XL CILAMCE
IBERO-LATIN AMERICAN CONGRESS ON COMPUTATIONAL METHODS IN ENGINEERING
NOVEMBER 11-14, 2019
Praiamar Natal Hotel & Convention
Natal, RN-BRAZIL

FEM PARALLEL FRAMEWORK USING OPENCL AND MULTIPROCESSING APPLIED TO COMPRESSIBLE TURBULENT REACTIVE FLOWS ON ROCKET ENGINES WITH THE NEW SUBGRID CLOSURE MODEL

Ruhan Ponce
Emanuel Rocha Woiski
João Batista Campos Silva
Elaine Maria Cardoso
ruhan.ponce@unesp.br
woiski@gmail.com
jbcampos.silva@gmail.com
elaine.cardoso@unesp.br
UNESP –São Paulo State University, Post-Graduation Program in Mechanical Engineering
Av. Brasil, 56, 15385-000, Ilha Solteira, SP, Brazil

Abstract. The objective of this work is to develop a methodology for the numerical analysis of a turbulent compressible reactive transient flow of a homogeneous premixed mixture within a convergent-divergent nozzle, applicable to rocket engines. The equations of continuity, momentum, energy and conservation of chemical species are discretized by applying the Galerkin finite element method through the CBS (Characteristic Based-Split) stabilization procedure. The Flamelet/Progress Variable scheme is employed to simulate the combustion process and capture the flame front behavior. For the modeling of chemical kinetics Cantera® software is employed which uses GRI-3.0, a combustion mechanism that contains 325 reactions and includes 53 chemical species as combustion products. In the context of turbulence, the LES methodology with the novel subgrid closure model will be applied. For the temporal and transient resolution, the Euler explicit scheme was applied, while for the spatial behavior the Element by Element (EbE) method was used, based on the Biconjugated Gradient method for the linear systems resolution, incurring the low memory space associated to local full matrices. A solver was developed in Python, deploying Object Oriented Programming (OOP), with the algebraic system resulting from the temporal and spatial discretization of finite elements combined with homogeneous and heterogeneous parallelism, with CPUs and GPUs through the control of multiprocessing, multithreads and using the OpenCL library. to this type of analysis.

Keywords: LES, Multiprocessing, Combustion, CBS, Parallel Programming, Python

Symbols

ρ	Density	u	Velocity	δ_{ij}	kronecker delta
E	Total energy	Y	Mass fraction	V	Diffusion velocity
τ	Shear stress	$p*$	Static pressure	q_j	Heat source
$\overline{\square}$	Average scalar	$\widetilde{\square}$	Filtered variable	$\square^{sgs}$	Closure subgrid variable
$\dot{\epsilon}$	Strain rate	ν_t	Turbulent viscosity	C_ν	Smagorinsky constant
$\overline{\Delta}$	Characteristic length mesh	Sc_t	Turbulent Schmidt number	Pr_t	Turbulent Prandt
M	Mixture total mass	W_k	Mass specie k	N_s	Number of species
μ	Dynamic viscosity	e	Internal energy	E^*	Energy spectral distribution
κ	Fourier turbulent modes	$\mathbb{G}$	Non-normalized Progress Variable	ζ	Normalized progress variable
$\alpha^t_{\mathbb{G}_\zeta}$	Turbulent diffusivity	k^{sgs}	Subgrid kinetic energy	η	Kolmogorov scale
R	Ideal gas constant	R_u	Universal gas constant		

1 Introduction

With respect to the subsystems of a launch vehicle, the study developed by Chang [1] shows the failure frequency with respect to each component. The propulsion subsystem accounted for 62.3% of launch failures in the world between 1983 and 1988, 50% for the United States, 71.4% for USSR and 83.3% for Europe. In Brazil it is even more alarming, because the propulsion system was responsible for 100% of the failures that occurred in the launches. In this way, it seems necessary a continuous advancement in technologies and studies applied to the aerospace propulsion subsystem, in order to develop methods of prediction and simulations to identify possible failures long before they occur.

Sutton and Biblarz [2], studying the propulsion of aerospace vehicles, stated the high complexity of that subsystem requiring careful design and large production costs. Within the propulsion system, the combustion chamber, which is responsible for the production of thrust to accomplish the mission of the vehicle, still presents challenges in the modeling of the flow through it mainly due to three factors: combustion details[3]; interference of the turbulence on the process [4]; and, representation of the real conditions of the atmosphere [5] due to the high altitudes reached by the prototypes.

