# Development of High Level Software using Loosely Coupled Parallel Computers for the Optimal Design of Thermal Systems and Equipment. TIC2003-07970

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#### Abstract

The goal of the project is to get deeper understanding of the fluid dynamics and heat transfer phenomena taking advantage of the new computing resources in parallel computation using loosely coupled parallel computers (Beowulf clusters). According to the most appropriate techniques for their parallelization, the codes/software to be developed within this project for the treatment of the different phenomena of interest have been grouped into three main areas: i) detailed resolution of turbulent incompressible flows based on DNS and LES methodologies, ii) resolution of flows with (approximately) parabolic spatial structure (cases of combustion, free surfaces and flow between plates will be of special interest); iii) resolution of flows with elliptic structure (turbulent flow in general with RANS models and moving surfaces). Although the project has essentially a basic/fundamental nature, the potential applications are addressed to the simulation of thermal systems and equipment of industrial and social interest in which the milestones achieved in this basic research line are applicable. Thus, the experience acquired will allow not only to maintain and improve the technology transfer to the companies with which the Group collaborates in the framework of research contracts and/or national and European research projects, but also to increment the possibilities of application to other companies and industrial and social sectors.

Keywords: heat and mass transfer, turbulence, DNS, LES, RANS, combustion, radiation, free surfaces, moving grids/boundaries, numerical methods, CFD&HT, HPCN, paralelization, Beowulf clusters.

# 1 Project objectives

#### 1.1-Introduction

This project focuses on the continuation of the work that the Group is carrying out in the framework of its main research line: "Numerical simulation and experimental validation of heat and mass transfer phenomena; application to the design of thermal systems and equipment". Starting from the know-how and numerical facilities developed by the Research Group, and as a continuation of previous TIC projects, the goal of the project is to get deeper understanding of the

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fluid dynamics and heat transfer phenomena taking advantage of the new computing resources in parallel computation using loosely coupled parallel computers: Beowulf clusters.

Even though the project has a fundamental character, and the main achievements will be in the academic area (publications, doctorate thesis...), it will be essential for the applied studies of the Group in the development of high performance software for the simulation of specific thermal system and equipment of industrial and social interest.

#### 1.2-Strategy for parallel code development

According to the most appropriate techniques for their parallelization, the codes/software to be developed within this project for the treatment of the different phenomena of interest have been grouped into three main areas:

- 1) Detailed resolution of turbulent incompressible flows based on DNS and LES methodologies
- 2) Resolution of flows with (approximately) parabolic spatial structure (cases of combustion, free surfaces and flow between plates will be of special interest)
- 3) Resolution of flows with elliptic structure (turbulent flow in general with RANS models and moving surfaces).

The possibilities of using the most appropriate algorithms in every area without restrictions will compensate the large scope of the project in respect to the implementation, verification, validation and maintenance of the codes. The design of the algorithms and the structure of the three mentioned codes will assure their portability and efficient use in other architectural types, such as share memory and NUMA (Non-Uniform Memory Access) systems. The recent installation of the supercomputer Mare Nostrum, a distributed memory tightly coupled computer has confirmed that our initial strategy of total portability was appropriated.

### 1.3-Methodology

The general methodology of the work for the development of these algorithms and codes can be divided into the following levels (which present high inter-relationships):

- 1) Mathematical formulation of the physical phenomena.
- 2) Algorithms and techniques for the numerical resolution.
- 3) Development and verification of parallel software.
- 4) Resolution of different phenomena/configurations and analysis of the quality of the numerical solutions (discretization errors and convergence errors).
- 5) Validation of the mathematical formulations developed (modelization errors).

Although the project has essentially a basic/fundamental nature, the potential applications are addressed to the simulation of thermal systems and equipment of industrial and social interest in which the milestones achieved in this basic research line are applicable. Thus, the experience acquired will allow a technology transfer to the companies with which the Group collaborates in the framework of research contracts and/or national and European research projects. This will allow not only to maintain and improve these collaborations, but also to increment the possibilities of application to other companies and industrial and social sectors.

# **1.4-Project Development**

The work is being carried out without differing significantly from the anticipated plan. Concretely, the work is structured in three main areas of parallel CFD code development, plus a fourth area regarding know-how development concerning PC clusters.

