CEDRE Software

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This article gives a general description of the CEDRE® system. CEDRE® is a multi-physics platform working on general unstructured meshes intended to both advance research and process industrial applications in the fields of energetics and propulsion. The system includes a graphical user interface for data entry and a set of pre and post processing utilities. The code is organized as a set of solvers, each of which can be used to handle a particular physics, which are coupled together for the computations. Here, we briefly present the solvers: reactive gas CHARME, Eulerian dispersed phase SPIREE, Lagrangian SPARTE, conduction ACACIA, FILM for studying liquid films, radiation ASTRE and REA, as well as the Peul solver. Other programs can be used to handle other physics that are not part of energetics, such as mechanics, by means of external couplings, using in particular the in-house CWIPI library. We have made several general remarks on parallelism, as performance cannot be considered independently from the computing code. The organization of development and the importance of configuration management are highlighted and stress is put on the validation process, which is of the utmost importance for qualifying the quality of results.

Introduction

CEDRE® is a multi-physics platform on general unstructured grids, for both research and industrial applications, in the fields of energetics and propulsion. The software architecture follows a multi-domain, multi-solver approach. Solvers are considered for each physical system: gas phase, dispersed phase, thermal fields in solids and radiation. These solvers share the CEDRE architecture and libraries, and can be coupled to perform a multi-physics computation or be operated alone. This calculation chain, which includes a graphical interface for data input, geometrical pre-processing, the calculation itself and post-processing, has capabilities oriented towards research, as well as industrial users (Astrium-ST, MBDA, Snecma, SPS, etc.). The software must meet the needs of industrial partners: decreased cycle design time, increased geometrical complexity, unsteady, multiphysical modeling and reduction of the costs. The application scope of the software includes jet engines, ramjets, rocket motors for missiles and launchers. Computations cover the fields of aerodynamics, aerothermal coupling (heat transfer), combustion, water ingestion, icing, propulsion, and aeroacoustics (jet noise, combustion instabilities). For application examples see [29].

Process description

There are relatively few developers, given this ambitious objective. Every one of them has an expertise limited to just one or to a few technical domains (numerical analysis, modeling, graphical interfaces, meshing, computer science, parallel computing, etc.) with little overlap between individual skills. Moreover, contributors belong to several departments and sites, and often share this activity with other tasks. Some of them are PhD students for whom CEDRE is primarily a test facility for numerical methods and physical models.

A large fraction of developers also use the code in the frame of research projects. In all cases, it is expected that newly implemented methods and models will become quickly available for Onera and for industrial users. The development process has been designed to meet the above constraints.

All the elements of the project (source code, test cases, documentation, etc.) are stored in a single database, and are accessible to all developers, which facilitates exchanges and collaboration. The limited number of developers does not allow for lengthy specification documents. Instead, specifications are based on one or several

scenarios, including the desired functionalities, numerical methods or physical models, which are divided into simple development cases, included in the project database prior to any development. The results given by the code for these scenarios evolve along with the developments, until they meet the expected functions and results. All along the development process, frequent interactions between users and developers allow the appropriate match between needs and work to be checked. At the end of the development, scenarios can be used as a part of acceptance tests, and are later kept in the project database as non-regression tests.

Every development is split up into several tasks, each lasting only a few days: the size of a task depends on the nature of the development and developer preferences, but each must fulfill all non-regression tests. Besides new methods or implementation models, many tasks may include or even be entirely devoted to code refactoring, which generally aims at simplification, optimization, safety or better error handling.

Development and integration can thus follow a very short cycle, with one version per week approximately. This version meets all non-regression requirements on the development machine, and runs on the two main high performance computers of Onera. This continuous development and integration process prevents divergence between individual versions of the project, and hence facilitates integration of a large flow of new models and methods. Furthermore, it allows a very fast feedback from Onera developers and users, so that most bugs are generally fixed fairly quickly. In the same way, a rapid feedback from users is optimal for model and method improvement. In addition, annual releases are also delivered for users who need to run it on specific machines or stable versions according to their internal processes, and β versions are designed for industrial users in case of urgent need for new functionalities.

The above process shares several features with Agile software development as XP (eXtreme Programming) (test based and iterative development, collaboration with users, frequent deliveries, regular refactoring etc.) without corresponding precisely with any officially formalized method because of the specificities of the project [11].

Configuration Management

Configuration management is the backbone of the project, because of specificities of the same: multi-departments, multi-sites, and multi-profiles developers. The software is mainly developed by several departments of the Onera, and involves three geographical sites although, from a computer network point of view, we can consider that we are in the presence of a single set, all the sites being interconnected with each other by a fast network.

