.

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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.

4.3 Globally convergent evolution strategies for constrained optimization.

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We propose, analyze, and test algorithms for constrained optimization when no use of derivatives of the objective function is made. The proposed methodology is built upon the globally convergent evolution strategies previously introduced by the authors for unconstrained optimization. Two approaches are encompassed to handle the constraints. In a first approach, feasibility is first enforced by a barrier function and the objective function is then evaluated directly at the feasible generated points. A second approach projects first all the generated points onto the feasible domain before evaluating the objective function. The resulting algorithms enjoy favorable global convergence properties (convergence to stationarity from arbitrary starting points), regardless of the linearity of the constraints. The algorithmic implementation (i) includes a step where previously evaluated points are used to accelerate the search (by minimizing quadratic models) and (ii) addresses the particular cases of bounds on the variables and linear constraints. Our solver is compared to others, and the numerical results confirm its competitiveness in terms of efficiency and robustness.

4.4 Parallelisation in the Time Dimension of Four-Dimensional Variational Data Assimilation.

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The current evolution of computer architectures towards increasing parallelism requires a corresponding evolution towards more parallel data assimilation algorithms. In this study, we consider parallelisation of weak-constraint 4DVar in the time dimension. We categorise algorithms according to whether or not they admit such parallelisation, and we introduce a new, highly parallel weak-constraint 4D-Var algorithm based on a saddle-point representation of the underlying optimisation problem.

4.5 Low rank updates in preconditioning the saddle point systems arising from data assimilation problems.

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The numerical solution of saddle point systems has received a lot of attention over the past few years in a wide variety of applications such as constrained optimization, computational fluid dynamics and optimal control, to name a few. In this paper, we focus on the saddle point formulation of a large-scale variational data assimilation problem, where the computations involving the constraint blocks are supposed to be much more expensive than those related to the (1, 1) block of the saddle point matrix. New low-rank limited memory preconditioners exploiting the particular structure of the problem are proposed and analysed theoretically. Numerical experiments performed within the Object Oriented Prediction System (OOPS) are presented to highlight the relevance of the proposed preconditioners.

4.6 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.

4.7 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 Lorenz96 system, the latter one being of special interest because of its similarity with numerical weather prediction systems.

4.8 Hybrid Levenberg-Marquardt and weak constraint ensemble Kalman smoother method.

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The ensemble Kalman smoother (EnKS) is used as a linear least-squares solver in the Gauss–Newton method for the large nonlinear least-squares system in incremental 4DVAR. The ensemble approach is naturally parallel over the ensemble members and no tangent or adjoint operators are needed. Furthermore, adding a regularization term results in replacing the Gauss–Newton method, which may diverge, by the Levenberg–Marquardt method, which is known to be convergent. The regularization is implemented efficiently as an additional observation in the EnKS. The method is illustrated on the Lorenz 63 model and a two-level quasi-geostrophic model.

4.9 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.

4.10 Correlation operators based on an implicitly formulated diffusion equation solved with the Chebyshev iteration.

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Correlation operators are used in the formulation of background-error covariance models in variational data assimilation (VDA) and for localizing low-rank sample estimates of background-error covariance matrices in ensemble VDA. This article describes new approaches for defining correlation operators based on diffusion operators. The starting point is a two-dimensional (2D) implicitly formulated diffusion operator on the sphere, which has been shown in previous works to support symmetric and positive-definite smoothing kernels that are closely related to those from the Matérn correlation family. Different methods are proposed for solving the 2D implicit diffusion problem and these are compared with respect to their efficiency, accuracy, memory cost, ease of implementation and parallelization properties on high-performance computers. The methods described in this article are evaluated in a global ocean VDA system. An iterative algorithm based on the Chebyshev iteration, which uses a fixed number of iterations and pre-computed eigenvalue bounds, is shown to be particularly promising. Techniques for improving the parallelization aspects of the algorithm further are discussed.

Propagation

5.1 A symmetric Trefftz-DG formulation based on a local boundary element method for the solution of the Helmholtz equation.

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This paper is devoted to a general symmetric Trefftz Discontinuous Galerkin method, for solving the Helmholtz equation with piecewise constant coefficients. The used method is built by integration by parts and addition of consistent terms. The construction of the corresponding local solutions to the Helmholtz equation is based on a boundary element method. The numerical experiments, which are presented, show an excellent stability relatively to the penalty parameters, and more importantly an outstanding capacity of the method to reduce the instabilities known as the “pollution effect” in the literature on numerical simulations of long-range wave propagation.

5.2 Approximation by Multipoles of the Multiple Acoustic Scattering by Small Obstacles in Three Dimensions and Application to the Foldy Theory of Isotropic Scattering.

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The asymptotic analysis, carried out in this paper, for the problem of a multiple scattering of a time-harmonic wave by obstacles whose size is small as compared with the wavelength establishes that the effect of the small bodies can be approximated at any order of accuracy by the field radiated by point sources. Among other issues, this asymptotic expansion of the wave furnishes a mathematical justification with optimal error estimates of Foldy's method that consists in approximating each small obstacle by a point isotropic scatterer. Finally, it is shown how this theory can be further improved by adequately locating the center of phase of the point scatterers and taking into account of self-interactions.

Qualitative Computing

With the ongoing financial support of Total/Direction Scientifique, the Qualitative Computing group is following its work on hypercomplex algebras. The main topics addressed concern some of the problems encountered in Scientific Computing and Industry (nonlinearity, coupling, information processing), from theoretical modelling aspects to a mid term numerical resolution in these algebraic structures. The PhD thesis of Jean-Baptiste Latre has started on 15/10/1. The recent advances on spectral coupling have been submitted in a paper to LAA (currently under revision). These results made a basis for the improvements concerning the link between bireal numbers and Mohr's Circle in continuous mechanics (called Arbelos in mathematics). This ongoing work has been presented at the conference Total-Mathias (Paris, Oct. 16) and will constitute a strong part of the Phd thesis.
The technical work done by the Qualitative Computing group can be found in the technical reports. Pr Chatelin has also been invited to contribute to the book "The Human face of Computing" of C. Calude (Univ. of Auckland, NZ) which is presented as "Written as a series of conversations with influential computer scientists, mathematicians and physicists, this book provides access to the inner thinking of those who have made essential contributions to the development of computing and its application".

Publications

7.1 Books

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[ALG2] I. Duff, A. Erisman, and J. Reid, (2016), *Direct Methods for Sparse Matrices. Second Edition.*, Oxford University Press, Oxford, England.

7.2 Conference Proceedings

[ALG3] Z. Bai and I. Duff, (2015), Practical methods and rigorous theories in numerical algebra and scientific computing, In *Preface to Special Issue Devoted to the 4th NASC 12 Conference in Dalian, PRC*, 1–2.

[ALG4] H. Barucq, A. Bendali, M. Fares, and S. Tordeux, (2016), A low dispersive Trefftz DG method based on a local BEM for the solution of the Helmholtz equation, Paris, Ecole Polytechnique.

[ALG5] H. Barucq, A. Bendali, M. Fares, and S. Tordeux, (2016), A non-dispersive discontinuous galerkin method to solve the Helmholtz equation in heterogenous media, Pau, JOSO 2016. Wave Days in South West, PAU.

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7.3 Journal Publications

[ALG10] E. Agullo, P. R. Amestoy, A. Buttari, A. Guermouche, J.-Y. L'Excellent, and F.-H. Rouet, (2016), Robust memory-aware mappings for parallel multifrontal factorizations, **38**, C256–C279.

[ALG11] P. R. Amestoy, R. Brossier, A. Buttari, J.-Y. L'Excellent, T. Mary, L. Métivier, A. Miniussi, and S. Operto, (2016), Fast 3D frequency-domain full waveform inversion with a parallel Block Low-Rank multifrontal direct solver: application to OBC data from the North Sea, *Geophysics*, **81**, R363–R383.

[ALG12] P. Amestoy, I. S. Duff, J.-Y. L'Excellent, and F.-H. Rouet, (2015), Parallel computation of entries of A^{-1}, *SIAM Journal on Scientific Computing*, **37**, C268–C284.

[ALG13] M. Arioli and I. S. Duff, (2015), Preconditioning linear least-squares problems by identifying a basis matrix, *SIAM Journal on Scientific Computing*, **37**, S544–S561.

[ALG14] H. Barucq, A. Bendali, J. Diaz, M. Fares, V. Mattesi, and S. Tordeux, (2015), A non-dispersive discontinuous Galerkin method for the simulation of acoustic scattering in complex media, *Journal of the Acoustical Society of America*, **138**, 1765.

[ALG15] H. Barucq, A. Bendali, M. Fares, V. Mattesi, and S. Tordeux, (2016), A Symmetric Trefftz-DG formulation based on a local boundary element method for the solution of the Helmholtz equation, *Journal of Computational Physics*.

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2

Climate and Environment

Introduction

This “Climate and Environment” chapter gathers the activities of three teams: GLOBC (Climate Modelling and Global Change), AE (Aviation and Environment) and part of ALGO (Parallel Algorithms). These activities cover the research axes of the CERFACS-CNRS joint research center (UMR 5318) CECI (Climate, Environment, Coupling and Uncertainties).

The present report has been written having in mind the presentation that is required for a scientific evaluation by the HCERES (Haut conseil de l’évaluation de la recherche et de l’enseignement supérieur) that regularly audits the CECI joint research center.

For this reason, this presentation does not include as it should the strength of the transversal synergies existing inside Cerfacs as put forward in other documents such as the three year CERFACS research strategic plans or the annual team sheet to be validated before each civil year. For example, sections such as “Uncertainties and Data Assimilation” in this chapter do not gather all the CERFACS activities in this domain since the present chapter only deals with the tasks performed in the framework of climate and environment.

This chapter is organised into five research axes :

- Climate Variability and Climate Change;
- Modeling Environnement and Safety;
- Couplers and Coupling Applications;
- Data Assimilation and Uncertainties;
- High Performance Computing and Data.

Climate Variability and Climate Change

2.1 Introduction

With emerging public awareness of human-induced climate change, a major challenge is to understand and communicate the causes of recent observed climate trends, particularly at local and regional scales. Such trends are often interpreted in the context of rising anthropogenic emissions of greenhouse gases (GHGs) and sulfate aerosols associated with the burning of fossil fuels. However, internally generated variability may also contribute to regional climate changes over periods of several decades and longer. In the context of adaptation to the impact of climate change, it is important for a broad range of stakeholders and decision makers to know how the mix of the response to anthropogenic forcing and the impact of natural variability will shape the near term evolution of climate on regional scales.

This goal remains very challenging in spite of decades of study, extensive progress in climate system modeling and improvements in the availability and coverage of a wide variety of observations. Considerable obstacles in applying this knowledge to actual predictions remain. This is in particular the case for the impact of the internal component of decadal climate variability, whose nature and physical origins and interaction with external forcing are still not fully understood. These obstacles test our ability to attribute past variations to the combined role of internal variability and external forcing, as well as predict the future near-term climate evolution on global and regional scales. To achieve credible regional climate predictions/projections, it is thus essential to understand underlying physical processes, reduce model biases, evaluate their impact on predictions/projections, and adequately account for internal variability ([CE147]). In the extratropics and especially over Europe, the weight of the latter introduces substantial uncertainty while exacerbating risks associated with extreme events.

The interdisciplinary endeavor to characterize, understand, attribute, simulate, and predict the slow, multi-annual variations of climate on global and regional scales, is the backbone of the research carried out by the Global Change and Climate Modeling (GLOBC) group; it is inserted within the CERFACS DECLIPP challenge. Details about the GLOBC 2-year achievements are structured below into 3 main sections. Section 1 is devoted to the characterization and understanding of decadal variability and predictability over the North Atlantic based on a suite of CNRM-CM model configurations. Section 2 specifically focuses on the added value of increased model resolution in terms of both physical processes and representation of the variability. Section 3 presents results on climate change over North America, Europe, the Sahel and the Mediterranean basin based on a diversity of analysis tools and models. A special attention is laid on the alteration of the hydrological cycle while climate is warming.

2.2 Decadal variability and predictability over the North Atlantic-Europe

2.2.1 Origin of the Atlantic Multidecadal Variability in the CNRM-CM5 model

The physical processes underlying the internal component of the Atlantic Multidecadal Variability (AMV) have been investigated from a 1000-yr pre-industrial control simulation of the CNRM-CM5 model. The low-frequency fluctuations of the Atlantic Meridional Overturning Circulation (AMOC) are shown to be the main precursor for the model AMV. The full life cycle of AMOC/AMV events relies on a complex time-evolving relationship with both North Atlantic Oscillation (NAO) and East Atlantic Pattern (EAP) that must be considered from a seasonal perspective in order to isolate their action; the ocean is responsible for setting the multidecadal timescale of the fluctuations.

More precisely, AMOC rise leading to a warm phase of AMV is statistically preceded by wintertime NAO+ and EAP+ from Lag -40/-20yrs. Associated wind stress anomalies induce an acceleration of the subpolar gyre (SPG) and enhanced northward transport of warm and saline subtropical water. Concurrent positive salinity anomalies occur in the Greenland-Iceland-Norwegian Seas in link to local sea-ice decline; those are advected by the Eastern Greenland Current to the Labrador Sea participating to the progressive densification of the SPG and the intensification of ocean deep convection leading to AMOC strengthening. From Lag -10yrs prior an AMOC maximum, opposite relationship is found with the NAO for both summer and winter seasons. Despite negative lags, NAO- at that time is consistent with the atmospheric response through teleconnection to the northward shift/intensification of the Inter Tropical Convergence Zone in link to the ongoing warming of tropical north Atlantic basin due to AMOC rise/AMV build-up. NAO- acts as a positive feedback for the full development of the model AMV through surface fluxes but, at the same time, prepares its termination through negative retroaction on AMOC. Finally, advection of fresher water from the tropical basin created by local atmosphere/ocean anomalous circulation on one hand and from the Arctic on the other hand due to large-scale sea ice melting leads to decrease of density in the SPG and contributes terminating the model AMOC/AMV events.

All together, the combined effects of NAO and EAP, their intertwined seasonal forcing/forced role upon/by the ocean and the primary role of salinity anomalies associated with oceanic dynamical changes acting as an integrator are responsible in CNRM-CM5 for an irregular and damped mode of variability for AMOC/AMV that takes about 35-40 (15-20) years to build up (dissipate). This work is described in [CE133].

2.2.2 Model diversity in the simulation of the Atlantic Multidecadal Variability

To test the robustness of the results and physical understanding related to the AMV simulated in the CNRM-CM5 model (see above), we have used the preindustrial control simulations of 28 models from the CMIP5 archive and computed several metrics to characterize the AMV in each model. A very large diversity is found between models in terms of spatial fingerprint over the North Atlantic basin, preferred timescale and strength of associated teleconnection over Europe. We conclude that the larger scale the AMV, in other words, the stronger the correlation between SPG and Tropical North Atlantic SST anomalies, the longer the AMV preferred timescale and the greater the teleconnection over Europe. Whatever the model, it is found that all the AMV fingerprints are not stationary in time when considering chunks of 115 years to match the 1900-2015 observational temporal window. This considerably hampers the understanding of the AMV from the sole observations as well as the evaluation of the climate models.

Despite considerable diversity, very few models are able to capture the observational AMV properties. The tropical-extratropical link between the subpolar gyre and the north tropical Atlantic basin is underestimated as well as the strength of the teleconnection over Europe. Sensitivity experiments are currently being performed with CNRM-CM5 to specifically address these issues, as part of DCPP-C/CMIP6 (Decadal Climate Predictability and Prediction, componentC) framework ([CE95]). As co-chair of the DCVP (Decadal Climate Variability and Predictability) panel of CLIVAR, CERFACS has played a leading role in proposing common modeling protocols and providing both guidelines and input files to conduct coordinated simulations to better understand the physical mechanisms of the atmospheric response to AMV ([CE96]). These targeted simulations will help better understanding why all decadal prediction systems in CMIP5 rapidly lose predictability over land whereas AMV oceanic imprints (AMOC, SST and heat transport anomalies) are reasonably well predicted up to 7-8 yr leadtime. This work is done as part of Said Qasmi's PhD thesis within DCPP and the ANR-MORDICUS project.

2.2.3 Predictability of the Atlantic Multidecadal Variability

In [CE91], within the FP7-EU-COMBINE project, evidence is provided for significant long-term skill in predicting the AMV when oceanic conditions are initialized and despite considerable drift in the coupled model. Drifts are always present in models when initialized from observed conditions because of intrinsic model errors. Model drifts are usually removed through more or less sophisticated techniques for skill assessment, but they are rarely analyzed. Beyond statistical predictability issues, the dynamical study of model drift and associated bias adjustment is crucial, since the rate and the spatial pattern of the bias development can provide useful information on physical processes connected to model systematic errors that potentially affect the skill scores. Within the FP7-EU-PREFACE and GICC-EPIDOM projects, we conducted a process-based analysis to understand the development of the errors in the Atlantic in the CNRM-CM suite of model configurations with the ultimate goal to provide guidance for model improvements. Within EU-FP7-SPECS, we evaluated the level of decadal predictability using hindcasts over the $1993-2009$ period based on a higher resolution of the model.

2.2.3.1 Model drift in decadal forecast

In [CE134], we provide a detailed physical and dynamical description of the drifts in the CNRM-CM5 coupled model using a set of decadal retrospective forecasts produced within CMIP5. The scope of this study is to give some physical insights and lines of approach to, on one hand, implement more appropriate techniques of initialization that minimize the drift in forecast mode, and on the other hand, eventually reduce the systematic biases of the models. We have proposed a novel protocol for ocean initialization where initial states for starting dates of the predictions are obtained from a preliminary integration of the coupled model where full-field ocean temperature and salinity are restored to observations through flux derivative terms at the surface while full-field subsurface fields (below the prognostic ocean mixed layer) are nudged towards NEMOVAR reanalyses through Newtonian damping. Nudging is applied outside the 15^oS-15^oN band allowing for dynamical balance between the depth and tilt of the thermocline and the model intrinsic biased wind in the deep tropics.

Drifts are analyzed in the Tropical Pacific and North Atlantic basins. In the Pacific, we show that the first year of the forecasts is characterized by a quasi-systematic excitation of El Nino Southern Oscillation (ENSO) warm events whatever the starting dates. Through ocean-to-atmosphere heat transfer during El Nino events, this can be viewed for the coupled model as an efficient way to rapidly adjust towards its own biased mean state characterized by discharged tropical Pacific. Weak cold ENSO events tend to occur the second year of the forecast and the spurious oscillatory behavior is progressively damped after 4 years. Associated atmospheric teleconnections interfere worldwide with regional drifts, especially in the North Pacific and more remotely in the North Atlantic.

In the latter basin, the drift can be interpreted as the coupled model adjustment to local intrinsic atmospheric circulation biases as found in the stand-alone atmosphere component of the model. Errors project onto the negative phase of the North Atlantic Oscillation. A fast adjustment (up to $5-year$ leadtime) occurs leading to a rapid slackening of both the vertical (Atlantic Meridional Overturning Circulation - AMOC) and horizontal circulations, especially in the Subpolar gyre. Slower adjustment of the entire water masses distribution in the North Atlantic then takes over involving several mechanisms. We show that a weak feedback is locally present between the atmospheric circulation and the ocean drift that controls the timescale of the setting of the coupled model biases.

Additional work on drift correction methods derived from the MOS (Model Output Statistics) approach and traditionally applied in weather forecasting, has been carried out as part of Y. Leauté Master training of the École Nationale de la Météorologie. We use the decadal hindcasts produced at CERFACS within CMIP5 and found that the MOS technique slightly improved the predictive skill of the AMV and also in the Pacific.

2.2.3.2 Model biases in the Tropical Atlantic

Model systematic errors are particularly strong in the Tropical Atlantic basin and very poor improvement has been achieved going from CMIP3 to CMIP5. This makes coupled models less reliable to study the climate variability and predictability, as well as climate future projections, over the adjacent continents.
Within the EU-FP7 PREFACE project and following on a process-based approach, we have studied the links between model errors in the mean-state and in the simulated variability. The goal is to diagnose the relative importance of the different processes for model bias development and targeted model-specific experiments have been conducted. A new coupled model based on ARPEGE-Climat (v5.3) in its T359L31 (about 0.5 deg.) configuration and NEMOv3.2 at 0.25 degree resolution has been implemented. This high-resolution coupled model, referred to as CERFACS-HR, has been also used for decadal forecasts in the EU-FP7-SPECS project (see below). Errors grow extremely fast in the Tropical Atlantic (a few months) and seasonal integrations are sufficient to address drift issues at the first order. Ensembles of seasonal hindcasts initialized in February 1st and May 1st have been performed over the 2000-2009 period. Full-field initialization is adopted using ERAI and Glorys2V3 reanalyses products for the atmosphere and the ocean respectively.
To assess the added value of the increased resolution, even if model versions and components are not strictly the same, results of CERFACS-HR are contrasted to twin experiments conducted at Météo-France using the standard resolution of CNRM-CM5 (T127L31 in the atmosphere and ORCA1 in the ocean). The analysis of the Tropical Atlantic SST bias development shows that a similar bias setting is found in HR and LR models, except over the Angola-Benguela region, in which a strong reduction of the bias in CERFACS-HR is noticeable. We provide evidence that such an improvement is due to a better representation of fine-scale atmospheric and oceanic processes controlling the coastal upwelling.
To confirm the physical mechanisms leading to coupled error growth, additional sets of seasonal hindcasts in which the model wind stress is replaced in the course of the forecast by ERAI values, have been carried out. Three key regions have been tested: the Tropical Atlantic Equatorial band, the entire tropical Atlantic ($30^oS - 30^oN$) and the Angola-Benguela region. To analyze in details the processes associated with the SST bias development in both control and sensitivity experiments, a heat budget analysis of the upper-ocean mixed layer has been performed. We show that the initial growth of the SST bias in the Angola-Benguela region (two-month leadtime) is associated with an excessive solar radiation (underestimation of low cloud cover) and weaker than observed wind stress. In the following months, SST errors are due to remote oceanic processes. Among them, spurious warm meridional advection from the Equator to the Southeastern Tropical Atlantic, that penetrates southward as far as of 25^oS and that is related to a reversed thermocline east-west gradient associated with westerly wind biases in spring season in the deep tropics, is the dominant one.

2.2.3.3 Predictability over the North Atlantic using the CERFACS-HR model

As an additional step within the DECLIPP challenge and within the EU-FP7-SPECS project, we have performed a set of decadal hindcasts with the CERFACS-HR model. The ability of the model to predict the annual means of temperature, precipitation, sea-ice volume and extent is assessed based on initialized hindcasts over the $1993 - 2009$ period. The ocean initialization is based on the GLORYS ocean reanalysis developed by the MERCATOR group. All observed natural and anthropogenic forcings were prescribed during the observed period (see [8]). The needed computing time was provided through the HiResCLIM PRACE project on the BSC supercomputing center in Barcelona.
Significant skill in predicting SST is obtained, especially over the North Atlantic, the tropical Atlantic and the Indian Ocean. The Sea Ice Extent and volume are also reasonably predicted in winter (March) and summer (September). The model skill is mainly due to the external forcing associated with well-mixed greenhouse gases. A slight decrease in global warming rate associated with a negative phase of the Pacific Decadal Oscillation is simulated by the model over a suite of ten-year periods when initialized from starting dates between 1999 and 2003. The model ability to predict regional change is also investigated

by focusing on the mid-90's Atlantic Ocean subpolar gyre warming. The model simulates the North Atlantic warming associated with a meridional heat transport increase, a strengthening of the North Atlantic current and a deepening of the mixed layer over the Labrador Sea. The atmosphere plays a role in the warming through a modulation of the North Atlantic Oscillation: a negative sea level pressure anomaly, located south of the subpolar gyre is associated with a wind speed decrease over the subpolar gyre. This leads to a reduced oceanic heat-loss and favors a northward displacement of anomalously warm and salty subtropical water that both concur to the subpolar gyre warming. In agreement with previous studies, the sub polar gyre warming seems to be mainly triggered by ocean dynamics with a possible contribution of atmospheric circulation favoring its persistence. Larger ensemble size would be needed to confirm a possible atmospheric role.
Additional experiments with the same model were also performed to assess a possible impact of post-2005 volcanic eruptions on the global mean temperature evolution. The results suggest that the contribution of volcanic activity (related to the emission of stratospheric aerosols) to the global mean surface temperature evolution between 2003 and 2012 is that of a slight but significant cooling (0.08^oC) in agreement with other studies.

2.3 Added value of increased ocean-atmosphere model resolution for the Atlantic Climate

Recent studies in literature based on both observations and models have provided evidence that meso-scale features may have a larger than anticipated impact on large-scale variability. Associated physical processes such as internal ocean variability, air-sea interaction in storms at midlatitudes etc. appear to be the key ingredients. This section presents fundamental research carried out by GLOBC, as part of several international initiatives to revisit the role of both atmospheric and oceanic eddies, and in preparation of climate model future generation that will inevitably include an eddy-permitting/eddy-resolving ocean component in a near future.

2.3.1 Intrinsic variability of the chaotic ocean and its signature in observed changes

So-called mesoscale eddies are ubiquitous in the ocean, and are well-known examples of small-scale (from a few tens or hundreds of kilometers, from weeks to months) intrinsic ocean variability: they emerge from the instability of the main currents without any atmospheric variability. This mesoscale variability is highly chaotic: just as their atmospheric counterparts, oceanic cyclones and anticyclones are turbulent, which makes their evolution difficult to predict. Can this intrinsic ocean variability influence low-frequency oceanic variability and make it less deterministic than previously thought?
The LGGE and CECI/CERFACS OCCIPUT project is targeted to answer this question. For the first time, we have performed a large initial condition ensemble with an eddy-permitting ocean model ([1]). This is based on a new, probabilistic version of the NEMO ocean/sea-ice modeling system. Ensemble simulations with N members are running simultaneously within a single executable, and interacting mutually if needed. This design is made possible through an enhanced MPI strategy including a double parallelization in the spatial and ensemble dimensions.
A large ensemble of 50 global ocean/sea-ice hindcasts is performed over the period $1960 - 2015$ at eddy-permitting resolution (0.25 deg.) for the OCCIPUT project (the large amount of required computing time was obtained through a PRACE project and the computation ended in summer 2016). This application aims to simultaneously simulate the intrinsic/chaotic and the atmospherically-forced contributions to the ocean variability, from meso-scale turbulence to interannual-to-multidecadal time scales. Such an ensemble provides a unique way to disentangle and study both contributions, as the forced variability may be estimated through the ensemble mean, and the intrinsic chaotic variability may be estimated through the

ensemble spread. Initial results confirm that the spread cascades from short and small (mesoscale) scales to large and long scales. The imprint of intrinsic chaotic variability on various indices turns out to be large, including at large spatial and time scales. For instance, the Atlantic Meridional Overturning Circulation (AMOC) chaotic variability represents about 30 per cent of the atmospherically-forced variability at interannual time scale. These preliminary results illustrate the importance of low-frequency oceanic chaos and advocate for the use of such probabilistic modeling approaches for future oceanic and coupled simulations that will incorporate eddying-ocean components. Regional diagnostic studies on ocean heat content changes and Arctic sea-ice ocean interaction are on-going and will be pursued in 2017.

2.3.2 Influence of sea surface temperature fronts on the free atmosphere

Mechanisms of mid-latitude air-sea interaction have been studied since several decades for their potential impact on large-scale climate. As supported by many observational and modeling studies, the current view is that mid-to-high latitude climate variability is mainly reflecting the passive response of the ocean to atmospheric forcing on time scales ranging from weeks to decades. However, recent satellite observations and high resolution atmospheric and coupled simulations have suggested that the potential strength of the oceanic forcing might have been underestimated in the previous generation of climate models.

To confirm a possible influence of the ocean at small spatial scale and short time scale (seasonal), we use the high-resolution version of the ARPEGE model (T359L31) to investigate the influence of the representation of small-scale North Atlantic SST patterns on the atmosphere during boreal winter ([CE125], [CE188]). Two ensembles of forced simulations are performed and compared. In the first ensemble (HRES), the full spatial resolution of the SST is maintained while small-scale features are smoothed out in the Gulf Stream region for the second ensemble (SMTH). The impact of small-scale SST patterns as depicted by differences between HRES and SMTH shows a strong meso-scale local mean response in terms of surface heat fluxes, convective precipitation, and to a lesser extent cloudiness. The main mechanism is that of a simple hydrostatic pressure adjustment related to increased SST and marine atmospheric boundary layer temperature gradient along the North Atlantic SST front. Significant changes are also simulated with regard to the North Atlantic storm track, such as a southward shift of the storm density off the coast of North America towards the maximum SST gradient. A storm density decrease is also depicted over Greenland and the Nordic seas while a significant increase is seen over the northern part of the Mediterranean basin.

2.3.3 Characterizing the Mediterranean Cyclones with regional Climate Models

Regional climate models (RCMs) are used to study and understand climate variability and change at local scales. Nevertheless, to correctly interpret regional climate simulations, a number of uncertainties need to be considered. In [11], we focus on the so-called Internal Variability (IV) that can be defined as the degree of irreproducibility of an RCM solution when driven by the same lateral boundary conditions (LBCs) but initialized from different states. Within the HyMeX program framework using the MedCORDEX simulations performed with the ALADIN-Climate RCM at 50 km resolution, we have investigated how IV affects the cyclone tracks over the Mediterranean. For standard variables such as sea level pressure, 2m temperature and precipitation, IV is found (i) to be stronger at the easternmost part of the domain where the control exerted by the LBCs is weaker, and (ii) to exhibit a strong seasonal dependence reaching larger values in summer than in winter. In addition, we found that the IV level is much higher for quantities such as the density of cyclone tracks than for the other documented variables, reaching more than 50% of the estimated total variability. Long travelling tracks as well as fast moving cyclones are associated with greatest IV. A secondary IV maximum is observed for static cyclones with short travelling distances (thermal lows) during the warm season.

In line with the previous article, we have also participated to the inter-comparison exercise of tracking methods to assess the reliability of RCM to simulate the Mediterranean Cyclones ([5]). We use the Météo-France tracking tool that is found to capture a large number of cyclone tracks compared to the

other algorithms, because of its ability to detect weak cyclones. Besides, long lifetime cyclones are better identified with the Météo-France method but the frequency of extreme cyclone tracks is underestimated.
Additional analyses have been carried out to evaluate the added value of increased resolution from 50km to 12km in ALADIN for the simulation of precipitation extremes in Southern France. This study was part of E. Harader's PhD thesis ([CE186]) and has been also conducted in the frame of the HyMeX and MED-CORDEX programs. During cold season, results show that the high-resolution configuration improves the simulation of intense rainfall event where small-scale topographical features are a key external forcing for the precipitation. The added value is more questionable over flat terrain. During warm season, differences originate from enhanced subgrid precipitation triggering in the 12km-resolution configuration. These differences are significant for extreme precipitation only, since the added value is not detectable in the mean 30-year precipitation climatology.

2.4 Climate variability and climate change

2.4.1 Attribution of temperature change at continental-scale

Distinguishing between anthropogenic and internal influences on time scales of less than 50 years and spatial scales smaller than continental remains an outstanding issue. We seek to elucidate the physical mechanisms underlying internal and forced components of winter surface air temperature (SAT) trends over North America during the past 50 years (1963 – 2012) (see [CE103]). To address this challenge, we use a combined observational and modeling framework based on a large initial condition ensemble (30 members) with the Community Earth System Model (CESM). All simulations are subject to an identical scenario of historical radiative forcing but starts from a slightly different atmospheric state. Any spread within the ensemble thus results from unpredictable (at time scale of a decade or more) internal variability superimposed on the forced model response to anthropogenic forcing.
We develop and use a dynamical adjustment method to estimate the dynamical contribution to forced and internal components of SAT trends: thermodynamic contributions are obtained as a residual. Internal circulation trends are estimated to account for approximately one-third of the observed wintertime warming trend over North America and more than half locally over parts of Canada and the United States. Removing the effects of internal atmospheric circulation variability narrows the spread of SAT trends within the CESM ensemble and brings the observed trends closer to the model radiatively forced response. In addition, removing internal dynamics approximately doubles the signal-to-noise ratio of the simulated SAT trends and substantially advances the time of emergence of the forced component of SAT anomalies. The methodological framework proposed and applied here provides a general template for improving physical understanding and interpretation of observed and simulated climate trends worldwide and may help to reconcile the diversity of SAT trends across the models from future phases of CMIP. This work is done in collaboration with the Climate Analysis Section of the National Center for Atmospheric Research (NCAR).

2.4.2 Attribution of season length changes over Western Europe

Temperatures over Europe are largely driven by the strength and inland penetration of the oceanic westerly flow. The wind influence depends on season: blocked westerlies, linked to high-pressure anomalies over Scandinavia, induce cold episodes in winter but warm conditions in summer. In [CE96], we propose to define the onset of the two seasons as the calendar day where the daily circulation/temperature relationship switches sign. According to this meteorologically-based metric assessed from several observational datasets, we provide evidence for an earlier summer onset by 10 days between the 1960s and 2000s (Figure 2.1).
Results from the CNRM-CM5 climate model show that this calendar advance is incompatible with solely internal variability and can be partly attributed to anthropogenic forcings. The modification of the zonal

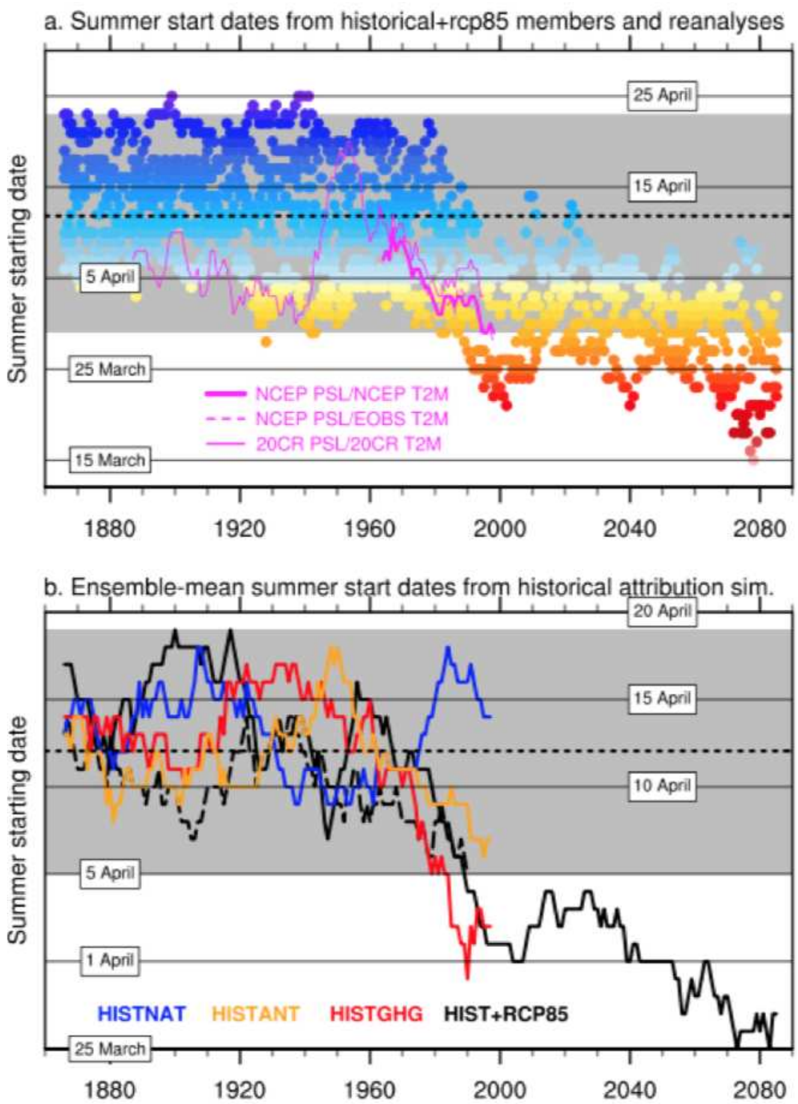

Figure 2.1: Advance of summer onset under warming climate. Temporal evolution of the summer starting date from observational datasets (magenta curves and labels) and from historical and scenario individual ensemble members (dots) computed over running 30-year periods. Blue (red) color of the dot (10 per year from 10 available historical simulations over 1850-2012, 5 from 5 RCP85 ones after 2012) stands for later (earlier) summer starting dates given by thin horizontal lines. The range of variability from pure internal dynamics as computed from 1000 random drawings of 30-yr period from piControl is represented in gray (5th and 95th percentile); the mean piControl summer starting date is superimposed (thick dashed). Formal detection is obtained when the index gets outside the gray envelop. b. Ensemble mean summer starting dates from 5-member attribution experiments where external forcings are applied individually over the historical period, namely natural (solar+volcanoes) forcing only (HISTNAT, blue), anthropogenic (GHG+aerorols) only (HISTANT, orange) and GHG only (HISTGHG, red). For HIST (black), because of 10-member availability over 1850-2012, the complementary 5-member estimate is provided (dashed line). Gray shading is computed here from 1000 random drawings of 5-averaged 30-year periods in piControl to match the 5-member ensemble mean.

advection due to winter snow earlier disappearance over Eastern Europe, which reduces continentality, is mainly responsible for the present-day and near-future summer advance in Western Europe. Our findings agree with phenological-based trends (earlier spring events) reported for many living species over Europe, for which we provide an alternative interpretation beyond the traditionally evoked local warming effect. Based on RCP8.5 scenario, a summer advance of 20 days compared to preindustrial climate is expected by 2100, while no clear signal arises for winter onset.

2.4.3 Respective roles of direct GHG radiative forcing and induced Arctic sea ice loss on the Northern Hemisphere atmospheric circulation

Arctic sea ice decline in recent decades has been reported from observational studies. Although such a trend can be partially explained by internal climate variability, modeling studies confirmed that it is mainly caused by the increasing GHG concentrations in the atmosphere. Arctic sea ice is expected to disappear by the middle of the 21st century in the business as usual scenario, yielding an ice-free region during boreal summer season (see IPCC-AR5 report).
Within the ANR-MORDICUS as part of T. Oudar PhD thesis ([CE187]), the large-scale and synoptic-scale Northern Hemisphere atmospheric circulation responses to projected late twenty-first century Arctic sea ice decline has been investigated using the CNRM-CM5 coupled model. An original protocol, based on a flux correction technique, allows isolating the respective roles of GHG direct radiative effect and induced Arctic sea ice loss under RCP8.5 scenario. Results show that in winter, the surface atmospheric response to GHG increase and Arctic sea ice loss respectively are opposite and cancel each other leading to no significant pattern in the total response. A dynamical approach based on Eady growth Rate parameter (a measure of the baroclinic activity) shows that Arctic sea ice loss is responsible for weakened low-level meridional temperature gradient, causing a general decrease of the baroclinicity at mid-to-high latitudes. Direct impacts of GHG increase are located more in the mid-to-high troposphere affecting the wind vertical shear leading to increased baroclinicity. Changes in flow waviness in the free atmosphere as evaluated from sinuosity and blocking frequency metrics, are found to be small relative to interannual internal variability ([9]).