Activities	First Year										Second Year											Third Year														
1. Code 1: Incompressible Turbulent Flows-DNS-LES	1	2	3	4	5	6	7	8	9	1	01	11	2	12	3	4	5	6	7	8	9	10	)11	12	1	2	3	4	5	6	7	8	9	10	111	12
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1.1a Discretization																																			T	-
1.1b 2nd order Poisson eq. Solution																																				_
1.1c Time average functions implementation									Γ																											_
1.1d Extension to non-periodic situations																																			Т	
1.2 4th order spectro consistent discretization																																				
1.2a Spatial and temporal discretization implementation																																				_
1.2b 4th order Poisson eq. Solution																																				_
1.3 LES models implementation																																				
1.4 Validation and Applications																																				
2. Code 2: Flows with parabolic spatial structure 2.1 Mathematical formulation	1	2	3	4	5	6	7	8	9	1	01	11	2	12	3	4	5	6	7	8	9	10	)11	12	1	2	3	4	5	6	7	8	9	101	<b>11</b> 1	2
2.1a Chemical reactions: Combustion																																			Т	
2.1b Two-phase flows with phase separation																																	Т			
2.1c Flows in channels of arbitrary geometry																																				
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2.2a Chemical reactions: Combustion																																				
2.2b Two-phase flows with phase separation																																				
2.2c Flows in channels of arbitrary geometry																																	Т			
2.3 Parallel software development & code verification																																				
2.4a Application and verification of numerical results																																				
2.4b Experimental validation																																				
3. Code 2: Turbulent flows with elliptic structure	1	2	3	4	5	6	7	8	9	1	01	11	2 ·	12	3	4	5	6	7	8	9	10	)11	12	1	2	3	4	5	6	7	8	9	10	111	12
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3.2a Grid techniques																																	Т			
3.2b Discretization																																				
3.3 Implementation of code			l					ſ	l	l	1																						T	Τ	T	
3.4 Code validation and verification of numerical results																										_						T	T	Т	T	_
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4. Tools for cluster administration																																				

1.4.1-Code for detailed resolution of incompressible turbulent flows by means of DBS-LES methods (Code1)

- The three-dimensional discretization of Verstapen and Veldman has been implemented in its second and fourth order versions.
- A parallel direct solver for second and fourth order Poisson equations, optimized for low-cost clusters, which permits the resolution of each Poisson equation with just one message, has been developed and implemented.
- Time average functions have been implemented.
- Work on implementation of a new turbulence model analog to LES models is being carried out.
- Direct simulations of natural convection in closed enclosures have been performed.

- The algorithms for the solution of the Poisson equation is being adapted to the new Mare Nostrum computer, in order to use effectively its major computing power. This task, which is of great interest, was not anticipated since neither this equipment existed nor the intentions of its installation were known in the beginning of the project.
- The code is still to extend to non-periodic situations in none of the axis, the implementation of LES models is to finish, and the code is to apply to more situations of interest.



Illustrative results obtained with Code1. From left to right, three instantaneous temperature fields at  $Ra_z = 6.4 \times 10^8$ ,  $2 \times 10^9$  and  $10^{10}$ , respectively, with Pr = 0.71 (air); the turbulent kinetic energy, the turbulent kinetic energy dissipation and the turbulent kinetic energy generation for  $Ra_z = 6.4 \times 10^8$  and Pr = 0.71. Bottom: Instantaneous pressure field for flow past a square cylinder at Re=22.000.

1.4.2-Code for the resolution of flows with approximately parabolic structure (Code2)

- Turbulence coupling formulations, generation ratios on the basis of Eddy break-up models and flamelet models have been carried out and implemented in the code.
- Radiation in participating media and its solution by means of the DOM technique and the Optically Thin Limit approximation have been formulated.
- Parallelization of DOM and its integration to the combustion code are pending.
- Regarding two-phase flows, the modeling has been carried out by means of a VOF model, implementation and application are performed in the design context of the absorption refrigeration systems using the parallel code for flows with parabolic structure.
- Regarding flows in channels of arbitrary geometry, the implementation of pressure and periodic boundary conditions, and the RANS models is completed.
- Coupling radiation in participating media (DOM) with combustion is pending. To do so, it is necessary to modelize the behavior of gas mixtures, implementing a multiband model.



Sample of Code2 results: CFD simulation of a Multifunctional thermal energy storage prototype (in black the streamlines).



Comparison of experimental results and CFD simulations using Code2. Testing of a Multifunctional thermal energy storage. Left: experimentally measured average and outlet temperature. Right: CFD results, also with average temperature (discontinous blue line). Note (i) the good agreement (ii) that CFD simulations provide more data than experiments, the average temperature in this case.

1.4.3-Code for flows with elliptic structure (Code3). The following goals have been achieved:

- Implementation of two-equation turbulence models, introducing anisotropy and nonlinearity
- Implementation of Explicit Algebraic Reynolds Stress Models
- Comparative study of different RANS formulations
- Generalization of RANS models for turbulent flows with moving boundaries
- Studies on the discretization of compressible flow equations. Numerical implementation.
- Generalization of RANS for compressible flows (Favre-averaging)

Sample results of Code3. Pollutant formation. Mole fraction isopleths for: nitrogen oxide, NO (top); nitrogen dioxide, NO<sub>2</sub> (bottom).

Implementation of the Differentially Reynolds Stress Models is pending.