The developer profile is either permanent, occasional, or PhD students. It is necessary for all developers to be in the same environment, because one main target of the project is the production of a competitive code for our industrial partners, that is, of a software that integrates the latest results of the advanced research, as quickly as possible. For this reason, it is necessary to have a friendly and successful tool, and the choice was made of a known commercial product, CM-SYNERGY® [32]. The interface allows the state and the history of an object to be displayed all the time (an object being in practice a file). The color associated with an object defines its state of development, predefined in the process (working, integrate, release, etc.). This product was chosen because it proposes a task based approach, which represents a logical change (evolution or correction) brought to the software. All the objects modified within the framework of a task are automatically associated to it. The integration is thus made by blocks of objects consistent with a task. A set of tasks is then included in a folder, which contains a set of new features that can be delivered to the users. This tool, which uses an Informix database, is more than a configuration management, it is a change management tool that integrates the traceability of the requests of the users (playing the role of problem report, or bug tracking, according to various used terms). It is very easy to obtain all types of statistics (by date, by user, by type of requests, by severity, or by element of the chain of calculation). Some figures show the necessity of such a tool: for the 3.1 release, the base size was 53 GB, the number of tasks created since the beginning of the implementation of this approach was 7900, and the number of Change Requests was of the order of 1000. The development of the code represented 4500 Fortran procedures just for the numerical solver part.

Mesh pre-processing

The calculation chain can use mesh data from many academic and industrial meshers. Some of these have direct output in the CEDRE format (Icem®, Centaur®, Harpoon®, Hexpress®, Star-ccm+®), whereas CEDRE provides a conversion utility from standard output for Gmsh, Gambit®, Cgns© formats, etc.

Geometrical pre-processing also includes many useful features, such as topological and metric verification, mesh connection calculation and mesh merging along a common surface. However, the key pre-processing is mesh partitioning with Metis [23] or Splitmesh (internal development), which is the basis for splitting the workload on the available calculation cores. Today, there is no sophisticated approach in the software to consider calculation/communication costs while assigning subdomains per processor. In the future, it is necessary to work to define the most optimal strategy.

CEDRE and its solvers

Common levels and solvers

The code itself consists of several solvers dedicated to physical subsystems: fluid calculation, Lagrangian and Eulerian solver for dispersed or diluted particles, heat conduction in solid walls, thermal radiation, stochastic reaction models, liquid films, etc. Many functionalities and models are common to several or all solvers, and are fulfilled by common libraries, for instance:

- all geometric calculations (cell volumes, surface vectors, Gauss points, wall distances, etc.) are performed at the common level for all solvers. This includes kinematics in the ALE case and mesh intersections for overlapping grids, general polyhedral mesh, etc.;
- thermophysical properties are calculated by a common library called Thermolib. The thermophysical model of CEDRE includes all the data and the procedures allowing the thermodynamic properties and transport coefficients of any material environment susceptible to participate in the multiphysical system, such as it was defined by the

user, to be calculated. This part is described in [8] and includes real gas of various state equations.

Finally, the common level of course includes interactions between solvers.

The fluid solver Charme

The continuum is a mixture of an arbitrary number of species, each species having its equation of state. The state of the mixture is defined by the densities of the species, together with the total energy and the momentum per unit volume. Governing equations are:

- mass conservation for every species, including source terms if chemical reactions are present;
- energy balance for the mixture;
- momentum conservation equation for the mixture.

In practical applications, velocity may cover a very wide range, from low Mach numbers to hypersonic speeds. Turbulence is present in most simulations and is taken into account in the LES (Large Eddy Simulation)[2] or RANS (Reynolds Averaged Navier-Stokes equations) approach. In the latter case, additional scalar quantities and balance equations are added to the aerothermochemical system to describe the macroscopic properties of turbulence. For most models, these quantities include the mean kinetic energy of turbulence, and an additional scalar may be dissipation, length scale or frequency.

Many types of boundary conditions are available, including:

- inlet-outlet with various sets of imposed fixed variables and options for swirl, radial equilibrium, mixing plane, non-reflection etc.;
- symmetry, axis, no-slip;
- spatial periodicity;
- walls with various heat transfer boundary conditions, and variants for porous walls or solid fuel motors.

Space discretization is described in [3]:

- the general framework is the cell-centered finite volume approach, on possibly moving and deformable control volumes (ALE formulation);
- interpolation follows a MUSCL type methodology. For each degree of freedom, space derivatives are evaluated algebraically from some neighborhood of the current cell, which allows a polynomial reconstruction on each cell;
- this reconstruction gives rise to two distinct evaluations of each variable at every point along the interface between two cells. After limitations for monotony, these evaluations are used as input for approximate Riemann solvers;
- cell reconstruction is also the basis for interface gradient and Navier-Stokes flux evaluation.