2.4.4 Characterizing future climate projections for the Sahel Precipitation

Based on studies using both CMIP3 and CMIP5 databases, there is a high level of uncertainty in future climate changes over the Sahel region; this is critical for adaptation strategies. Within the EU-FP7-PREFACE project, the future evolution of the West African Monsoon is studied by analyzing 32 CMIP5 models under the RCP8.5 emission scenario ([8]). A hierarchical clustering method based on the simulated pattern of precipitation changes is used to classify the models. Four groups are obtained; their differences are such that they could even differ by the sign of the changes. We find that the inter-group differences are mainly associated with large spreads in (i) temperature increase over the Sahara and North Atlantic basin and (2) strengthening of low-to-mid-level winds over Africa. A wetter Sahel is associated with a strong increase in temperature over the Sahara ($> 6^oC$), a northward shift of the monsoon system and a weakening of the African Easterly jet (AEJ). A dryer Sahel is associated with local subsidence anomalies, strengthened AEJ, and moderate warming over the Northern Hemisphere.
Additional analyses have been conducted to evaluate the link between model mean biases in temperature and precipitation for present climate and modeled changes in the RCP8.5 scenarios of the Sahel precipitation. The ultimate goal of this approach is to provide to the downscaling community a list of few models that are representative of the multi-model uncertainties in terms of ensemble mean and ensemble spread for Sahel precipitation. We examined several methods for subsampling and show that the mean bias is not a reliable metric for the model selection. We propose a so-called ”diversity” and ”pattern selection” methods, which turn out to be more reliable to choose 3-4 models representing the full CMIP5 ensemble mean and spread.

2.4.5 Modification of the ENSO teleconnection over the North Atlantic in a warmer world

Enso connections over Europe throughout the 20th and early 21st century are rather weak and not stationary in time. The alteration of the connection in a warmer word (typically the mean climate expected at the end of the 21st century under the RCP8.5 scenario) is investigated using so-called "pacemaker experiments" conducted within the ANR-MORDICUS project using the CNRM-CM5 model. 30 years of climate that are representative of ENSO observed variability are selected from the 1000-yr preindustrial control simulation of CNRM-CM5. A set of two 10-member ensembles of 30-yr simulations is conducted in which the model SST is restored towards the selected anomalies over the sole Eastern Tropical Pacific region while the rest of the model is kept freely coupled. The two ensembles differ by the mean state, either preindustrial or RCP85, on top of which the selected SST anomalies are superimposed. By construction, ENSO variability is strictly the same in both ensembles and computing their difference allows investigating the changes associated with the sole background mean climate.

We found that ENSO teleconnections over Europe are considerably increased in RCP85 mean climate and become quasi-systematic in winter. This contrasts with the non-stationary link between ENSO and North Atlantic dynamics in preindustrial climate. The enhanced teleconnection is related to the mean acceleration and southeastward shift of the westerly upper-level jet over the North Pacific that more efficiently connects with the entrance of the North Atlantic jet stream acting as waveguide. Warm (cold) ENSO events are associated with negative (positive) North Atlantic Oscillation leading to significant precipitation and temperature anomalies over the European continent. By contrast, because of the eastward shift of the entire teleconnection patterns over the North Pacific, connectivity is reduced between ENSO events and the western American continent.

2.4.6 Changes in extreme temperature events

Impacts of climate change are not solely experienced through the increase in global mean temperature but also by an increased occurrence and severity of extreme temperature events. Extreme temperature events have a long history in the global assessment of climate change impacts because of their potential high consequences. Record-breaking temperature events are by definition extreme events that have never occurred. Under the assumption of a stationary climate, the record occurrence should decrease as $\frac{1}{n}$, n being the number of time steps (years) since the beginning of the record counting. M. Bador PhD main objective within the ANR-SEEN, is to compare this theoretical evolution with the observed one in order to detect and attribute changes due to external factors ([CE88], [CE89] and [CE182]). A particular goal was to fully account for the possible influence of low-frequency climate variability in the detection and attribution process.

Main results from M. Bador PhD ([CE182]) are as follows: observations suggest that Europe has recently experienced numerous record-breaking temperatures that take place among a global and sustained change in temperature record statistics. Furthermore, observational analysis of Europe summer record-breaking temperatures suggests that their occurrence differs from that expected in a stationary climate since the late 1980s. The observed cold and warm record evolution is also well simulated by the ensemble mean of 27 coupled models from CMIP5. This suggests that the observed evolution could be partially forced by external forcings. However, we find that this evolution is still today within the range of internal variability derived from the full range of CMIP5 preindustrial simulations. We then estimate a time of emergence of the summer record anthropogenic influence in a world under a business as usual greenhouse gas emission scenario. We suggest a time of emergence around 2020 for the cold records and 2030 for the warm ones with an uncertainty of $\pm$ 20 years. By 2100, the multimodel ensemble mean indicates a tenfold increase of the number of warm records compared to the first half of the twentieth century and the quasi-disappearance of cold records.

2.4.7 Changes in hydrology

2.4.7.1 Emerging constraints to better assess uncertainties in climate projections over Europe and France

In [CE94], we have done some work to better understand the physical mechanisms responsible for the large uncertainties in current climate projections regarding the continental hydrological cycle over Western Europe in summer. We show that anthropogenic aerosols have a major impact on summer evapotranspiration, and to lesser extent precipitation, leading to discernible anthropogenic changes in evapotranspiration over western Europe as soon as the early 20th century in some climate models. In other models, virtually no impact of anthropogenic aerosols on evapotranspiration is seen on the entire historical period. The differential behavior of these two groups of models continue in the future climate, especially in the coming decades, with much less severe changes in summer evapotranspiration and precipitation projected by the former than the latter. This differential behavior is largely explained by the combination of two properties of the climate models: the sensitivity of shortwave radiation to anthropogenic aerosols and whether summer evapotranspiration over Western Europe is primarily soil-moisture or energy limited.

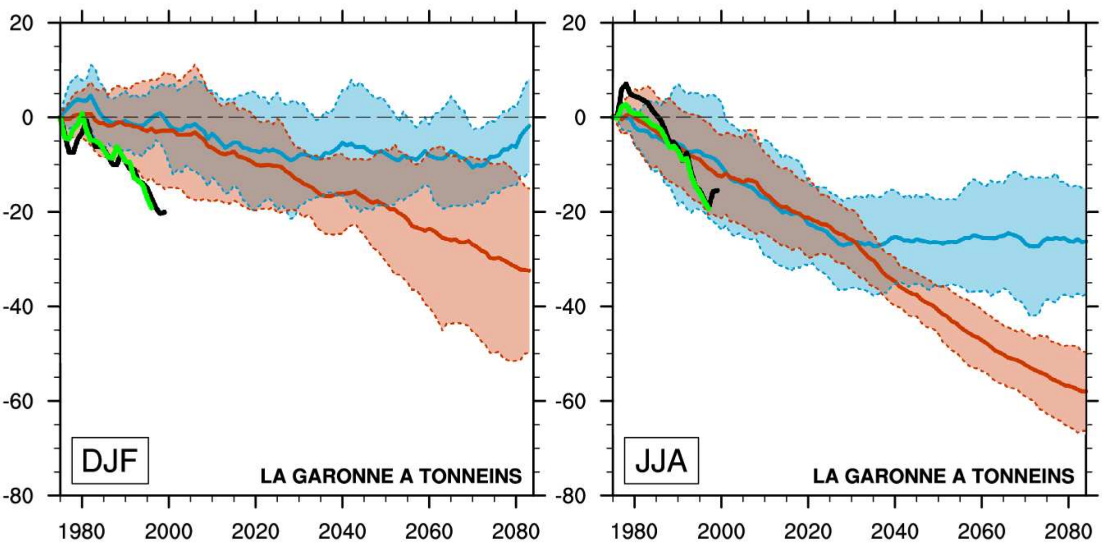

Figure 2.2: Changes in seasonal flow of the Garonne River with respect to the 1960-1990 reference period, as simulated from ISBA-MODCOU forced by downscaled CMIP5 Global Circulation Models for the RCP2.6 (blue) and RCP8.5 (red) greenhouse gazes emissions scenarios. Shading stands for total uncertainties and ensemble means are given in solid lines. Observations are in black and SIM river flows over the historical period are in green for the winter (left) and summer (right) seasons.

Within the ANR-ECHO project, the new statistical downscaling method previously developed and described in [CE102] has been applied to downscale a large multi-model, multi-member, and multi-scenario ensemble of climate projections from CMIP5 and do the corresponding hydrological projections over France with the ISBA-MODCOU model (Figure 2.2). Projections with the MORDOR hydrological model in collaboration with J. Gailhard from EDF have also been done for some river basins. Their results have been analyzed and described in the PhD thesis of G. Dayon [CE184]. As an example, we show that even with an emission scenario compatible with a limitation of global warming to 2K, a decrease in the summer river flows of the Garonne as large as 30% might still occur. We also have shown that at annual time scales, the uncertainties due the hydrological model are weak, but they are large in summer. These uncertainties are related to an important extent to the representation of slow sub-surface flows associated in the reality with aquifers. Our analyses also suggest that internal multi-decadal variations tend to be underestimated in current hydrological projections, likely because of climate models, resulting in the under-estimation of related uncertainties.

In line with this overall conclusions, work has been done, notably within the LEFE-VITESSE project and the PhD thesis of R. Bonnet, to better characterize and understand the past multi-decadal to centennial variations in the continental hydrological cycle over France thanks to the analysis of observations and hydrological reconstructions. Weather stations were very sparse in the early 20th century and specific approaches have to be developed to obtain a meteorological forcing suitable for hydrological modeling. We have developed a method to combine the results of the statistical downscaling method of [CE102] applied to two long-term atmospheric reanalyses and sparse long-term homogenized precipitation or temperature series in order to obtain the meteorological forcing necessary for hydrological modeling on the entire 20th century. Corresponding hydrological reconstructions have been done with the ISBA-MODCOU model. Different methodological variants have been tested and evaluated, and the interest and usefulness of our approach demonstrated. We have begun to use these reconstructions to study multi-decadal hydrological variations over France, and in particular the role of snow and soil moisture to extend the impact of spring multi-decadal climate variations to summer hydrological variables.

2.4.7.2 Evaluation of uncertainties in extreme future precipitation changes over northwestern Mediterranean watersheds from high-resolution regional models

During the first year of the A. Colmet-Daage PhD thesis, the impacts of climate change on extreme precipitation events have been studied by using an ensemble of regional climate models (RCMs) simulations at high resolution ($\sim$ 12 km) provided by the CORDEX program. In this study, performed in collaboration with Meteo-France, WSP and HSM, we have evaluated the RCM performance in terms of extremes of precipitation over complex watersheds located in the northwestern Mediterranean basin (France and Spain). RMCs are evaluated and intercompared by using direct measures of precipitation ([CE157]), as well as high resolution reanalysis products as SAFRAN-France and SAFRAN-Spain provided by Meteo-France and Observatorio del Ebro.

RCMs have been interpolated to a common grid for comparison purposes ([CE156]). Results show that extreme precipitations are underestimated in all seasons by all the models for actual climate, including in the fall when the majority of the Mediterranean flash floods occur. Future extreme precipitation change uncertainties have been evaluated from the multi-model ensemble, by using two GHG emission scenarios (RCP4.5, RCP8.5) and over two time-slice periods (mid and late 21st century). Though strong uncertainties exist, the RCM ensemble mean projects an increase in precipitation intensity from the 90th to 99.9th quantile under both scenarios and for all time periods. Additional work focuses on the characterization of an extreme flash flood episode in future climate conditions by using the future extreme precipitation projections as a initial condition for several hydrological models. The methodology is similar to the one implemented in the E. Harader PhD thesis but in this case uncertainties are better evaluated from a multi-model ensemble projections under two different emission scenarios.

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Modeling Environment and Safety

3.1 Introduction

MODEST (Modeling for Environment and Safety) is an emerging challenge at CERFACS (initiated mid 2014) to tackle issues related to the prediction of industrial risks (fire, explosion, pollutant dispersion) and environmental risks (inundation, wildfire) that could be induced by natural disasters, human activities and/or industrial accidents. These issues are of great importance for public safety, industrial plant safety as well as environmental protection. CERFACS, in synergy with the research activities conducted among its shareholders, is an ideal place to address these questions since the expertise in high fidelity numerical modeling and high performance computing is already present in AE, GLOBC (CECI) and CFD teams.
Over the last few years, CECI has become an active research institution in the following areas that have contributed to the emergence of the MODEST challenge: natural hazards monitoring (floods/inundations, wildfire spread); anthropogenic impacts on the environment (aviation, rocket launch); and environment surveillance (regional-/global-scale air quality). MODEST is thus multidisciplinary and addresses a wide variety of objectives (surveillance, early warning system, monitoring, reanalysis, scenarios, forecasting), spatio-temporal scales (from flame scale, meso-scale to regional and global scales), simulation tools (CFD, hydrodynamics, front tracking, aerodynamics, surface emissions) and algorithms (data assimilation and optimization, uncertainty quantification, code coupling, high performance computing).
This chapter is divided into two sections: one section related to the design and application of large eddy simulations (LES) for air quality predictions; and a second section related to the design and application of data assimilation algorithms for environmental surveillance.

3.2 Air quality predictions using large eddy simulations

3.2.1 The impact of aviation on atmosphere and climate

The main activities of the AE team of CERFACS have been focused during the last two years on the climate impact of aviation. This is still an open question since the non-CO_2 forcing due to contrail and cirrus-contrail formation, and the ozone perturbation due to the emission of NOx are still very uncertain. The main effort has focussed in past years on the development of a computational tool to represent the physico-chemical processes occurring in aircraft plumes based on high-resolution large-eddy simulations [CE121]. The focus has been laid on ice microphysics for the purpose of simulating the formation of contrails and their development into contrail-cirrus with the atmospheric model Méso-NH. The model outputs have been compared to in-situ aircraft measurements obtained during the TC2 campaigns. The TC2 (Traînées de condensation et climat) project has been funded by the DGAC. Figure 3.1 shows the distributions of ice diameter as a function of the concentration of ice particles obtained during the campaigns (in black) and calculated by Méso-NH. Overall the distributions are comparable, although the measurements tend to show larger concentrations from the largest particles.
Those results have led to the implementation of a parameterization of the contrail effects in the global CNRM-CCM (the climate model of Météo-France). Within the IMPACT project (initiated by the CORAC with funding from DGAC) update evaluations of the impact of aviation on climate using the CNRM-CCM with the aircraft plume effects are foreseen. First results (Fig. 3.2) show the distribution of the cloud fraction

covered by contrails using this new parameterization. Overall the mean global fraction is in the range of 0.38 %, but local values can reach 10 % in regions of dense traffic.

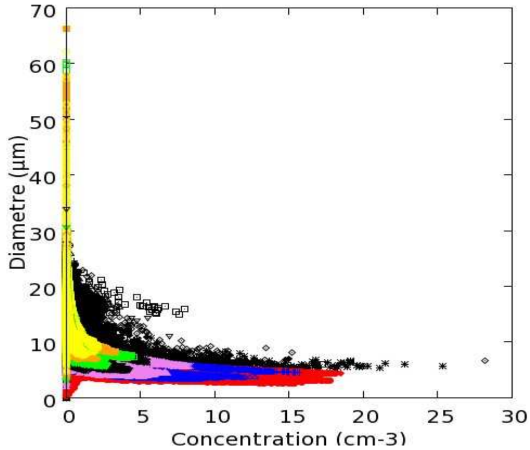

Figure 3.1: Mean diameter of ice particles as a function of particle concentrations. From the TC2 campaign measurements in black, from the Méso-NH simulation in color (after 5 min in red, 20 min in purple, 30 min in black, 50 min in orange and 60 min in yellow)

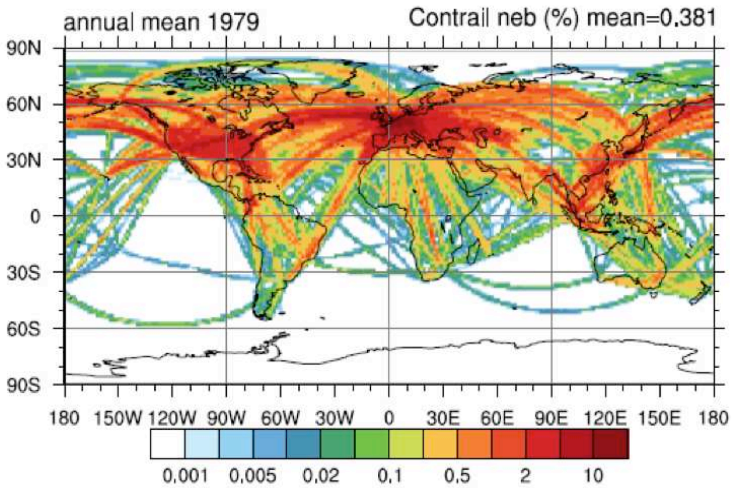

Figure 3.2: Map of the distribution of the fraction of sky covered by contrails on the 250 hPa level for a simulation of one year of the CNRM-CCM model.

3.2.2 Atmospheric impact of launcher

In response to CNES inquiries CERFACS has conducted studies on the atmospheric impact of rocket launcher emissions. The objective is to evaluate the impact on the stratospheric composition of rockets launched from the Kourou facility. Rockets have an impact on the chemical composition of the atmosphere, and particularly on stratospheric ozone. Among all types of propulsion, Solid-Rocket Motors (SRMs) raised concerns since their emissions are responsible for a severe decrease in ozone concentration in the rocket plume during the first hours after a launch. The main source of ozone depletion is due to the conversion of hydrogen chloride, a chemical compound emitted in large quantities by ammonium perchlorate based propellants, into active chlorine compounds, which then react with ozone in a destructive catalytic cycle, similar to those responsible for the Antartic ”Ozone hole”. This conversion occurs in the hot, supersonic exhaust plume, as part of a strong second combustion between chemical species of the plume and air.

In a first step, the active chlorine concentration in the far-field plume of a SRM has been evaluated using LES [CE128]. The gas is injected through the entire nozzle of the SRM and a local time-stepping method based on coupling multi-instances of the fluid solver is used to extend the computational domain up to 400 nozzle exit diameters downstream of the nozzle exit. The methodology is validated for a non-reactive case by analyzing the flow characteristics of the resulting supersonic co-flowing under-expanded jet. Then the chemistry of chlorine is studied off-line using a complex chemistry solver applied on trajectories extracted from the LES time-averaged flow-field. Finally, the online chemistry is analyzed by means of the multi-species version of the LES solver using a reduced chemical scheme. To the best of our knowledge, this represents one of the first LES of a reactive supersonic jet, including nozzle geometry, performed over such a long computational domain. By capturing the effect of mixing of the exhaust plume with ambient air and the interactions between turbulence and combustion, LES offers an evaluation of chemical species distribution in the SRM plume with an unprecedented accuracy.

These results have been used to initialize atmospheric simulations on larger domains, in order to model the chemical reactions between active chlorine and ozone and to quantify the ozone loss in SRM plumes during the first 30 minutes of the plume diffusion. This work has been realized with the atmospheric research model Meso-NH. Two chemical schemes have been considered. A scheme which represents the evolution of 2 species, active chlorine and ozone, using mean parameterizations of (i) active chlorine deactivation by ozone and methane, and (ii) ozone destruction by active chlorine. An advantage of this simple scheme is the low computational cost. In order to evaluate the accuracy of this scheme, the simulation have been reproduced with 8 species chemical scheme:

$$Cl + O_3 \rightarrow ClO + O_2$$

$$Cl_2 + hnu \rightarrow 2Cl$$

$$ClO + ClO \rightarrow Cl_2O_2$$

$$Cl_2O2 + (M) \rightarrow ClO + ClO$$

$$Cl_2O_2 + hnu(M) \rightarrow Cl_2 + O2$$

$$Cl + CH_4 \rightarrow HCl + CH3$$

$$ClO + O \rightarrow Cl + O2$$

$$O + (O2 + M) \rightarrow O_3 + M$$

$$O_3 + hnu \rightarrow O_2 + O$$

The comparison of the results obtained with the two chemical schemes brought to light that the methane and ozone total destruction must be considered by chlorine deactivation parameterization in the simple scheme to correctly evaluate the ozone destruction by active chlorine (Figure 3.3). Furthermore, the simulation with the 8 chemical species scheme highlighted the ambiguous role of atmospheric turbulence on ozone destruction. Two processes have been identified. Firstly, the increase of the turbulence induces an increase of the plume diffusion and leads to an increase of the ozone destruction. Secondly, an increase of the turbulence goes along with an increase of the shear, which induced a greater deformation of the plume. The increase of plume deformation restrains the overlapping of the plume on the vertical and, consequently, limits the vertical overlapping of regions where ozone destruction occurs. Hence, increasing the turbulence induces two opposite effects on vertical ozone destruction.

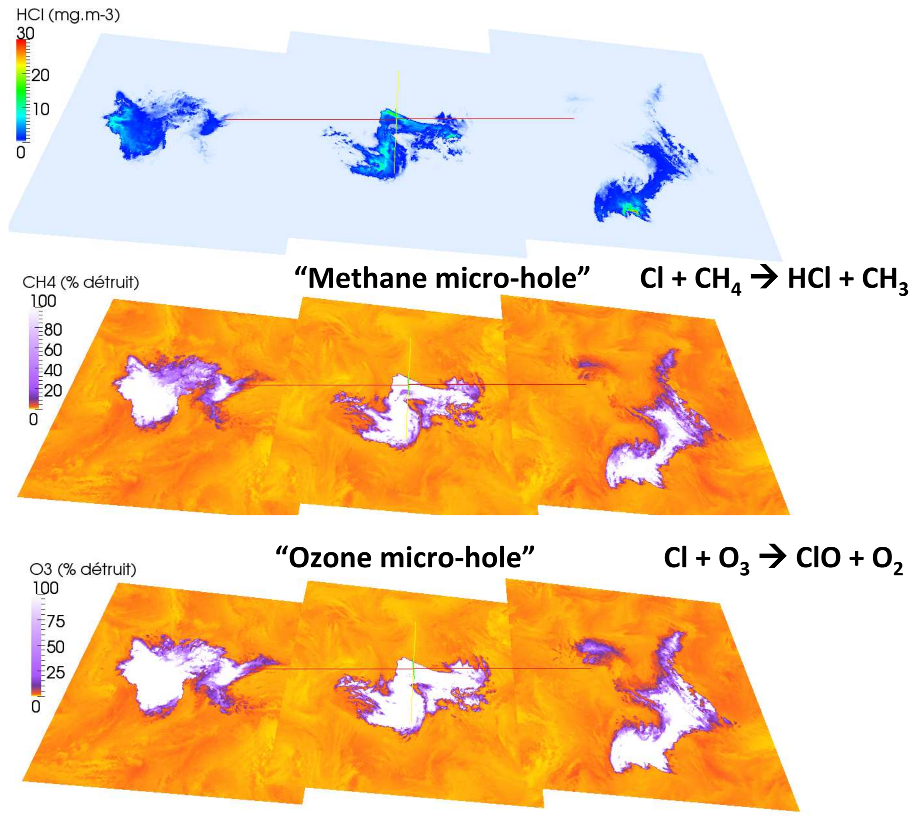

Figure 3.3: Distribution of HCl, CH_4 and O_3 after 30' of a solid propellant rocket launch (booster). The large amount of chlorine radicals leads to the destruction of CH_4 and O_3 within the rocket plume.

It is now important to determine which process (the plume diffusion or its deformation) controls the vertical ozone destruction during the first hour after the plume emission. The simulations are in progress in the context of a GENCI project. Theses calculations are performed at different altitudes in order to diagnose ozone destruction over the entire atmospheric column.

3.2.3 Modelling of the emission transport: the MUST case

CERFACS initiated in 2016 in the frame of the DEMODEST project (DEMO for MODEST - funded by the Initiative At Cerfacs project calls), a CFD code benchmark study, with the objective to demonstrate the added value of LES to represent pollutant emissions and short-to-medium-term smoke plume evolution. This new project will develop and strengthen in the coming year through the 2017-2018 RTRA-STAE initiative (chantier MIRAP, Modélisation et Incertitudes pour l'évaluation du Risque de dispersion Atmosphérique de Polluants), piloted by CERFACS and led in collaboration with Météo-France/CNRM and Observatoire Midi-Pyrénées. The key idea is to investigate how LES (possibly combined with UQ techniques) could contribute in the long term to the improvement of effective crisis management tools. A demonstration case will be carried out in the context of operational Ariane rocket launch at the Guiana Space Centre (Centre Spatial Guyanais CSG), Kourou, managed by ESA and CNES.

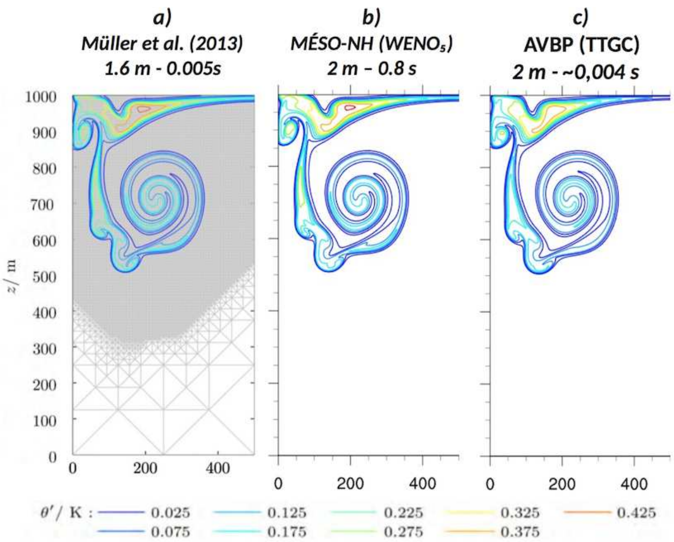

Figure 3.4: Comparative results of the rising thermal bubble test case between LES solvers, MesoNH, AVBP and literature reference at $t = 1000$ s.

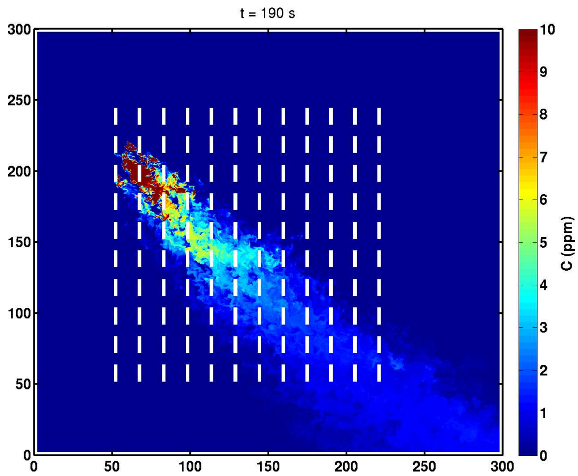

Figure 3.5: Horizontal cross-section of concentration fields (ppm) at $z = 1.6$ m for the MUST trial 2681829 with an inflow wind direction of -41 degree.

A code intercomparison study has been initiated in 2016 to evaluate the potential benefits of LES (with the codes AVBP, MesoNH) compared to RANS (G. Réa, Post-doc). Both academic test cases (rising thermal bubble) and idealized urban cases (MUST experiment) were investigated. First, an intercomparison of AVBP and MesoNH was investigated on a simple low-Mach number case, the rising thermal bubble, to test spatial and temporal integration schemes and boundary conditions in a non-confined environment where buoyancy effects are predominant (which is not the case in AVBP main applications). Here the motions are due to buoyancy induced by a 0.5-K temperature perturbation. The bubble evolution has been simulated over 1100 s with the two codes. The implementation of buoyancy effects in AVBP showed

good results compared to MesoNH and the literature (Fig. 3.4). Second, the intercomparison has been extended to the MUST experiment, which aimed at mimicking urban canopy via a series of containers. They constitute a large database of nonreactive gas leak cases, each case corresponding to different near-surface wind conditions and gas leak location. In 2016 one configuration has been simulated using AVBP and an upgraded version of Meso-NH (with IBM, see precedent section). This configuration (trial 2681829) had an inflow wind direction of -41 degree and a wind 4-m high amplitude of 7 m/s. Figure 3.5 shows a snapshot of the tracer 190 s after the beginning of the release, in the Meso-NH simulation at 0.2 m of resolution.
The analysis of the results is ongoing to evaluate the domain of feasibility and validity of each LES code. Additional comparisons will be made with the low-Mach LES code YALES-2 and CODE-SATURNE (in collaboration with Bertrand Carissimo, CEREA/EDF) to analyze the benefits of LES for a large panel of codes. The main objective for 2017 is to extend the inter-comparison to the study of Ariane launch at the Guiana space center (CSG/CNES) and to design suitable uncertainty quantification strategies.

3.3 Environmental and atmospheric monitoring using data assimilation

3.3.1 Wildland fire, spread and emissions

Because wildfires feature complex multi-physics occurring at multiple scales, our ability to accurately simulate their behavior at large regional scales remains limited. The mathematical models proposed to simulate wildfire spread are currently limited because of their inability to cover the entire range of relevant scales (i.e., from biomass pyrolysis to atmospheric dynamics), and also because of knowledge gaps and/or inaccuracies in the description of the physics as well as knowledge gaps and/or inaccuracies in the description of the controlling input parameters (i.e., vegetation, topographical and meteorological properties). For this purpose, the uncertainty in regional-scale wildfire behavior modeling must be quantified and reduced.
Wildfire spread is typically modeled using a front-tracking simulator relying on a semi-empirical parameterization of the front speed/direction, which is subject to significant uncertainties. A data-driven wildfire spread modeling prototype (FIREFLY) was designed to sequentially integrate remote sensing (typically infrared imaging) measurements and to translate the differences in the observed and simulated fire front locations into a correction of the input parameters of the wildfire spread model or directly of the fire front location.
The objective of the FIREFLY data-driven modeling prototype is two-fold, i.e. forecasting both wildfire dynamics and plume emissions. On the one hand, the use of a data assimilation algorithm allows to produce more reliable forecasts of wildfire spread at future lead times. Details on the data assimilation methodologies are provided in the dedicated section "Uncertainties and Data Assimilation". Figure 3.6 illustrates the application of data assimilation to the RIM fire that occurred during the 2013 California wildfire season on the edge of Yosemite National Park; it started on August 23 from illegal campfire in a remote canyon in central-Sierra Nevada and extended up to 1040 km^2 (the third largest wildfire in California's history). The use of state estimation allows the retrieval of more accurate fire front positions that can be used to initialize forecasts [25, 13]. Ongoing work aims at combining the state estimation approach to a spatially-distributed parameter estimation approach to increase the forecast performance by addressing and reducing model bias. On the other hand, FIREFLY is useful to provide time-series of the pollutant emissions released by wildfires at high resolution. Data assimilation allows to provide more accurate predictions of the burning area and therefore of the resulting emissions. Ongoing work aims at showing the benefits of using a data-driven wildfire spread model to produce an inventory of fire emissions at regional scales (1 to 50 km), which is then used by chemistry-transport models for air quality predictions (ongoing LEFE/INSU project and CHARMEX program).

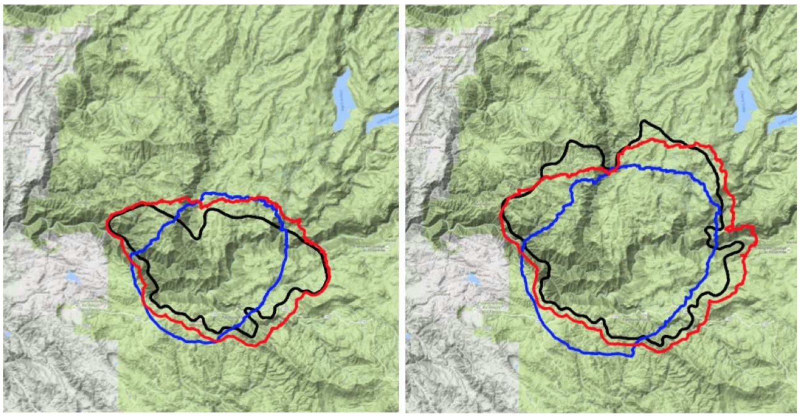

Figure 3.6: Accidental RIM fire (20-25 August, 2013, 1040 km^2 - Sierra Nevada, California). Comparison of observations (black curve), forecast estimate providing the FARSITE (US Forest Service) model prediction (blue curve) and analysis estimate resulting from the sequential assimilation of the observation (red curve).

3.3.2 Hydraulics/hydrology

Flooding causes important social, environmental and economic losses and is likely to be aggravated by climat change over the next decades. For example, flooding of the Var River in the South-East France in 2010 resulted in a 700-million-euro loss and 25 victims. Worldwide, national or international operational flood forecasting centers are in charge of providing water level predictions and flood risks at short- to medium-range lead time that are of great importance for civil protection. To this end, operational centers (SCHAPI in France) aim at providing an accurate forecast of the hydraulic variables (i.e. water level and discharge) along the monitored network. This forecast relies on the complementary use of numerical models and observations. The capacity for real-time anticipation of extreme flood events remains limited due to uncertainty in hydrological forcing, hydraulic parameters and description of the river geometry.

As illustrated in Fig. 3.7, data assimilation, based on an extended Kalman filter algorithm, of water level observations allows to sequentially correct hydrologic boundary conditions, hydraulic model parameters and hydraulic state. This strategy is implemented in DAMP (Data Assimilation with Mascaret Prototype) and integrated in the POM (Multi-model Operational Platform) used at SCHAPI. It leads to a significative improvement of flood forecasting for short- to medium-range lead time [23, CE110]. The cost of the data assimilation is reduced with a surrogate model used in place of the direct model, also efficient for sensitivity analysis and uncertainty quantification. Data Assimilation and Uncertainty Quantification studies are also implemented on a 2-D model on the Gironde estuary with the objective of providing a flood alert system (V. Laborie PhD's 2015-2018). A sensitivity analysis with respect to maritime and fluvial boundary conditions, friction coefficients, atmospheric forcing and wind transfer coefficient highlighted that water level is driven by different source of uncertainty from upstream to downstream.

Even with data assimilation, 1-D modeling is limited when the flow becomes complex (for instance flood plains or confluences). While multi-dimensional modeling makes the most of High Performance Computing, it requires significant computational resources that are not always compatible with operational constraint. Coupling between a full 1-D model and a local 2-D model where the flow is complex, offers a convenient solution with a limited computational cost. It also allows for a complementary use of data assimilation capabilities already implemented with the model 1-D model and the multi-dimensional coupling approach [CE183]. Several coupling strategies are proposed depending on the catchment with longitudinal, lateral and overlapping approaches, to be used for real-time flood risk management and water resources management.

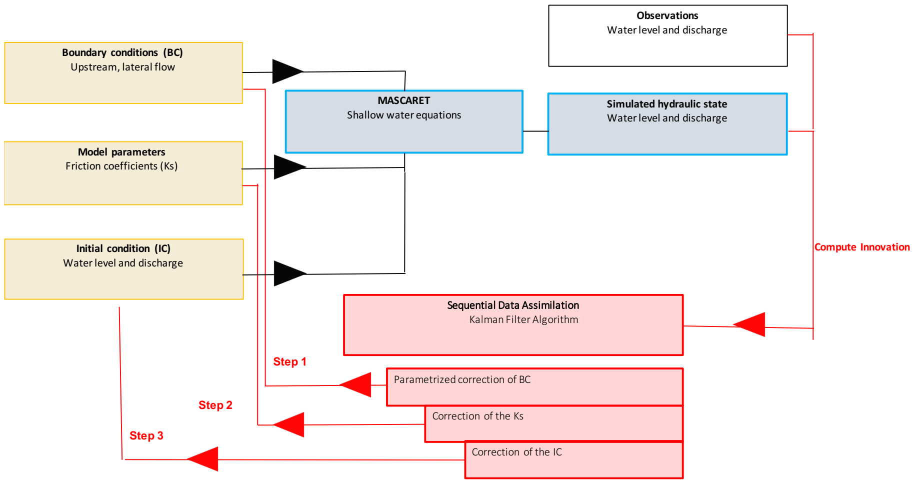

Figure 3.7: Data Assimilation with Mascaret Prototype scheme for correction of model paremeters, state and boundary conditions with Kalman Filter algorithm.

3.3.3 Modeling and assimilation of atmospheric composition

3.3.3.1 Assimilation of trace gases from satellites

This activity covers the work done using the CERFACS chemical assimilation suite (DAIMON) both at regional (MACCIII, ADONISS, SURVEYOZONE projects) and at global scale (TOSCA project, H. Peiro PhD). The common denominator of these projects is the exploitation of data from the Infrared Atmospheric Sounding Interferometer (IASI) onboard MetOP satellites for ozone reanalyses. In 2015-2016 the research efforts have focused on the following axes:

- **Decadal reanalyses of tropospheric ozone.** The long-term availability of high quality radiometric measurements from IASI provides a great opportunity to compute climate reanalyses of the tropospheric composition. A first long-term reanalysis (2007-2014) of global tropospheric ozone was performed assimilating both IASI Level 2 (L2) tropospheric ozone columns (SOFRID product from LA-OMP) and MLS stratospheric profiles. The time series of analysed ozone have been validated against ozonesondes and confirmed previous findings about the difficulties of assimilating current IASI L2 products at high latitudes. Hence, the focus has been oriented to the tropical region (15° S - 15° N) in the Indian and Pacific Ocean regions (80° E - 100° W). The objective was to investigate the monthly and yearly variability of the tropical ozone column. This variability is a result of ENSO, QBO and MJO oscillations, as documented in previous studies. The DAIMON reanalysis is able to capture the main features of the ENSO variability (Fig. 3.8), showing for the first time the interest of IASI tropospheric retrievals for long-term ozone monitoring. This work has been presented at the IASI 2016 conference and a manuscript is in preparation. Future work may concern the analysis of variability at shorter time scales.