2 Study of the Art

As for the discretization method

Of all the references analyzed, most used the FVM[1] with some softwares such as Ansys CFX® [6], FLUENT® [7], FIRE® code [8], AVBP® [9], NTMIX-3D® [10]. A few have used the FDM[2] such as Martin et al. [9] and there LES/CAA[3] coupling analysis with the existing AVSP® code. Must be mentioned the theoretical work of Oefelein [11] and Albayrak and Polifke [12], the latter with laminar flow. Note that it has not being possible to determine the kind of numerical solution method presented by LIU et al. [13], Huo and Yang [14] and Lipatnikov et al. [15].

[1]Finite Volume Method
[2]Finite Difference Method
[3]Computational Aeroacustic

Among the severals methods of discretization, is extremely difficult to identify the most suitable method. In books like Chung [16] and Hirsch [17], for example, although they use all three methods for the same combustion problem, there is no comparison between them under the same conditions, especially for problems with available experimental data in the literature.

It has been verified that the FVM was a preferred initial choice for solving flow problems due to its robust way to deal with the inherent non-linearities present in the Navier-Stokes equations, which were not easily solved by using the classical Galerkin approach of the FEM due to some unstability, and, therefore, FEM was initially applied only to conduction cases. With respect to the FDM, its reduced utilization is associated with its difficult application to problems with complex geometries and with unstructured meshes.

One of the most contrasting differences between the FVM and FEM is the conservation property, considered essential to respect when solving flow problems. FVM includes this property by construction, both locally and globally [18]. On the contrary, the FEM yields only global conservation of the equations – the local conservation is not guaranteed when multipling the equations by the weight function [19].

Also FEM uses the weak formulation of the equations then yielding the disappearance of the derivatives of higher order during the integration process, leading to an easier modeling and, consequentely, programming, if compared with the FVM, which uses the strong formulation of the conservation equations.

Therefore, FEM was assessed as more suitable for the analysis of the problem proposed in this scope. However, due to the instabilities caused by the pure Galerkin method, it is necessary to employ a proper stabilizer method, and the CBS or Taylor-Galerkin method has been found to be adequate to the problem. Moreover, due to the robustness of the CBS method, it can be applied for both incompressible and compressible problems with the same general formulation [20].

As for the turbulence model

Although most of the references analyzed employed the LES methodology with the kinetic energy subgrid (SGS) closure method, Schlimpert et al. [21] and Mühlbauer et al. [6] used the RANS[4] methodology, the last with the closing model $\kappa - \epsilon$. In the work of Schlimpert et al. [21], the low-dissipation AUSM[5] was applied to the spatial discretization of the advective terms and for discretization in time a third-order Runge-Kutta scheme. The DNS[6] method was selected by Boger et al. [10], Lipatnikov et al. [15] and LIU et al. [13]. In particular Domingo et al. [22] compared results between DNS and LES, whereas Potturi et al. [23] used the hybrid model of LES/RANS with the least squares closure model [24].

Since the accuracy of a method is related to its ability to discretize the behavior of small scales, or Komolgorov scales, the different turbulence analysis methodologies are distinguished by this aspect. Therefore, the methodologies may be classified in descending order of accuracy by DNS, LES and RANS.

However, the discretization ability of the small scales is directly linked to the computational cost, resulting in the non-applicability of the DNS methodology for the present work. From the analyzed works that apply DNS, as a way to counteract the excessive computational cost, their authors have employed some simplifications for the problem, such as isotropic turbulence and homogeneity [10] or statically planar turbulence [13, 15].

An alternative to DNS is the LES methodology, in which the average flow is obtained through an analysis of both the small and large vortices, evaluating with some precision the energy contained in the flow. In this methodology the small scales are not simulated as in the DNS, but they influence the rest of the flow. This influence occurs in a passive way, such that the large vortices usually contain greater energy values, which increase their importance in the simulation. In short, the success of the LES methodology is related to the fact that the energy and other information from the flow travels from

[4]Reynolds-averaged Navier–Stokes

[5]Advection Upstream Splitting Method

[6]Direct Numeric Simulation

the largest to the smallest vortex scales, a phenomenon known as the energy cascade, but never in the opposite direction [25].

The RANS model provides results for the average flows with engineering precision employing moderate cost of computing, as a comparison, about 1% to 10% of the cost employed in LES, the latter requiring a much more refined mesh. However, for anisotropic vortex flow situations, the mean quantities are less satisfactory with RANS. In addition, LES provides instability in the data that is indispensable for modeling a chaotic flow as is the case of real turbulence, but LES cannot be used for symmetric flows in space [26].