Time integration is described in [3]:

- classical Runge-Kutta methods are used in many unsteady simulations. In some cases (low Mach number flows for instance), implicit generalizations of these methods can be useful;
- Euler implicit method can be used at large time intervals when a steady solution is expected.

For implicit schemes, large sparse linear systems are solved at each time interval with the help of the Generalized Minimal Residual method (Gmres).

The conduction solver ACACIA

This solver is used for conductive heat transfer in solid walls, which are considered as an incompressible medium without deformation. The only state variable is thus temperature, which is governed by energy conservation:

- the heat flux is subject to the isotropic Fourier law, conductivity and specific heat being given functions of temperature. More general models are planned, for example, to deal with anisotropic media;
- sources can be considered to simulate the Joule effect, or other energy inputs.

Several types of boundary conditions are available, the most useful one being a quasi-linear relationship between heat flux and boundary temperature:

- this condition can simulate convective and radiative heat transfer in an environment with prescribed temperature;
- it can also be used as the basis for fluid-solid coupling when the fluid is calculated via the flow solver Charme.

Numerical methods are very similar to those defined for the fluid solver:

- finite volume space discretization is based on a linear reconstruction on each cell, temperature gradient being calculated through a least-squares formula. Interface gradients between two cells are computed through an interpolation formula, using state variables and gradients in both cells;
- various explicit and implicit time integration schemes are available, for instance the Euler implicit method with Gmres resolution.

The Eulerian dispersed phase solver SPIREE

The Eulerian solver called SPIREE is devoted to the computation of dispersed two-phase flows which is of major importance for many applications in the aerospace context. In the case of dispersed flows, one phase is assumed to be diluted (typical values of the volume fraction lie between 10^{-5} and 10^{-2}) and the influence of the inclusions on the carrier phase is taken into account through the introduction of source terms on the solver CHARME.

As we mentioned, SPIREE is based on the Eulerian resolution of conservation equations for some particular moments of the number density function. These equations can be formally derived from the kinetic equation introduced by Williams in [39] or [40] by assuming particular closure assumptions. Two general options are possible in the code. The first one is the sampling method, in which the number density function presumed can be written under a sum of Dirac in size. The second one, recently implemented into the code, is called the “multi-fluid” model or sectional method and has been introduced in [15].

A system of conservative equations is derived for each class or section, and then solved by a classical Finite Volume Formulation on unstructured meshes. Now, we describe the principal ingredients concerning physical modeling and numerical method implemented into the solver.
Concerning the numerical method, the convective part of the system is solved using upwind schemes based on Flux-Difference-Splitting, or on the resolution of the Riemann problem for particles [4]. The second order accuracy for spatial discretization is obtained thanks to MUSCL techniques [37]. Both explicit and implicit are used for time integration, based on Runge-Kutta method of order 1 or 2. Recent developments

concern kinetic schemes for the spatial discretization of the convective part of the system, as well as splitting method in the time integration, in order to have specific algorithms for stiff source terms.

Concerning the modeling of forces acting on particles, Drag force is implemented in the solver with different correlations. If we consider a Stokes regime, the expression of the drag force is very simple. However, if the Reynolds number increases, the Schiller-Naumann correlation [30] for example, has to be employed. For compressible regimes, a specific correction based on the relative Mach number is applied on the drag coefficient. Gravity and Unsteady acceleration source terms are also implemented in the code.

Evaporation phenomena and Heat transfer are of course implemented in the solver, and are a key issue for combustion problems in aerospace applications. Thermal transfer is implemented. Several evaporation models derived from the d2-law [31], such as for example the Abramzon-Sirignano model [1], are implemented. A N-layer model that allows the description of the detailed internal temperature distribution inside the particle is in preparation. Specific models for Aluminum combustion are also implemented.

In the sectional approach, interactions between particles are taken into account. Coalescence phenomena are still implemented, while secondary break-up is in the final step of implementation.
In regard to boundary conditions, the solver includes: inlet-outlet with various sets of imposed variables, symmetry, axis, slip conditions and spatial periodicity.

The solver is principally used in Liquid and Solid propulsion. Some recent applications of the solver also concern the prediction of ice formation on aircraft [26] [24].