- **Assimilation of satellite radiances.** A possible approach to reduce IASI biases at high latitudes and more in general to solve some of the incoherencies due to the two-step assimilation of satellite data (radiances - L2 retrieval - assimilation) is to assimilate directly satellite radiances in the chemistry transport model. As first step, we replaced the reference input climatology in the SOFRID 1D-Var retrieval algorithm with MOCAGE simulated ozone. All other retrieval parameters were kept constant. This preliminary work has been conducted in collaboration with the LA-OMP and permits a first assessment of the potential advantages of radiance assimilation. Initial tests on a small selection of ozone profiles confirmed the importance of the a-priori and its error covariance matrix for infrared ozone retrievals. Better agreement with ozonesondes was found in the troposphere when using the dynamical information of the model as input for the IASI retrieval. Since the MOCAGE configuration used does not reproduce tropospheric processes (linear ozone scheme) the increased accuracy is probably due to correctly accounting for the tropopause dynamics when using the modeled fields. A global map of retrieved ozone with the reference SOFRID algorithm and with the updated a-priori is shown in Fig. 3.9. The maps show that more information can be extracted from infrared measurements when using a more accurate a-priori than a constant climatology. For example, the maximum sensitivity of the retrieval is increased, a larger number of pixels and more detailed tropospheric structures are retrieved. Note that those structures were not present in the a-priori field. A full validation of the new retrieval has been done for a 2-year long period (2008-2009) and showed promising results. For example the original retrieval bias found in the Southern hemisphere has been reduced from 33% to 6% thanks to the model a-priori. This work will be presented at the 2016 AGU conference. Further work has to be done concerning the parameterization of the a-priori error covariance.

- **Data assimilation for European air quality.** Regional reanalyses of ozone over Europe have been computed in the context of French [CE158] and European projects. The objective was to assess the capacity of satellite observations to improve air quality analyses. A regional configuration of the model (corresponding to Copernicus air quality operational forecasts) has been used for this activity and both satellite (IASI, IASI+GOME2) and surface measurements (AIRBASE) have been assimilated during a summer and a winter month. In general, results have shown a limited impact of satellite measurements for air quality applications. The main reason is the small sensitivity of tropospheric satellite retrievals to the boundary layer concentration. Nevertheless, IASI retrievals improve the free-troposphere ozone concentration of the model. A multi-instrument (surface, IASI and MLS) regional reanalysis has been computed to provide an accurate *nature run* for observing systems simulation experiments conducted at LISA (manuscript in preparation).

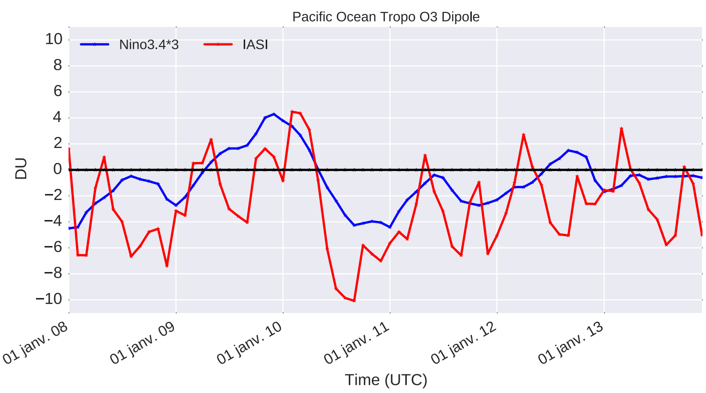

Figure 3.8: In red: time series of the ozone ENSO index (difference between the tropospheric ozone column in the 110° W - 180° W and the 70° E - 140° E regions, in Dobson units) computed with DAIMON. In blue: ENSO index (rescaled to fit the ozone units).

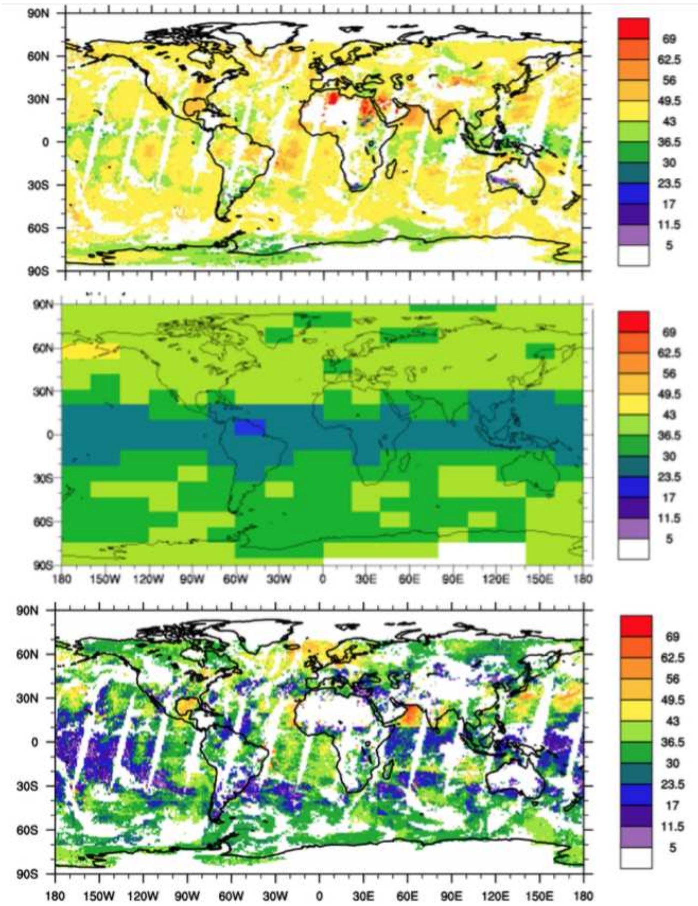

Figure 3.9: IASI-SOFRID ozone retrievals (in ppbv) at 750 hPa for one day in 2008. Top: reference retrieval (climatological a-priori). Middle: MOCAGE modeled a-priori on the selected day. Bottom: new retrieval (modeled a-priori).

3.3.3.2 Desert dust emission inversion in the chemical-transport model MOCAGE

Saharan desert dust is responsible for repeated strong episodic peaks in aerosol concentrations in Europe. The main physical mechanism governing mineral dust, the wind-driven saltation, is still poorly understood. This process depends on the soil and terrain characteristics and it is triggered only at wind speeds higher than a threshold wind speed. The large uncertainties are still present in the dust modelling and dust emission schemes, with the unknowns related to the actual process and its description in the emission scheme, and inaccurate soil and wind data. The increasing availability of aerosol products from satellites provides a strong asset for the improving the dust modelling and possibly forecasts by means of the data assimilation. We implemented a variational inversion algorithm in the the assimilation suite VALENTINA around the global chemical-transport model MOCAGE developed. Further, we applied it to the estimation of the desert dust emissions and here, we present briefly its development and impact on the modelled dust emissions.
We invert the dust emissions, by assimilating the aerosol optical depth (AOD) or lidar observations, within the standard 4D-VAR framework. The control variable, which the system tries to correct, is the 3D aerosol emission flux field (2D spatial + 1D time). Connection between the observations and the emission fluxes is assured by the observation and model operators. The 4D-VAR method was applied to permit the aerosol

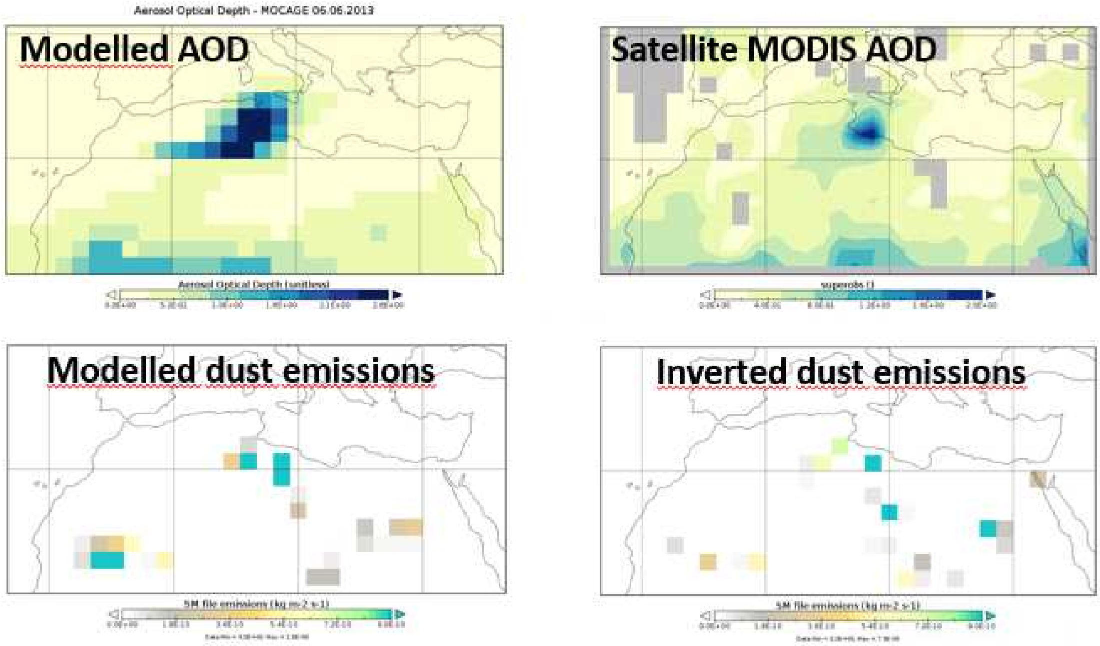

Figure 3.10: An example of the desert dust source inversion. The modelled AOD **(a)** differs from the MODIS satellite AOD **(b)**. The assimilation of the observed AOD into the model modifies the modelled dust emission flux field **(c)** and results in the inverted emission flux field **(d)** which corresponds better to the observations.

backward propagation in the adjoint, which is necessary for the inverting the emissions. Sensitivity tests are performed to determine the influence of the dust physical processes on the inversion scheme, and as a result, the vertical diffusion and the surface dry deposition are included in the adjoint code.
We used observing system simulation experiments (OSSE) to evaluate the performance of the system and impact of each characteristics or approximation used in the system, like number of the bins in the system, accuracy of the tangent linear model, interpolation order in the advection adjoint code, including/excluding different physical processes in the adjoint, effect of the turbulences in the emission, model resolution, window length, degree of the temporal correlation, etc.
The inversion scheme results indicate that the inversion scheme allow significant adjustments of the modelled emissions and the inverted emissions have improved the performance against AOD observations. Equally important, the emission inversion can be very usefull as a benchmark to evaluate the degree of uncertainties in the modelled emissions, since direct dust flux observations are rare.
In the assimilation of the satellite AODs different dust sources are corrected significantly, and, an additional correction can be applied by knowing a model mismatch only for a part of a certain dust event and propagating it to the whole event. Such inferred correction can improve results even in region where there are no observations.

3.3.3.3 The DAIMON project

The DAIMON project has been conducted in collaboration with Météo France CNRM and its objective was to improve the data assimilation capabilities in the MOCAGE Chemistry and Transport Model with a particular focus on the observation of the aerosol content of the atmosphere. The demand for better

observations and predictions of the aerosol concentration has increased in the last years since the eruption of the Iceland volcano Eyjafjöll in 2010 and also due to the greater societal concern about air quality and health impact. The VALENTINA assimilation system developed more than 10 years ago with the PALM Research coupler is able to assimilate some aerosol observations in a former version of MOCAGE since the work of Sic. The Aerosol Optical Depth (AOD) measured from satellite or the retro-diffusion signal of ground or airborne lidars can be used in this system to correct the various components of the aerosols. The DAIMON project has enabled to update this system, to improve its efficiency and to extend its capabilities for future use and developments.
UPDATE: The assimilation system is now available in the supported open-PALM MP framework and includes the most recent version of the CTM MOCAGE which is much better parallelized and optimized (CERFACS-CNRM OPTIMAL project) and benefits from a more complete aerosol modeling.
PERFORMANCE: Higher performance is achieved due to the upgrade of the MOCAGE model but also to a great simplification in the organization of the system, and a reduction in the amount of communication needed during the assimilation process. In addition, the various operators have been optimized and a new library for the resolution of the linear systems arising during the minimization loop has been implemented in collaboration with Inria (PaStiX, Parallel Sparse matriX package).
CAPABILITIES: A great effort has been made to simplify the assimilation system which was a necessity for the planned upgrade. The VALENTINA system was not designed to allow the assimilation of several quantities over several domains. This will be possible in a near future with the new DAIMON system, which is better structured and more open to inclusion of future developments, in particular those of the PAE team in the field of data assimilation for the monitoring of the air composition.

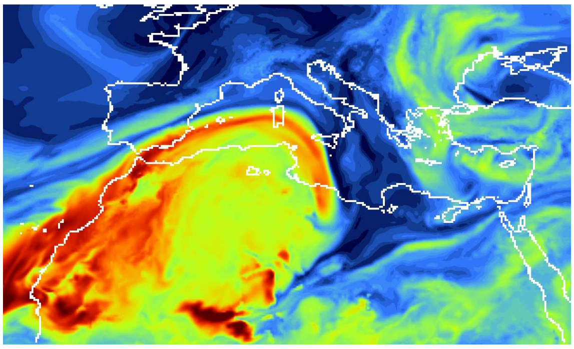

Figure 3.11: Desert dust concentration in a DAIMON analysis assimilating L1.5 exctinction coefficients from CALIOP/CALIPSO LIDAR observations (July 8th 2012).

References

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[13] M. Rochoux, A. Collin, C. Zhang, S. Ricci, A. Trouvé, and P. Moireau, (2017), 2016 CEMRACS research project - Front shape similarity measure for data-driven wildfire spread modeling, tech. rep., CECI, CERFACS-CNRS, 42, av. G. Coriolis, 31057 Toulouse Cedex France.

Couplers and Coupling Applications

4.1 Introduction

Code coupling is an important research and applicative topic in which Cerfacs has been involved 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 Earth System models, data assimilation platforms, multi-physic and multi-component coupled systems or design optimization. In this field, Cerfacs carries on research in order to improve the methodologies and performance of its open source couplers OASIS3-MCT (including the MCT library developed by the Argonne National Laboratory) and OpenPALM (co-developed with ONERA). A coupler is a library of functionalities that facilitate the sequential or concurrent execution of existing component codes as well as the exchange and the regridding of data between these components. The coupling is achieved in part via primitives called in the codes as well as via more complex mechanisms for application workflow. Cerfacs also plays a key role of networking at the international level, especially in the framework of the European project IS-ENES2 (InfraStructure for the European Network of Earth System Modelling) and of ESiWACE, the Centre of Excellence (CoE) in Simulation of Weather and Climate in Europe. For example, Cerfacs launched in Toulouse in 2010 the series of "Coupling Technologies for Earth System Modelling" workshops [CE140] and is now actively participating in the organisation of the fourth workshop planned in Princeton (USA) in March 2017.

4.2 OASIS3-MCT

The OASIS3-MCT 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 OASIS3-MCT coupler is used by about 45 climate modelling groups in France and in Europe but also in many other countries around the world.

The main functions of OASIS3-MCT are to interpolate and exchange the coupling fields between the components of a coupled system. It forms a library to be linked to the component codes and supports coupling of 2D 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, the Model Coupling Toolkit (MCT) developed by the Argonne National Laboratory in the USA implements fully parallel regridding, as a parallel matrix vector multiplication based on pre-computed weights and addresses, and distributed exchanges of the coupling fields.

The latest version of OASIS3-MCT, i.e. OASIS3-MCT_3.0, was released in May 2015. OASIS3-MCT_3.0 supports coupling exchanges between components deployed in much more diverse configurations than with previous versions [CE176]. It is of course possible to implement coupling exchanges between two components corresponding to two different executables running concurrently on separate sets of tasks, as before, but also between two components running sequentially on separate or overlapping sets of tasks within one executable. It is also now possible to have some or all tasks of a component not participating to the coupling exchanges. OASIS3-MCT_3.0 also includes a new tool, Lucia, to analyse the coupled model load balance and comes with a Graphical User Interface based on OpenTEA. The next version of the coupler, OASIS3-MCT_3.1 is planned in 2017 in the framework of ESiWACE.

The performance of OASIS3-MCT_3.0 was evaluated and compared to the performance of OASIS3-MCT_2.0 to make sure that the added flexibility of OASIS3-MCT_3.0 does not have any detrimental effect regarding its efficiency.

Tests were done with a "toy" model coupling two codes reproducing real coupling exchanges but no physics or dynamics. The codes use respectively the NEMO ORCA025 grid (1021x1442 grid points) and the Gaussian Reduced T799 grid (843 000 grid points). Figure 4.2 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 on the TGCC Bullx Curie thin nodes with OASIS3-MCT_3.0, OASIS3-MCT_2.0 and also with the old non parallel OASIS3 version. These tests show the good behaviour of OASIS3-MCT_3.0 at high number of cores. Indeed it can be inferred from these tests that the coupling overhead for one-year long simulation with 1 coupling exchange every 3 hours in each direction between codes with O(1 M) grid points running on O(10K) cores/component would take $\sim$7 minutes for the coupling initialisation (not shown) and $\sim$5 mins for the data exchanges, which is small compared to the time needed by a real coupled model at that resolution to run one simulated year.

Other modifications were done recently to improve the quality or the performance of the interpolation weight calculation, e.g. using a variable number of interpolation neighbours [CE166] or introducing a level of OpenMP parallelism in the weight calculation [CE162].

Since its first release in May 2015, more than 250 downloads of OASIS3-MCT_3.0 were registered from most major climate modelling groups in Europe but also in Canada, USA, Mexico, Peru, Brazil, Chile, Australia, New Sealand, Indonesia, India, Singapore, Japan, China, Russia, Saudi Arabia, Algeria, South Africa, Egypt, Iran, etc. During the last two years, Cerfacs has provided active user support to many

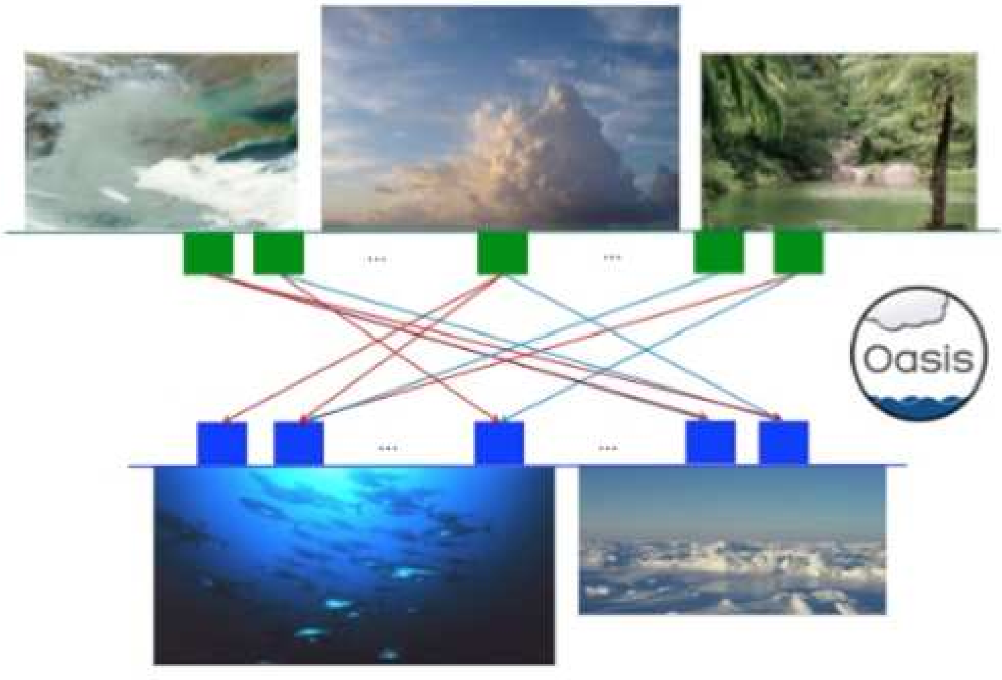

Figure 4.1: Figurative representation of a coupling managed by OASIS between an atmospheric code (including physic and dynamic parts and a land scheme) and an ocean code including a sea-ice model

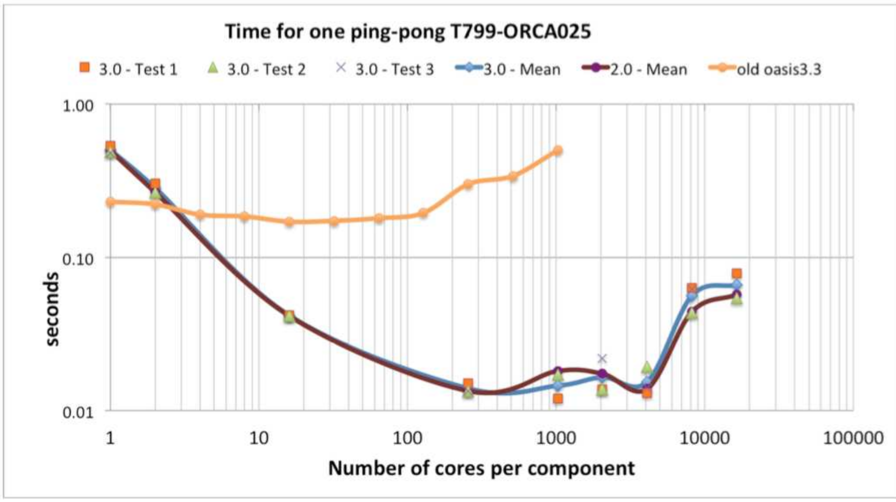

Figure 4.2: Time of a back and forth exchange between the two codes using respectively the ORCA025 grid and the Gaussian Reduced T799 grid as a function of the number of cores used to run each code on the TGCC Bullx Curie thin nodes with OASIS3-MCT_3.0, OASIS3-MCT_2.0 and with the old non parallel OASIS3 version.

of these groups through mail or phone exchanges and forum discussions. A three-day general training session on OASIS3-MCT_3.0 gathering 5 participants was also offered in January 2016. Finally, Cerfacs has also provided in-person support to DWD (Germany, 2 days), BTU-Cottbus (Germany, 4 days), IFREMER (France, 2 days).

In particular, OASIS3-MCT_3.0 is used at the Centre National de Recherches Météorologiques (CNRM) of Météo-France to assemble different climate models in the framework of various national, European or international projects and CNRM benefits from the coupling expertise and user support of our team in the realisation of these coupled systems.

The last climate coupled model developed at CNRM, with help and support from Cerfacs, is CNRM-CM6 based on the atmospheric model ARPEGE-Climat V6.2.4 including the surface module SURFEX V8 and on the ocean model NEMO 3.6 integrating CNRM GELATO sea-ice model. The low-resolution version of CNRM-CM6 (T127 i.e. ∼150 km horizontally and 91 vertical levels for the atmosphere and ∼1-degree horizontally and 75 vertical levels for the ocean) has been technically developed and scientifically validated and the high-resolution version CNRM-CM6_HR (i.e. T359 or ∼50 km horizontally and 91 vertical levels for the atmosphere and ∼0.25 degree and 75 vertical levels for the ocean) is under developement. CNRM-CM6 will be used in particular by the CNRM-Cerfacs group in the 6^{th} international Coupled Model Intercomparison Project (CMIP6), by CNRM in the CRESCENDO European project and by Cerfacs in the PRIMAVERA European project.

In 2015-2016, CERFACS participated to the implementation of many other OASIS based coupled systems, among which one can cite for example:

- CERFACS-HR, assembling ARPEGE-Climat V5 at T359 horizontal resolution and 31 vertical levels with NEMO-LIM V3.4 at a ∼0.25 degree resolution and 75 vertical levels, which was used at Cerfacs for decadal prediction in the EU SPECS project [CE40] and for studying the tropical atlantic biases mechanism in the EU PREFACE project [CE31];
- the 3D global-regional coupled system developed at BTU-Cottbus (Germany), used for regional climate studies, into which OASIS3-MCT ensures exchanges of 6 3D coupling fields every timestep

between the COSMO-CLM regional atmosphere model and the global ECHAM atmosphere model, and also 2D coupling exchanges with the MPI-OM ocean model [34];

- the PULSATION HR tropical system coupling the atmospheric WRF model and the NEMO ocean model with zooms in both models reaching resolution of 27 to 9 kms; PULSATION benefited from a 19 Mhours allocation on TGCC Bullx Curie in the PRACE 9^{th} call in 2015, in particular to study the impact of small-scale processes on large-scale climate [16].

Besides the permanent manpower ensured by Cerfacs and CNRS, the IS-ENES2 project, the ESiWACE CoE and the ANR CONVERGENCE project were the main sources of external funding for the development and maintenance of the OASIS3-MCT coupler in the 2015-2016 period.
More details on OASIS event, source downloads and users can be found on its web site at https://verc.enes.org/oasis.

4.3 OpenPALM

OpenPALM is a general tool allowing to easily integrate high performance computing applications in a flexible and evolutive way while complying with performance, software reuse and numerical accuracy criteria. OpenPALM is mainly composed of 3 complementary components, (1) the PALM[1] library developed by Cerfacs, (2) the CWIPI[2] library developed by ONERA and (3) the graphical interface PrePALM developed by Cerfacs. As the application programming interface is available in Fortran and C/C++, OpenPALM can couple codes written in different languages. In the context of the Cerfacs/ONERA collaboration, the coupler has become open source since January 2011.
PALM has originally been designed for oceanographic data assimilation algorithms, but its application domain may extend to every kind of scientific applications [14]. In the framework of PALM, applications are split into elementary components that can exchange data though MPI communications. The main features of PALM are the dynamic launching of the coupled components, the full independence of the components from the application algorithm, the parallel data exchanges and redistribution, and the possible combination of physical modules with algebraic operations offered by the PALM algebra toolbox. It can be defined as a dynamic coupler for its ability to deal with situations where the component execution scheduling and the data exchange patterns cannot be entirely defined before execution.
Based on FVM (EDF's "Finite Volume Mesh" library under LGPL licence), CWIPI [15] provides a fully parallel communication layer for mesh based coupling between several parallel codes with MPI communications. The library takes into account all types of geometrical elements (polygon, polyhedral) with an unstructured description. CWIPI ensures the construction of the communication graph between distributed geometric interfaces through geometrical localization, the interpolation on non coincident meshes, the exchange of coupling fields for massively parallel applications and the generation of visualisation files to be used for a verification of the coupling interface.
The Graphic User Interface, called PrePALM, is a portable Tcl/Tk application. The relevant coupling features are described in the component source codes in identity cards that are loaded by PrePALM to construct the coupled applications. The user describes the execution scheduling, the parallel sections, the data exchange patterns and the algebraic treatments, entirely through the user interface. PrePALM then provides the input file for the coupler executable and the source code for the wrappers of the coupled component. These input file and wrappers take entirely care of the set-up of the communication context with no need of change in the component source code. The same graphic tool can be used at run-time to monitor the simulation status and to provide post-mortem some statistics on the memory and CPU time resources used by the different components.

[1]Projet d'Assimilation par Logiciel Multiméthodes
[2]Coupling With Interpolation Parallel Interface

The main points investigated during the period 2015-2016 are:

- Many installation tests on current HPC architectures: Nemo (Cerfacs/France), Beaufix and Prolix (Météo-France/France), Marenostrum III (BSC/Spain, rank 106 machine on Top500), Turing (IDRIS/France, rank 81 machine on Top500), Cobalt (CEA-CCRT/France, rank 63 machine on Top500), Occigen (CINES/France, rank 53 machine on Top500), Titan (Oak-Ridge/USA, rank 3 machine on Top500). The scalability of the CWIPI library has been tested on coupled applications in turbomachinery for up to 131 000 cores on Titan and Turing. Figure 4.3 illustrates the performance of this latter application on Titan by showing the time requested by the initialization step of the coupling (routing of processes) and by a ping-pong (back and forth) exchange between two instances of the AVBP code for a compressor simulation as a function of the total number of cores involved in the coupling.

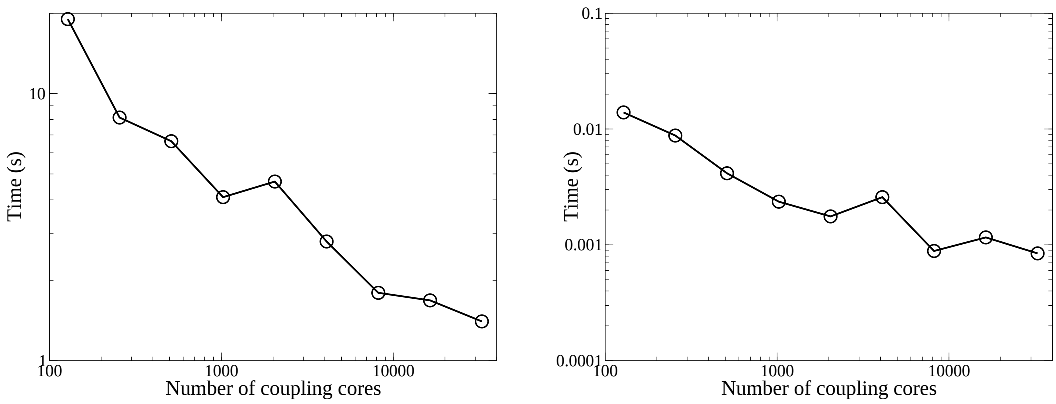

Figure 4.3: Time requested by the initialization step of the coupling (a) and by a ping-pong (b) exchange between two instances of the AVBP code for a compressor simulation as a function of the total number of cores involved in the coupling for up to 130 000 cores on Titan.

- Integration of dynamic distributors for PALM parallel communications in collaboration with KIT (Karlsruhe Institute of Technology).
- Development of a TCL script to automatically generate PrePALM coupling files.
- Development of a preliminary version of automatic mesh check in CWIPI.
- Add the possibility to run an OpenPALM application without the driver when possible (mainly for multiphysic and multicomponent simulations with CWIPI library).
- Development of a save and reuse (in memory or disc) strategy of mesh localisations and interpolation weights in CWIPI for periodic simulation such as in turbomachinery applications.
- Development of a preliminary version of an inline update of the localisations for moving mesh applications such as turbomachinery and fluid/structure interactions.
- Integration of an interface for Python codes for the PARASOL functionality.

The OpenPALM coupler is used in the framework of Data Assimilation (DA) for several geophysical applications by Cerfacs and its partners.

In the context of atmospheric chemistry, the variational DA suite for the Météo France chemistry transport model MOCAGE (DAIMON) is currently based on OpenPALM, which is used to schedule the DA tasks and monitor their execution. DAIMON provides operational air-quality forecasts for Météo France and is used for a number of scientific applications at Cerfacs, which include decadal reanalyses of tropospheric ozone and Saharan dust source inversion. In the coming year, the possibility of parallel coupling offered by OpenPALM will be exploited for the inclusion of costly radiative transfer computations, which should enable the assimilation of satellite radiances within a reasonable execution time.

In the context of wildfire modeling, the ensemble-based DA suite FIREFLY aims at forecasting wildfire behavior through the assimilation of time-evolving fire front position derived from mid-infrared imaging. FIREFLY is designed in collaboration between Cerfacs, the University of Maryland and Inria. One key aspect of FIREFLY is to rely on a front shape similarity measure to represent the distance between observations and simulated fire front at a given time. FIREFLY is currently based on OpenPALM, which is used to schedule the DA tasks and monitor their execution. OpenPALM ensures the integration of an ensemble of fire spread models for varying scenarios of near-surface wind and biomass state that is required in the ensemble Kalman filter to specify stochastically the error variances of the input parameters and of the fire front position as well as their correlations. The ensemble runs are specifically monitored by the PARASOL functionality in OpenPALM. In the coming year, the ensemble-based DA will be further developed and evaluated against real-world wildfire events. Simulating an ensemble of potentiel fire behaviors at different lead times should remain cost effective. For this purpose, the use of uncertainty quantification methods in the frame of the ensemble DA will be investigated. This will be managed by using the OpenTURNS uncertainty quantification python library within OpenPALM.

In the context of hydrology, OpenPALM was used, during the 2015-2016 period, as a task parallelism manager to handle communications and data exchanges between hydrodynamics solvers (1D, 2D hydraulic solvers, small-regional and large scale hydrology solvers) and the mathematical units required to sequentially perform the DA and Uncertainty Quantification (UQ). PALM-PARASOL is used to integrate independent runs of MASCARET (1D hydraulic solver) in parallel when a Monte-Carlo approach is implemented. The OpenTurns UQ-dedicated python library is used for the formulation of a Polynomial Chaos (PC) surrogate model, thus reducing the cost of stochastic estimation of hydraulic state statistics as well as sensitivity analysis (N. El Mocayd PhD, EDF/CNES). DAMP (Data Assimilation with MASCARET Platform) is used operationnaly at SCHAPI[3] and at SPC SAMA[4] for real-time flood forecasting with sequential assimilation of water level in-situ observations that allow for the correction of the upstream and lateral inflow, the friction coefficient as well as the hydraulic state (PhD J. Habert). The DA algorithm is a filter implemented following extended as well as ensemble-based formulations. PALM-PARASOL is used for the ensemble integration in the forecast and analysis steps. The cost of the covariance matrix estimation is reduced when the PC surrogate is used in place of the direct model.

OpenPALM is also used for multidimensional coupling between 1D and 2D hydraulic solvers. When the flow is 1D, MASCARET is used and coupled with TELEMAC 2D in areas where the flow is more complex (confluence, flood plains). An iterative Rieman solver was implemented with three different implementations of the coupling (PhD S. Barthélémy, SCHAPI/MiPy): a longitudinal coupling based on boundary condition exchanges, a lateral coupling where only the flood plain are solved in 2D and provide lateral inflow to the 1D river bed dynamics and an overlappling coupling where a local 2D patch model provides inflow to the 1D model when activated. In this latter formulation, the 1D network remains unchanged and this approach makes the most of the expertise available on both models, especially on the 1D model, for which DA is implemented. As such, a multidimensional coupling with DA was implemented between MASCARET and TELEMAC. In the coming year, the lateral coupling approach will be further developed and a coupling platform for operational used will be implemented (EoCoe EU project, S.

[3]Service Central d'Hydrométéorologie et d'Appui à la Prévision des Inondations'

[4]Service de Prévision des Crues Seine Amont Marne Amont

Barthélémy Post-Doc). A UQ and DA dedicated python library will be implemented with OpenPALM for hydraulic applications with MASCARET and TELEMAC API as well as for CFD-oriented applications.
In climate and environmental domains, a number of modeling systems rely on the OpenPALM coupler. In 2015-2016, efforts have concentrated on two multi-physic applications:

- AquiFR (http://www.metis.upmc.fr/ aqui-fr/), which aims to monitor and forecast groundwater resources in France as well as to facilitate climate change impact assessments. OpenPALM makes it possible to manage the various hydro-geological applications of the 3 models (computing codes) integrated to date (Gadenia, Marthe and Eau-dyssée). Cerfacs provided PALM support to the laboratories in charge of the development of Aqui-FR (BRGM, Meteo-France, UPMC,...);

- The modeling platform for urban climate, ACCLIMAT, running at Cerfacs and Météo-France, benefited from major improvements in 2016. In particular, it now takes fully advantage of the CWIPI library, replacing the Dscrip interpolation library, for coupling MesoNH with SURFEX. This leads to gains in performance, code and PrePalm scheduling simplifications and robustness of the application. MesoNH version was upgraded and the applicability of the platform to different French cities was demonstrated.

Finally, as a code coupler, OpenPALM is intensively used in many multi-physic and multi-component studies in the Computational Fluid Dynamic team of Cerfacs. Firstly, an important axis deals with aerothermal simulations 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 is solids and PRISSMA for the radiation) was developed with OpenPALM (Fig. 4.4). OpenPALM is also used by Cerfacs academic partners such as CORIA to develop conjugate heat transfer with the YALES2 Large Eddy Simulation solver. 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 the 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. In this context, the TurboAVBP system that couples several instances of the AVBP code with OpenPALM is intensively used for compressor, turbine and integrated combustion chamber/turbine simulations (Fig. 4.4). All these applications lead to an important number of publications increasing the notoriety of OpenPALM.

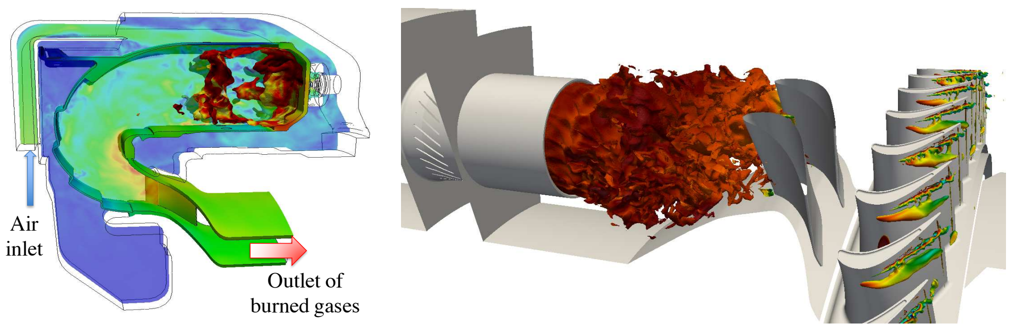

Figure 4.4: View of fluid and solid models of an industrial combustor Conjugate Heat Transfer simulation (left) and example of an integrated combustor/turbine simulation (right).

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, Airbus-Group, ONERA, CNES, CNRM (Météo France), EDF and about 70 other institutions. An important part of industrial use was supported via the FUI project COSMOS+ (2012-2015), which objective was to develop and implement

multiphysics coupling to meet the needs of industry and research in the aerospace field. This project provided resources to develop the OpenPALM Cerfacs-ONERA coupling environment and to define a coupling strategy for diverse application domains (aerodynamics, thermodynamics, convection, radiation, etc.)
Over 2015-2016, three 3-day training sessions on OpenPALM coupler were held at Cerfacs for a total of 28 trainees. A 2-day training session on the use of OpenPALM coupler for DA and UQ applications was also given.

4.4 Coupling technology benchmarks

Evaluating the performances for different coupling technologies used today in climate modelling within a standard benchmarking environment is one major objective of IS-ENES2. Within this EU project, Cerfacs is leading the corresponding task into which 3 other partners are contributing. This evaluation is mandatory in order to better define the best bases for the development of a next-generation exascale coupler.
The work began by defining Earth System Modelling (ESM) coupling characteristics during the ≪ 2nd Workshop on Coupling Technologies ≫ held in 2013 in Boulder, USA. This definition was finalized by IS-ENES2 partners interacting with colleagues from the US Earth System Bridge project. From these coupling characteristics (the component grids, the number of MPI ranks used to run the components, the number of fields exchanged between the components, the frequency of exchange), the main features of a benchmark suite were then defined [CE177] The first implementation step was to develop stand-alone components running on different grids. These components were then assembled using the different coupling technologies in well-defined coupled configurations.
Today, four simple coupled configurations are available for testing. The components of these configurations run on regular latitude-longitude grids with up to 3000x3000 grid points. All configurations implement the same coupling algorithm (i.e. fields are sent back and forth between the components) using the OASIS3-MCT, OpenPALM, ESMF[5], MCT only or YAC [6] coupling technologies. The time for the coupling initialization and for the coupling exchanges is measured for the configurations running with up to O(10000) cores on three different platforms: Bullx at CINES in France, a Cray XC40 at the UK Met Office, and the Broadwell partition of Marconi at CINECA in Italy. These results and any lessons learned from this first benchmark experience will be analysed shortly and will be presented at the Fourth Coupling Technologies for Earth System Modelling in Princeton (USA) in March 2017.