Considering the strengths of RANS and LES methodologies, it was natural for some authors to combine both to ally the computational speed of one with the applicability and reliability of the other through hybrid models [23] a it is the case of Thakur et al. [27] with DES[7], a hybrid model used in FVM for axissymetric flow. Nguyen et al. [28] used the same DES, also for axissymetric flows with chemical multispecies, but with FDM associated to a variation of the classical JST[8] method.

Finally, the applicability of each methodology must be consistent with the level of accuracy and computational cost that should be previously established for each problem. With this in mind, and taking into account the strengths presented, the LES methodology will be used in the present work. In addition, both LES and RANS, because of the application of the filters and averages to the modeling, demand some way of closing the system of equations. The novel closure that will be proposed in the present work is a variation of the subgrid scale model involving the concept of turbulent kinetic energy [4, 11, 29].

As for the turbulence-chemical integration

Due to its simplicity and ease of implementation, the G-Equation model that detects the flame front was employed in the great majority of works analyzed [8, 12, 21, 30, 31]. The works of Lipatnikov et al. [15], Boger et al. [10], Domingo et al. [22] employ the Flame Surface Density (FSD) model. The Thickened Flame model[9, 32]. Merk et al. [33] used Linear Eddy Model (LEM), whereas Flemming et al. [34] worked with Flamelet Model; Bui et al. [35] with Steady Flamelet Model; Mühlbauer et al. [6] and Cecere et al. [36] applied Flamelet/Progress Variable. Oefelein [11] compared the models Laminar Flamelet Model [37], Transported Probability Density Function [38] and LEM [39], whereas Huo and Yang [14] compared Flamelet Model and Flamelet/Progress Variable and Zong et al. [40] compared Conserved Scalar and the Direct-closure approaches.

Despite the progress in turbulent combustion studies, a truly predictive, universal, multi-regime and multi-application model is still undefined. The main models analyzed in this literature review are the Flamelet models – including Steady Flamelet Model, Flamelet/Progress Variable and Unsteady Flamelet/Progress Variable Model [41] – LEM and Filtered Density Function (FDF) [13], wich all employ the LES methodology.

The Flamelet models, wich are limited by the reduction in the number of chemical species, do not produce good results for flows of pure substances. Still, the simplest Flamelet model is the Steady Flamelet, in which the turbulent combustion can be characterized by the chemical kinetics of some reaction [42]. To circumvent such limitations of the model, one has the most robust model of Flamelet/Progress Variable, to be further discussed.

For the LEM, the molecular diffusion is considered directly along some directions within the flow. However the strong multidimensional nature of the flames and the turbulent convection of the sub-grid scale acting on the set-level function of mapping of the flame front, which limits the characterization of the flame, do not easily justify that procedure [29].

In the FDF model with LES the source terms of the set-level transport equation are naturally closed, which limits the performance, due to modeling difficulties of the filtered conditional diffusion, or the filtered conditional dissipation in the reactive flows. In fact, there may be substantial differences in behavior within distinct locations in space, among regions of high and low variance of turbulent small scale closure [29].

[7]Detached Eddy Simulation

[8]Jameson–Schmidt–Turkel

In the Flamelet models, the LES transport equations for the fraction of the filtered mixture and/or progress variables can converge to their exact equations; however, combustion will always be dictated by a suitable flamelet library, not by the solution of the detailed coupled chemistry. As a way to bypass such limitation some authors have used the opensource GRI 3.0 (also called GRI-Mech 3.0) library [4, 14, 32], that aggregates 325 reactions and 53 chemical species[9].

For this work, the Flamelet/Progress Variable model will be used in conjunction with Cantera® – a Python developed library – that includes GRI 3.0.

As for the premixed mixture

Most references used homogeneous premixed mixture prior to combustion. However, non-premixed combustion was also detected in the works by Mühlbauer et al. [6], Oefelein [11], Huo and Yang [14], Flemming et al. [34], Bui et al. [35]. Finally, Dekena and Peters [8] and Lipatnikov et al. [15] worked with partially premixed blends.

As for fuel and oxidizer

Most of the references used methane as fuel and molecular oxygen as oxidizer. Potturi et al. [23], Martin et al. [9], Angelberger et al. [32] and LIU et al. [13] worked with the propane/oxygen ratio. Cao et al. [7] and Huo and Yang [14] applied hydrogen to molecular oxygen. Some reserarchers chose more elaborate mixtures of fuel, such as the hydrogen-nitrogen mixture with molecular oxygen in Bui et al. [35] and Flemming et al. [34] and the mixture of dilute nitrogen in methane-hydrogen with application of oxygen as oxidizer in Mühlbauer et al. [6]. Finally, Dekena and Peters [8] analysed the behavior of gasoline-air mixture during the combustion process.