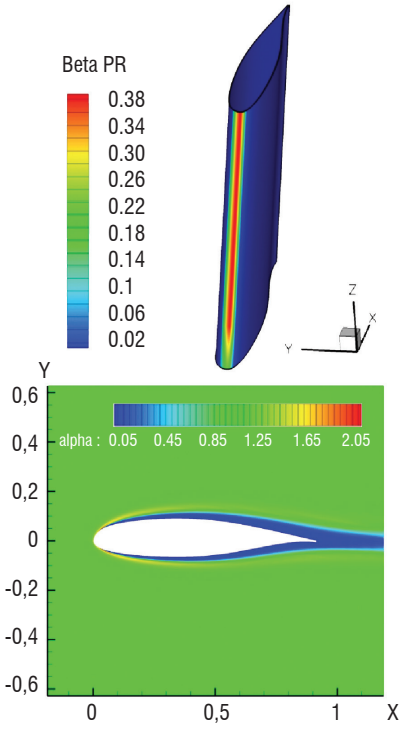

Figure 1 – Water catch collection coefficient (top) and droplet flux of mass (bottom) on the wing

The Lagrangian dispersed phase solver SPARTE

The SPARTE solver is devoted to the simulation of a dispersed phase (composed of solid particles or droplets) suspended in a gas flow. It is based on a Lagrangian approach which means that the particulate phase is simulated by solving the motion of a large number of numerical particles (parcels) in space equipped with variables of time, position, velocity, size and temperature, or other relevant quantities. The mean dispersed phase properties are obtained by averaging over a representative sample of parcels that cross a defined volume, within a certain time interval.

The particulate phase can be composed of particles of different physical states (solid or liquid) and of different chemical composition. Specific models (for heating, phase change …) may be chosen independently for each type of particle. In the present version, the following models are available:

- drag force, inertial forces (rotating frame);
- heat exchange;
- fusion/solidification, evaporation/condensation, multi-component evaporation/ condensation;
- collision/ coalescence;
- droplet secondary break-up;
- complex particle/wall interactions : inelastic bouncing, splashing, deposition, etc.;
- turbulent dispersion.

Most of these models are described in [25].

Two variants of the stochastic particle method can be used depending on the particle mass loading, and on whether the flow is stationary or not: the steady particle method (very efficient but with a limited range of applications) and the unsteady particle method (much more expensive but with a wide range of applications). The principles of these two methods are explained in [25].

As regards the boundary conditions, the following are currently available:

- walls with various interaction models;
- inlet with particle emission;
- outlet (free boundary);
- spatial periodicity;
- mixing plane (for a surface separating a rotating domain from a fixed one).

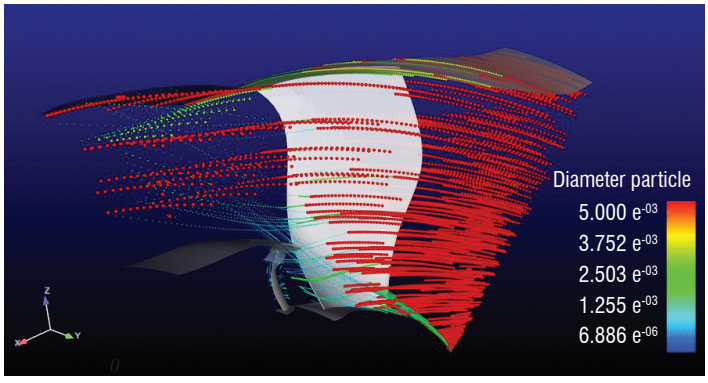

Figure 2 – Example of hail particle trajectories colored by their diameter through a turbojet engine (fan and IGV)

The FILM solver

The so-called "FILM" solver is devoted to the computation of wall liquid films formed under multi-physics configurations (Figure 3). The solver uses an Eulerian approach to solve film equations over a three dimensional complex surface. The FILM geometry (a surface mesh) is built beforehand from the CEDRE geometry (a volume mesh).

The liquid film equations are written in an integral form (integration across the film thickness of the Navier-Stokes equations, with a no-slip condition at the bottom), and solved using a 2D finite-volume scheme [1]. The liquid Reynolds number is assumed to be small enough for the film flow to be laminar. The film thickness is obtained by solving the integral continuity equation. If the film thickness is small enough to neglect the inertial forces in comparison with the other forces (gas shear stress, film viscosity, etc.), the flow rate can be expressed as a function of the thickness. This model is called the "one-equation model" because it only requires the integral continuity equation to be solved. A second model is foreseen to treat the case where the mechanical equilibrium is not verified locally. It is called the "two-equations model" because in addition it solves the integral momentum equation (see shallow water equations).

The FILM solver is coupled with the gas phase solver CHARME for modeling the shear driven force and the pressure effects on the film motion. The disperse phase solver computes the source terms for modeling the film formation by spray impingement [27]. The FILM solver is currently coupled with the Lagrangian solver SPARTE, in which models for droplet-wall interactions have been implemented (splashing, deposition, etc.). Coupling with the Eulerian disperse phase solver SPIREE is possible as well. The FILM solver is parallelized in the same way as the other solvers. The FILM sub-domains are the surface projection of the 3D-geometry sub-domains. Therefore, there are not external exchanges between processors for data transfers between solvers.