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[5]https://www.earthsystemcog.org/projects/esmf/
[6]https://doc.redmine.dkrz.de/YAC/html/

Data Assimilation and Uncertainties

5.1 Introduction

Data Assimilation (DA) is a transversal axis at CERFACS that gathers ALGO, AE and GLOBC teams. It is also one of the major research axis for CECI. It is mostly developped for applications in geosciences. It closely relates to Uncertainty Quantification (UQ) theme (also a transversal axis at CERFACS and for CECI) as the uncertainties once identified and quantified can then be reduced with Data Assimilation algorithms.
The activity in DA and UQ are reported in the "Parallel Algoritms Project" report (Part 1) for methodological aspects, in the "Modeling Environment and Safety" chapter (Chapter 2.3) for risk related aspects and finally in the present section for an overview of application related aspects. Interaction with the Couplers and coupling applications chapter are also described in "Couplers and Coupling Applications" chapter (Chapter 2.4) regarding the use of the OpenPALM coupling software for UQ and DA implementation.
This chapter is divided into four sections corresponding to UQ and DA applications ofr oceanography, hydrology, wildland fires and atmospheric chemistry.

5.2 Oceanography

This activity concerns global ocean DA developments for NEMOVAR, a variational data assimilation system for the NEMO model, developed jointly by CERFACS, ECMWF, Met Office and INRIA, for research and operational applications. The period covered by this report saw NEMOVAR consolidate its position as one of the world's leading ocean DA systems for operational forecasting and reanalysis. The Met Office operational implementation of NEMOVAR is described in [CE145], while the ECMWF implementation is described in an earlier publication. Results from NEMOVAR have also figured prominently in two ocean DA review articles: [CE120], which covers operational ocean forecasting activities within the framework of the international programme GODAE OceanView; and[CE138], which focuses on ocean DA related to climate applications, such as reanalysis and seasonal forecasting. NEMOVAR forms the ocean DA component of the coupled ocean-atmosphere reanalysis system developed at ECMWF as part of the ERA-CLIM2 project, a project in which CERFACS is also a partner.
In parallel with progress on applications, a significant effort has been devoted in the reporting period to develop the next-generation version of NEMOVAR. This work has been motivated by two factors: 1) the need to improve estimates of uncertainty (background and analysis error) through the use of ensembles; and 2) the need for improving specific algorithms for high-resolution applications on high-performance computers. CERFACS has played a leading role in the development of the new version of NEMOVAR, notably through its expertise in covariance modelling and iterative methods.
Two ways have been developed to use ensemble perturbations to define the background error covariance matrix ($\mathbf{B}$). The first method uses the ensembles to estimate parameters (variances and local correlation tensor) of the covariance model. The second method uses the ensembles to define a sample estimate of the covariance matrix. Optimally based techniques have been developed to filter the covariance model parameters and to localize the sample covariances. This is essential since practical ensemble sizes are small and hence sampling error is large. A hybrid formulation of $\mathbf{B}$, involving a linear combination of

the covariance model and the localized sample covariance matrix, has also been developed, as well as a procedure to optimally determine the weights given to each term.
Central to the *hybrid* $\mathbf{B}$ formulation in NEMOVAR is the "diffusion" algorithm that is used for spatial filtering and localization of the ensemble covariances, and for defining the correlation component of the covariance model. The diffusion-model formulation has been entirely revised to make it more general and flexible for representing complex correlation structures. Furthermore, significant improvements to computational aspects of the algorithm have been made, notably through the use of an implicit solver based on the Chebyshev iteration, as described in [CE146].
The ocean DA activity is supported by projects funded by the EU (ERA-CLIM2), RTRA-STAE (AVENUE), and LEFE-MANU.

5.3 Hydraulics/hydrology

A summary of the main achievements in hydrology/hydraulic UQ and DA over 2015-2016 is given below. The work has been conducted within the framework of several projects, PhDs and post-doctorate: EoCoE (H2020) - Energy Oriented Center of Excellence; LEFE-MANU (HYDRAU-SWOT); TOSCA-CNES; J. Habert PhD (SCHAPI, defense Jan. 2016), S. Barthélémy PhD (SCHAPI/MiPy, defense June 2015) and Post-doctorate (EoCoE, until Nov. 2017), N. El Moçayd (EDF/CNES, defense planned early 2017), C. Emery (CNES/LEGOS, defense planned early 2017), V. Haflinger (CNES/CNRM, defense Nov. 2015), V. Laborie (CEREMA). This work has been carried out in close collaboration with EDF (LNHE, LHSV), CNRM, SCHAPI, CNES and LEGOS. This research axis relates to the MODEST challenge at CERFACS, it also relates to the "Coupling" activity at CERFACS, especially regarding the use of the OpenPALM coupling software. It finally also related to the "Algorithmic" activity at CERFACS, especially regarding DA methods and to the "CFD" activity at CERFACS regarding UQ methods.

5.3.1 Uncertainty quantification (UQ) and sensitivity analysis (SA) for hydraulic model

River water level and discharge simulated by numerical solvers suffer from uncertainties related to the approximate description of physics equations, hydraulic parameters, meteorological, hydrological and geographical data; thus limiting the predictive capacity of the deterministic approach. In the framework of flood forecasting or water resource management, these uncertainties should be quantified to provide a range of uncertainty along with the water level forecast, for instance for threshold exceed estimation. SA allows to identify the most significant sources of errors in the model quantities of interest, that they could thus be reduced with DA. Ensemble-based approaches are favored for SA and uncertainty propagation as they make the most of increasing computational resources and remain non-intrusive for the solver.
A UQ study has been carried out in the framework of N. El Moçayd's PhD [18] to quantify the errors in water level due to errors in the description of friction coefficients and upstream flow boundary conditions for stationary flows with the 1D hydraulic model MASCARET developed at EDF. The study was carried out over the Garonne catchment. The algorithm was implemented with OpenPALM, making the most of the resource management with PALM-PARASOL for the ensemble integrations as well as making the most of the UQ-dedicated OpenTURNS library. It should be noted that the SALOME-HYDRO platform was also used. So far, a polynomial surrogate model was set with respect to up to 4 aleatory variables. We have demonstrated the ability of Polynomial Chaos surrogate to evaluate the probabilistic features of the simulated water level with the same accuracy as a classical Monte Carlo method but at a reduced computational cost. It was shown that the water level probability density function and covariance matrix are better estimated with the Polynomial surrogate model than with a Monte Carlo approach on the direct model given a limited budget of direct model evaluations. An alternative method based on Proper Orthogonal Decomposition (POD) and Kriging was also investigated in the context of a collaboration with the CFD

team (P. Roy M2 internship described in CFD related section 2.4 of Part 3). This work should be extended to uncertain aleatory fields when the flow is unstationary. This is a crucial step for the use of surrogate model within DA algorithms as the main objective is real-time flood forecasting.

The hydrodynamics of the Gironde estuary is simulated with the 2D solver TELEMAC. The 7000 nodes model is forced upstream with hydrological inputs, downstream with maritim state and with meteorological wind and pressure fields at the surface. In the framework of V. Laborie's PhD (2016-2019), a univariate sensitivity analysis highlighted that the downstream part of the estuary is mostly under the influence of the maritim boundary conditions and local friction coefficient; in contrast, the upstream part is under the influence of hydrological inflows and local friction coefficient. A global SA with respect to spatial and time varying forcing should be carried out in order to identify a reduced dimension control vector for DA. The UQ analysis with both MASCARET and TELEMAC are developed making the most of the available API functions that allow for a non-intrusive implementation,

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

The DAMP (Data Assimilation with MASCARET Prototype) data-driven flood forecasting system has been implemented for the past few years at CERFACS in collaboration with SCHAPI and EDF. Built in the OpenPALM framework, this system relies on the sequential assimilation of in situ observations through Kalman filtering to correct the simulated hydraulic state as well as the upstream and lateral inflow to the model [23]. The background covariance matrix for the state correction is stationary with anisotropic correlation length scale. The observation operator for parameter (parametric correction of the forcing) is computed with a finite diffenrence scheme. Following this strategy, over the 2015-2016 period, the definition of the control vector and the implementation of the DA algorithm were improved. First, the sequential assimilation of in-situ water level enabled the correction of the friction coefficients ([CE110], [CE185]) to account for error in friction but also to account for local imperfect description of the bathymetry. This approach appears like an indirect, thus efficient way of correcting errors in the water level-discharge model relation. An ensemble-based Kalman filter was also implemented to provide a flow-dependent propagation of background error covariances ([CE183], [17]. It was demonstrated that the river network and the bathymetry significantly influences the shape of the spatial univariate and multivariate covariances functions for water level and discharge. These new developments increase the computational cost of DA, still, it remains within the limits of operational constraint as a localisation and inflation solution were proposed to limit the size of the ensemble to 50 members. These developments resulted in the improvement of our modeling/forecasting capability of river hydrodynamics at short to medium lead-time (from 1h to 36h).

DAMP is used for real-time forecast at SPC SAMA (Flood forecasting service, Seine Amont-Marne Amont) since January 2015 and is currently being implemented for operational use at SCHAPI within the POM platform (Multimodele Operational Platform). DAMP uses the OpenPALM-PARASOL functionality to integrate independent MASCARET runs in parallel within the ensemble making the most of available computational resources. The MASCARET API are used for a non-intrusive implementation of DA with respect to the numerical solver.

Complementary to ensemble-based approach, a parametric formulation of the Kalman Filter is also being investigated. The dynamics of the variance and the diffusion tensor which is related to the correlation length scale are approximated and propagated along the analysis and forecast cycles. This work published in [21] on 1D advection-diffusion equations should be further extended to multi-dimensional and complex hydraulic equations.

5.3.3 Investigating the use of remote sensing data for hydraulic and hydrology modeling

The Surface Water and Ocean Topography (SWOT) satellite mission planned for launch in 2020 will map river elevations and inundated area globally for rivers > 100 m wide. Present work aims at demonstrating the benefits of up-coming remote sensing missions such as SWOT 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 the framework of a collaboration with LEGOS and CNRM, two PhDs ([22], [19], CNES funding) were carried out to investigate the potential of SWOT data for parameter optimization for large scale river routing models which are typically employed in Land Surface Models for global scale applications. The method consists in applying an EKF and an EnKF algorithms, to correct the Manning roughness coefficients of the ISBA-TRIP Continental Hydrologic System, over the Niger and the Amazon. Following this path, synthetic SWOT data are assimilated in order to improve a regional hydrometeorological model [CE111] that represents the dynamics of continental waters over the Garonne catchment as detailed in [20]. The river bed roughness coefficient and thus the simulated water levels are corrected, assimilating SWOT-like data in the context of Observing System Simulation Experiments. It was showed that the corrected roughness coefficient values and the associated river water levels tend to be close to the "truth" with a reasonable error of 5 cm.
The possibility of estimating discharge in ungauged reaches using synthetic SWOT measurements was investigated by [CE104]. Discharge is derived from hydraulic models using five discharge algorithms designed for SWOT for nineteen rivers spanning a range of hydraulic and geomorphic conditions. We found at least one algorithm able to estimate instantaneous discharge to within 35% relative RMSE on $14/16$ non-braided rivers despite out of-bank flows, multi-channel planforms, and backwater effects. The DAMP system currently relies on the assimilation of in situ data that are sparse along the hydraulic network and needs to be extended to the assimilation of SWOT-like remote sensing data. For this purpose, the SWOT-HR simulator was used with input simulated data from MASCARET or TELEMAC-2D. The DA algorithm will be extended to this type of data generated by the SWOT-HR simulator that is now able to provide SWOT-like observations over time. A major issue lies in the spatial and temporal averaging of these data in order to compare them with the model outputs. This work will be carried out in the framework of a TOSCA funded position (IR to be hired end of 2016), focusing on the Garonne catchment.

5.3.4 Multidimensional coupling in hydraulic with data assimilation

In order to more accurately represent complex flows such as in confluence areas and flood plains, while keeping an affordable computational cost in an operational perspective, a multi-dimensional (1-D/2-D) coupling system was designed with longitudinal, lateral and overlapping methods. This coupling system was combined with the assimilation of water level in situ observations on the 1-D domain; its positive impact was shown over the 2-D computational domain for a set of flood hazards on the Adour catchment [CE183]. Different interface coupling strategies have been implemented to provide adapted solution for various catchment and dynamics in the frame of Barthélémy's Postdoctorate (EU-EoCOE and SCHAPI). Three different coupling algorithms were implemented with the three different coupling methods: the longitudinal coupling is based on boundary conditions exchanges; the lateral coupling applies where only the flood plains are solved in 2D and provides lateral inflow and boundary conditions respectively to the 1D and the 2D models; the overlapling coupling applies where a local 2D model provides lateral inflow to the 1D model while the 1D model provides boundary conditions for the 2D model. In this last formulation, the 1D network remains unchanged and this approach makes the most of the expertise available on both models, especially on the 1D model, for which DA is implemented. With this strategy, a multidimensional coupling with DA was implemented between MASCARET and TELEMAC. The lateral coupling approach has been developed in the framework of the CEMRACS project in 2016 (collaboration between LNHE, INRIA and CERFACS) and will be further developed with S. Barthélémy Post-Doc funded by EoCoe EU project. In this context, the longitudinal and overlapping coupling methods are also being integrated into an operational platform at SCHAPI.

5.4 Wildland fires

Real-time forecast of wildfire behavior (spread and emissions) remains a key challenge for fire emergency response. Whether used as a planning tool prior to prescribed burning or as an operational tool to predict the growth of current or potential uncontrolled wildfires, the accuracy of wildfire spread models and their ability to provide useful information in a timely manner are of paramount importance. This is particularly true in the perspective of climate change that tends to favor extreme drought and to alter precipitations, thus dramatically increasing the risk for the growth of large, long-term, highly destructive fires known as *megafires*, with strong implications for public safety and air pollution far away from 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 based on the assimilation of wildfire remote sensing data becomes essential. Current operational wildfire spread simulators simulate large-scale wildfire hazard as a front that self propagates normal to itself into unburnt vegetation. They use simplified models to calculate the front propagating speed, or rate of spread (ROS), as a semi-empirical function of biomass fuel properties, topography and near-surface wind. To overcome the large uncertainties associated with the ROS model as well as the aleatory environmental/meteorological conditions, a data assimilation prototype named FIREFLY has been designed at CECI in close collaboration with the University of Maryland since 2010 [24, 25, CE132].
A summary of the main achievements in wildfire behavior UQ and DA over 2015–2016 is given below. This research has been carried out

- within the framework of several projects, i.e. LEFE/INSU national program (MANU *Méthodes mathématiques et numériques*, 2015–2016); LabEx AMIES (PEPS *Projet Exploratoire Premier Soutien*, 2016); and NSF–WIFIRE US funding (2014–2018) through C. Zhang's PhD (University of Maryland, 2014–2018);

- in close collaboration with CNRM, LA, SPE (CNRS/University of Corsica), Inria (the new ANR–FireCaster – FIRE, foreCASTing and Emergency Response platform – project will start in 2017), LIMSI and the University of Maryland.

From CERFACS' perspective, this project relates to the "MODEST" (MODeling for Environment and SafeTy) challenge on the applicative side. It also relates to the "Coupling" activity (especially regarding the use of the OpenPALM coupling software) and "Algorithmic" activity (especially regarding the development of cutting-edge DA algorithms) for methodological issues.

5.4.1 Extension of ensemble Kalman filter to regional-scale fires

Operationally oriented fire spread models can be used to simulate fire growth using forecasted vegetation maps and wind-weather scenarios but offer no information on the probability of an area being impact in the short term under multiple vegetation and weather scenarios. Ensemble-based modeling overcomes this limitation by generating hundreds of potential vegetation and weather scenarios, leading to the prediction of thousands of individual fires through the integration of a Level-Set or Lagrangian front-tracking simulator. The ensemble-averaged predictions result in probabilities for fire growth. DA then offers to take advantage of real-time data to reduce the spread of the ensemble around a more realistic fire scenario and to build upon this correction to produce more reliable forecasts. The FIREFLY system deploys this idea using an ensemble Kalman filter (EnKF) featuring either a parameter estimation approach (in which the estimation targets are the ROS input parameters such as near-surface wind speed/direction and biomass moisture content) or a state estimation approach (in which the estimation targets are the fire front positions). These two approaches are implemented based on the OpenPALM dynamic coupler combined with the PARASOL functionality for effective ensemble generation (task parallelism).

Previous work was limited to the evaluation of FIREFLY on reduced-scale controlled burnings [25, CE132]. We extended the FIREFLY system to a spatially-distributed parameter estimation approach to cope with the spatial variations of environmental conditions (in particular near-surface wind conditions) and to address the anisotropy in wildfire spread at regional scales. The estimation targets are thus treated as functions of space and time on a grid that is coarser than the forward model grid (roughly by a factor of 10). To generate a reliable ensemble and ensure an accurate correction, the EnKF algorithm requires sampling truncated probability density functions as well as localizing, i.e., dynamically selecting the areas where the wind parameters are corrected.

The potential of FIREFLY for dynamically estimating the interactions between the near-surface wind and the fire was evaluated in simulations of a field-scale prescribed-burn experiment, the 30-hectare FireFlux experiment [26]. The spatialized parameter estimation approach retrieved accurate fire front position and shape at observation times, and led to a substantial improvement in the forecast performance compared to the standalone wildfire spread model. The variability of the forecast error is determined by the temporal and spatial variability of the near-surface wind conditions. We note in particular that the forecast error can be decreased by providing a more accurate wildfire spread model (the present ROS model has limitations on the flanks and in the rear of the fire and therefore negatively impacts the FIREFLY performance) and/or by coupling the wildfire spread model to a meso-scale atmospheric model to have more representative dynamically-evolving near-surface wind fields (incoming ANR–FireCaster project based on the coupled FOREFIRE/Meso-NH simulator and ongoing NSF–WIFIRE project in collaboration with the University of Maryland).

5.4.2 Front shape similarity measure to assimilate fire imaging data

One key issue in the EnKF algorithm is to compute the innovation term, i.e. the discrepancies between simulated fire fronts and observations. The wildfire remote sensing data usually provide (binary) images showing the areas where the mid-infrared radiance is high and thus corresponding to active fire areas. FIREFLY initially treated the observed fire front as a discretized contour with a finite set of markers and therefore used a Lagrangian-type innovation. The observed fire fronts were extracted in a preprocessing step, from the binary images as the boundary of the burning area. The distance between the simulated fronts and the resulting observations was computed by pairing each observed marker with its closest neighbor along the simulated front. This selection procedure was questionable since the resulting observation operator is not the same for all members of the ensemble. It also became unsuitable when moving to real-world wildfire events with complex front topology.

To overcome this issue, we proposed a new method to represent the distance between observed and simulated fronts (2016 CEMRACS Summer Program). This method – deriving from object detection in image processing theory and already adapted in the context of electrophysiology data assimilation – formulates a shape similarity measure based on the Chan-Vese contour fitting functional at a given time. The shape similarity measure decomposes into two terms, one term quantifying the overlap area between the observed burning area and the simulated burning area, a second term quantifying how much of the observed burning area is outside of the simulated burning area. This provides a signed local discrepancy between the simulations and observations. The burning area is thus represented as a coherent structure (or object) that shall be deformed to steer the model prediction towards the observation. The new innovation term based on the front shape similarity measure is adapted to both Level-Set (e.g. SFIRE) and Lagrangian (e.g. FARSITE, FOREFIRE) wildfire spread models, which are representative of the panel of models available in the wildfire community [13]. It can be used in the context of state estimation to directly correct the fire front position at a given time (see Fig. 5.1), or parameter estimation to retrieve input parameters of the ROS model leading to improved fire front location forecast at future lead times. The application and evaluation of the front shape similarity measure in the context of the EnKF algorithm is ongoing. Further analysis of the behavior of the front shape similarity measure and comparison with alternative distances formulations are required for different test cases (from synthetic experiments to real-world wildfire hazard events). This is part of an ongoing LEFE/INSU project in collaboration with Inria.

5.4.3 Surrogate for cost-effective parameter estimation

The EnKF algorithm is a sequential two-step procedure made of a prediction step to compute the ensemble of fire front trajectories and an analysis step that provides a corrected ensemble at observation times. A reduced-cost EnKF strategy based on polynomial chaos (PC) expansion was designed. The key idea is to build a polynomial surface response mapping the uncertain input parameters of the ROS model (e.g., biomass moisture content, biomass fuel aspect ratio) onto the uncertain fire front location. We investigated the ability of a PC surrogate to mimic the wildfire spread model in the EnKF prediction step at reduced cost and without loss of accuracy. The resulting PC-EnKF algorithm was shown to significantly reduce the computational cost of the EnKF-based parameter estimation approach (by a factor of at least 10 in the reduced-scale controlled burning), and thereby to provide access to accurate error statistics on both model inputs and outputs for the formulation of the Kalman gain matrix. Future plans include the extension of the proposed PC-EnKF approach to regional-scale cases with spatially varying biomass fuel conditions and time-varying wind conditions to further validate and optimize this strategy in terms of computational cost.
We also used the PC surrogate to study in a systematic way, the sensitivity of the innovation term to changes in the input parameters of the ROS model [13]. This opens the possibility to change the parameters that are included in the control vector between the assimilation cycles, according to the level of information available (uncertainties in the surface wind and in the biomass fuel properties are not time-invariant); automatic sensitivity tests could be performed inline to focus the EnKF update on the most uncertain parameters over a given time period. Ongoing work relates to deploying this type of sensitivity analysis for parameter estimation based on the new front shape similarity measure (ongoing LEFE/INSU project in collaboration with Inria and LIMSI).

5.4.4 Cost-effective state estimation: Kalman filtering vs. Nudging

To address anisotropy in wildfire spread and especially track the fire front topology, we impemented and tested two different state estimation approaches. On the one hand, we designed a standard EnKF algorithm. The results on the reduced-scale controlled burning showed that even with a relatively small number of members in the ensemble, the EnKF was able to retrieve the actual shape of the fire front. This approach was also found relevant for observations made with significant errors and/or cases in which the observations are incomplete (e.g., when only a section of the fireline is informed), in order to reconstruct a complete, reliable initial condition for FIREFLY restart. On the other hand, we implemented a state estimation based on direct nudging correction combined with the front shape similarity measure [13]. This approach has the advantage to avoid the formulation of the Kalman matrix, whose size increases with the burning area. Results on the 2012 RxCADRE nearly full-scale controlled burning (see Fig. 5.1) and on the Rim fire hazard (see "MODEST" section) showed that the front shape similarity measure allowed to accurately track fire fronts and identify fire spread conditions. Ongoing work is required to test the front shape similarity measure within the framework of the EnKF algorithm for state estimation. The objective is to analyze the advantages and drawbacks of the EnKF and of nudging, in a standalone way or in combination with EnKF-based parameter estimation (ongoing LEFE/INSU project in collaboration with Inria and the University of Maryland).

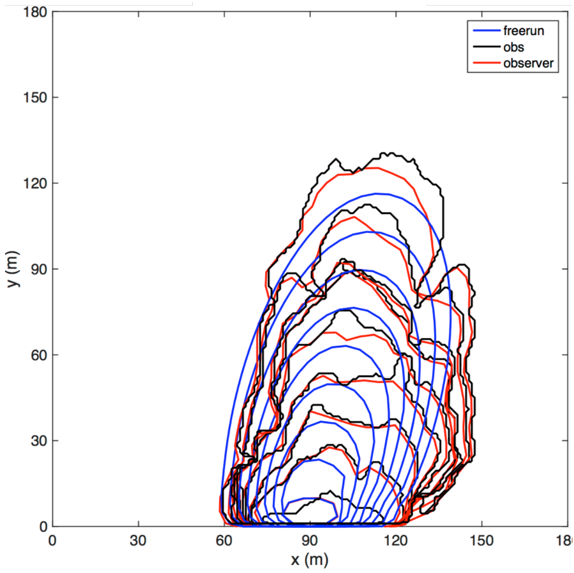

Figure 5.1: RxCADRE controlled burning experiment (3.2 hectares) – Assimilation of observations at 100-s time intervals (black curves) for nudging-based state estimation with front shape similarity measure. The time-evolving free run simulated with the standalone FARSITE (US Forest Service) Lagrangian model is in blue curves. The time-evolving nudging correction is in red curves.

Over the past few years, DA has demonstrated the potential of dramatically increasing wildfire simulation accuracy. New features have been tested in the frame of the NSF–WIFIRE project (Zhang's PhD co-supervised by CECI) and of the 2016 CEMRACS Summer Program (funded by LEFE/INSU and AMIES) through a new collaboration with Inria to develop DA methodologies adapted to front-tracking problems. While DA is at an early stage of development for wildfire applications, it is envisioned that they will eventually be similar to current weather forecast capabilities, providing real-time fire forecasts including a description of both wildfire dynamics and plume emissions. This is the target of the incoming ANR–FireCaster project.

5.5 Ensemble methods for atmospheric chemistry data assimilation

Model errors play a significant role in air quality forecasts. Accounting for them in the data assimilation (DA) procedures is decisive to obtain improved forecasts. We address this issue using a reduced-order coupled chemistry-meteorology model based on quasi-geostrophic dynamics and a detailed tropospheric chemistry mechanism, which we name QG-Chem. This model has been coupled to the software library for the data assimilation Object Oriented Prediction System (OOPS) and used to assess the potential of the 4DEnVar algorithm for air quality analyses and forecasts. The assets of 4DEnVar include the possibility to deal with multivariate aspects of atmospheric chemistry and to account for model errors of a generic type. A simple diagnostic procedure for detecting model errors is proposed, based on the 4DEnVar analysis and one additional model forecast. A large number of idealized data assimilation experiments are shown for several chemical species of relevance for air quality forecasts (O_3, NO_X, CO and CO_2) with very different atmospheric lifetimes and chemical couplings. Experiments are done both under a perfect model hypothesis and including model error through perturbation of surface chemical emissions. Some key elements of the 4DEnVar algorithm such as the ensemble size and localization are also discussed. A comparison with results of 3D-Var, widely used in operational centers, shows that, for some species, analysis and next-day forecast errors can be halved when model error is taken into account. This result was obtained using a small ensemble size, which remains affordable for most operational centers. We conclude that 4DEnVar has a promising potential for operational air quality models. We finally highlight areas that deserve further research for applying 4DEnVar to large-scale chemistry models, i.e., localization techniques, propagation of analysis covariance between DA cycles and treatment for chemical nonlinearities. QG-Chem can provide a useful tool in this regard.

This study is supported by a LEFE project coordinated by CERFACS (HERMES, 2016-2019) and was published in [CE106].

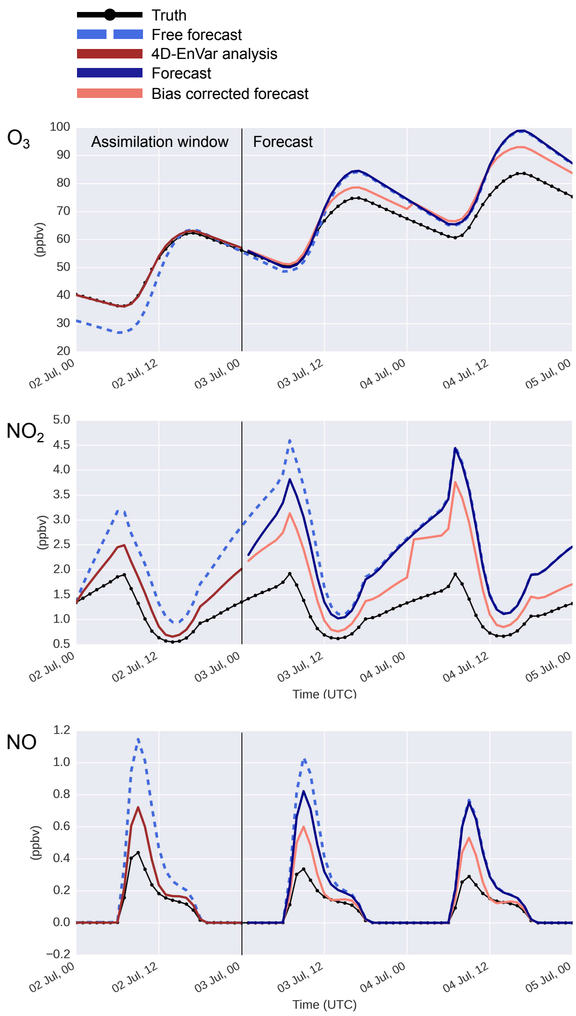

Figure 5.2: Impact of model bias correction on 48 h chemical forecasts. Temporal trajectory of free forecast (3 days), analysis (24 h), truth and 48 h long forecasts initialized from the latest available analysis, for a model grid point and three reactive species (O_3, NO_2, NO). Only ozone measurements are assimilated during the first 24 h.

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High Performance Computing and Data

6.1 Introduction

High Performance Computing (HPC) activities for climate and environement has been undertaken in several ways:

- Development of a high resolution climate model and runs on the PRACE supercomputers;
- Implementation of the IBM methods in a mesoscale model to represent complex terrains;
- Development of new numerical scheme for the simulation of atmospheric chemistry.

Data management and services is complementary to HPC, especially for the processing of climate simulations. This activity has benefited from strong implications in European projects.

6.2 High Performance Computing of Climate Models

Climate modelling based on High Performance Computing is a constant activity at Cerfacs. The developments, described in this paragraph, contribute to adapt the models of our community to top-end supercomputers and enhance their performances on these machines. At the same time, these models are used in their most advanced configurations to perform simulations required by our scientific studies. In particular, we ran, during the last two years, the following models on Météo-France and PRACE supercomputers:

- CERFACS-HR model, assembling ARPEGE-Climat V5 at T359 horizontal resolution and 31 vertical levels with NEMO-LIM V3.4 at a $\sim$0.25 degree resolution and 75 vertical levels; CERFACS-HR was used for decadal predictions (HiResClim PRACE project, [CE40]), and studies of SST fast growing biases in Tropical Atlantic (PREFACE project, [CE31]),
- its ocean component (NEMO) for probabilistic ocean modelling (OCCIPUT PRACE project,[1])

The scientific results obtained with with these models has been detailled in Section 2.

The present evolution of supercomputing technology drives us to increase the parallelism of our applications in all possible ways and to reduce as much as possible their disk access. Particular care was taken to increase task parallelism: the traditional sequence of computations, inherited from legacy codes, can, under some conditions, be split in independent tasks and their processing be mapped to different computing cores. We found that our OASIS3-MCT coupler was particularly well suited for an efficient implementation of this task parallelism. In NEMO model, ocean and sea-ice computations were separated into 2 different executables and run concurrently coupled through OASIS3-MCT. The resulting algorithmic changes were validated and the implementation included in the NEMO reference code ([CE160]).
Also, computing performances with parallel applications cannot be achieved without a strict balance of the computing load onto available resources. Strategy to reduce the imbalance of OASIS based coupled applications was studied in [34], among which those plotted in Figure 6.1.

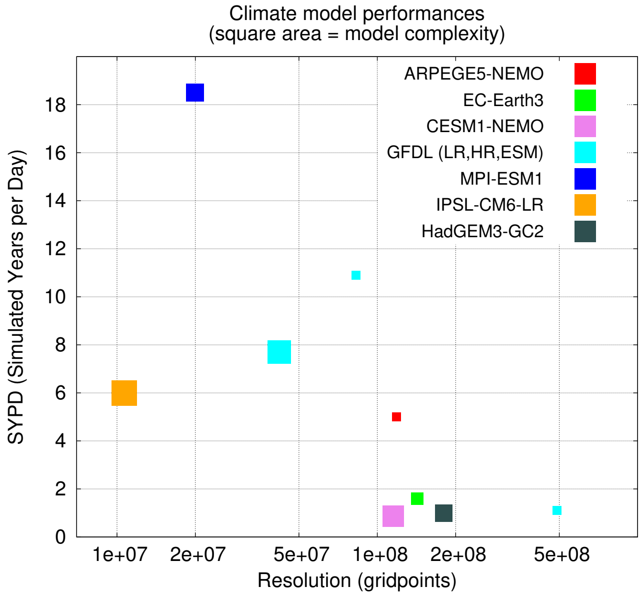


Figure 6.1: Performance, resolution and complexity for ESMs in production mode.

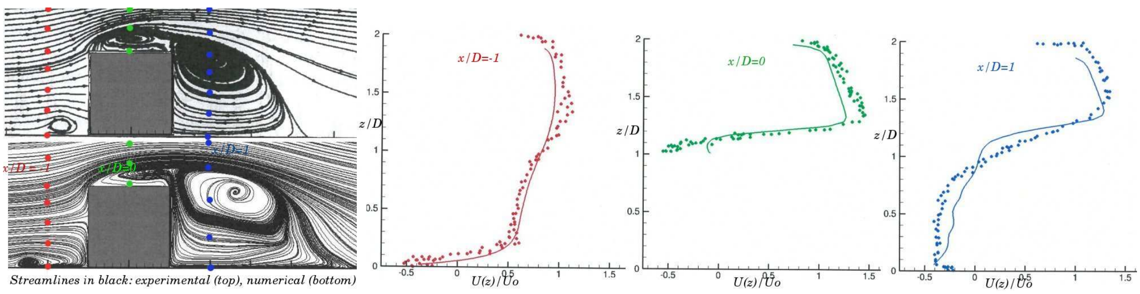
To improve the performance of coupled models, operations like diagnostic outputs can also be performed on separated computing resources (IO servers). The IPSL XIOS server was adapted to the size of our multi-decadal ensemble runs (running on 7,000 cores in one job) and high output frequency (some hourly diagnostics, see [1]). To prepare XIOS configuration at such high resolution without involving the full complexity models, simple XIOS clients with HR-realistic output were developed ([CE165]).
Finally, some modifications were included in Météo France atmospheric model ARPEGE-Climat V6 to improve its stand-alone performance. The crucial question of reducing disk access was addressed by removing the constraint of the monthly restart frequency; ARPEGE-Climat V6 can now be run for an entire year without restarting. Finally, a better vectorization of this model, a key aspect on emerging many-core processors, was ensured by reducing the number of non automatically vectorized routines ([CE164]).
The correct evaluation of the impact of these improvements requires an accurate picture of the characteristics of our model performances. In the framework of the IS-ENES EU project, Cerfacs actively participated in a community effort to define a comprehensive list of these key numbers ([29], Figure 6.1).

6.2.1 An IBM method for the Meso-NH model

The processes occurring in the lowest few kilometers of the Earth's atmosphere are dominated by the interaction with the surface and its characteristics. Complex terrains such mountains or cities strongly affects the dynamic of the surrounding fluid merely with the surface shape. As a second step exchanges (moisture, temperature, aerosol) between surface and atmosphere boundary layer (ABL) could be impacted by the topography: to illustrate this, we can cite the restricted air movement due to the mountains presence which participates on the often observed pollution episode and temperature anomaly in the Grenoble Valley. Therefore the impact of anthropogenic activities (and the estimate of this impact) are closely tied to the topography.
Currently, the european and international directives claim that ecology takes a significant place in politic decisions and anthropogenic behaviors (climate conference COP21-2015). To achieve a way to brave the global climate change the first step is to follow and understand the key processes of the pollutant transport

in the ABL. In that context, meteorological research plays a major role and the numerical modeling is one way to approach that chemical and physical problems encountered in meteorology. For these reasons and for the covered scientific themes, the AE team of the CERFACS has to intervene and participate. Supported by the Midi-Pyrénées region and by the CERFACS, attached to the UMR5318-CECI, Franck Auguste was recruited as CNRS researcher (two years contract) in November 2014.

The improvements in the computational fluid dynamics allow the Numerical Weather Predictions (NWP) to approach multi-scale problems such as the impact of perturbations due to urban canopies (set of buildings with spatiotemporal scales of about the meter and the second) on the mesocale behaviors of the ABL (with spatiotemporal scales of about the kilometer and the hour). The employed meteorological model is Meso-NH (MNH): non-hydrostatic, 3D and unsteady, incompressible, massively parallel, developed by the French community (jointly by the Laboratoire d'Aerologie UMR5560 and the CNRM-GAME UMR3589). This model has the ability to simulate the high number of physical and chemical processes operating in the ABL. Our objective was/is to develop and implement a numerical method which allows to model the topography impact in MNH. The topography is considered as a part of the resolved scales and therefore we decide to implement an immersed boundary method (IBM). The success of such method is based on the well recover of the fluid-solid interface embedded in the structured numerical domain. The first works were dedicated to the characterization of that interface in respect of its geometric characteristics by the use of a LevelSet function (LS) and an associated smooth technique. Then we worked on the IBM forcing of the explicit numerical schemes (advection, diffusion,..) appearing in the MNH conservation laws (momentum, energy, conservative scalar) by the use of a ghost-cell technique (GCT). Our GCT choice is original by the definition of several image points (and not the classic mirror point) which permits a better recover of the fluid information near the interface. We focus after our attention on the implicit resolution of the pressure problem (incompressible version of MNH, associated step projection). We propose an alteration of the Poisson equation second member coupled to an iterative procedure (Richardson or Gradient Conjugate type) to satisfy the non-permeability hypothesis at the fluid-solid interface. The numerical method had been presented to the scientific community during the Eighth Meso-NH user's meeting in 2015. It was also the subject of workshop/meeting with E. Pardyjak (Professor at the University of Utah) and L. Lacaze and M. Mercier (IMFT researchers).



(a) (b) (c) (d)

Figure 6.2: Experimental (Martinuzzi and Tropea, JFE 1993) and numerical (IBM-MNH) results: Streamlines in the vertical symmetry plane of the cube and definitions of three longitudinal locations, (a); Vertical profile of the mean horizontal velocity depending on the three longitudinal locations (b,c,d).

After tests and validations of our numerical method on different academic cases (potential and inviscid flows around simple obstacles) we investigate the cases of flows in presence of stratification and turbulence (characters of the atmospheric flow). This investigation has required an adequacy between the IBM (resolved scales) with the turbulence scheme (unresolved scales) and the externalized surface scheme often coupled with MNH (SURFEX). That investigation led to propositions of wall models based on a roughness

scale. The validation of the complete IBM (dynamic part of the flow) was done by the comparison of our results with previous results (experimental and LES approaches) on a popular case: a turbulent flow around a surface surmounted by a cube (see Figure 6.2). Currently the studied case the dispersion of NO2 pollutant over Toulouse and after the explosion of the AZF factory in Toulouse the 21 September 2001 (see Figure 6.3).
The MNH-IBM is also used in the CERFACS-MODEST challenge (The 'Mock Urban Setting Test' experiment, see the dedicated section). In a near future (2017) we will dedicate a significant part of our work to the adequacy of the IBM with the radiative effects: that next evolution will open the access to a others applications: airport pollution in a convective atmospheric situation (DGAC-CORAC project), urban heat island effect (Eurequa-Capitoul project).