Intensive work has been carried out on non-structured grids and actually a sequential prototype code (in C) to resolve the threedimensional and transient Navier-Stokes equations is available. Other parallel C++ code is being developed, all the basic classes to contain the grids, communications, etc. have been written.

Finishing the sequential prototype for non-structured grids in C, transferring the code to the parallel C++ version, and implementing additional models in this new code, like the RANS-type models, are pending.



This is essentially what is anticipated in the project, except for the delay in the initial phase caused by the use of C++, but the result is expected to be more robust and modular.

1.4.4-Tools for the administration of the PCs

Different codes in order to facilitate the installation and management of the cluster are developed. The selection and implementation of software for parallel queue management is pending.

# 2 Indicators of Results

Information on different indicators that can show the relevance of the results obtained up to now has been included. These indicators consider at least: staff in formation, achieved publications, technology transfer, patents, participation in international projects (especially in the EU), and collaborations with national and foreign groups.

# 2.1 Participation in projects

A narrow collaboration is maintained with the companies that supported this project: Unidad Hermética of Electrolux Group (nowadays CUBIGEL S.A. (Unidad Hermética)); Radiadores Cerezo, Tefrinca. Below are the collaboration projects with the above-mentioned companies, for which the achievements of this project are fundamental:

- Research project n° C04749, Company: CUBIGEL, S.A. (Unidad Hermética)., Period: 2002-2005, Funding: 365.000 Euro, Title: Study of the viability and development of hermetic compressors prototypes working with CO2 as fluid refrigerant.
- CRAFT Programme (ref. CRAFT 1999 71024 "COMHEX"), European Commission, Directorate-General XII. The CTTC is the Research Project Co-ordinator. Period: 2002-2004; Funding corresponding to the CTTC: 351.060 Euro. Title: Optimisation of Gas-Liquid Compact Heat Exchangers Considering Their Interaction with the Rest of the System.
- Research project nº C05652, Company: CUBIGEL S.A., Period: 2005 2006; Funding:108.000,00
  Euro. Title: Optimization of Hermetic Reciprocating Compressors Based on Numerical Simulation
  and Experimental Validation Methodologies. Detailed Study of the Flow through Valves and the
  Piston-Cylinder Leakages.

• CRAFT Programme (Contract No. COOP-CT-2004-513106-EFROST). The CTTC is the Research Project Co-ordinator. Period:2005-2006; Funding corresponding to the CTTC: 476.051,00 Euro. Title: Efficient Refrigerated Food Storage.

The Group maintains contacts and carries out collaborations with various centers/universities and companies, with the common link being the numerical resolution of heat and mass transfer and fluid dynamics phenomena. The majority of these projects is of European scope and performed under our leadership. The most relevant projects are given below:

- CRAFT Programme (ref. CRAF-1999-70878-"STATIC II")(ref. CTT n° E00694), European Commission, Directorate-General XII, Period: 2002-2004; Funding corresponding to the CTTC: 372.562 Euro, Title: Stagnation Proof Solar Collectors Transparently Insulated Flat Plate Collectors - II. CTTC is the research coordinator.
- CRAFT Programme (ref. CRAF-1999-70967-"ASFIC")(ref. CTT n° E00695), European Commission, Directorate-General XII, Period: 2002-2004, Funding corresponding to the CTTC: 396.592 Euro, Title: Advanced Solar Facades with Integrated Collectors-Accumulators for Domestic Hot Water and Space Heating Applications. CTTC is the research coordinator.
- CRAFT Programme (ref. CRAFT 1999 71024 "COMHEX"), European Commission, Directorate-General XII. The CTTC is the Research Project Co-ordinator. Period: 2002-2004; Funding corresponding to the CTTC: 351.060 Euro. Title: Optimisation of Gas-Liquid Compact Heat Exchangers Considering Their Interaction with the Rest of the System.
- CRAFT Programme (ref. CRAFT 1999 70604 "OPICS"), European Commission, Directorate-General XII. The CTTC is the Research Project Co-ordinator. Period: 2002-2004; Funding corresponding to the CTTC: 336.500 Euro. Title: Optimised Integrated Collector Storage: low-cost solar thermal systems for houses and offices.
- CRAFT Programme (Contract N°: ENK6 CT 2002 30033), GREENFACADE. The CTTC is the Research Project Co-ordinator. Period: 2003-2004; Funding: 311.200 Euro. Title: Vegetation for cooling advanced glazed facades: Arquitectural integration, gardening technology, numerical simulation.
- CRAFT Programme (Contract No. 1999 72475), HYDRA. The CTTC is the Research Project Coordinator. Period: 2003-2005; Funding 333.400 Euro. Title: Hybrid latent/sensible compact storage devices for combined thermal solar energy applications: refrigeration, heating and air – conditioning (HYDRA).
- CRAFT Programme (ref. CRAFT 1999 71217 "COMPACT"), European Commission, Directorate-General XII. The CTTC is the Research Project Co-ordinator. Period: 2003-2005; Funding corresponding to the CTTC: 244.168 Euro. Title: Low-cost compact solar heaters made of plastic materials and composites.
- CRAFT Programme (Contract No. COOP-CT-2004-513106-EFROST). The CTTC is the Research Project Co-ordinator. Period:2005-2006; Funding corresponding to the CTTC: 476.051,00 Euro. Title: Efficient Refrigerated Food Storage.