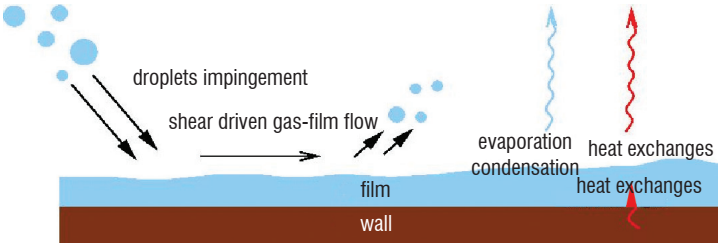

Figure 3 – Wall liquid films formed under multi-physics configurations

Radiation solvers

In the CEDRE code, two radiation solvers have been developed: one, called REA [18], is based on a discrete ordinate method, while a Monte Carlo method is implemented in the other, named ASTRE [7][33][34]. These two methods are complementary.

The discrete ordinate method is based on a discrete representation of the directional variation of the radiative intensity. Thus, the radiative transfer equation, the integro-differential equation describing the evolution of the spectral directional radiative intensity, is replaced by a system of partial differential equations involving intensities that are angularly averaged over each ordinate direction (one equation for each ordinate direction). Integrals over a range of solid angles are approximated by weighted sums over the ordinate directions within that range (use of a numerical quadrature).

Applied to thermal radiation problems, the Monte Carlo method consists of following a finite large number of energy bundles (an energy bundle is a discrete amount of energy, which can be thought of as a group of photons bound together) through their transport histories, from their point of emission to their point of absorption. Bundle characteristics (wavelength, initial direction, point of emission) and physical events along bundle trajectories (absorption, scattering, reflection on walls) are chosen according to probability distributions by drawing random numbers.

That is why Monte Carlo simulations are often referred to as direct simulations of radiative transfer by statistical distributions of energy over space, direction and wavelength, and results obtained with Monte Carlo methods are often considered as reference solutions. Since Monte Carlo methods are statistical, exact results can be approximated if enough bundles are followed. Another advantage of Monte Carlo methods is that even the most complicated problem can be solved with relative ease.

At the present time, REA is dedicated to radiative transfer calculation in solid propellant rocket motors. Gas radiative properties (H_2O, CO_2, CO and HCl) are approximated by a box model. Two sets of parameters are available in REA for this model: the set used by Joumani [18], and the one obtained by Duval [9]. Radiative properties of alumina particles (Al_2O_3) are calculated from the Mie theory. REA is coupled with the CHARME and SPIREE solvers. A domain decomposition technique is used to parallelize REA: each core involved in the simulation deals with only one part (which consists of one or several sub-domains) of the whole domain.

Three kinds of gas radiative property model can be used in ASTRE: Correlated-K model (CK), Statistical Narrow-Band model (SNB), and box model. Several sets of parameters for these three kinds of model are available in ASTRE. Moreover, soot, alumina and water particles, and turbulence-radiation interaction can be taken into account. All these models allow radiative transfer calculations in a wide range of applications: air breathing combustion (laboratory flames at atmospheric pressure [33][35][36] and aeroengine combustors [22]), solid propellant rocket motors, atmospheric (re-)entries [5][6][8], glass forming [5], etc. On the one hand, ASTRE is a solver of CEDRE coupled with the CHARME, PEUL and SPIREE solvers; on the other hand, ASTRE is an independent radiative transfer code able to be coupled to other codes (ZeBuLoN [5], CELHYO [17][19][28], ABAQUS [22], ANSYS [22], N3S [22], etc.) according to the considered application. Since all the bundles are statistically independent, the parallelization of ASTRE is carried out by distributing the bundles over the cores: N_{core} bundles are followed simultaneously, where N_{core} is the number of cores involved in the simulation. It is easy to implement such a parallelization, but memory storage problem may be encountered when the mesh is composed of a very large number of cells. Because there is no required communication among parallel cores during bundle history generation, the parallelization efficiency is close to 100%. Recently, this property of ASTRE was checked for various numbers of cores (from 16 to 2048 cores).

To obtain more information about these two solvers, the reader may refer to [19] dedicated to radiative transfer modeling used at Onera in CFD simulations.

Box 1 - External coupling

For the simulation of domains not included in the CEDRE package, such as aeroelasticity or solid mechanics for instance, external coupling with other software is available. Thus, CEDRE can be coupled with various finite element analysis solvers, such as ABAQUS, MARC, and ZeBuLoN [B1-01]. Among large Fluid-Structure Interactions (FSI), the system coupling methods make it possible to solve steady or unsteady thermal problems, as well as structure deformation problems.