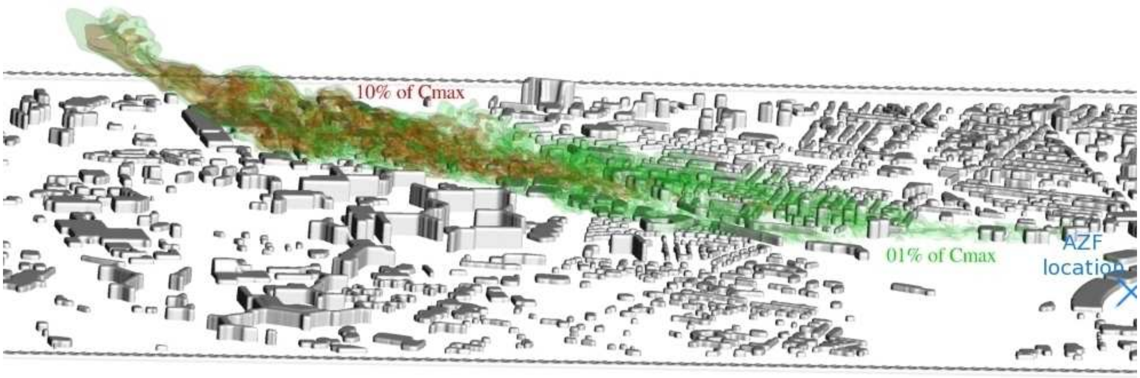


Figure 6.3: The AZF plume ten minutes after the explosion and over Toulouse districts: two NO2 concentration levels.

6.2.2 The ASIS solver

During the past years CERFACS has developed and tested the Adaptative Semi-Implicit Scheme (ASIS) solver for the simulation of atmospheric chemistry. To solve the Ordinary Differential Equation systems associated with the time evolution of the species concentrations, ASIS adopts a one step linearized implicit scheme with specific treatments of the Jacobian of the chemical fluxes.
The ASIS solver has been designed to cope with the various situations encountered within the numerical simulation of the atmospheric chemistry. The main properties of the solver are mass conservation, an approximation of the Jacobian matrix of the chemical fluxes that stabilizes the associated system of differential equations, a time stepping varying module to control accuracy, and a code implementation that allows an easy adaptation to various chemical schemes. In box model test cases, the numerical solutions obtained with the ASIS solver were found in good agreement with those of multi-step algorithms like Rosenbrock's and Gear's methods.
The ASIS solver has been implemented in two 3D models of the Earth (MOCAGE) and Mars (LMD model) planets. The results with MOCAGE using ASIS reveals two weaknesses of the original semi-implicit solver. One is related to the calculation of the partionning of the NOx species at the surface and the other to an overestimation of the ozone depletion in the Antarctic stratospheric vortex in Spring (see figure below). In the simulation of the Mars atmosphere ASIS gives more accurate simulations during day-night transitions and at night for the HOx species. These results stress the importance of having accurate enough numerical solutions, otherwise differences between model simulations and observations could be wrongly attributed to missing chemistry or misrepresentation of some physical processes.

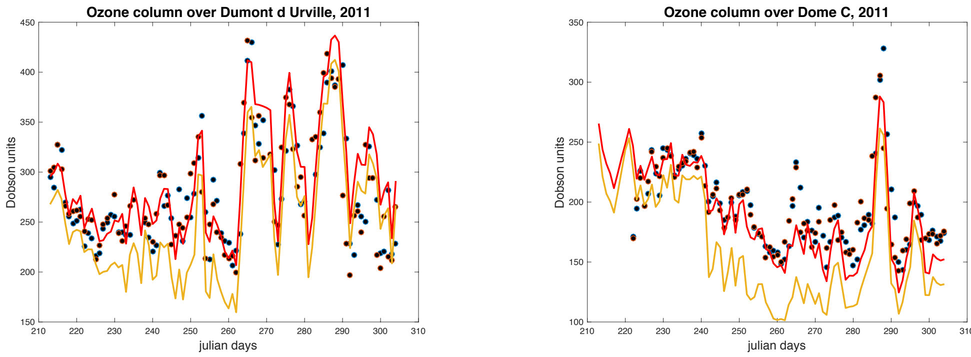


Figure 6.4: Evolution of the total ozone column over the Dumont d'Urville and Dome C antarctic stations. The dots are the observations of the SAOZ instrument, the orange line is the evolution calculated in the reference simulation, and the red line the same output from the simulation using the ASIS solver.

The model simulations show the benefit of using a chemical solver with good properties such as mass conservation and controlled accuracy. This objective can be achieved using multi-step high order algorithms but the computational cost of those schemes increases rapidly with the number of species considered. Since ASIS is implicit and one step, a single linear system has to be solved for each iteration. For this, direct or iterative algorithms can be used. The direct methods based on LU decomposition see their computational cost increasing at least quadratically with the number of species, whereas the cost of iterative solvers increases rather linearly. Within ASIS we found that the GMRES iterative algorithm is stable and efficient, and is competitive in terms of CPU cost compared to the direct DGESV algorithm.
In atmospheric models the computational cost is a key issue and parallelisation of the computations must be efficient to reduce the elapse time spent for the simulations. As pointed out earlier the amount of computation spent by ASIS to solve the chemical system can vary significantly from one grid point to another. This renders the equilibrium of tasks more difficult if a domain decomposition strategy is adopted to implement the parallelisation. One possibility to diminish the number of iterations and the heterogeneity in the CPU used at each grid-point is to account for non chemical tendencies in the species continuity equations. Rather than updating the concentrations after each process the resulting tendencies could be added and integrated within ASIS.
The present version of the ASIS solver adresses the evolution of the concentrations in gas phase only. For some applications the aqueous phase associated with the presence of clouds must be also considered. The chemistry module has to solve both gaseous and aqueous phases chemistry as well as mass transfer reactions between gas and liquid phases.
In conclusion, the ASIS solver can deal with many situations encountered in modeling atmospheric chemistry for a computational cost affordable by CTMs and GCMs that include comprehensive chemical schemes. A complet description of the ASIS solver has been submitted to publication in the GMD revue [30].

6.3 Data management and services

Research and development activities related to data aspects have emerged within the past few years at Cerfacs because of rapidly increasing needs of data management and processing in Climate Modeling field. This rapid increase is explained by the recent model developments that make model more complex, and

by HPC facilities and storage capacities that enable to perform large ensemble of simulations, at higher resolution. An other important factor is the evolution of the intercomparison project framework (WCRP Coupled Model Intercomparison Project) that is getting larger, from one Phase to a next one, both by the number of numerical experiments to perform and the number of outputs required (the so-called “Data Request”, herafter refereed as DRQ).
The strategy on data, is structured on 4 tightly inter-connected themes: data production, data description, data infrastructure, data access and data analytics.
Climate modeling activity does not restrict to model numerical integration (physics and dynamics computation) but also requires to handle the ensemble of data produced, both “dynamically” on the course of each run, and “statically” once the run ended. Data processing and management, from model output to distribution to the community of end-users, form the so-called “data workflow” that emerges in the last years as a crucial piece of the of the overall modelling (”production”) workflow.
Data management happens at different stages of the production (in the following, ”data” implicitly refers to ”output data”) :

- data preparation: configuration of the model outputs prior to simulation run;
- data writing: I/O strategies and tools;
- data monitoring: runtime visualization and control of the results of ongoing simulations;
- data post-processing: deriving diagnosis, reformatting and gluing metadata to the data files so as to conform to the community standards (CMOR - Climate Output Rewritter), relying on CF-conventions) and remapping to comply with the DRQ grid requirements;
- data storage : storage of model runtime data on local archives (raw outputs, restarts);
- data preservation : archiving data in their definitive shape (CMOR) on long-term storage solutions (data centers, ESFG – Earth System Grid Federation - data nodes);
- data distribution : quality control and publication through the ESG federated network.

For the near coming climate modeling projects, climate modeling groups have to face the scale factor challenge, data volumes undergoing a strong increase: from [2-5 PB in the community/ 20 TB for Cerfacs contribution] for the CMIP5 database to [100 PB in the community/ 600 TB for Cerfacs contribution] for the next CMIP Phase (CMIP6). Consequently, conceptual view and technical implementation of data workflow have to be revised (see Figure 6.5). Previous data post-processing and management tools are not sufficiently efficient and robust to be reused for the next generation of climate modeling systems: requiring too many data movement, a lot of manual intervention in the processing chain, sequential treatments.
These last two years can be seen has a transition period during which we had both to maintain and make evolve previous generations of data workflow for ongoing projects (EU-FP7/SPECS, ANR/MORDICUS, PhDs in the Globc team) and prepare the next generation for future ones (WCRP/CMIP6, H2020/PRIMAVERA).
The old generation of data workflows are the one used to process CNRM-CM5 and CERFACS-HR model output. These two distinct workflows, we maintained and ported on Cerfacs HPC infrastructure (neptune BullX and nemo Lenovo) and support has been provided to Cerfacs users. For CERFACS-HR, new tools were developed to ensure CMORisation of data with the CMOR2 library.
In 2016, efforts were dedicated to rethink, together with our Météo-France/CNRM partner, the overall data workflow. Main idea is to reduce at most the chaining of operations and manual intervention and disk access within the data workflow. An important part of this reshaping try to avoid the use of CMOR library to produce CMIP6-compliant data since it requires heavy I/O traffic and is a long time consuming process. To reach this objective, XIOS was implemented by the CNRM in each component of the coupled CNRM-CM6

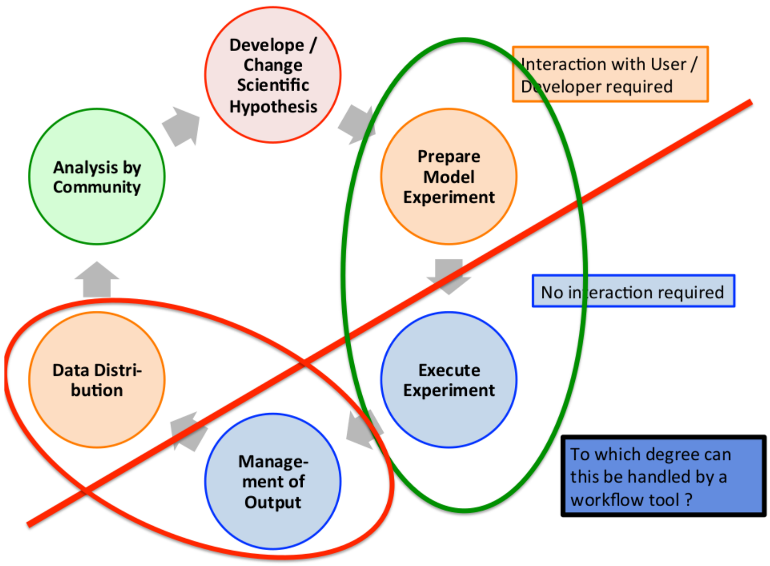


Figure 6.5: Rethinking the data workflow and its articulation with the overall climate modeling workflow, from K. Fieg (DKRZ), R. Budich (MPI) talk at the Joint IS-ENES2 Workshop on Workflows and Metadata Generation, Lisbon 27-29 September 2016.

model (ARPEGE, SURFEX, TRIP - NEMO being since a long time XIOS-enabled). Given the size and complexity of the CMIP6 Data Request, 6-fold increase in both the number of experiments and diagnosis, a particular effort was focused on this latter to gain expertise with the DRQ python API developed at STFC/BADC. Cerfacs also contributed to the development of a python tool ([33]) to automatically configure the XIOS server in each component of the coupled model so as to directly output data that comply with the DRQ and with CMIP6 file naming and metadata conventions (work still under progress).
For preservation of data produced by the Cerfacs these last years, we have been working with external data center: CINES for MORDICUS (12 TB) and CMIP5 database rescuing (20 TB), Jasmin/BADC for SPECS (15 TB) and future PRIMAVERA database. We also prepared the local and ESG storage and distribution solutions for hosting future CMIP6 data that will be produced by th Cerfacs (coordinated work with the Météo-France CNRM/CTI and Cerfacs/CSG teams). For CMIP6, as it was the case for CMIP5, Cerfacs will benefit from the ESG datanode infrastructure hosted and administrated at Météo-France/CTI.
To support efficient data access and analytics, developments have been done on the underlying infrastructure to cope better with larger data volumes. Several important "building blocks" have been developed in 2015 and 2016:

1. The main international infrastructure for the dissemination of climate data is the Earth System Grid Federation (ESGF). It is a federation of peer-to-peer data nodes that distribute climate datasets (a data node is running at Météo-France). A Compute Working Team (CWT) has been initiated by US partners to design, specify, and prototype the future ESGF computing nodes that will enable users to perform on-demand data reduction when accessing data on the ESGF data nodes. Cerfacs is an active member of this CWT, with support from the European projects FP7-IS-ENES2 and H2020-EUDAT2020. In 2015 the API has been designed, and the first prototypes of the implementation have been tested in late 2016.

2. Most science domains have strong needs in data analytics and, because of large data volumes, it is getting mandatory to get away from the "download-analyze" traditional workflows. To this extent,

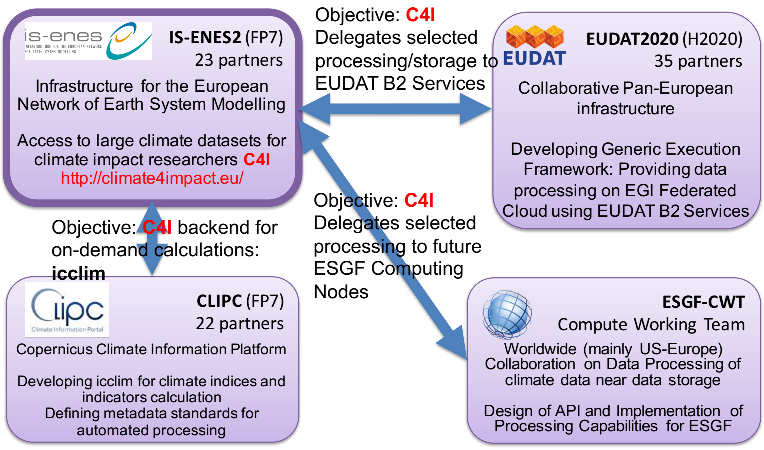


Figure 6.6: Integration of several building blocks at the European scale.

Cerfacs has contributed to the design of a generic API (GEF) to perform data processing within the EUDAT e-infrastructure, which is currently getting connected to the ESGF (work done by DKRZ). The EUDAT GEF implementation is currently being extended to access European Grid Infrastructure (EGI) Federated Cloud resources, in order to perform on-demand data processing. This work is lead by Cerfacs, and it is embedded in the EGI-EUDAT Interoperability Working Group involving several scientific communities and representatives of data centers (EUDAT) and EGI. The outcomes of this work will be used in the design of the future European Open Science Cloud (EOSC), a large initiative driven and funded by the European Commission (EC).

3. Numerous backends can be used to implement data processing and data analytic functions, and expose them to the user through APIs and portals. Cerfacs has lead, within the FP7-IS-ENES2 and FP7-CLIPC projects and especially in collaboration with SMHI, the development of a climate indices and indicators calculation software package written in python, with some specific parts optimized in C. The open-source software is called icclim and is available on github. The python language has been chosen because it can be efficiently integrated in Web Processing Services (WPS) used in the interfaces.

4. Automating data analytics, distribution, and processing, requires standards in data organization and description. There are several existing standards thanks to the international CMIP experiments, but still, no standard were available to organize and describe properly climate indices and indicators. Pushed forward by the needs of the FP7-CLIPC project, two joint international workshops were organized by Cerfacs within the CLIPC and IS-ENES2 projects in 2016. The objectives were to define a Data Reference Syntax (DRS), variables names, and metadata descriptions of the files and variables, for climate indices and indicators. Those were based on extending the already existing standards, and also to ensure that most of the representative international community was involved, such as Australia, Canada, US, several European countries, etc. The outcomes of this work is already being used outside the scope of the partners involved in the initiative, and it is important to note that the FP7-CLIPC project outcomes are aimed at feeding into the C3S Copernicus operational suite of services.

All those components are essential to the building of end users' services, through tailored web portals, platforms, frameworks, and re-usable standard OGC services such as WPS. In 2015-2016, Cerfacs has participated actively to build those end users' services:

- The climate4impact.eu (C4I) platform and services has been extensively developed with major IS-ENES2 partners: KNMI, SMHI, UC, WUR. Cerfacs is leading this initiative since 2009. This platform is integrating the icclim software as a backend. In the near future it will integrate the ESGF CWT API as well as the EUDAT e-infrastructure services such as EGI-GEF.
- The climate4impact standard services (OGC WPS and WMS) have been used to built the CLIPC portal, tailored at the impact and adaptation communities. It is an example of the successful implementation of the climate4impact platform services to built a tailored portal, thanks to the development and use of international standards.

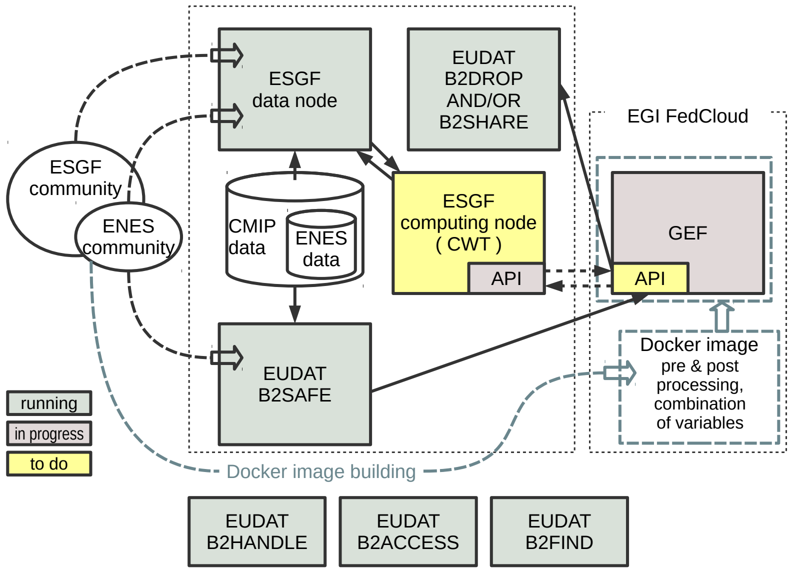


Figure 6.7: EUDAT architecture to support on-demand end users' climate data analytics.

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3

Computational Fluid Dynamics

Introduction

Computational Fluid Dynamics (CFD) is a strong activity at CERFACS. It is obviously the main research topic within the CFD team but many other teams use CFD too: GlobC for example develops flow solvers even if they address totally different types of flows. CFD is also the field which has the most direct contacts with industry, especially in the field of aeronautics. More than 60 researchers work in the CFD team now. For 2015 - 2016, the CFD report is split in three main parts (Fig. 1.1):

- Numerical methods
- Physical models
- Applications

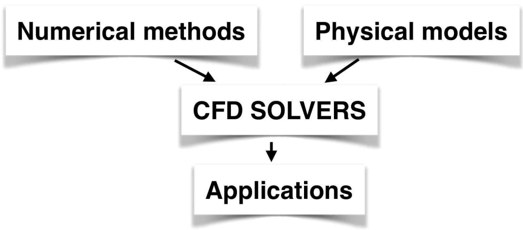


Figure 1.1: The CFD team organization: three activities around CFD codes.

These three parts describe the necessary ingredients to construct efficient CFD solvers which are then used by laboratories and by CERFACS shareholders. Note the importance of modeling and applications: the development of efficient solvers requires specialists of numerical methods to address real applications and therefore to deal with models which represent the physics to simulate.
This presentation reflects also the evolution of the team: part of the CFD research addresses questions which are purely numerical and focus on the development of novel algorithms for flow simulation. This activity directly connects and actually is often challenged by the second one (applications) where these algorithms are brought into real life by writing codes which are used to solve real problems for real applications. This requires the development of physical submodels (turbulence, combustion, near wall phenomena, plasmas, pollutant formation) which are needed for these real applications in addition to the algorithms and the code itself. This explains the three roots of the CFD team: numerical methods, physical models and applications.
The application field addressed by the CFD team keeps growing: in addition to the classical domains of expertise of the team (aircraft aerodynamics, combustion), the CFD team is now developing new fields of application in turbomachinery (compressors and turbines), kinetics (pollutant formation such as CO, NO and soot, petrochemistry), aeroacoustics (of aircraft and helicopter), plasma physics (for combustion control or for satellite electric propulsion). For all these activities, multiphysics (and therefore code coupling) and quantification of uncertainties have become major research topics too.
The following sections provide a summary of the most remarkable results obtained by the CFD team since 2014. A few salient points are pointed out here:

Academic excellence
The CFD team continues to publish in the best journals and to produce around 10 PhDs per year. Table 1.1 provides the number of papers published per year in A journals as well as the number of PhDs 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
2015	27	11
2016	20	9

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

published per year and permanent researcher is 2. The team has also won an ERC grant (see below) and its leader has given the Hottel plenary lecture at the 36th Symp. (Int.) on Comb. (Seoul 2016) which is the most famous lecture in the field. Many PhDs work in the team, confirming the importance of formation: more than 35 PhD students were present in the team in 2016. Many of these PhDs have received prizes (M. Bauerheim, A. Misdariis: L. Escande prize, M. Bauerheim: Aerospace Valley prize) and all have found positions in industry or academia rapidly.

The ERC advanced grant INTECOCIS on combustion instabilities
IMF Toulouse and CERFACS have won an ERC (European Research Council) advanced grant in the field of thermoacoustics (intecocis.inp-toulouse.fr). This 2.5 Meuros grant will run until 2018 and is allowing the development of a joint thermo-acoustics team in Toulouse where IMFT and CERFACS teams collaborate to study combustion instabilities in multiple systems from small laboratory burners to full rocket engines. This group is probably the largest thermoacoustics team worldwide today (11 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 CFD for plasma flows
Satellite electric propulsion has recently gained attention in the context of the competitive commercial market of satellite launching and control. SAFRAN proposes a series of Hall effect thrusters, and has identified numerical simulation as a key tool to design and optimize such systems. In collaboration with the Laboratoire de Physique des Plasmas (Ecole Polytechnique), CERFACS has engaged in the development of a code to simulate plasma flows in the presence of an electric field in the complex geometry of real engines. Such tools do not exist today and represent an important challenge, due to both the complex physics and the computing requirements.

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 turbomachinery 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 thousands processors). The strategy elaborated by CERFACS has been to explore a first solution based on the solvers used for the LES of reacting flow (AVBP and YALES2, order of accuracy 3 to 4) while developing a new class of higher-order codes (order of accuracy larger than 4) in a spectral difference tool called JAGUAR in collaboration with Cenaero.

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 or 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 them all in a single solver because industry applications will clearly go into this direction.

The introduction of new topics
Two new fields of research have been open in the last years with the support of Total. The simulation of explosions in buildings has been quite successful, leading to an INCITE project in 2013 and 2014 and renewed projects in the field of safety. Petrochemistry also provided exciting new topics where CERFACS studied the reacting flow inside a ribbed duct in collaboration with VKI, Stanford and ISAE Toulouse. Plasma flows have also become an important new field with two main applications: understanding the initial phase of spark ignition and modeling plasma satellite engines.

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 (4 to 6) while still being able to handle unstructured meshes is growing fast and the development of the JAGUAR solver at CERFACS (spectral differences) as well as the collaboration with CENAERO on DG (Discontinuous Galerkin) techniques are becoming important 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 training on LES, combustion, mesh generation, numerical methods, acoustics, etc.

Numerics

Certain CFD solvers of the Cerfacs CFD team like AVBP have been used for academic and applied purposes with great success over the last ten years: this multi-species, hybrid meshes, LES, high-order code has been the workhorse and the reference code of the team for a long time but new approaches are being tested now to prepare the code which will replace AVBP on the long term. This section presents CERFACS work on these future numerical methods. Numerical approaches are discussed first before presenting methods to control errors (Uncertainty Quantification). Then, research on High Performance Computing for our solvers is described. The efficient use of high-fidelity CFD to simulate multi-physics flows implies to work on all parts of the CFD workflow. For this reason, CERFACS has developed tools to deal with Interfaces (to set up a computation), Coupling tools (to couple several solvers) and Post-Processing.

2.1 High-order CFD solver for unsteady flows on unstructured grids (J.-F. Boussuge, G. Puigt, G. Marait, A. Balan, V. Joncquières, J. Vanharen, M. Lemesle, W. Stachura, R. Dray, W. Hamri, B. Cuenot)

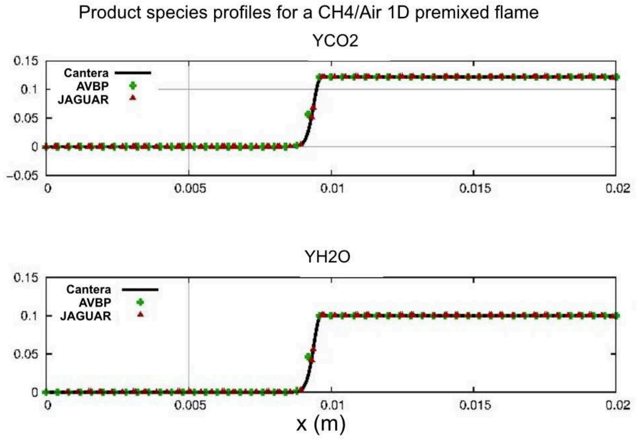
A promising context for the next generation of CFD solvers is to perform Large Eddy Simulation (LES) on complex geometries with unstructured grids and very high-order schemes. Classical high-order approaches for unstructured grids need a large stencil (more than 100 cells for a 5th order WENO approach), leading to many data exchanges in a parallel framework and poor HPC performance. A more appropriate solution consists in switching the considered paradigm.

Several possibilities exist to do this [35], and CERFACS has started employing the Spectral Difference (SD) approach in a solver called JAGUAR. Navier-Stokes equations are solved in their strong form, as in Finite Difference method and this point justifies the name of the approach. The principle of the SD method is to define a polynomial representation of the conservative quantities inside each cell and to take into account the discontinuity at cell boundaries by mean of a Riemann solver. The approach is locally continuous (inside the cell) and globally discontinuous (from cell to cell). It uses a limited stencil making it effective in a parallel HPC framework.

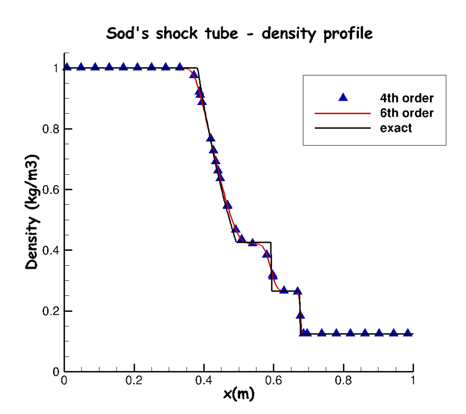
During 2013-2014, CERFACS initiated the development of the JAGUAR solver during the Safran CN2020 programme. Comparisons of results from JAGUAR and other software were performed, and the solution accuracy and low-sensitivity to mesh elements of poor quality were highlighted. During the last two years, several key points were addressed. First, High Performance Computing capabilities were developed including MPI, OpenMP and hybrid OpenMP-MPI techniques [CFD160]. A new theoretical spectral analysis of the numerical schemes was proposed based on an eigenvalue problem. Aliasing was shown to occur for wavenumber above π, but it may only be visible depending on the polynomial degree p, the time integration procedure and the wavelength. Finally, the required number of points per wavelength was compared with standard finite difference schemes. The sixth-order spectral difference method was found as accurate as the sixth-order compact scheme of Lele [32].

Since 2015, CERFACS is involved in the European project TILDA which aims at showing the exascale capability of high-order spectral discontinuous methods for LES and DNS. CERFACS must extend the

capability of JAGUAR with $h-$ (space) and $p-$ (accuracy) refinements following Mortar elements [28], while keeping parallel efficiency. The final application will concern jet aeroacoustics.
In 2015, V. Joncquières investigated the use of the spectral difference method for combustion. Results for standard 1D flames showed that the accuracy of the method is in agreement with the requirements of the combustion team [CFD176]. Multi-species equations were also introduced in JAGUAR as shown in Fig. 2.1-a, and results were compared to reference solutions from Cantera and AVBP.



(a) 1D laminar premixed flame, comparison of Cantera (detailed chemistry solver), AVBP and JAGUAR solutions for the species profiles



(b) Sod shock tube - effect of the shock capturing technique on the density.

Figure 2.1: Spectral differences (JAGUAR) results for combustion (a) and shock (b) test problems

Handling thermochemistry in a SD solver needs to address specific key points to ensure monotonicity of species mass fractions. The research area regarding the coupling of combustion and spectral discontinuous schemes is new, and only addressed by a few scientific leading groups: University of Stanford [26], CORIA and CERFACS.
Finally, several shock capturing techniques were investigated in JAGUAR [24, CFD193] (Fig. 2.1-b), specifically focusing on the approach of Persson and Peraire [30].

2.2 Lattice-Boltzmann Methods (C. Coreixas, G. Wissocq, J.-F. Boussuge, G. Puigt, L. Muscat)

Over the past few years, Lattice Boltzmann Methods (LBM) have become an attractive alternative to standard Navier-Stokes solvers for the simulation of isothermal and weakly-compressible flows around very complex geometries. Indeed, for these configurations, the interest in LBM is threefold:

- The volumetric mesh generation, based on the coupling of the octree refinement method (embedded cartesian grids) and Lattice-Boltzmann boundary conditions, is almost automatic and allows to drastically reduce the time allocated to this process.

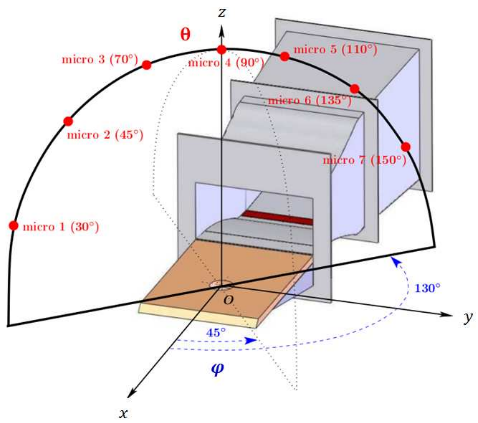
- The wall-clock time of LBM is almost one order of magnitude shorter than standard CFD methods at least for low Mach number flows.

- The numerical dissipation of LBM is very low. Thus, the generation and the propagation of small disturbances of the flow can be simulated over long distances without loss of information.

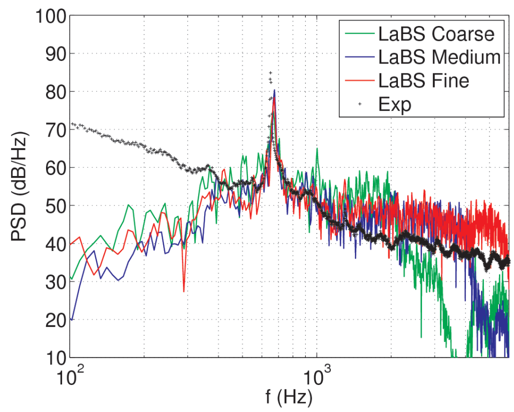
CERFACS is involved in the French project around the LBM-based solver named "LaBS" (Lattice Boltzmann Solver) since 2014. This code has been developed within a consortium of industrial companies (Renault, Airbus, CS), academic laboratories (UPMC, ENS Lyon) and strong partnerships with other entities (Onera, Gantha, Paris Sud University, Alstom, Matelys) from 2010 to 2014. First CERFACS activity was to estimate the capability of this solver for aeroacoustic simulations of isothermal and weakly-compressible flows. Since 2015, CERFACS is also involved in the development of high-order LBM dedicated to the simulation of high-Mach number flows including discontinuities such as shocks.

Validation of LBM for Computational AeroAcoustics (CAA)

The capability of the LaBS solver for CAA was investigated *via* two very different simulations: (i) direct computation of the sound generated by a grazing flow around a round cavity and (ii) prediction of the sound emitted by the flow over a generic two-wheel nose landing gear through the coupling of LaBS and a Ffowcs-Williams-Hawkings solver (KIM). LaBS gives the pressure fluctuations to the solver KIM of ONERA and KIM estimates the pressure fluctuations in the far-field. Figures. 2.2 and 2.3 show a satisfying agreement between experiments and numerical simulations [CFD18, CFD82].



(a) Experimental array of microphones

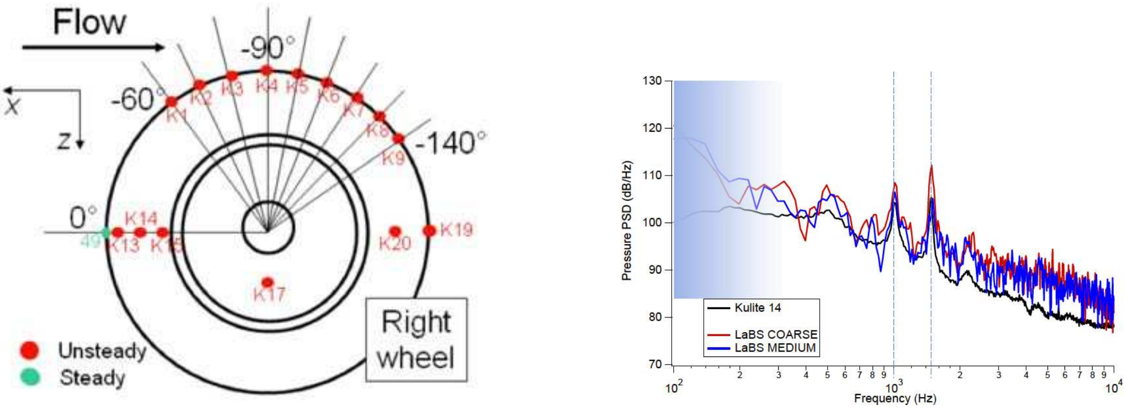


(b) Data at microphone 4

Figure 2.2: AEROCAV configuration [CFD18]. LaBS results vs experiments

Extension of LBM for the simulation of highly-compressible flows

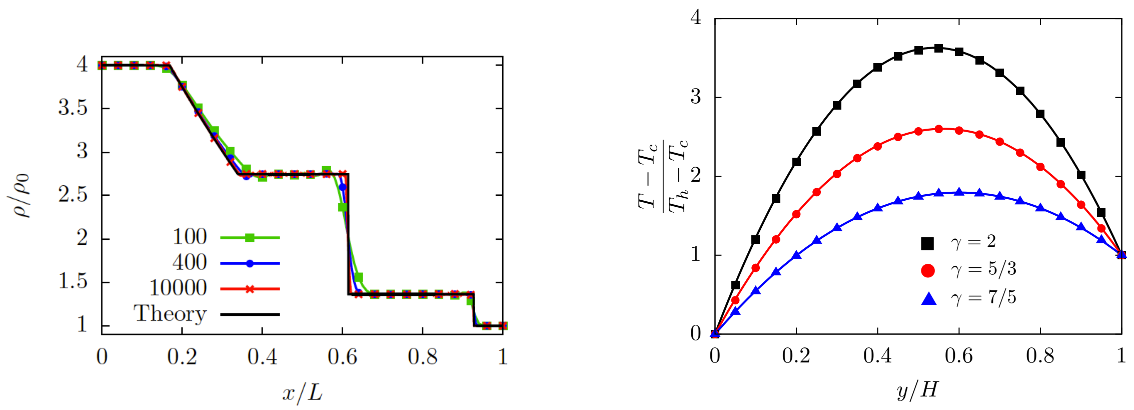
A first step towards high-Mach number simulations has been made by CERFACS by coupling a high-order LBM with a shock-sensor. This new model allows to properly recover the evolution of the three characteristic waves encountered in Sod shock tube testcases: the rarefaction wave, the contact discontinuity and the shock discontinuity (see Fig. 2.4(a)). To improve the CPU time consumption and the scalability of this new high-order LBM, a coupling between two standard LBM is ongoing. This approach is still restricted to weakly-compressible flows, but first improvements allowed to extend it to variable specific heat ratio γ (see Fig. 2.4(b)).



(a) Location of the Kulites sensors

(b) Data comparison at K15

Figure 2.3: LAGOON configuration computed with LaBS [CFD82]



(a) Sod shock tube

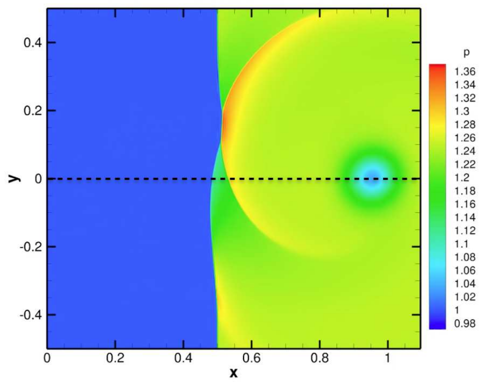
(b) Thermal Couette flow

Figure 2.4: Validation of high-order LBM (symbols) on two standard compressible testcases including analytical solutions (solid lines)

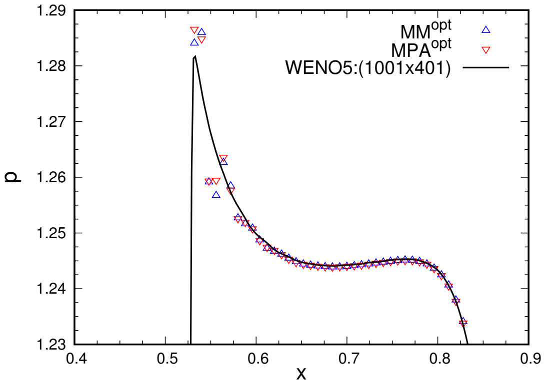
2.3 High-order CFD solver for unsteady flows on structured grids (C. Perez Arroyo, S. Bidadi, G. Puigt, G. Daviller, J.-F. Boussuge)

Numerical ingredients were developed in the elsA solver of ONERA to perform aeroacoustics simulations on structured grids using a compact finite volume solver [15] and dedicated boundary conditions. Such a scheme, even if it is stabilized with the filter of Visbal and Gaitonde [33] to remove grid-to-grid oscillations in smooth regions, is unable to deal with shocks. As a consequence, accurate solutions can be computed for subsonic flows but not for dual-stream under-expanded jets. Such dual stream jets are responsible for the noise transmitted to the cabin in cruise condition and on the passenger confort during the flight.
Within the Marie-Curie European project Aerotranet-2, CERFACS proposed and analysed a new adaptive nonlinear filtering technique to capture sharp discontinuities in the flow [6]. Knowing that the compact scheme and the filter are numerically efficient and optimized, a nonlinear filter was proposed leading to a minimum impact on the basic numerical schemes. First, the sensors of Bogey and Ducros [7, 11] were employed to control the dissipation of the nonlinear filter. Within the shock/dissipation region, the second-

order minmod and fifth-order Monotonicity Preserving Approach (MPA) reconstruction algorithms were used to provide the required dissipation. The dispersion and dissipative properties of the scheme were analysed with the approximate dispersion relation. The dispersion-dissipation condition of Hu *et al.* [21] was used to optimize the spectral properties of the nonlinear filter. This approach was applied to standard test cases: Sod'shock tube, Shu-Osher tube, shock / vortex interaction (Fig. 2.5) and shock / shear layer interactions. The proposed method is now under evaluation for performing aeroacoustics simulations of supersonic jets.