#### **2.2 Publications**

- J. Castro, L. Leal, C.D. Pérez-Segarra, P. Pozo, "Numerical study of the enhancement produced in absorption processes using surfactants", *International Journal of Heat and Mass Transfer*, Vol. 47, p.3463 3476, 2004.
- G. Colomer, M. Costa, R. Cònsul, A. Oliva, "Three dimensional numerical simulation of convection and radiation in a differentially heated cavity using the discrete ordinates methods", *International Journal of Heat and Mass Transfer*, Vol. 7, n° 2, p.257 269, 2004.

- O. García-Valladares, C.D. Pérez-Segarra, and J. Rigola, "Numerical simulation of double-pipe condensers and evaporators", *International Journal of Refrigeration*, Vol 27, p.656-670, 2004.
- M. Soria, X. Trias, C.D. Pérez-Segarra, A. Oliva, "Direct numerical simulation of the threedimensional natural convection flow in a differentially heated cavity of aspect ratio 4", *Numerical Heat Transfer. Part A: Applications*, Vol 45, 2004.
- K. Claramunt, R. Cònsul. C.D. Pérez-Segarra, A. Oliva, "Multidimensional Mathematical Modelling and Numerical Investigation of Co-flow Partially Premixed Methane/Air Laminar Flames", *Combustion and Flame*, Vol. 137, p.444 457, 2004.
- J. Rigola, G. Raush, C.D. Pérez-Segarra, A. Oliva, "Detailed experimental validation of the thermal and fluid dynamics behavior of hermetic reciprocating compressors", *Int. Journal of Heating, Ventilating, Air Conditioning and Refrigerating Research, Vol.* 10, p.291-306, 2004.
- R. Cònsul, I. Rodríguez, C.D. Pérez-Segarra, M. Soria, "Virtual prototyping of storage tanks by means of three-dimensional CFD and heat transfer numerical simulations", *Solar Energy*, Vol. 77, p.179 – 191, 2004.
- G. Raush, J. Rigola, C.D.Pérez-Segarra, A. Oliva, "A novel Sigma-Delta ADC application oriented to test hermetic reciprocating compressors. *Measurements Science and Technology*, Vol. 15, p.2207-2214, 2004.
- C.D.Pérez-Segarra, J.Rigola, M. Soria, A. Oliva, "Detailed thermodynamic characterization of hermetic reciprocating compressors", *International Journal of Refrigeration*, Vol. 28, No.4, p.579-593, 2005.
- J.Rigola, C.D. Pérez-Segarra, A. Oliva, "Parametric studies on hermetic reciprocating compressors", International Journal of Refrigeration, Vol. 28, No.2, p.253-266, 2005.
- F.X.Trias, M.Soria, C.D.Pérez-Segarra, A.Oliva, "A direct Shur-Fouriere decomposition for the efficient solution of high-order Poisson equations on loosely coupled parallel computers", *Numerical Linear Algebra with Applications*. In press.
- C.D.Perez-Segarra, C.Farre, J.Cadafalch, A. Oliva, "Analysis of different numerical schemes for the resolution of convection-diffusion equations using finite volume methods on three-dimensional unstructured grids. Part I: Discretitzation schemes", *Numerical Heat Transfer. Part B: Fundamentals*. In press.
- C.Farre, C.D.Perez-Segarra, M.Soria, A. Oliva, "Analysis of different numerical schemes for the resolution of convection-diffusion equations using finite volume methods on three-dimensional unstructured grids. Part II: Numerical analysis", *Numerical Heat Transfer. Part B: Fundamentals*. In press.

#### 2.3 Doctoral thesis

Two doctorate thesis have been performed within the framework of the present TIC project and the last period of the previous one. The maximum qualification have been obtained in the two theses: Kilian Claramunt Altimira (February 2005), "Numerical simulation of non-premixed laminar and turbulent flames by means of flamelet modelling approaches", and Jesús Castro Gonzàlez (May 2005), "Simulation of heat and mass transfer phenomena in the critical elements of H2O-LiBr absorption cooling machines. Experimental validation and application to design". In September, the thesis "Development of experimental and numerical infrastructures for the study of compact heat exchangers and liquid overfeed refrigeration systems" by Stoyan Viktorov Danov will be read. Three more thesis will be read within the next year.