In the coupled approach used, the FSI is achieved by partitioning the problem into fluid and solid parts solved separately with boundary conditions calculated by the other part. In this partitioned procedure, the coupled problem is numerically solved using a Conventional Serial Staggered approach. In all these FSI computations, matching grids between fluid and solid are employed and therefore no non-matching load transfer scheme needs to be used.

The transfer of the physical data is performed by the coupling library MpCCI™, developed at the Fraunhofer Institute. Among all the benefits, we can report software interchanging, independent modelling and various integrated interpolations. MpCCI™ can also be used on heterogeneous distributed platforms. It allows the coupling of more than 2 codes through surface or volume.

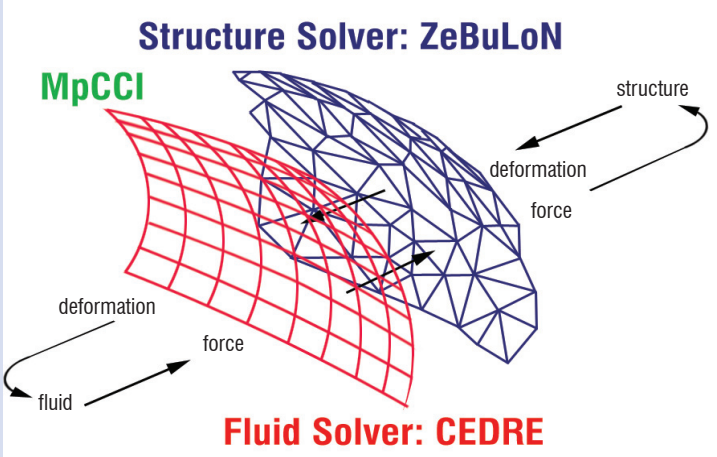

Figure B1-01 – CEDRE - ZeBuLoN coupling

Still, in a near future, the SDK version of MpCCI™, which is implemented in the CEDRE and ZeBuLon codes, may be replaced by a less flexible version named Code Adapter. Given this uncertainty, Onera has decided to develop its own coupling library CWIPI.

The PEUL solver

The PEUL model "Probabilistic Eulerian Lagrangian model", consists, on the one hand, in solving the balance equations of mass, momentum, energy, k (turbulent kinetic energy) and ε (dissipation rate of k), using a usual Eulerian discretization method and, on the other hand, in solving the thermochemical composition PDF (Probability Density Function) equation, by means of a stochastic Monte Carlo method. The characteristics of the stochastic particles are the same as those of the reactive turbulent flow. The trajectory and the composition of the gas particles are described by the equations:

$$\frac{dx_i}{dt} = < V_i > + V_i'$$

$$\frac{dY_a}{dt} = \frac{< Y_a > - Y_a}{\tau} + w_a$$

where $< V_i >$ is the average velocity given by the Eulerian resolution of the balance equation; V_i' is a velocity fluctuation calculated by a turbulent dispersion model. Y_a stands for the mass fraction of the ath chemical species $(1 \le a \le n)$, or for the enthalpy of the particle $(a = n+1)$. $< Y_a >$, the average value of Y_a, is provided by the Eulerian calculation. τ is a microscale mixing time evaluated from the turbulence model. w_a is the chemical source term of a a^{th} species.

A PEUL calculation provides information about velocity, temperature, production rate and mass fraction of species of the particle, as means Lagrangian quantities. Thus, the PEUL model can treat different combustion regimes, and it is particularly adapted to calculate complex kinetics. It can be used in many applications in the domain of aircraft combustors, ramjet and scramjet and rocket engines.

The PEUL model is written as a solver of the CEDRE. This enables many physical phenomena (combustion-radiation, combustion-two phase flow, etc.) to be taken into account, thanks to solver coupling (PEUL-ASTRE-CHARME, PEUL-SPIREE-CHARME, etc.). Actually, the PEUL solver is coupled with the CHARME solver (one way coupling) and can calculate the production of pollutants in multi-domain configurations. Future work concerns the parallelization of the PEUL solver in order to simulate complex industrial configurations.

Validation procedure

The validation database is a key component of the project: it capitalizes a large number of computations performed with CEDRE, and compares

Box 2 - CWIPI

CWIPI (Coupling With Interpolation Parallel Interface) is a library that makes it possible to couple n parallel codes with MPI communications. Coupling is made through an exchange zone that can be discretized in a different way on any coupled code. Linear, surface or volume couplings are available. CWIPI takes into account all types of geometrical elements (polygon, polyhedral); there is no requirement about the mesh nature. CWIPI contains the following functionalities: control of coupled processes, geometrical location, interpolation, field exchange and visualization file building. The application programming interface is available in Fortran and C/C++. CWIPI can thus couple codes written in different languages. Some functionalities are called from the FVM library [13].