(a) Pressure representation of a shock/vortex interaction, computation with the Bogey filter on a mesh of 251x101 nodes



(b) Comparison of pressure profiles for Minmod and MPA filters with reference WENO5 scheme at Y=0.0

Figure 2.5: Interaction between a steady shock and a moving vortex, computed with elsA.

2.4 Uncertainty Quantification and Sensitivity Analysis (J.C. Jouhaud, P. Roy, M. Montagnac, J.-F. Boussuge)

JPOD Tool

Uncertainty Quantification (UQ) has recently become a major topic in Computational Fluids Dynamics (CFD): identifying and characterizing critical thresholds for operating systems (e.g. gas turbine) is a key issue for industrial risk assessment. Despite significative advances in turbulence modeling, the diversity of uncertainties on boundary or initial conditions, just like on the parameters of the models (empirical coefficients), forces CFD users to get out of the deterministic context in order to quantify uncertainties. Moreover, the computing power available now makes a large number of parallel simulations possible, which permits the implementation of algorithms able to compute the sensitivity of uncertainties and their propagations.

Today, non-intrusive approaches in UQ are preferred for (large) industrial solvers because the solver is kept unchanged, and UQ is managed out of the CFD solver. Furthermore, to limit the calculation time, a solution consists in replacing the direct simulations over the sampling by a surrogate model. Since 2008, the CFD Team develops the JPOD (Jack-POD) tool. This tool, based on a kriging technique coupled with POD (Proper Orthogonal Decomposition), provides response surfaces to perform the propagation of uncertainty sources. The strategy consists in a hybridization between response surfaces and design of experiments [8]. The Python language was chosen in order to favor the coupling between codes and to benefit from the developments realized by the scientific community (e.g. Scikit-learn library).

The latest developments concern the implementation of propagation methods to treat the sources of uncertainties. In fact, JPOD was recently coupled with OpenTURNS (Open source Treatment of Uncertainty, Risk oN Statistics) software [3], the UQ software developed by EDF, to benefit from features such as the analysis of the sensitivity (computation of Sobol indices) and the estimation of PDF (Probability Density Functions).

Application to heat transfer over the LS89 turbine blade

In the CASCADE project (FUI funding), the JPOD tool was applied to the LS89 turbine blade to analyze its response to inflow conditions. Such a case is known to be highly sensitive to inflow conditions: shock location and intensity are especially difficult to assess as they result from a complex interaction between the boundary layer (either laminar or turbulent) and the blade wake. These flow patterns depend on both the flow operating point and the inflow specifications such as the turbulent intensity, Tu, entering the domain or the flow angle, α, relative to the blade orientation.
The objective of this study was to assess the sensitivity of the heat transfer coefficient, noted H, to two uncertain inflow parameters: Tu and α. A surrogate model was built on the parameter space $[-5°, +5°] \times [0\%, 30\%]$ and the corresponding PDF of H was obtained considering uniform probability distributions (Fig. 2.6). Turbulence intensity was shown to be the major parameter [CFD190].

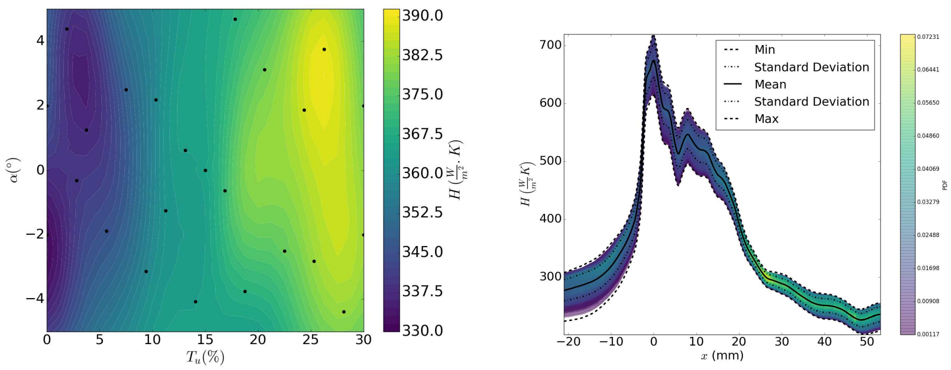


Figure 2.6: LS89 turbine blade: surrogate model obtained with 25 snapshots (left) and Probability Density Function (PDF) of the heat transfert coefficient (right)
.

2.5 High Performance Computing (G. Staffelbach, C. Fournier, G. Marait, A. Cassagne, J-F. Boussuge, G. Puigt)

A specificity of Cerfacs is to maintain a very intense HPC work force on each solver to keep up with computer evolution. This is viewed as a critical issue for the long term development of our solvers.

AVBP solver

Current work on AVBP is focused on improving parallel and computational efficiency with the support of the Intel Parallel Computing Center program (IPCC). CERFACS has been a member of IPCC for the two last years.

Using advanced methods and code profiling tools, the efficiency of the code has been improved on all Intel-based architectures (without negative effects on competitor architectures). Figure 2.7 highlights the time per iteration observed between AVBP 6.2.1 and the latest release 7.0.2 for an industrial gas turbine test case[1] from Safran Helicoper Engines. This data was extracted from the CCRT architectures using the Sandybridge AIRAIN system up to the newest Broadwell COBALT system. The data reflects the

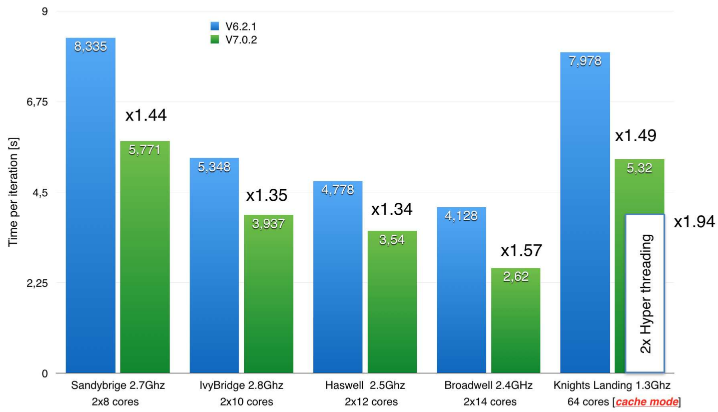


Figure 2.7: AVBP Time per Iteration per Architecture for a Safran Helicopter Engine test case

important optimisation work to increase computational efficiency by tapping the vectorisation potential of these chips. The efficiency of the code (for this test case) was increased by at least 30%. Besides providing tools and support to improve the computational efficiency of the code, IPCC provided access and advanced knowledge on future architectures. For example, the recently unveiled knights landing platform (KNL) was also benchmarked in Fig. 2.7 thanks to IPCC support.
While the increase in efficiency is clear, it is also found that it does not affect the parallel efficiency of the code as shown in Fig. 2.8. A 75% strong scaling efficiency is maintained from 200 to 40000 cores on a

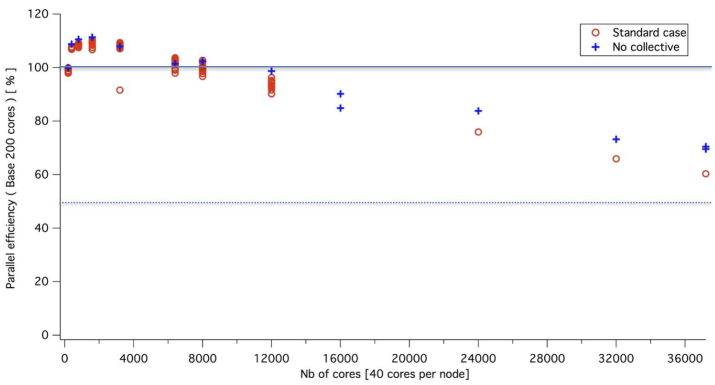


Figure 2.8: AVBP Strong scaling efficiency on the E5-2698 v4 @ 2.20GHz PROLIX machine. LES of an explosion in a confined space. 150M tetrahedra

[1] Acceleration factor will vary from simulation to simulation and should be seen as a global trend and not fixed general figures.

dual socket broadwell system with 20 cores per socket (Météo France PROLIX system) allowing a time to solution reduced by 150. This figure also highlights the impact of collective operations on scalability and singles out the need to reduce global MPI communications by introducing hybrid OpenMP/MPI parallelism in the code.
Work on the hybridisation of AVBP for MPI+OPENMP parallelism continues and an alpha release of the solver is available with over 50% of the computing code parallelised using both MPI and OpenMP. This work is on-going to increase the parallelisation ratio of OpenMP in AVBP.

JAGUAR solver

During the last two years, the performance of the JAGUAR solver has been extensively analysed and optimized on many-core supercomputers. Two aspects were highlighted.
First, concerning the performance of JAGUAR with the flat MPI paradigm, a perfect speedup was reached up to 131 072 cpu cores on a BlueGene platform. Second, CERFACS worked in close collaboration with CINES (Montpellier) on the performance of the solver using a hybrid OpenMP/MPI approach in a PRACE (Partnership for Advanced Computing in Europe) project [CFD160]. In the new version of the solver, the OpenMP threads are created only once, just before the time loop of the code. The subroutines dedicated to MPI communications are intrinsically sequential and "OpenMP master zones" were used for them. Except for these subroutines, the whole solver (inside the time loop) has been entirely parallelised. In order to reduce the cost of task creation, it is mandatory to allocate more than one mesh cell to a single task. The number of cells associated to one task depends on the size of the cell representation in memory: the size of the different types of cells is pre-computed to create cell packs smaller than the L3 cache size. This allows the code to perform cache blocking so that the number of tasks is drastically reduced (by limiting tasks management overhead). The performance of full MPI and hybrid MPI/OMP approaches is compared in Fig. 2.9.

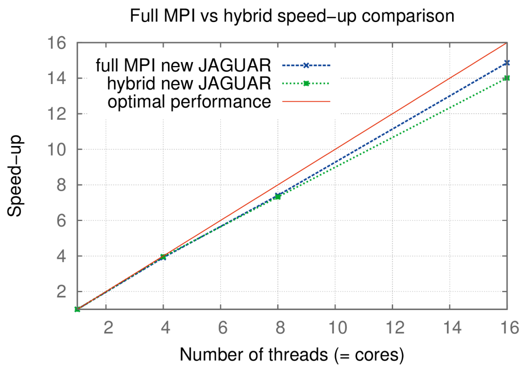


Figure 2.9: Spectral differences (JAGUAR): comparison of full MPI and hybrid MPI/OpenMP versions on Curie supercomputer (any node is composed of two sockets and each socket contains an Intel Sandy Bridge with 8 cores)

2.6 Graphical User Interfaces (A. Dauptain)

The diffusion of HPC tools outside specialized centers is not controlled by the quality of the code but by the quality fo the GUIs that experts can propose to non expert users. This statement has been inspiring CERFACS actions in this field for many years now, as shown below.

Aeronautical Engines

This activity is mainly built around C3Sm, which is a software suite installed at SAFRAN and in operation since 2012. C3Sm incorporates all the “know how“ linked to the LES tools of Cerfacs and CORIA.
The biggest achievement of 2016 is the decision of SHE to use systematically a breakthrough method in effusion cooling models for day-to-day combustion chamber CFD simulations. This change was critical: 90 percent of SHE CPU time goes to combustion chambers. In these devices, almost all the air flow is injected in the combustion chamber through effusion plates, involving 10 to 100 thousands of sub-millimeter holes. Until now, the numerical setups using effusion cooling were using homogeneous injection, where the holes are not meshed and the wall is modeled as a porous plate so that only 100 Degrees of Freedom (DoF) are needed to describe the effusion cooling. The new setup includes the hole shapes and uses millions of DoF to map each hole individually. Six months separate the model presentation at the PhD defense of D. Lahbib in Dec. 2015 and its effective use by Safran engineers. This evolution is a turning point for reduced model

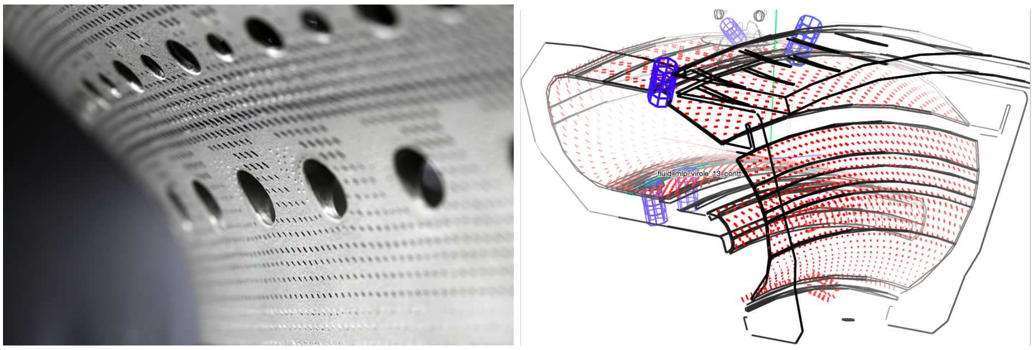


Figure 2.10: Left, close-up of multiperforated plate for aeronautical engine. Right, matching the perforation database (red) with a CFD domain (black) through an OpenTEA dialog

applications. For example, the wall temperature can be extracted from an adiabatic LES computation within one minute. All these tools are controlled through the GUIs of the C3Sm Suite.

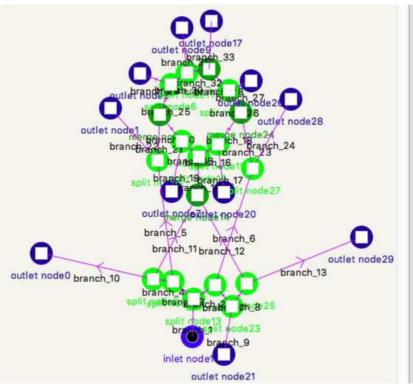
Blood Circulation

An interesting collaboration on C3Sm was led with Prof. F. Nicoud (UM2-Montpellier). Parts of human blood circulation can be described by a network of mono-dimensional arterial models. Canonical networks with typical measurements can be found in anatomy textbooks. For example, a model of the brain circulation can be obtained from a 33 branches description of the Willis polygon. A data assimilation (DA) step is added to move on to a tool for the physician. The monitoring of a patient is provided to transform the textbook version into a patient-specific model.
CERFACS developed a GUI focusing on the network creation since beyond 5 branches the connectivity cannot be managed with text files. A graphical dialog (Fig. 2.11(a)) was created to interactively create the network with a real-time computation of the connectivity.

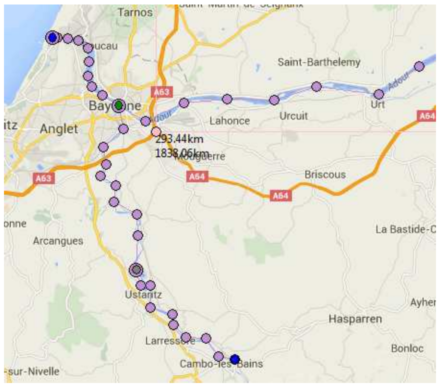
Flood Forecast

In our regions, climate change is expected to increase extreme rain events. The flood risk is therefore a major concern for future public safety. Flood forecast is done in France by the French hydrometeorological flood forecasting center SCHAPI, with the software MASCARET from the french electric power company EDF. As a 10 cm water elevation matters, the fluvial network model can be improved using data assimilation

(DA). CERFACS works on DAMP which is a data-driven river hydrodynamic simulator dedicated to real-time flood forecasting.
The first step of this data assimilation is to identify the elements of networks that should be improved: missing profiles, coarse description of Stricklers zones, etc. A specific GUI has been developed at CERFACS (Fig. 2.11(b)), in collaboration with CNES, to help the DA preparation. In particular, a GIS-like dialog allows to manually geo-reference the network. Thank to this dialog, a position defined in MASCARET as ”2300 to 2500m downstream branch 3” can be linked to ”the 3 channels of La Nive spreading near Ustaritz”. This work will be presented to Artelia, the company in charge of the future developments of MASCARET and its interface FUDAA-Mascaret.



(a) The 33 branches Willis polygon



(b) Geo-reference of a MASCARET network

Figure 2.11: OpenTEA dialogs

Activity Evolution: the MOSAIC project

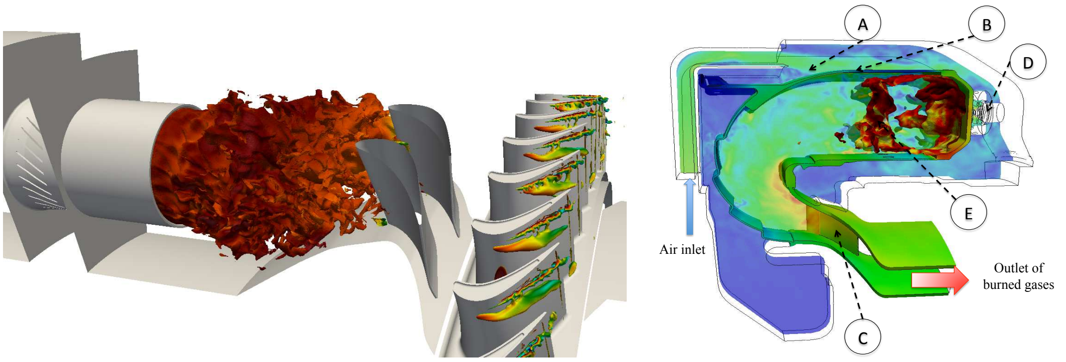
In 2016, Safran selected OpenTEA as one of the basic elements for its CFD platform MOSAIC. The C3Sm software suite will be integrated into MOSAIC and extended to other CFD tools by Safran Tech. This activity will move from the CFD team to the CSG team to share these competences with other teams and shareholders.

2.7 Coupling (D. Lahbib, S. Berger, L. Gicquel, F. Duchaine)

The design of gas turbines requires to consider strong interactions between different physics as well as the components of the engine. As a result, integrated simulations involving multiphysics and multicomponents are performed both at the research level as well as in industry. With the constant increase of computing power, numerical simulations of the interactions between the compressor, combustion chamber and turbine, as well as of the thermal interaction between fluid flows and solids offer new design paths to diminish development costs through important reductions of the number of experimental tests. In these fields, the main idea is to jointly simulate the different parts of the coupled problems with a high level of fidelity limiting hypotheses on the boundary conditions:

- for the interactions between turbomachinery parts and combustor, inlet and outlet models of the component interfaces can be avoided by resolving the full system at once (Fig. 2.12-a),
- to determine mean heat loads on structures, Conjugate Heat Transfer (CHT) allows to solve the fluid and solid equations simultaneously to predict temperature and heat flux distributions in the system (Fig. 2.12-b).

Recent works have shown the ability of Large Eddy Simulation (LES) to provide reliable results in the context of combustors and turbomachinery. Using an unsteady LES flow solver to resolve coupled problems raises several complexities such as : adequate resolution methods to avoid computing useless thermal transients, stability / convergence criteria of the coupled schemes, high performance computing issues when running the coupled applications with highly loaded codes on massively parallel machines where the solvers exchange a large amount of data at a high frequency.



(a) (b)

Figure 2.12: Example of an integrated combustor/turbine simulation (a), view of fluid and solid models of an industrial combustor Conjugate Heat Transfer simulation (b).

Among the ongoing numerical problems addressed within CERFACS, the following ones have received special attention during the period:

Conjugate heat transfer of steady laminar flows

In collaboration with ONERA, the performance of coupling coefficients of a Dirichlet-Robin transmission procedure was tested in the context of steady conjugate heat transfer. Particular emphasis was put on the optimal coefficients highlighted recently in a theoretical study based on normal mode stability analysis [13]. The stability and convergence properties predicted by the model problem were compared to those obtained in the CHT computation, showing an excellent agreement. Moreover, for all the Fourier numbers considered in the numerical experiment, the numerical solution is stable and oscillation-free when the optimal coefficient of the model problem is used. This suggests that the one-dimensional normal mode analysis can provide relevant coefficients directly applicable to real CHT problems [CFD33, CFD109].
The role of initial thermal conditions on the converged solution of a CHT problem has been studied based on a square cylinder flame holder [CFD10, CFD9]. Due to the interaction between the flame and the flame holder wall, a bifurcation in the convergence process is observed as a function of the initial thermal state of the bluff body (Fig. 2.13). For initial conditions with low wall temperatures, the joint problem converges towards a lifted flame while a bowed flame is obtained for high initial temperatures. Interestingly, the thermal state at which the bifurcation occurs depends on the conductivity of the solid medium. Aside from the bifurcation between two different converged solutions, a good initial guess of the coupled converged solution allows significant saving of CPU time. This is of foremost importance since fully turbulent complex geometry applications are targeted and CPU demanding. Such strategies however should not come at the expense of physics, care should be taken in the choice of the initial guess in light of the potential flow bifurcations and interactions between physics, modeling and coupling algorithms. Here, the reproducibility of the present results is assessed through the realization of two specific CHT computations with a different approach derived from the chaining methodology proposed [CFD33]. These new computations exhibit the

exact same converged solutions of the coupled problems further highlighting the accuracy and robustness of the coupling strategy employed for this specific problem.

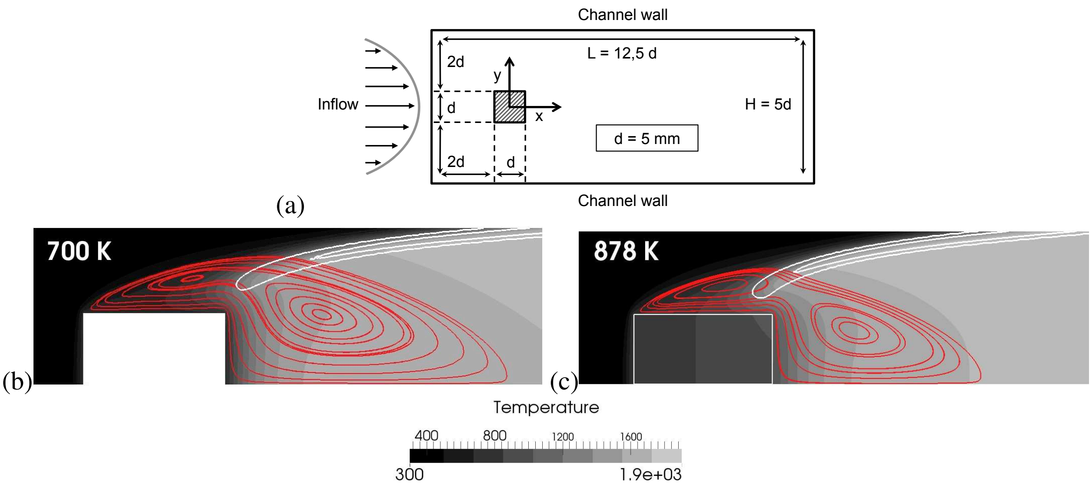


Figure 2.13: Typical flame-holder combustor problem: (a) configuration for a fully premixed mixture of methane/air at an equivalence ratio of 0.7 and a bluff-body Reynolds number of 500. Views of the flame front location (white iso-contour of heat release) and temperature field obtained with (b) a 700 K isothermal bluff-body wall condition and (b) the CHT-based coupled result for which the mean solid temperature reaches 878 K.

Multicomponent simulations for gas turbines

In the context of the overset grid method MISCOG developed at Cerfacs since 2011 to perform massively parallel LES of turbomachinery stages on unstructured grids, a high-order interpolation method has been introduced in AVBP [CFD30, CFD25]. This interpolation relies on 1-D Hermite interpolators and has been implemented for various types of 2-D and 3-D elements. It provides third order accuracy even in the most detrimental case: non-matching cells at the interface, coarsened cells in all directions and moving interface It is highly recommended to use this method whatever the numerical convective scheme, for the following demonstrated reasons: it preserves the global accuracy of the scheme; it limits amplitudes of spurious waves generated at the interface; it accurately transfers diffusive fluxes and SGS tensor and its cost is identical to the one of the original method. Current perspectives and potential subjects of interest still to be probed today are the effective impact of the SGS discontinuity on a LES prediction and the risk of spurious numerical waves generated at the moving interface.

2.8 CFD Data Processing (M. Montagnac, M. Daroukh, J.-F. Boussuge, G. Marait, G. Daviller)

Since 2012, Cerfacs develops a generic data-processing library called Antares. The project is managed with the web application Redmine (issue tracking, documentation, etc.), the source code management is Git, and the documentation and tutorials are disseminated thanks to a website (`www.cerfacs.fr/antares`).
The library can be used to process CFD data at large. It can be used all along the CFD process both to set up a CFD computation (initialization) and to post-process data generated during simulations. If the steering process of the CFD computation is written in python, this library can also be used to co-process data (in situ) during massively parallel simulations to reduce the amount of generated data. This library provides a

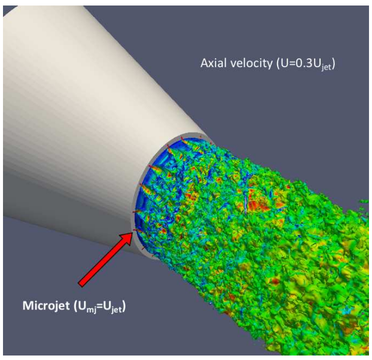
python application programming interface. The large choice of features available within the Python/NumPy framework enables to write complex data analysis procedures. Thus, CFD users can develop their own numerical tools on top of Antares data structures.
Finally it is free for research purposes so that users have a clear view of the library contents, and can modify them if necessary. This library is currently provided to many research labs and industries (`www.cerfacs.fr/antares/partners.html`).

Developments

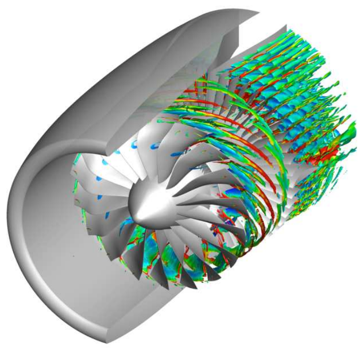
During the past two years, the library version went from 1.5 to 1.8. During this period, a large number of functionalities has been developed for Cerfacs specific needs in Antares such as allowing numerous readers and writers, providing capabilities to handle file formats or geometric algorithms.
The parallelism based on distributed memory paradigm was recently introduced in the framework of the PIA project ELCI.
In collaboration with Safran AE specific post-treatments have been introduced for turbomachinery application. Concerning aircraft application, in collaboration with Airbus Group, CERFACS developed an Antares module to analyze aerodynamic and thermal boundary layers from CFD computations.
In the context of the European Horizon 2020 project TILDA, a task has just started to extend Antares to high-order polynomial solutions (as given by DG or SD techniques). Indeed, Antares only deals up to now with one degree of freedom per vertex or control volume as done in standard CFD solvers.
Antares library has also been modified to include a Ffowcs-Williams-Hawkings analogy module in the context of the European project AeroTranet-II. More generally, discussions have started with Airbus and Safran to elaborate a post-processing tool based on the Antares library for production purposes.

Examples of Application

Among all applications treated with Antares, two of them are illustrated here. First in 2015, Antares was used to co-process a LES computation of a subsonic jet configuration with an axisymetric nozzle controlled by eight pairs of microjets, using a multi-block structured mesh containing around 2 billions of points, and run on 4096 cores in the context of a Grand Challenge CINES/Airbus during the test of the CINES/occigen supercomputer (Fig. 2.14-a). Second, Fig. 2.14-b shows an example of Antares use for turbomachinery applications to visualize fan/Outlet Guided Vane (OGV) interaction.



(a) Isosurface of axial velocity for jet noise simulation.



(b) Q-criterion isosurface colored by the vorticity modulus for a Nacelle/FAN/OGV simulation

Figure 2.14: Co-processing with Antares [CFD105, CFD24]

Modeling

The flow solvers developed at CERFACS would have a limited field of application if they would not integrate sophisticated physical sub-models for critical phenomena such as turbulence near walls, flame / turbulence interaction, plasmas or instabilities. These models are described in this Chapter.

3.1 Near Wall Turbulence Modeling

Wall flows remain a key fundamental CFD modeling issue irrespectively of the turbulent modeling context. Although near-wall flow modeling and understanding has benefited from many years of fundamental developments while considering it either fully turbulent, laminar or transitioning, with or without weak / favorable / unfavorable main stream pressure gradients... such issues still remain at the heart of simulations especially if LES or multi-physics applications are targeted. Indeed, the wall flow boundary layer state is crucial in determining both friction and heat transfer between solid walls and the flow. It also determines the performance of wing profiles and turbomachinery blades, flame stabilization processes. As such, many CFD complex application predictions rely on the model introduced to treat the near wall flow.

CERFACS is studying near-wall flows in two different frameworks:

- Near-wall flow dynamics
- Heat transfer and multi-physics.

3.1.1 Near-wall flow dynamics (M. Catchirayer, L. Troth, J. Delaborderie, O. Vermorel, F. Duchaine, J.F. Boussuge, L. Gicquel)

Pure aerodynamics as well as heat transfer require fine predictions of the flow boundary layer, which in LES and more broadly in CFD can be addressed in a wall-resolved or a wall-modeled manner: *i.e.* with a grid resolution that either respects the near wall scaling of the flow dynamics or provides the necessary quantities (wall shear stress and heat flux) at a low grid resolution level (and therefore at a lower computational cost).

- For wall-resolved LES around profiles, the near-wall grid resolution must represent the flow state around and prior to the blade so as to trigger the proper flow mechanisms controlling the spatial and temporal evolution of the near wall dynamics. Such requirements are not easy to master due to uncertainties in measurements or in numerics as well as implementations of boundary conditions in fully unsteady CFD solvers. For turbomachinery, the CN2020 SAFRAN project has been a driving component of code, numerics and modeling assessment around the prediction of the flow over the LS89 cascade from VKI. CERFACS codes as well as other codes have been benched for the LS89 test case where different grid size and operating conditions were computed, Fig. 3.1(a). In parallel, for fully turbulent operating conditions reported experimentally, dedicated turbulent inflow specifications and models have been built to capture the effect of free stream turbulence. This is obtained by running the blade simulation simultaneously with a *Precursor* simulation generating a physically reliable turbulent flow field which is used to feed the *Main* simulation by providing temporally and spatially evolving inflow conditions, Fig. 3.1(b). This exchange is performed thanks to code coupling through OpenPALM.

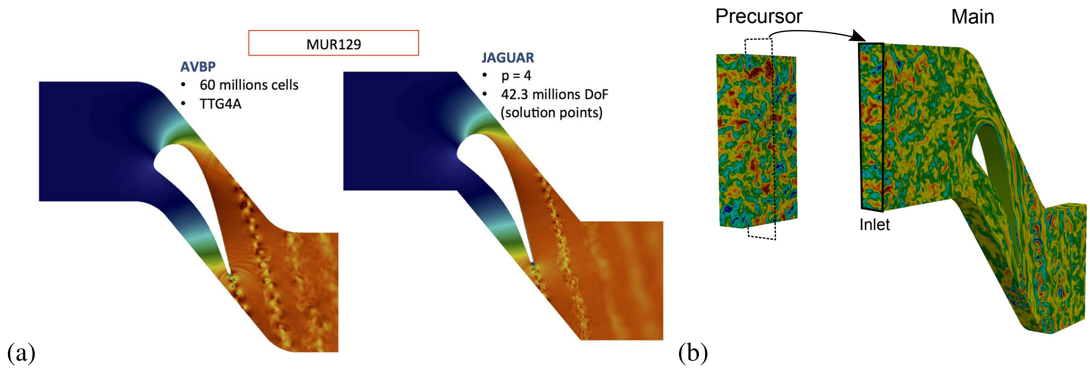


Figure 3.1: LES predictions of the LS89 cascade (experimentally studied by VKI [1]): (a) direct comparison of the flow field obtained for the MUR129 operating condition obtained with AVBP and JAGUAR to evaluate the impact of numerics and high-order schemes, (b) development of a coupling procedure dedicated to the generation and injection of a physical turbulent field applied to the MUR235 operating condition.

- For wall-modeled LES, the wall boundary layer is assumed to be in a generic state that is often far from the true industrial problem. Moreover, numerical implementations of the laws to be inverted analytically or numerically may yield different solutions depending on the procedure. Classical law-of-the-wall models are also extended to account for pressure and large temperature gradients encountered in combustion applications.

3.1.2 Heat transfer and multiphysics (S. Berger, T. Grosnickel, P. Aillaud, F. Duchaine, L. Gicquel, D. Maestro)

Heat transfer and multi-physics applications strongly rely on the capacity of CFD to deal with near-wall flows. However this requires accurate wall conditions, like wall temperatures for example. These temperatures can be obtained only through coupled LES / Heat-transfer-in-walls simulations. In this context, the development of LES-based CHT tools have been pursued as discussed below.

The primary interest of LES-based CHT solutions is to provide wall temperatures by using a fully unsteady approach to predict mixing of cold and hot fluids within the bulk flow as well as near the walls. For internal cooling systems encountered in turbomachinery applications for example, local flow Reynolds numbers are adequate for wall-resolved LES. Typical examples include impacting jets on flat and curved plates [CFD2], Fig. 3.2(a), or ribbed channels in static and rotating situations [17, 18, 16], Fig. 3.2(b). Combined with the efforts invested for LES of turbomachinery vane flows, convergence towards fully coupled CHT-based predictions of the internal / external / solid problem is arising and is part of the COUGAR CERFACS Challenge and of the CASCADE PIA project.
Developing dedicated aerothermal wall models is also the subject of on-going research in the context of combustors. The temperatures reached in today's combustors are far above any metal melting temperature, and film cooling is heavily used to shield combustor walls from the hot stream. The efficiency of so-called multiperforated liners must be carefully evaluated to design real systems and ensure durability of the combustor walls. This requires precise estimates of the solid temperature (typically with an error smaller than 25 K) and henceforth a multi-physics approach. On the other hand, hole sizes of multiperforated liners

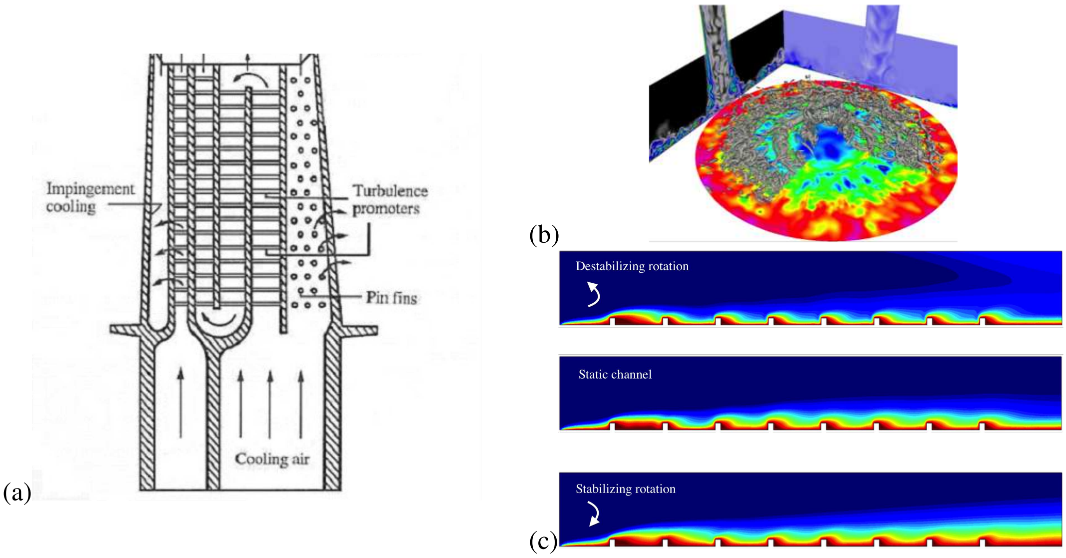


Figure 3.2: Typical view of the cooling system present in turbine blades (a) and associated LES-based CHT studied for isolated flow technological cooling components: (b) jet impacting on a hot flat plate and (c) ribbed channels in static or rotating operative conditions.

are usually too small, and the flow Reynolds numbers are too high, to allow the use of a wall-resolved approach and modeling of the local near-wall flow features is required. To address these issues, fully coupled solid / fluid simulations are used to complement existing experimental data [CFD52, CFD203, 23]. The developed wall models can then be applied in the LES-based, multi-physics combustor simulations, *i.e.* coupling reacting flow / conduction / radiation [CFD96, CFD10, CFD195, CFD12].

LES allows to go beyond the analysis of mean temperature fields, for example by quantifying the PDF of temperature of the exhaust gas of gas turbine chambers [CFD6, CFD49, CFD201, CFD125, CFD124, 22], or of impacting jets [CFD2]. A multi-physics environment is also mandatory for turbulent reacting flows as it greatly influences the temperature distribution of the hot gas at the combustor exit, prior to its ingestion by the turbine. More importantly, multi-physics impact flame stabilization mechanisms, where chemistry, flow dynamics and heat transfer tightly interplay to determine the flame position downstream of flame holders. Such key features have been observed to also influence the thermo-acoustic stability of burners [CFD199, CFD116].

3.2 Turbulent Combustion

Turbulent combustion is the source of energy production in most industrial systems. It combines turbulence and chemistry, two complex and highly non-linear phenomena, which strongly interact. The resulting turbulent flames are delicate to predict and are still the subject of numerous research works. For years, combustion chemistry and turbulence have been studied separately, leading to detailed chemical schemes on one side and accurate numerical models for turbulence on the other side. Today the available computing power, allows to begin including both accurate chemistry and accurate turbulence models in the same simulation. This significantly increases the prediction capacity of the numerical solvers, in particular in the case of strong flow inhomogeneities and transient conditions. In addition, it gives access to gaseous pollutants and soot precursors, whose emission and control have become a critical issue for industry.