The coupled applications must be launched in the same MPI environment. During the initialization phase, CWIPI creates an internal communicator for each code. For every coupling defined by the user, inter communicators are created between coupled codes. From the user point of view, the inter-application communications become completely transparent even if the applications are parallel.

The user can define coupling algorithms by the use of the control parameters. These parameters are global variables that are synchronized and shared between coupled codes. By default, no variable is defined. For example, the user can define some control parameters to exchange the convergence state or the simulation time.

The field projection from a mesh A to a mesh B is carried out in three steps. The first one is the location of degrees of freedom of mesh B in mesh A. Three levels of location are defined, the first one is the partition number of the mesh, the second one is the cell number in the selected partition, and the next one is the mean values [16]computed in the selected cell. The second projection step is based on the interpolation mean values. This method is linear; the user can customize the interpolation with call-back definition. The next projection step is the interpolated field exchange.

CWIPI exports all result to Ensight™ gold format files to visualize exchanged interpolated fields.

them whenever possible with the experiments carried out at Onera or other organizations, for example see [6].

The validation procedure was defined in an Onera quality report, which is partly based on the work of [14] and illustrated in [38]. A validation report is generated at each new release version of CEDRE.

CEDRE validation is based upon test case computations. A test case may feature several subcases, which consist in changing physical model parameters. In CEDRE version 3.2, the test cases fall apart in the database in 4 distinct levels according to their complexity:

- Level 1 is divided into 9 cases and 17 subcases, and refers to “academic” test cases, where simple geometry and well known physics are implied. In many cases, an analytic solution allows precise comparison with calculations;
- Level 2 features 11 cases and 13 subcases, and deals with basic functions in a simple physical context. Analytical solutions are generally not available, but comparisons between several approaches are often possible;
- Level 3 comprises 9 cases and 14 subcases, it deals with elementary well instrumented technical devices. Physical models tend to be more complex, but the quality of the measurements allows significant comparisons with experiments;
- Level 4 includes 6 cases and 7 subcases, and is concerned with complete industrial configurations. Detailed measurements are generally not available, but global results can still be compared with the actual device.

Until now, test case database organization was rather historical (aggregation of user issues), with no physical classification. Furthermore, subcases were not systematic, and some physical models were under represented. All this contributed to an opaque validation procedure.

Thus, a new structured database must be built. Other validation logics are available worldwide, such as for instance the institutional Ercoftac database [10], or Craft Tech software editors CRAVE database [21]. These databases are split into main physical problems and applicative challenges.

To apply this structure on CEDRE, we must identify the main scopes of CEDRE applications:

- aeroacoustics;
- aerodynamics;
- aerothermics;
- combustion.

Each of these disciplines relies on a main basis physics, for instance, for aerodynamics:

- free flows;
- wall flows;
- confined flows;
- flows around bodies;
- ...

All of these main basis physics may then be combined into one complete list, which will be used as a second entry on the test case matrix. On the line corresponding to a test case, ticks will mark the basis physics implied. For instance, rib test case is classified horizontally as sub-level 3, and vertically matches 3 aspects of basis physics (wall flows, imposed detachment, and heated wall).

This way, it increases the benefits of the existing database structure: each test case will be located once horizontally (according to the sublevel) and one or more times vertically (according to the basis physics). Finally, another asset of this new database is to clearly emphasize the missing cases in the actual one.

Parallel Performance

CEDRE has proven for long to be a successful parallel code. Parallel computing uses the MPI library on the computational domains. On the former Onera cluster, usual computations would use up to 64 processors (the limitation was due to the batch class structure), while CEDRE is computed on 256 sub-domains, with 4 sub-domains on each processor. The process of distributing several sub-domains per calculation core makes it possible to take into account the memory available on various machines. An example of such a divided domain is given in Figure 4, with 256 small domains.