CERFACS has been very active in the past years in the field of turbulent combustion modeling, and is continuing its effort to address more complex combustion phenomena. The research is mostly based on Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES) of turbulent reacting flows with the code AVBP jointly developed with IFPEN, or with YALES2 developed by CORIA . The main innovation in the past two years has been the development of an original methodology, in collaboration with Cornell University (Pr. P. Pepiot), to include realistic chemistry in LES of turbulent combustion. This potentially impacts all combustion phenomena and allows to address chemistry-driven mechanisms such as pollutant emissions.

3.2.1 Combustion chemistry and pollutant emissions (A. Felden, T. Jaravel, F. Collin-Bastiani, B. Cuenot, E. Riber)

Combustion proceeds through complex and highly non-linear chemical processes that involve up to hundreds of different chemical compounds. To describe such chemistry in 3D flow computations, it is common to use pre-tabulated 1D laminar flame solutions, using two chemical variables (progress variable and mixture fraction). This constrains the flame state to evolve along these simple flame structures and does not allow to fully account for flow-combustion interactions in complex turbulent flames. An alternative is to considerably simplify the chemistry and use reduced schemes. Globally fitted chemical mechanisms, based on 1 to 4 global reactions, are able to reproduce macroscopic flame characteristics such as burnt gas state or flame speed. They are however limited to a small range of operating conditions around the derivation states and do not give access to the chemical flame structure and its pollutant emission. On the contrary, as the result of a knowledge-based reduction approach, Analytically Reduced Chemistry (ARC) accurately describes combustion phenomena by retaining the most important species and reactions (Fig. 3.3). ARC is derived at CERFACS with the tool YARC of P. Pepiot (Cornell Univ., USA). Benefits of using ARC, combined to the Thickened Flame (DTFLES) turbulent combustion model, have been demonstrated when used in the LES of realistic swirl-stabilized aero-engine combustors [CFD36, CFD200]. The flame structure (velocity, temperature, combustion regimes, CO and OH species) obtained with ARC is closer to measurements in comparison with other methods, at a reasonable computational cost. The ARC approach was also successfully extended to multi-component real fuels [CFD37].

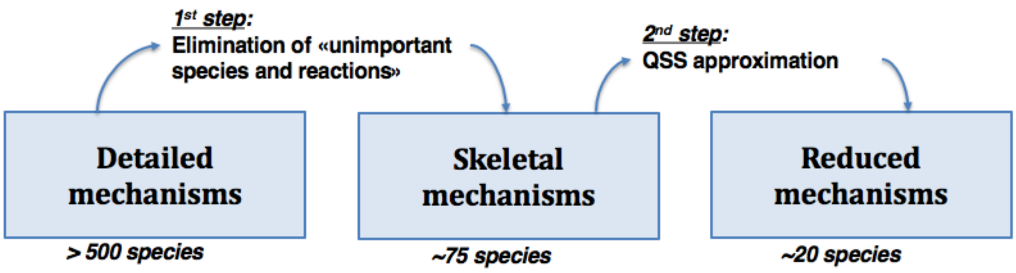


Figure 3.3: Principle of the ARC approach. The final reduced mechanisms can be directly integrated in LES codes.

Another direct application of ARC is the prediction of pollutant concentrations, both inside the combustor and at the engine exit. Stringent regulations of pollutant emissions now apply to new-generation combustion devices. To predict nitrogen oxides (NOx) and carbon monoxide (CO) emissions simultaneously, ARCs with accurate CO and NO prediction were derived, validated on canonical laminar flames and implemented in AVBP. The accuracy of this approach was demonstrated with a highly resolved simulation of the academic turbulent Sandia flame D, for which excellent prediction of NO and CO was obtained [CFD200].

The methodology was also applied to two swirled burners: the SGT-100 is a lean partially-premixed gas turbine model combustor studied experimentally at DLR, in which LES with ARC highlighted the chemical processes of pollutant formation and provided qualitative and quantitative understanding of the impact of operating conditions [CFD47]. The second target configuration was a liquid-fueled prototype of an ultra-low NOx, staged multipoint injection aeronautical combustor developed in the framework of the LEMCOTEC European project and studied experimentally at ONERA [CFD8]. Results again showed the excellent performances of ARC, for both the flame characteristics and the prediction of pollutants.
The very promising results of ARC were presented in an Invited Lecture at the *Second International Workshop on Combustion Chemistry Models of Real Liquid Fuels* by T. Poinsot, at Arlington (USA) in June 2016. They will be consolidated in the framework of the European project JETSCREEN (submitted in 2016) and the PhD of F. Collin-Bastiani.
Thanks to the accurate prediction of soot precursors, ARC is also a promising method for soot prediction in industrial systems because it provides correct levels for soot precursors. The gaseous ARC chemistry was coupled to a two-equation empirical model for soot prediction [25] and assessed against experiments in laminar sooting flames. It was then applied to an experimental burner studied at DLR [19] at 3 and 5 bars in the context of the International Sooting Flame (ISF) workshop (http://www.adelaide.edu.au/cet/isfworkshop/). The research work on soot prediction will be intensified with the European project SOPRANO, started September 1st, 2016 and coordinated by SAFRAN-Tech. The objective is to include the calculation of the size distribution of soot particles, in order to allow a better description of the heterogeneous chemistry at the particle surface.

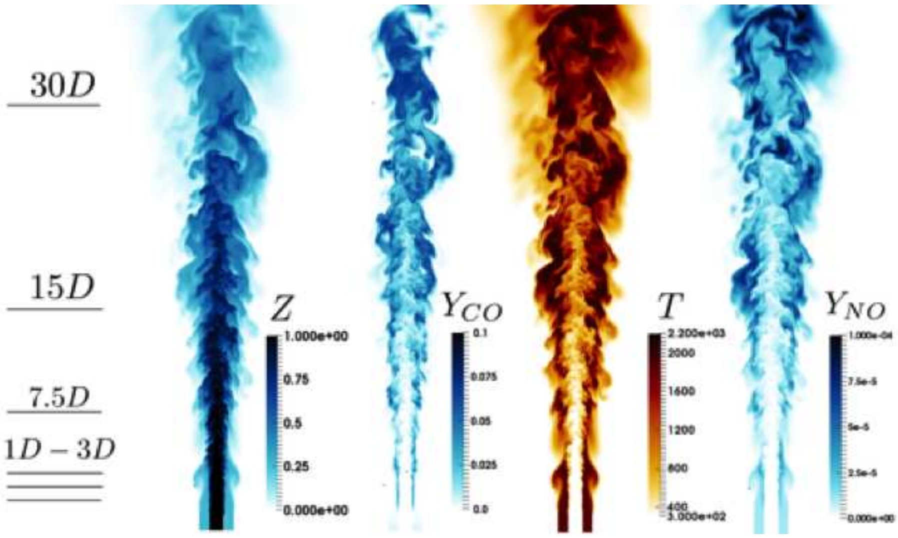


Figure 3.4: Instantaneous LES results of Sandia Flame D. From left to right : mixture fraction, CO mass fraction, temperature and NO mass fraction.

3.2.2 Ignition (L. Esclapez, F. Collin-Bastiani, B. Cuenot, E. Riber, O. Vermorel)

For safety reasons, in-flight relight of an aeronautical engine must be guaranteed over a wide range of operating conditions. However the current trends of engine design, complying with high efficiency, but low cost and low pollutant emission requirements, might be detrimental to ignition. The full ignition of an annular burner can be decomposed in three distinct phases, each being controlled by specific physical phenomena. First the spark discharge creates a plasma at very high temperature. This plasma rapidly cools down and triggers combustion chemistry, forming a flame kernel which then evolves to a turbulent flame. If favorable conditions are met, the turbulent flame propagates upstream to the injection plane where it stabilizes: this is the end of the second phase. Finally the flame of the first ignited burner propagates gradually to the next burners until full ignition of the combustor. It is now well recognized that LES correctly describes turbulent flames and the propagation phases of the ignition process [CFD141, CFD110]. However the first instants of ignition, ie., the kernel formation and development, are complex phenomena which remain difficult to predict and are the subject of current research at CERFACS.

The role of the spark discharge and its modeling were investigated in the ANR project FAMAC (automotive engines) and in the PhD of F. Collin-Bastiani (aeronautical engines). The effect of the discharge is threefold: first a shock wave induces a mechanical effect; the extremely high temperature (above 10000K) reached in the plasma induces a strong thermal effect; the plasma phase finally creates chemical radicals which may not be fully recombined at the start of combustion and induce chemical effects. To evaluate the relative importance of these three effects, numerical simulations of pin-to-pin discharge configuration are performed. This implies shock capturing techniques, high temperature thermodynamics, and accurate chemistry able to describe the chemical effect of plasma. An illustration is given in Fig. 3.5, where the shock wave is clearly visible 2 μs after ignition.

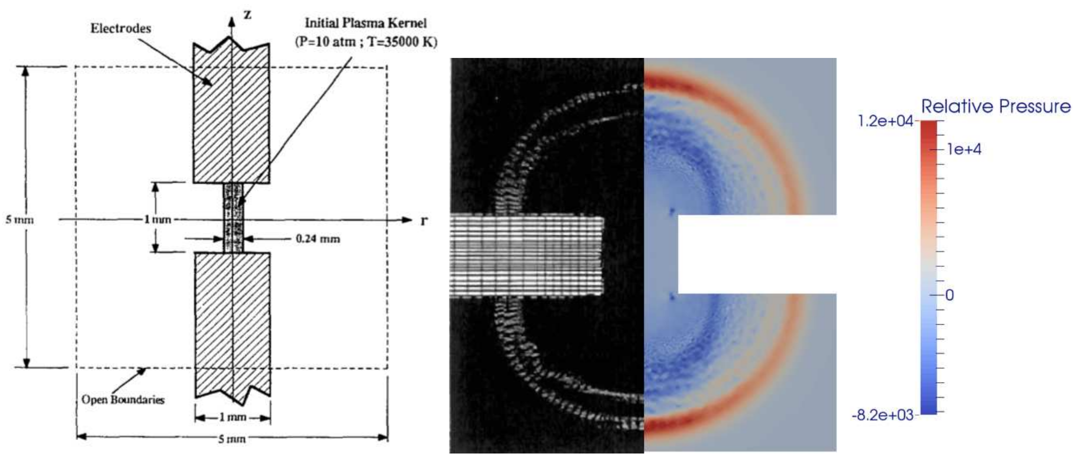


Figure 3.5: Pin-to-pin discharge configuration: geometry and comparison at 2 μs of experiment from [27] (left side) with the relative pressure field from the simulation (right side) [CFD181]

Another issue arising in the kernel phase of ignition is the uncertain evolution of the kernel subject to the turbulent flow. Depending on the local conditions met along its trajectory, the kernel may develop or reduce, and even be quenched. This process is responsible for the random nature of ignition in turbulent flows, usually quantified with a probability of success. In the work of L. Esclapez, this issue was investigated in two ways: first, ignition statistics in a single burner were reproduced by brute force LES, performing 20 ignition simulations at three different spark locations. The analysis of the simulation series allowed to identify the mechanisms controlling ignition success or failure, and to propose a methodology to predict ignition probability maps at a low computational cost using only non-reacting flow statistics [14]. Results of this low-order model proved to be very good in comparison with the experiment, as shown in Fig. 3.6.

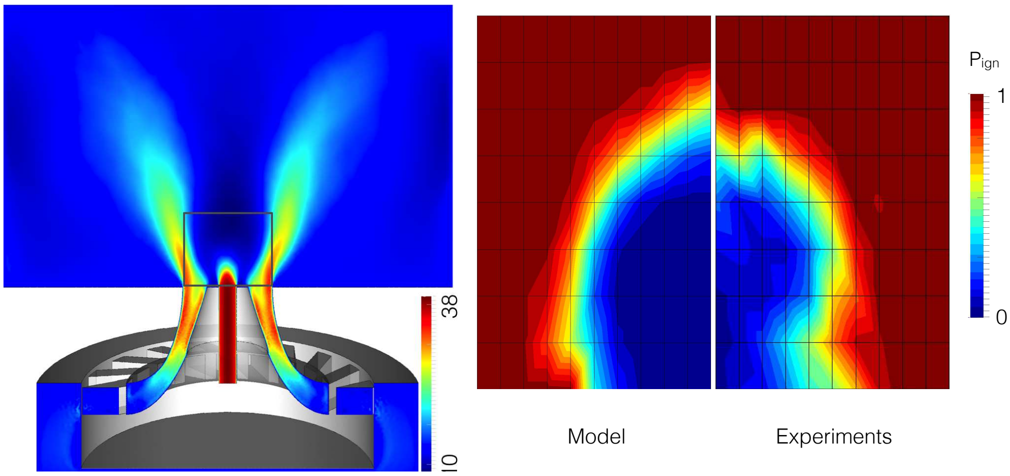


Figure 3.6: Ignition in a single premixed burner [CFD198]. Left : mean axial velocity fiels, the grey box corresponds to the zone where the ignition map was built. Right : comparison between the probability of ignition predicted by the low-order model (left side) and measured in the experiment (right side).

3.2.3 Spray combustion (D. Paulhiac, F. Shum-Kivan, B. Rochette, B. Cuenot, E. Riber)

Most industrial burners are fed with liquid fuel that is directly injected into the combustion chamber, generating a strong interaction between spray, turbulent flow and combustion. Although this interaction has been extensively studied in academic configurations, the modeling of spray combustion in the framework of LES for complex geometries, remains a difficult issue. CERFACS has developed two solvers for the liquid phase, based either on an Eulerian or a Lagrangian formulation. Both solvers are used to perform LES of two-phase combustion in realistic burners. In both models the two-phase flame is always considered in the so-called "evaporated" regime, where the droplet fully evaporates as a non-burning droplet and the flame only sees and burns the fuel vapor. This means that individual droplet combustion is ignored, although it can be the main combustion mode in some regions of the combustor. This modeling issue was addressed in the PhD of D. Paulhiac, who introduced various spray combustion regimes and proposed the Multi-State Algorithm for Reacting Droplets (MuStaRD) approach. The MuStaRD algorithm was validated on several academic configurations of growing complexity, then evaluated in a lab-scale burner (Fig. 3.7). Results showed the importance of individual droplet combustion as predicted by the MuStaRD model and its impact on the flame structure by comparison with the classical "evaporated" model. One practical result was the better prediction of unburnt hydrocarbons, which was significantly over-predicted without the MuStaRD model.

The capacity of droplets to evaporate also has an impact on the gaseous flame regime, which can be partially-premixed or even non-premixed. In order to better understand the spray flame structure, a joint experimental and numerical study has been performed on an n-heptane/air lab-scale jet spray burner (KIAI project [CFD84]). Both experiment and simulation showed a lifted flame exhibiting a double reaction zone, related to the spray distribution and burning in both partially premixed and non-premixed modes (Fig. 3.8left). The DTFLES turbulent combustion model can not be directly applied to diffusion flames and must be adapted. To this end, DNS of 3D methane/air diffusion flames in steady Homogeneous Isotropic Turbulence (HIT) are performed to evaluate the sub-grid scale wrinkling effect on the heat release (Fig. 3.8right). This work is performed in the framework of the PhD of F. Shum-Kivan, with the support of the ANR project NEXTFLAME.

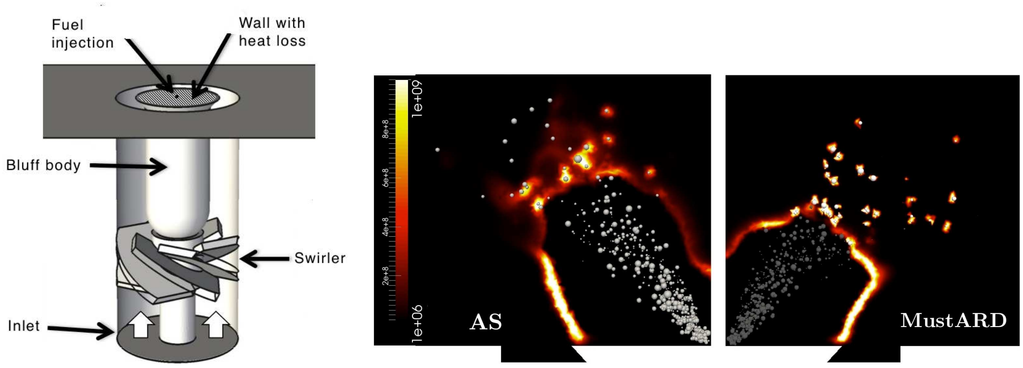


Figure 3.7: LES of the two-phase swirled burner of [9]: geometry (left) and field of instantaneous heat release with droplet visualisation, left : stantard evaporation model; right: MuStaRD model. [CFD211]

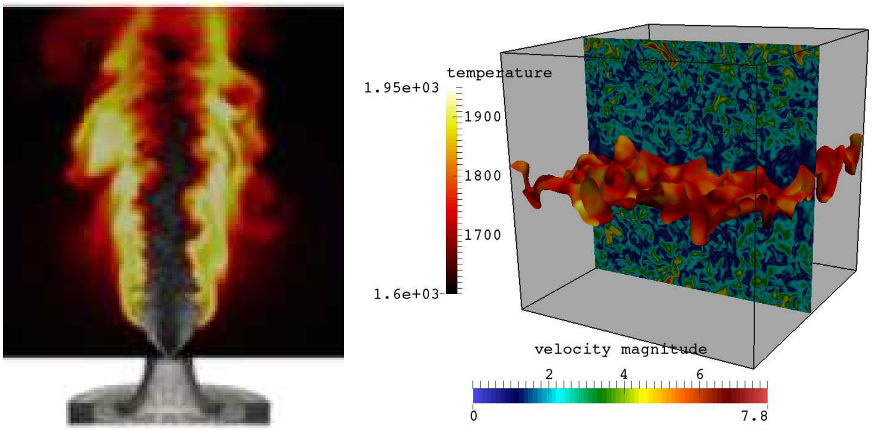


Figure 3.8: Left : LES of the two-phase KIAI burner: field of instantaneous temperature and droplet visualisation [CFD84]. Right: DNS of a turbulent diffusion flame : field of instantaneous vorticity with an isocontour of stoichiometric mixture fraction colored by temperature.

3.3 Plasma Modeling (F. Pechereau, V. Joncquières, O. Vermorel, B. Cuenot)

In an increasingly competitive satellite market, electric propulsion has recently regained attention. Among the various electric propulsion systems, Hall effect thrusters are one of the most promising technologies and Safran has been a major player in this sector for many years.
Hall effect thrusters have been extensively studied since their invention in the 1960s. However, the physics of magnetized plasmas typical of these thrusters is complex. Several plasma processes that have direct relevance to the thruster performance and lifetime are still poorly understood. Today, the design and development of Hall effect thrusters is still semi empirical with long and expensive tests. In the past years, many 1D or 2D structured codes were developed that greatly helped understanding basic features of a Hall thruster despite using inaccurate and basic models. However no tool exists today to simulate the plasma flow in the context of complex geometry of real thrusters.
With the support of Snecma, CERFACS is engaged in the development of such a numerical tool (AVIP), and first steps have been reached toward the computation of a model Hall effect thruster, as illustrated in Fig. 3.9.

The objectives are to: (i) better understand the complex plasma processes occurring in such systems; (ii) develop accurate, massively parallel and unstructured 3D numerical tools (AVIP) for the simulation of such problems and make them available to the industry (Safran); (iii) use these tools to improve the efficiency of existing systems and eventually to provide the foundation for breakthroughs in the design of new electric thrusters.

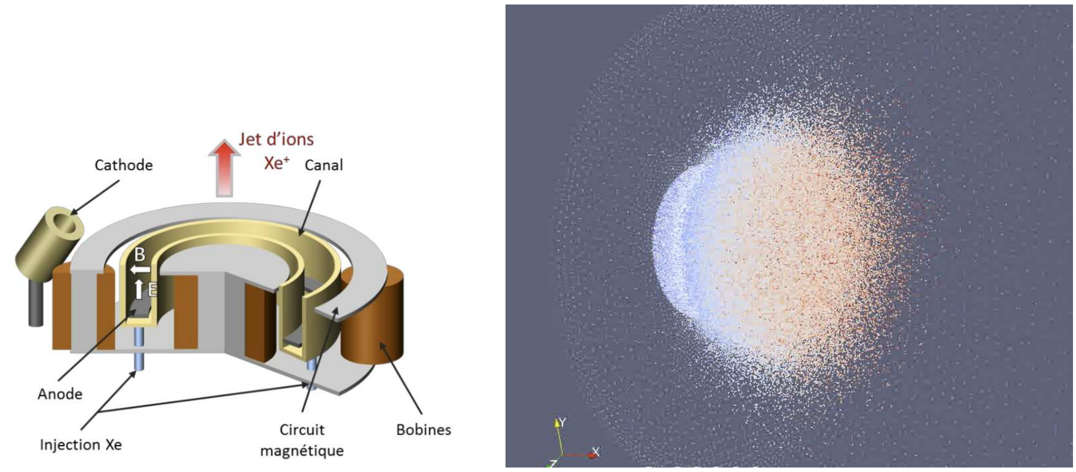


Figure 3.9: Hall effect thruster: geometry and visualization of particle injection.

Two approaches are classically used for plasma modeling, depending on the required accuracy level and the available computational resources: the Lagrangian approach (Particle-In-Cell (PIC) simulations) and the Eulerian approach (fluid simulations). In PIC simulations, different kinds of particles or macroparticles (electrons, ions and neutrals) are individually tracked and interact with each other and with the electromagnetic fields that are defined on a Eulerian mesh. Charges of particles are interpolated on the Eulerian mesh where the electric field is solved. Then the electric field force is interpolated back on the particles. Collisions are usually handled with a Monte-Carlo method. Those simulations are considered as the most accurate for low-pressure plasmas representative of Hall effect thrusters. On the other hand, they are very computationally expensive since they require tracking a very large number of particles (typically billions). Fluid simulations describe particles dynamics with macroscopic averaged variables. The set of equations to solve is very similar to the one solved in CFD for two-phase flows. These methods are less accurate than Lagrangian methods because they can miss some kinetic effects and are very sensitive to numerical methods, but they are also much less CPU consuming compared to PIC simulations.

The strategy adopted by CERFACS in AVIP is to use a hybrid approach, which combines the advantages of both PIC and fluid methods: slow particles (ions and neutrals) are treated in a Lagrangian framework to preserve accuracy and fast particles (electrons) are described in an Eulerian framework to limit CPU costs. Building such a code is an important challenge both in terms of numerical requirements and physical modeling. AVIP is based on the strong expertise of CERFACS for massively parallel codes. In particular, it is largely based on algorithms and numerical methods developed for the LES solver AVBP. For the physical modeling, AVIP benefits from the internationally recognized expertise of the Laboratoire de Physique des Plasmas (LPP Ecole Polytechnique), which closely collaborates to the project. CERFACS is also associated together with Safran to the ANR "Chaire industrielle" POSEIDON, coordinated by A. Bourdon at LPP.

The first step in the development of AVIP was the implementation of a Poisson solver for the computation of the electric field. A collaboration with INRIA (HiePACS team) has been developed on this topic through the MaPHys library (Massively Parallel Hybrid Solver for large linear systems), which is now available in the code. The development of the Lagrangian module of AVIP started in 2015 within the Post-Doc of

F. Pechereau. A new data structure was created to handle more than 2.5 billions particles in a full 3D PIC simulation. New numerical schemes were implemented to couple the dynamics of charged particles with the electric field. A Monte-Carlo method was implemented to handle the different types of collisions between particles (ionization, elastic). The Lagrangian module was thoroughly tested and validated on many test cases and is now being tested for scaling purposes. The development of the Eulerian module of AVIP started in January 2016 with the PhD of V. Joncquières, in parallel of the Lagrangian module. Data structures for the fluid equations were first created. Various high-order convective numerical schemes (3rd order in space and time) and boundary conditions derived from AVBP were adapted to the plasma fluid equations.
Although this new solver is dedicated to the simulation of plasma flows in Hall effect thrusters, this work may also be seen as a stepping stone for future other applications such as nanosecond pulsed discharges for plasma assisted combustion or flow control.

3.4 Combustion instabilities and combustion noise

Combustion noise is a major 'pollutant' created by combustion chambers and it is felt much more directly by the community than gaseous pollutants such as NO or CO. The 'Combustion noise' acronym has actually been a source of misunderstanding: today, combustion noise and thermo-acoustic instabilities are slowly being recognized as two sides of the same problem. While acoustic experts study combustion noise in the framework of broadband noise, a simple examination of most noise spectra produced by combustion chambers reveals that multiple discrete modes also appear in addition to broadband noise. Most of these modes are due to acoustic modes of the chamber. Generally, their amplitude remains small and they are simply additional contributions to noise. In certain cases however, their amplitude grows, exceeding the rest of the broadband noise by orders of magnitude, leading to what is called thermo-acoustic instabilities and increased noise. CERFACS has been heavily involved in combustion noise as well as thermo-acoustics studies over the last 15 years and this activity was strong in 2015 and 2016 with multiple PhDs, the end of the ANR DISCERN program, an EC (RECORD) project and the ERC Advanced Grant INTECOCIS collaboration with IMFT (intecocis.inp-toulouse.fr). Importantly, 2015 and 2016 have shown that the tools used for noise and thermo-acoustics were converging, leading to an integrated set of tools to study both the noise and the instabilities produced by an engine.
The beginning of the ERC advanced grant INTECOCIS (intecocis.inp-toulouse.fr) has been a major thrust since 2013: the collaboration of IMF Toulouse and CERFACS teams on thermo-acoustics makes Toulouse the world largest group in this field. This collaboration reaches also far beyond Toulouse and CERFACS collaborates actively on thermo-acoustics with EM2C, DLR, TU Munich, Cambridge, NTNU or Stanford, leading the research in this field as shown for example by the invited lecture on thermo-acoustics given by Dr Poinsot at the 2014 APS DFD meeting in San Francisco or the Hottel plenary lecture at the 36th Symp. (Int.) on Comb. in Seoul (2016). In France, CERFACS collaborates on thermo-acoustics with IMFT, EM2C, CORIA and ONERA, which use some or all of CERFACS tools for instabilities.

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

Rockets and aircrafts are the strongest noise generators on earth. Multiple mechanisms contribute to the noise heard in the far field of an engine. The noise created inside the combustion chamber itself is now a significant part of the total noise created by aircrafts or helicopters because other noise sources have been strongly reduced: understanding and decreasing combustion noise has become a major research theme.
Two mechanisms contribute to combustion noise: "direct" noise is due to unsteady combustion in the chamber acting like a monopole source; "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,

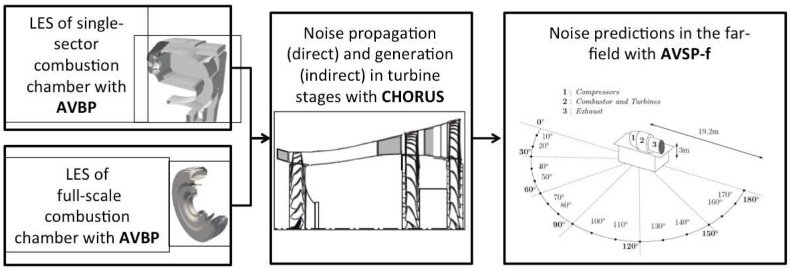


Figure 3.10: A fully deterministic chain to compute combustion noise: CONOCHAIN. LES (AVBP) is performed in the chamber; acoustic, vorticity and entropy waves are measured in the outlet planes and propagated into the turbine stages using actuator disk theory (CHORUS) to obtain both direct and indirect noise in the outlet nozzle; a far field propagation tool (AVSP-f) is then used to propagate noise to the far field.

additional indirect noise is produced and this is a major contribution in most gas turbines. CERFACS has been studying these phenomena in collaboration with Univ. Montpellier, ONERA, Univ. Sherbrooke, EM2C in Paris and DLR Berlin in two programs (ANR DISCERN and EC program RECORD) as well as two PhDs with SAFRAN. The objective of CERFACS is to stop using ad-hoc correlation-based models and build a fully deterministic method to predict combustion noise, including the noise of thermo-acoustic modes. The computation begins with a LES of the chamber and ends in the far field of the engine, coupling multiple tools shown in Fig. 3.10. This methodology has been applied successfully in two engines: (1) a helicopter engine by T. Livebardon (SAFRAN HELICOPTER ENGINES) [CFD129, CFD56], (2) an aircraft engine by M. Ferand (SAFRAN AIRCRAFT ENGINES). The method was also tested in the choked combustion chamber of EM2C (Centrale-Supelec) by C. Lapeyre (CERFACS) [CFD128] .

An interesting development associated to CHORUS is that this technique, developed for combustion noise, is also directly relevant for thermo-acoustics: CHORUS provides the transmission coefficients of noise through the turbine stages (required for noise studies) but also the reflection of these waves into the combustion chamber (the turbine impedance seen from the chamber, required for thermo-acoustics studies). Impedances of turbines and compressors are needed in the thermo-acoustics community and CHORUS can answer this request. In 2017 it should be compared to results obtained at Polimi (Milano) on impedances of a stator-rotor stage tested during the EC RECORD program.

Multiple publications have been produced in the last five years in RECORD, presenting the methods and their validations [CFD150, 12]. 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 challenge started at CERFACS in 2011, which aims at computing a full gas turbine. As the tools to do this have become available [CFD50, CFD125, CFD6, CFD124] thanks to the development of coupling techniques (based on the open source OpenPALM software of ONERA and CERFACS), the analytical method (an extension of the actuator disk theory) used for noise production and propagation through the turbine can be verified, improved and ultimately replaced by a full LES simulation. This evolution will be mandatory to compute the noise of new engine concepts such as 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. These systems can not be designed on a modular basis (chamber on one side and turbine on the other one): the design must be based on a coupled simulation of chamber and turbine together as envisioned with COUGAR.

3.4.2 Combustion instabilities (M. Falese, M. Bauerheim, A. Ghani, D. Maestro, S. Hermeth, F. Ni, A. Ndiaye, G. Staffelbach, T. Poinsot, L. Gicquel, J. Dombard, F. Nicoud)

Combustion noise is a one-way process where flames make noise and this noise is propagated away from the flame zone. If it is reflected towards the flame and can influence it with the proper phase and gain, then the system can become self-excited and the noise level increased by 20 to 40 dB, leading to combustion instabilities. These instabilities are not 'noise' only: they can destroy an engine in a few seconds and reach amplitudes of the order of the mean pressure. They 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: many of the companies contacting CERFACS (SPACE X, GE, SIEMENS, ANSALDO, ALSTOM, PRATT & WHITNEY), and the shareholder SAFRAN, are interested first in combustion instabilities. It is also an academic field where CERFACS is well known, as shown by the plenary lectures given on this topic by CERFACS at the APS meeting in 2014 and the 36th Symp. on Combustion in 2016 (Hottel lecture). CERFACS has developed a full chain of simulation tools for combustion instabilities called QUIET. These tools incorporate 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.

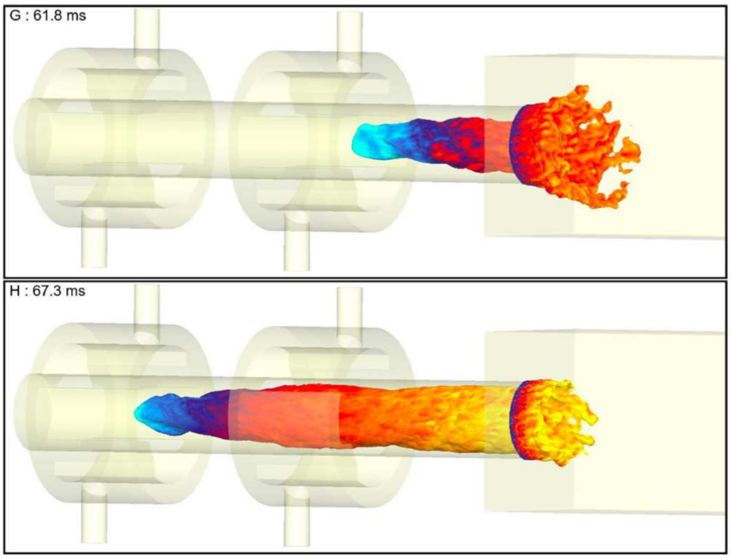


Figure 3.11: LES of flashback induced by thermoacoustic instabilities in the rig of EM2C. The flame position is visualized at two instants during the flashback of the flame [CFD128].

A new field of studies on instability is high-frequency transverse modes: these modes are the most destructive and CERFACS has been able to study them using various approaches. For the Volvo rig (premixed turbulent combustion stabilized behind a triangular flameholder), LES and acoustic analysis have allowed to isolate the mode responsible for the high frequency mode [CFD116]. For the ONERA Lotar rig (two-phase, swirled flame), transverse modes have also been identified with the same tools [CFD115].

Combustion instabilities do not only create oscillating flames: they can also lead to flashback as shown by the study of Lapeyre in the framework of the RECORD project [CFD128]: in this experiment, the coupling between acoustic waves and swirl can lead to a flashback mode where the flame penetrates the swirlers in the central region, pushed by acoustic waves (Fig. 3.11).

The interaction between thermo-acoustics and flame stabilization was also observed in another case: an industrial gas turbine studied for ANSALDO. In this turbine chamber, bistability is observed and bifurcations can lead the flame to one state or to another (Fig. 3.12). Here again, the flame is not only oscillating: it can change its stabilization point. For the Ansaldo case, the central part of the flame stabilized in the inner recirculation zone quenches and reignites only when a strong thermoacoustic mode takes place. These phenomena are believed to happen in other engines and CERFACS continues to investigate them.

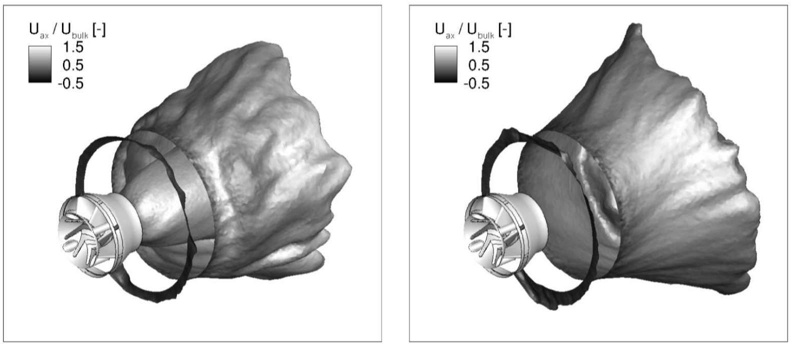


Figure 3.12: Example of bistable flame in an industrial gas turbine: the two states (attached, left and detached, right) can be observed for the same operating conditions, depending on the level of instabilities. [20].

Theory is also taking an important place in thermo-acoustics at CERFACS with the development of a purely analytical method (called ATACAMAC) dedicated to the prediction of unstable azimuthal modes in annular chambers. CERFACS actually wrote an invited review paper on analytical methods for instabilities in Phys. of Fluids in 2015 [CFD94] and these methods are developing rapidly to complement LES and acoustic solvers which have significant CPU costs. ATACAMAC has received a strong interest in the academic community [4, 5] because it allows to investigate problems which are far beyond the capabilities of simulation tools, for example to explore symmetry breaking mitigation methods in annular chambers [5]. Analytical methods also allow to introduce UQ (Uncertainty Quantification) methods into thermo-acoustics [CFD62] 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).

A specific field where instabilities are especially critical is rocket engines. The collaboration between IMFT, CERFACS, EM2C and DLR has allowed to analyze the high-frequency mode appearing in the 42 injector H2-O2 BKD engine of DLR Lampoldshausen. Figure 3.13 displays a field of temperature in the central plane of the engine, obtained from a LES of the full engine performed under a PRACE allocation [CFD152, CFD90]. This was the first time that such a complex engine was fully computed with LES. LES captures the first two modes observed in the experiment and allows to analyze their structures, showing that the first mode is a transverse mode of the chamber coupled to a 3/2L longitudinal mode of the oxygen feeding lines. The second mode is the radial mode of the chamber but is also combined to the longitudinal modes of the dome feeding lines. The combination of experimental and LES results in this 100 MW engine is a major breakthrough in the quest for instability control in these configurations.

All LES results presented above depend on the development of efficient massively parallel solvers for LES but also of three-dimensional acoustic solvers. CERFACS has worked with INRIA on AVSP solvers (the Helmholtz code of CERFACS) to improve its efficiency on massively parallel machines. In 2015 and 2016,

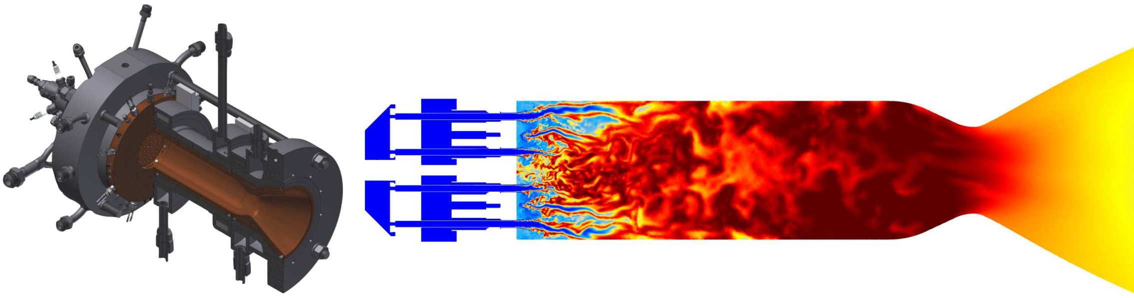


Figure 3.13: LES of combustion instability in the BKD H2-O2 engine of DLR [CFD152]. Left: configuration. Right: field of instantaneous temperature. Collaboration with IMF Toulouse and EM2C Paris.

the collaboration with INRIA has focused on run-time solutions for AVBP (with Dr L. Giraud) and on adaptive mesh for LES (with C. Dobrzynski).

Applications

Applications of CERFACS tools to real combustors is of course a primary driver of CERFACS CFD activity and past successes. Thanks to the link with CERFACS' partners as well as to external collaborations, many applications of industrial interests have been dealt with in the 2015-2016 years. Among others, the following fields of applications are detailed in this document:

- Space related applications,
- Aeronautical engine issues and demonstrations,
- Turbomachinery,
- Novel propulsion concepts,
- Safety,
- Chemical processes.

4.1 Space propulsion

Space propulsion covers various propulsion systems, including cryogenic liquid engines (like Vulcain or Vinci), solid propulsion for boosters or electric propulsion for satellites. Each of them involves different physics and raises specific technical issues. Cryogenic propulsion deals with supercritical flows, highly reactive mixtures such as H2-O2, and large wall heat fluxes as well as unsteady pressure loads. Cryogenic engines are prone to thermo-acoustic instabilities which shake the launcher and the satellite, and can even lead to their destruction. Combustion in solid propulsion boosters involves complex heterogeneous chemistry and is difficult to control too. These systems also generate hydrodynamic instabilities which are dangerous for the launcher. For cryogenic and solid propulsion systems, CERFACS has developed specific models and implemented them successfully in the code AVBP. The situation is somewhat different for satellite electric propulsion, based on plasma physics which are not fully understood and require long and costly experimental tests. In addition, a satellite engine must be reliable and able to operate for years during the whole life of the satellite. Unfortunately little is known about the real engine operation and wear, and the recent renewed interest in such systems now demands numerical tools to predict their behaviour. This is what CERFACS has started, supported by SNECMA and in collaboration with the Laboratoire de Physique des Plasmas (LPP, Ecole Polytechnique). First steps in modeling such systems were described in Section 3.3.

4.1.1 Liquid propulsion (R. Mari, L. Potier, D. Maestro, T. Bridel-Bertomeu, B.Cuenot)

One critical issue for the design of spatial liquid propellers is heat transfer, which directly impacts flame stabilisation and the thermal fatigue of the combustion chamber walls. The effect of heat transfer on flame behaviour was studied in the PhD of R. Mari, who performed coupled simulations with AVBP for the LES of supercritical flames and AVTP for the heat conduction in the chamber walls (Fig. 4.1). Based on coupled simulations of 1D flame-wall interaction [CFD131], the analysis of the flame stabilization clearly showed the role of chemistry in the mechanism of flame anchoring at the injector tip.

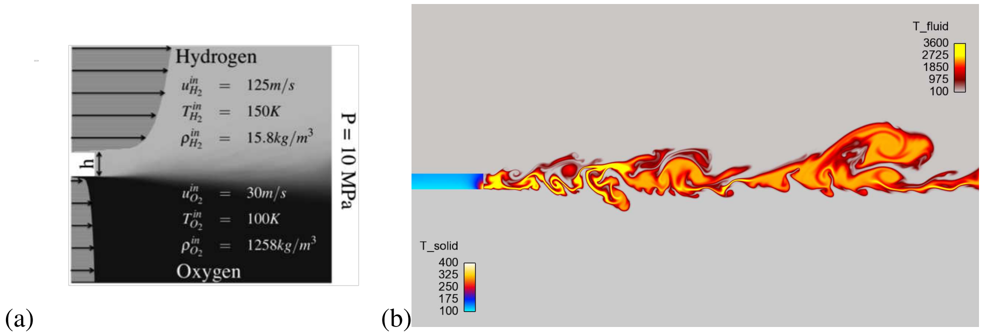


Figure 4.1: Coupled AVBP/AVTP slmulation of a cryogenic H2/O2 flame: (a) flow configuration and (b) instantaneous field of temperature in the gas and in the solid. [CFD207]

Heat transfer to walls is currently studied in various configurations. One is the CONFORTH configuration, tested on the MASCOTTE test bench at ONERA [31] in rocket engine representative conditions. The CONFORTH chamber uses gaseous hydrogen/liquid oxygen (GH2/LOx) propellants, injected through 5 coaxial injectors, and cooled by water circulation around the chamber walls. A subcritical case was simulated with AVBP to compare calculated heat fluxes to measurements and validate thermal wall laws (Fig. 4.2). Results showed that, due to the extremely high temperature of the burnt gas, a *coupled* wall law, where the dynamic and thermal wall models are coupled and solved together, is required [CFD71]. The same conclusion was obtained by D. Maestro (PhD funded by the COPA-GT project) who used a coupled wall law to recover the heat flux in a methane / oxygen gaseous burner experimentally studied at TU Munich [CFD58]. Using the same methodology, current work now focuses on the evaluation of the efficiency of longitudinal ribs, placed along the combustion chamber walls to reduce the heat load, as tested in the JAXA combustion chamber [29].

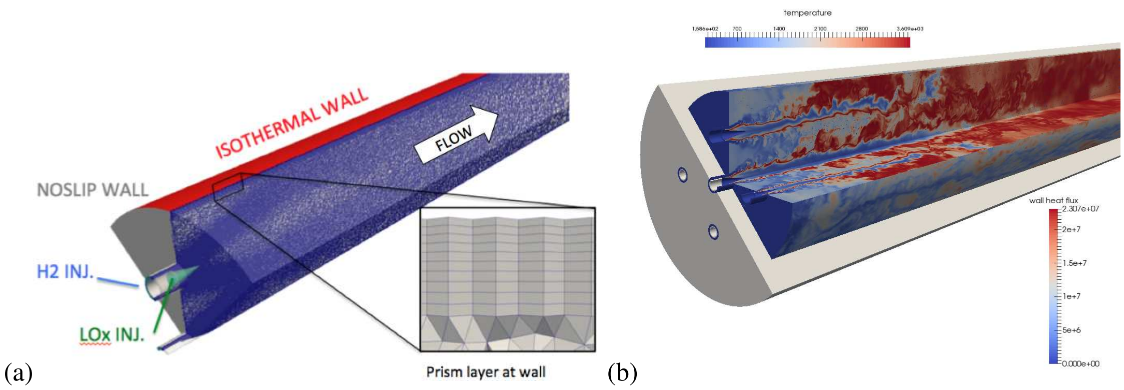


Figure 4.2: CONFORTH test configuration: (a) CFD computational domain and boundary conditions as well as (b) an instantaneous temperature field inside the fluid complemented by the wall heat flux at the cylindrical interface.

Another challenge in cryogenic propulsion is the transition between sub and supercritical conditions. In the first case, a classical two-phase flow is found, with a spray and a sharp interface between the liquid and the gas and surface tension forces. In the second case, only a dense and a light phase can be identified, with a smooth transition between the two. The transition from one case to the other is a complex thermodynamic problem and a numerical challenge. This is the topic of the ANR project SUB&SUPERJET, coordinated by EM2C (Ecole Centrale Paris).

Upstream of the combustion chamber, turbo-pumps are also a crucial element of liquid propulsion and are investigated in the framework of the PhD of T. Bridel-Bertomeu. Indeed, in such pumps, the flow stability must be ensured in the cavities between the fixed and rotating parts, to avoid large flow variations leading to miss-tuned operating conditions in the engine and a drastic loss of performance or life-span. LES was therefore applied to an enclosed rotor-stator (RS) configuration, leading to several interesting conclusions. It appeared that the unsteady pressure signals encountered in such systems stem from the instability of the stator boundary layer in which coherent patterns rotate at exactly the constituent frequencies of the pressure signals (Fig. 4.3). Furthermore, a DMD analysis showed that these coherent patterns extend throughout the cavity. These conclusions were found to hold also for a real space engine turbo-pump turbine cavity, in spite of the complexity of the geometry and the much higher rotation Reynolds numbers.

The simulation results were related to theory through Linear Stability Analysis (LSA) to establish a predictive strategy for academic RS-cavity flows, given the underlying mean flow field. The AVLP code, a Linearized Navier-Stokes Equations solver dedicated to axisymmetric mean flows was completed and thoroughly tested against test-cases from the literature. The generalization to various RS-cavities is still undergoing, but it was proven that seeking the most amplified spatial branch at the frequency of the instability (as given by DMD) yields the correct two-dimensional (r,z) organization of the mode.

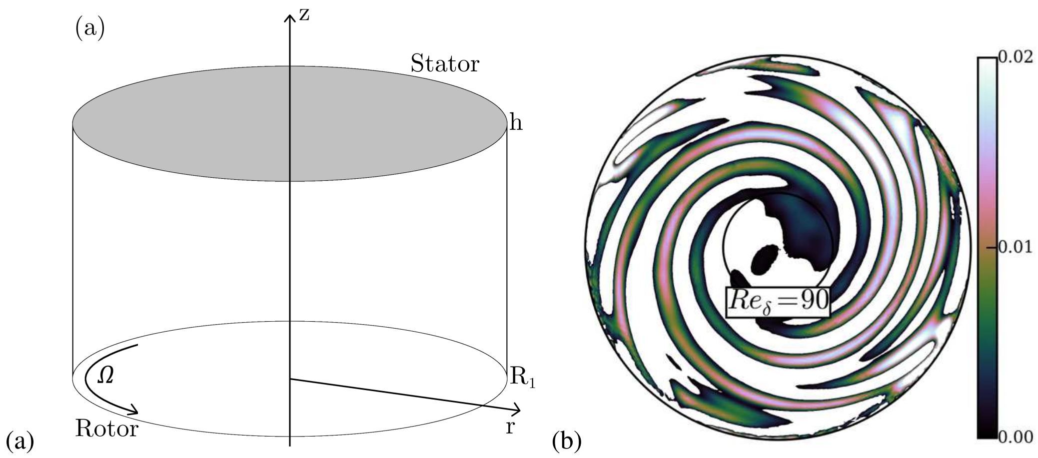


Figure 4.3: Rotor / stator cavity flow simulations: (a) domain simulated by LES (cavity with aspect ratio H/R=1.18 at radial Reynolds number 10^5) and (b) axial velocity fluctuation field at a given instant in a near stator plane.

4.1.2 Solid propulsion (L. Lacassagne, E. Riber, B. Cuenot)

Pressure oscillations are a major issue in solid rocket motor design, as very small pressure oscillations induce strong thrust oscillations, involving vibrations detrimental to carrying load. Extensive research has enabled to characterize several sources of instabilities. These instabilities can be divided into two main categories: combustion instabilities, linked to the propellant combustion and hydrodynamic instabilities due to vortex shedding phenomena. The objective of the PhD work of L. Lacassagne is to simulate vortex shedding mechanisms, corner vortex shedding (VSA), and the influence of the solid aluminum particles on this instability.

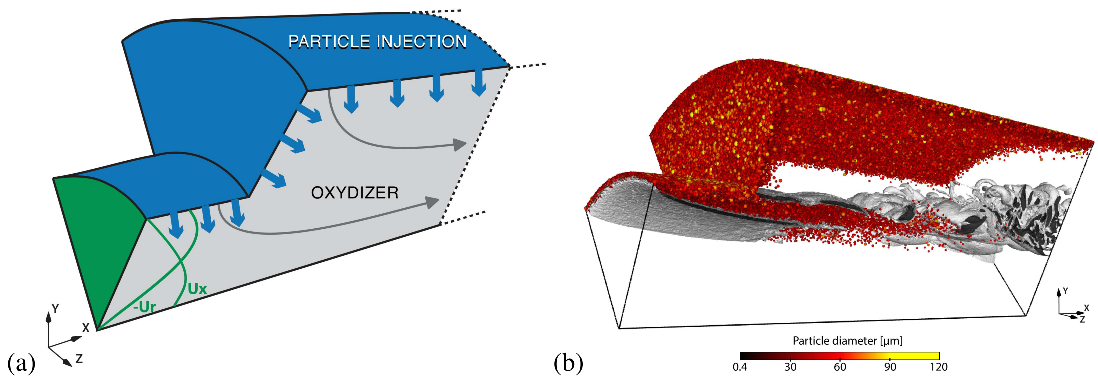
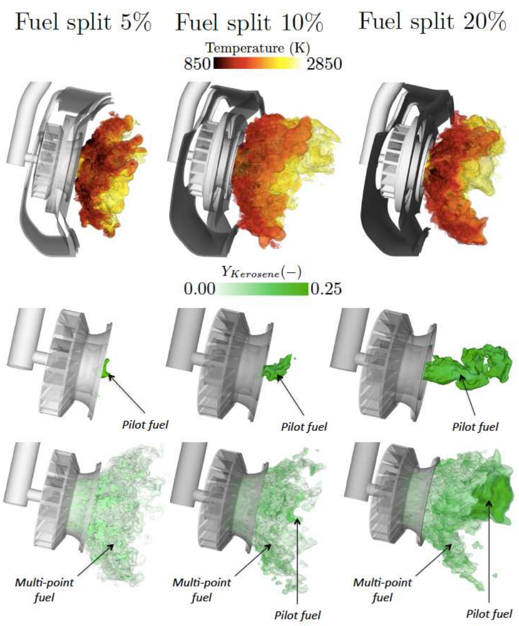


Figure 4.4: (a) Computational domain and flow problem description of an academic solid rocket motor: blue surfaces correspond to the solid propellant alimentation feed with aluminium particles while the green surface is the oxydizer gaseous flow. (b) Instantaneous two-phase flow. Particles in combustion colored and scaled by diameter and vorticity contours.

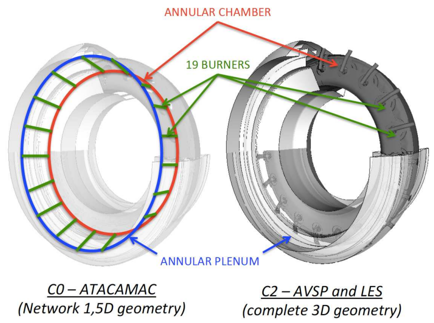
LES of a 3D academic configuration featuring only the VSA was performed with all the characteristics of a solid rocket motor flow, in particular including burning aluminum particles. The impacts of the numerical scheme, the spatial resolution or the turbulence injection were assessed. Results showed that particles burn very close to the propellant surface and that the associated heat release does not impact the shear layer. Moreover the presence of inert particles inside the vortices decreases the oscillation amplitudes [CFD51]. Another interesting result was the influence of the lateral blowing intensity on the instability. Lateral blowing coming from the surface mass flow rate was found to decrease the instability, and even stabilize the flow for sufficient blowing intensity. This result was confirmed theoretically thanks to linear stability analysis with the code AVLP. Finally, the impact of the scale was studied with a 3D simulation at a dimension close to the real engine dimensions in order to see if the instability characteristics are recovered at a full scale and if the aluminum particles have the same impact on the instability.

4.1.3 Aeronautical engines (G. Hannebique, L. Esclapez, T. Jaravel, L. Gicquel)

Aeronautical engine applications appeared very early on in the context of the CFD team. As a continuation of previous efforts and demonstrations, recent applications focused on new issues related to the development of the next generation of aeronautical and power generation engines. These relate to engine efficiency, reliability and pollutant emissions. Such industrial issues necessitate today to deal with multiphase turbulent reacting flow predictions as well as fully transient processes as encountered in an ignition sequence of the combustor.
To deal with pollutant emissions and efficiency, AVBP has been applied to the LEMCOTEC (standing for Low EMission COre-engin TEChnology) combustor. The specificity of this SAFRAN representative aeronautical burner is that it prefigures the next generation of ultra-low NOx technologies that rely on a multi-point and pilot fuel injection systems and for which experimental data is made available through



(a)



(b)

Figure 4.5: (a) LEMCOTEC burner LES predictions: Iso-contours of heat release colored by temperature (top), iso-contour of fuel mass fraction (rich, middle) and (lean, bottom) to visualize the flame shape as well as the pilot (middle) and multi-point (bottom) flames vs. the fuel split parameter: 5% (left), 10% (middle) and 20% (right) [CFD47, CFD200]. (b) Model reduction applied to the fully annular LEMCOTEC burner allowing the thermo acoustic stability analysis of the concept based on LES evaluation of the burner flame dynamics [CFD94, CFD95].

the European project. One specific issue was the ability for models to retrieve experimental data but also provide detailed characterization of the multiphase flow under different operating conditions or more specifically fuel-split ratios: *i.e.* amount of fuel injected through the multi-point system or through the pilot injector [CFD47, CFD200]. Such issues are of primary interest since these systems are known to be prone to thermoacoustic instabilities which can be triggered by the fuel split ratio [CFD94, CFD95], Fig. 4.5(a). Detailed chemical models based on the ARC procedure (see Section 3.3) have been used to study key processes in the production of Nox and CO. Likewise, an advanced thermoacoustic analysis making use of forced LES predictions for this fully annular burner has been produced, Fig. 4.5(b) [CFD94, CFD95].

4.1.4 Turbomachinery (L. Gicquel, J.-F. Boussuge, F. Duchaine, J. De Laborderie, C. Koupper, J. Dombard)

Turbomachinery is an essential component of aeronautical applications where compressors and turbines determine the overall power and operative limits of engines. Even though LES remains difficult for turbomachinery, CERFACS believes that it will become a standard tool (as it is for combustion chambers) in the next ten years. Using the same LES tools for the combustor and for the compressor / turbine flows is also a logical path to explore, and AVBP has been used now for engine turbomachinery components as detailed in the following three industrial applications:

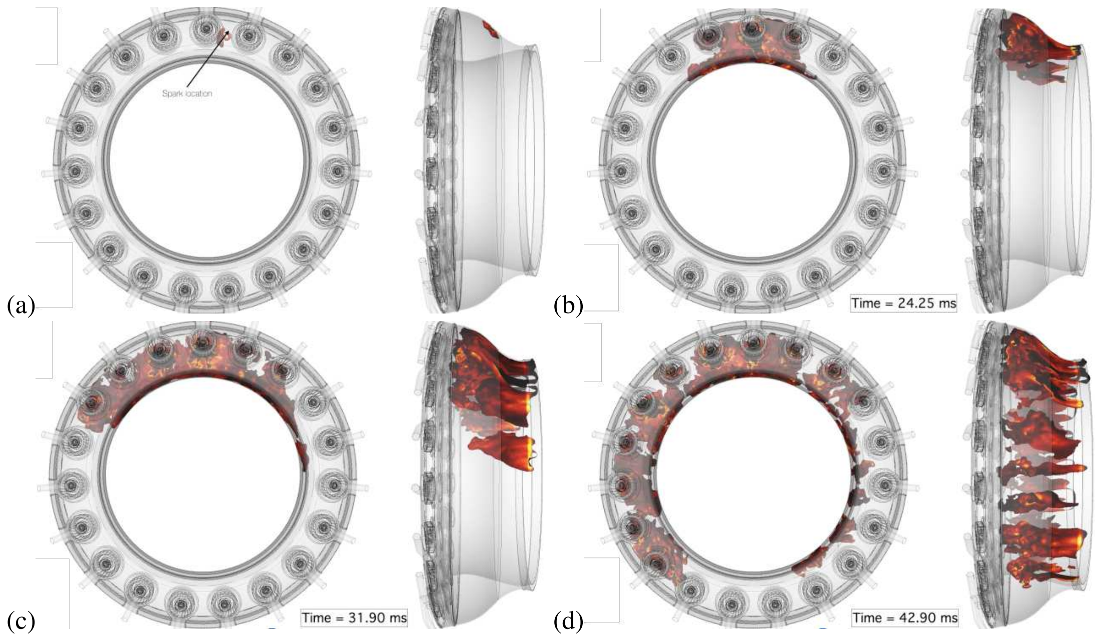


Figure 4.6: Ignition sequence of the LEMCOTEC full annular burner as obtained by LES at four distinct instant of the light-around process. [CFD8, CFD198]

- The CREATE demonstrator, Fig. 4.7 (a) & (b): a three and a half stage axial compressor representative of the next generation of design from SAFRAN and studied experimentally at Ecole Centrale de Lyon (LMFA team).
- The Pi9 radial compressor, Fig. 4.7 (c) studied experimentally at Ecole Centrale de Lyon and part of a PERICLES action between CERFACS and SAFRAN Helicopter Engines.
- The FACTOR demonstrator, Fig. 4.7 (d): a non-reacting combustor turbine component mounted at Florence University (UNIFI) dedicated to the study of the combustor turbine interactions in the European project FACTOR.

Although still under validation against experimental data, these turbomachinery LES predictions constitute today a world premiere. Thanks to dedicated CPU grants from a PRACE allocation as well as a GENCI 'grand challenge', they demonstrate the capacity of CERFACS to treat such problems with cutting-edge modeling approaches and CFD tools. Dedicated communications are respectively available in [CFD25, CFD30, CFD169] for CREATE whose results are part of the CN2020 project of SAFRAN Tech. and [CFD50, CFD126, CFD49, CFD125, CFD124] for the FACTOR application. Ongoing transfer toward industry on proprietary geometries is currently under investigation within PERICLES.

Similarly to compressors or turbines, fans and open rotors are turbomachinery components of importance not only in the generation of propulsive power but also because they create noise which can significantly contribute to the overall sound emitted by an aircraft. For this specific issue, again LES seems to be an interesting approach and ongoing analyses are pursued in collaboration with ISAE on the DGEN engine (COFFECCI RTRA project), Fig. 4.8(a), or with Pr. S. Moureau (LMFA and Sherbrooke University) around the NASA SDT fan databasis, Fig. 4.8(b).
Complementarily to fans, simulations of design issues related to the aircraft engine air intake geometry is addressed for real engine configurations by M. Daroukh: the full azimuthal complexity of the

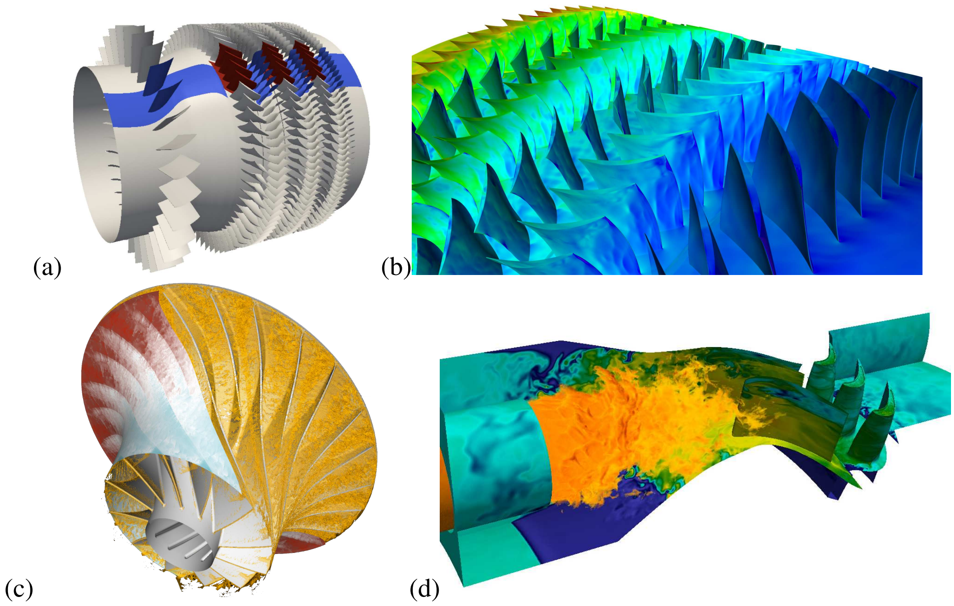


Figure 4.7: LES of compressors: CREATE three and a half axial compressor, (a) geometry and (b) LES instantaneous flow field [CFD47, CFD200]; (c) radial compressor Pi9 and (d) fully integrated LES simulation of the FACTOR combustor / turbine interaction demonstrator [CFD94, CFD95].

geometry is considered in a URANS computation to identify sources of noise while evaluating design changes and their impact on the fan performance [CFD24, CFD146, 10]. Note finally that computational domain size reduction relying on the phase-lag method has been investigated in the context of LES [CFD209, CFD135, CFD59] to alleviate CPU cost of turbomachinery computation which for real engines required full azimuthal domain simulations. These developments, applicable to both URANS and LES, seek numerical solutions where only single passage flow CFD domains are computed for each row, these passages being then coupled to represent the expected full wheel flow physics even for non proportional numbers of blade passages between rows.

4.1.5 Novel propulsion concepts (R. Bizzari, L. Labarrere, A. Dauptain, T. Poinsot)

Since 2013, CERFACS has been involved in the numerical study of various novel propulsion concepts for aeronautical applications. Most concepts target constant volume combustion in the chamber to increase the thermodynamic efficiency of the cycle. Two paths are possible to reach this objective: (1) subsonic constant volume combustion chambers using valves at inlet and outlet or (2) detonation engines where the flame speed (1.5 km/s) is so large that combustion takes place almost at constant volume.

In a collaborative work with Pprime (Poitiers) and COMAT, CERFACS has studied a subsonic chamber using valves (Fig. 4.9). The experimental prototype, developed in Poitiers, uses rotating valves at the inlet and the outlet to ensure constant volume combustion. The valve movement was taken into account in AVBP using the MISCOG method developed for turbomachinery [CFD137, 34]. The rest of the LES setup was identical to the machinery used for gas turbines or piston engines in AVBP. Results of LES (Fig. 4.10) show how the flame (ignited by a spark at each cycle) grows during the constant volume phase and show that intake and exhaust phases are difficult to tune to achieve high efficiencies in this configuration. LES

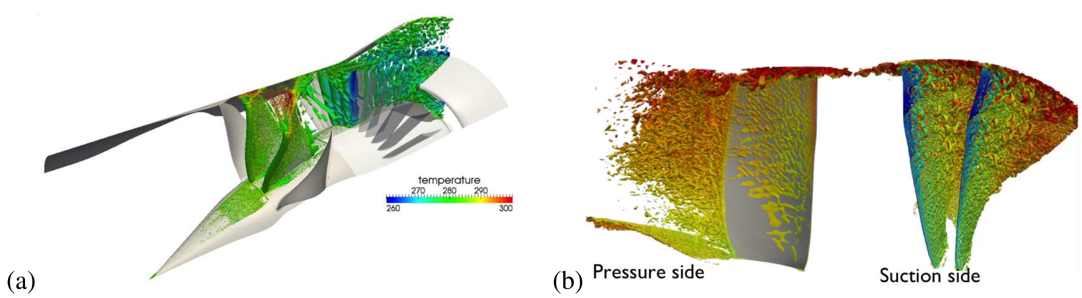


Figure 4.8: LES of fan geometries dedicated to the analysis and prediction of turbomachinery noise: (a) DGEN engine of PRICE Induction, (b) SDT NASA (iso surface of Q-criterion colored by the local). Both figures report flow details obtained by LES and evidenced by Q-criterion iso-surfaces colored by the local flow temperature value.

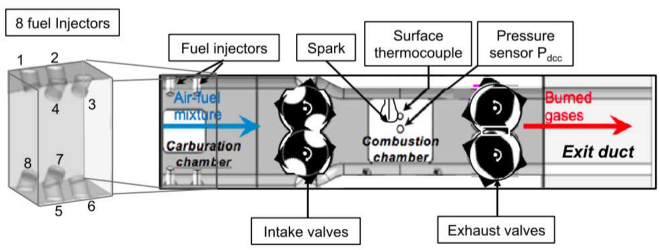


Figure 4.9: The constant volume chamber (CVC) of Pprime, Poitiers [2].

have also revealed the existence (confirmed by experiments) of significant cycle to cycle variations and highlighted the instability mechanisms which are due to coupling between consecutive cycles [CFD127].

Another promising path for future engines is rotating detonation engines (RDE) where combustion is performed in a fast (1.5 km/s) combustion wave associated to a shock. Unlike PDWE (Propagating Detonation Wave Engines), the detonation in a RDE is continuous and turns around in the annular chamber. RDE concepts are now studied worldwide and CERFACS has been preparing the tools needed for LES of such flows. This requires being able to capture shock and detonation as well as mixing and turbulence (which are important to compute reactants injection and mixing) within a LES context, a task which is obviously difficult but corresponds also to efforts lead in the team in the field of explosions in buildings and in DDT (Deflagration Detonation Transition). AVBP has been tested for detonating flows and the first computations of rotating detonation have been performed in 2015. As an example, Fig. 4.11 shows a LES of RDE performed by R. Bizzari. Using the Cook and Cabot model for shocks and a reduced scheme for H_2/O_2 chemistry, the structure of the detonation waves in a RDE was successfully computed. In 2016, a new breakthrough was achieved which allows to use ARC analytical schemes (see section) for detonation as well as for DDT (Deflagration Detonation Transition) cases. The high-order code of CERFACS, JAGUAR (spectral differences) was also prepared to compute these flows in the future.

For both CVC and RDE chambers, an interesting issue is linked to the unsteadiness at the chamber outlet due to its inherent pulsating character. This will obviously raise the question of the noise created by such engines but also of the operation of the turbine in pulsated regimes: strong fluctuations at the outlet of the chamber will lead to a degraded operation of the turbine. This can be studied only by coupling chamber and turbine flows and it opens a new field for CFD: computing an engine using a CVC or a RDE chamber can not be done in a modular approach anymore, where the combustion chamber is computed first and the

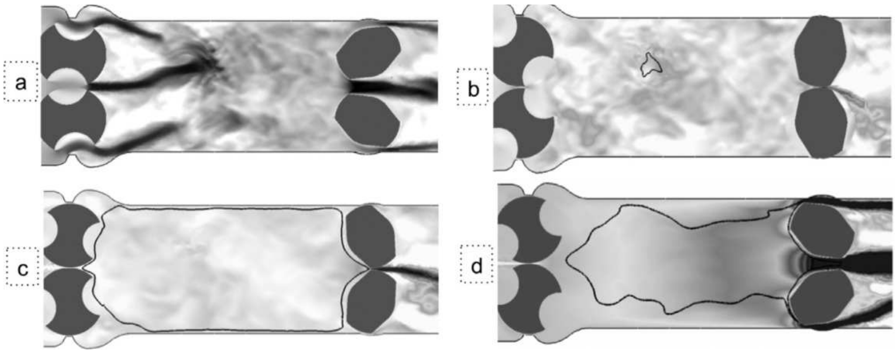


Figure 4.10: LES of the reacting flow in the Poitiers chamber [2]. Flame position (isolevel of temperature: T = 1800 K) superimposed to the axial velocity field (velocity magnitude from 0 to 100 m/s). (a) Intake ($\theta = 82deg$). (b) Ignition ($\theta = 125deg$). (c) End of combustion phase ($\theta = 161deg$). (d) Exhaust ($\theta = 13deg$)

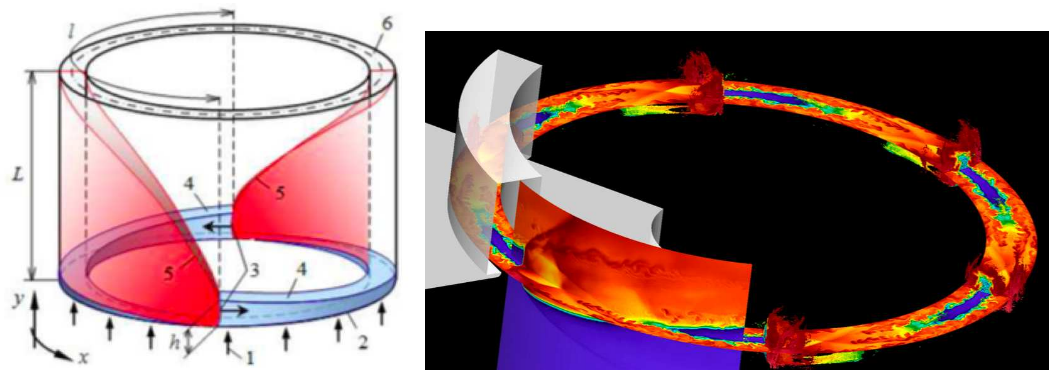


Figure 4.11: LES of a generic RDE engine. Left: geometry. Right: temperature field in a case with six fronts.

turbine is computed next in a separate task. Since the flow is fully unsteady, chamber and turbine will have to be computed simultaneously, a task which is exactly the goal of the COUGAR challenge, initiated at CERFACS five years ago which targets integrated simulations of turbine elements instead of the usual modular approach.

4.1.6 Safety (O. Dounia, D. Barré, 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. Controlling and reducing this over-pressure in case of industrial accidents is thus the key point in any safety related procedure. In this context, the main objective of the safety project at CERFACS is to further develop and improve the numerical tools to simulate gas explosion phenomena in realistic conditions. The pioneer work (for CERFACS) of P. Quillatre (PhD defended in 2014) showed that LES in general, and AVBP in particular, were the proper tools to tackle this challenge. This work, which focused on deflagration scenarios only, was continued by D. Barré (Post-Doc funded by Total, 2014-2015) to study upscaling effects in gas explosions. One of the main questions is to know how LES models (especially turbulent combustion models) behave when changing from laboratory small-scale configurations (a few centimeters) to realistic large-scale configurations (several meters). CERFACS collaborates actively with EM2C Paris and with Total on this topic (Dr. D. Veynante, PhD of P. Volpiani) to develop and validate new types of combustion models based on a dynamic procedure to automatically determine parameters used in flame wrinkling models.

More recently, two additional activities linked to gas explosions have started within the PhD of O. Dounia (funded by TOTAL, 2014-2017).

- The first one concerns the mitigation of explosions using chemical inhibitors, typically alkali metal compounds (Na, K) as proposed by P. Hoorelbeke at Total for example. In the context of LES, accounting for the detailed chemical mechanisms leading to flame inhibition is impossible because of their prohibitive computational cost. The strategy adopted at CERFACS consists in deriving analytically reduced chemical schemes, as described in Section 3.2.1, using the chemistry reduction tool YARC (collaboration with Dr P. Pepiot, Cornell University). First tests on methane-air-sodium bicarbonate (NaHCO3) mixtures have confirmed the great potential of such an approach.

- The second activity is related to the flame acceleration and deflagration-to-detonation transition (DDT) processes. This is of course a topic of prime interest in the context of safety since detonation is known to be much more devastating due to the higher levels of pressure produced compared to deflagration. 2D DNS and 3D LES of flame propagation in a closed configuration equipped with obstacles (TU Munich) have been performed with AVBP (Fig. 4.12). First comparisons with measurements show the capacity of LES to correctly predict the flame acceleration and the propagation mode, i.e. deflagration of detonation. This topic is directly connected to the study of RDE described in the previous section and is based on the same methods to capture detonation in LES.

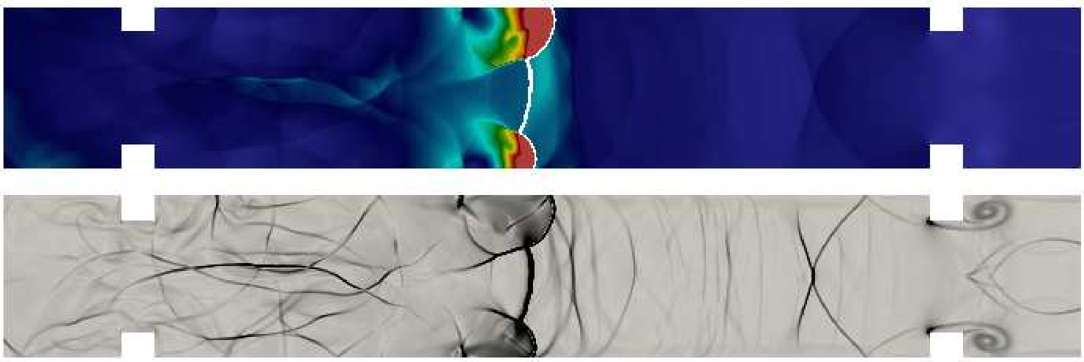


Figure 4.12: 2D DNS of DDT in a closed channel with obstacles (Gravent configuration, TU Munich). Top: pressure; bottom: density gradient normalized by density.

DDT is also the topic of a new PhD funded by Total (F. Pacaud, 2016-2019) starting in November 2016. Since 2015, CERFACS is a member of the Groupe de Travail Explosion project (2015-2017), led by INERIS. This collaboration with many other industrial and research partners (ENGIE, Air Liquide, Apsys, Fluidyn, CEA, IRSN) aims at testing and comparing various CFD solvers for the prediction of gas explosion phenomena. This consortium is a great opportunity to compare AVBP with different RANS and LES codes used in the field of safety, such as FLACS (GexCon) of Fluidyn-MP (Fluidyn).

4.2 Chemical processes (M. Zhu, R. Campet, E. Riber, B. Cuenot)

A critical factor for steam-cracking processes is heat transfer, as chemical conversion is most efficient in narrow temperature ranges. Introducing artificial roughness on the inner surface of the process tubes is known to increase the turbulence level of the flow: it is a passive method for heat transfer enhancement, which is why ribbed tubes are often used for cracking applications. However, this method also induces an increase in pressure loss that needs to be limited: gains in heat transfer may be offset by excessive pressure losses, leading to a subtile optimum point. The main goal of this work is to perform Large Eddy Simulations of the industrial steam-cracking process including the chemical transformation and to optimize the chemical selectivity of some produced species such as ethylene by modifying wall roughness of the cracking tubes for example by adding ribs on these walls.

Numerical simulations of the steam cracking process are challenging because of the size of the computational domain (cracking tubes can be tens meters long), the complex flow dynamics and the stiffness of the chemical mechanism. Large-Eddy Simulations (LES) over the full spatial configuration induce a huge computational cost and remain too expensive for a complete study of the reactor. Therefore, a methodology was developed in the framework of the PhD of M. Zhu, in order to perform LES of the steam cracking flow in ribbed tubes within a reasonable computational cost. It uses a periodic configuration of only one rib pitch length, the correct flow dynamics and thermochemistry being ensured by specific source terms added to the conservation equations [CFD214].

This methodology was implemented in AVBP, and validated in a ribbed tube configuration without chemical reactions against detailed experimental measurements performed at VKI, for both non-heated and heated walls. The mean velocity field as well as the wall friction coefficient were found in good agreement with the measurements. The simulation captures the recirculation zones upstream and downstream of each rib, as well as the rib-induced rotating motion of the flow (Fig. 4.13). The thermal behavior of the tubes predicted by LES was found also in good agreement with the measurements in terms of Nusselt number.

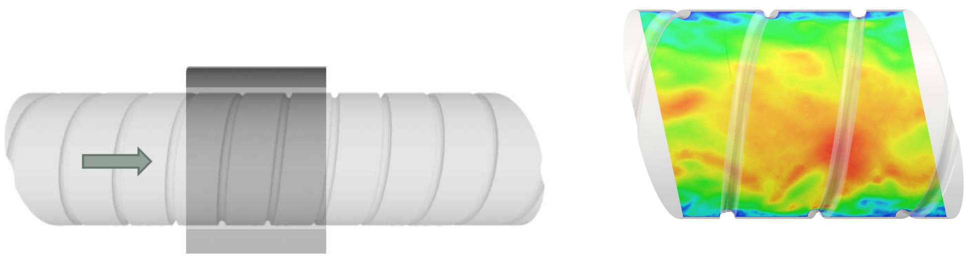


Figure 4.13: LES of ribbed tube. Left : configuration. Right: instantaneous flow velocity.

Once the flow dynamics and thermal behaviour were correctly captured, effort was put on the chemistry of steam-cracking. In collaboration with University of Ghent (Pr. K. van Geem), the chemical mechanism for butane cracking chemistry was implemented in AVBP and validated against simulations done with the CANTERA code in 0D reactor configurations. The chemical mechanism stiffness was reduced via a Quasi-Steady State Approximation (QSSA), allowing to perform LES of butane steam-cracking in real operating conditions. Current objectives are twofold: first it is necessary to increase again the complexity of the chemistry, starting from hexane. The second objective is to derive a methodology to perform shape optimization. These are the topics of the PhD of R. Campet (Total), started in october 2015.

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