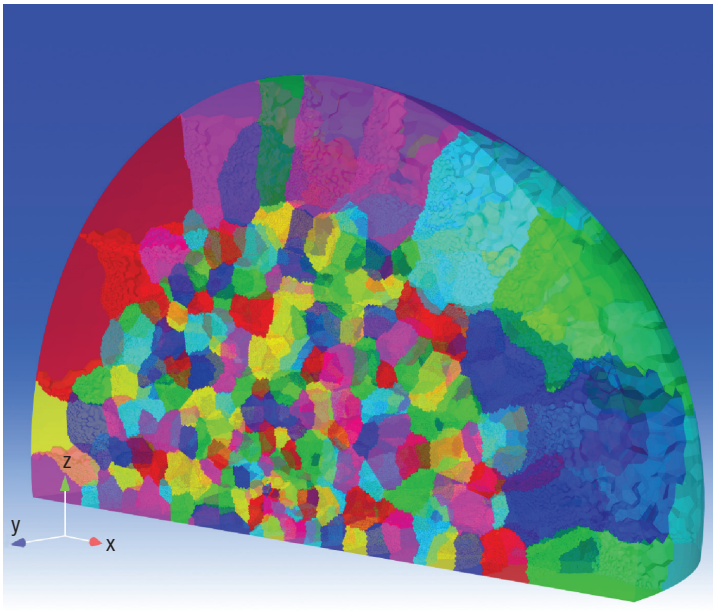

Figure 4 – An example of domain partition with CEDRE[29]

The constant increase in the need for computational power led to wonder whether CEDRE could be run on larger clusters. Recently, a computation was carried out on Onera's cluster (SGI cluster with 3000 Nehalem cores), and used 999 processors with success. The total restitution time is slightly inferior to the one obtained on previous computations (when applying scale factors corresponding to the difference in face number or the change of processors). CEDRE can be said to be supra-linear as illustrated in Figure 5 (the origin of the curve is 10 CPUS and not 1, because the case is too large to run on one processor). Two explanations are possible to explain this trend, first an effect of the processor architecture, the smaller the data to be treated are, the more they go into the cache of the processor. Second for implicit schemes, the major effect in the GMRES method is that the smaller the domains are, the less there is of calculation, because there are a fewer internal iterations, and we converge faster.

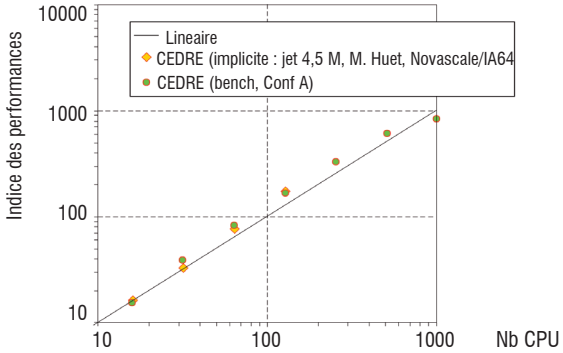

Figure 5 – Example of CEDRE performance on parallel computers

Project features

The project gives users an external Web site [41], but also an in-house directed site project for access to management configuration plan, project management and quality plan, rules of programming, and a large number of quality procedures. The software is protected by a key mechanism and offers the possibility of private functionality. Users are invited to participate in the CEDRE users conference, which is organized annually.

The user support set up is organized on two levels; the second level corresponds to problems that need an advanced knowledge of the code, of an application point of view, while the first level concerns installation or basic problems faced by users. Even if the number of users is restricted enough, one average year of support represents 1500 exchanged e-mails, more than 100 phone conversations and direct visits, to treat on average 270 requests.

The process of code porting is organized according to 4 phases: debug, which uses the lowest level of optimization and activates the most rigorous options of the compiler (not initialized variables, programming non-in compliance with the standard,…), optimization averages (of type -O2), which allows a reference base of non-regression to be obtained, then a final phase (type -O3) allowing to have an optimized code.

The non-regression is made on the output data; however, an additional phase defines some case tests, making it possible to ensure that there is no regression on the performance CPU of a version delivered to the other one. This operation is repeated on all of the code supporting machines (NEC SX-8, Intel Nehalem, Itanium, and IBM Power 6, x 86-64, etc.). The heart of the calculation of solvers is written in Fortran 95, a choice made because of the simplicity of the language, which contains all the features of modern languages (pointer, derived type, dynamic allocation, recursive procedure, overload of operator, module). Some Fortran 2003 features can be used if they are available on all of the available compilers (xlf95, pgi, ifort, sxf90), the portability must take into account all of the present machines, for our industrial partners.

The input/output part and certain utilities of the chain of calculation are written in C ++ there. The fact of having a standard language 'far from the system', and of reducing the number of languages, allows to limit the problems of code porting. The fast evolutions of the code made complex the management of the former versions of the input files (for example for the Graphical User Interface), to solve this problem, former ASCII files are today XML format files. This format was also retained for the thermodynamics data. The output files remain in a binary format owner, making it possible and guaranteeing a little endian/big endian portability ■

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Acronyms
LES (Large Eddy Simulation)
RANS (Reynolds Averaged Navier-Stokes equations)

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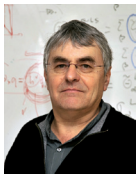

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