As for the code development

In all the publications analyzed, even those in which the use of some kind of commercial or open-source software in the various aspects of transport phenomena was informed, the authors omitted or somehow trivialized the solution methodology employed, as well as the choice of some important physical parameters involved directly in solving the specific problem, making it impossible to further analyze in detail or even to reconstruct their procedures.

3 Goals

The present research project has the objective of developing a parallelized modular framework to numerical simulate a compressible flow with turbulent combustion of homogeneous mixture in an convergent-divergent nozzle a known geometry, using the FEM with CBS stabilization and thermo-chemical apply Cantera® and turbulence models, which used LES subgrid model, characterization of all combustion zones, employing Flamelet/Progress Variable, as well as the analysis of the behavior of the flame front, as presented by Liang et al. [43].

4 Mathematical Model

The proposed problem is the characterization of the flame front and the effects generated by a turbulent compressible premixed combustion. For this, after the definition of the geometry and the coordinate system, the system of transport equations to be solved was obtained.

For the LES methodology, a spatial filter of Favré was applied and a model of subgrid closure was developed. For the subgrid terms an isotropic flow was assumed.

[9] `http://combustion.berkeley.edu/gri-mech/version30/text30.html`

For the combustion modeling, a premixed mixture of GCH_4/GO_2 was selected, and the flamelet/progress variable method was used to characterize the flame front. The following is the system of transport equations as well as the other hypotheses employed in the present work.

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho}\widetilde{u_i}}{\partial x_i} = 0 \tag{1}$$

$$\frac{\partial \overline{\rho}\widetilde{u_i}}{\partial t} + \frac{\partial}{\partial x_j}\left[\overline{\rho}\widetilde{u_i}\widetilde{u_j} + \overline{p^*}\delta_{ij} + \tau_{ij}^{sgs} - \overline{\tau_{ij}}\right] = 0 \tag{2}$$

$$\frac{\partial \overline{\rho}\widetilde{E}}{\partial t} + \frac{\partial}{\partial x_j}\left[\overline{\rho}\widetilde{u_j}\widetilde{E} + \widetilde{u_j}\overline{p^*} + \overline{q_j} - \widetilde{u_i}\overline{\tau_{ji}} + H_j^{sgs} + \sigma_j^{sgs}\right] = 0 \tag{3}$$

$$\frac{\partial \overline{\rho}\widetilde{Y_k}}{\partial t} + \frac{\partial}{\partial x_i}\left[\overline{\rho}\left(\widetilde{Y_k}\widetilde{u_i} + \widetilde{Y_k}\widetilde{V_{i,k}}\right) + Y_{i,k}^{sgs} + \theta_{i,k}^{sgs}\right] = 0 \tag{4}$$

closure

$$\begin{aligned}\widetilde{E} &= \widetilde{e} + \tfrac{1}{2}\widetilde{u_k u_k} \\ &= \widetilde{e} + \tfrac{1}{2}\widetilde{u_k}\widetilde{u_k} + \tfrac{1}{2}(\widetilde{u_k u_k} - \widetilde{u_k}\widetilde{u_k}) \\ &= \widetilde{e} + \tfrac{1}{2}\widetilde{u_k}\widetilde{u_k} + k^{sgs}\end{aligned}$$

$$\widetilde{e} = \sum_{k=1}^{N_s}\widetilde{Y_k}e_{f,k}^0 + \sum_{k=1}^{N_s}\widetilde{Y_k}\int_{T_0}^{\widetilde{T}} c_{V,k}(T)dT + \sum_{k=1}^{N_s}E_k^{sgs}$$

$$\overline{p^*} = \overline{\rho}\widetilde{R}\widetilde{T} + \overline{\rho}R_u T^{sgs}$$

$$\overline{\tau_{ij}} = 2\mu(\widetilde{T})\left(\widetilde{\dot{\varepsilon}_{ij}} - \frac{1}{3}\widetilde{\dot{\varepsilon}_{kk}}\delta_{ij}\right)$$

$$\overline{q_j} = -\kappa(\widetilde{T})\frac{\partial \widetilde{T}}{\partial x_j} + \overline{\rho}\sum\widetilde{Y_k}h_k(\widetilde{T})\widetilde{V_{i,k}} + q_j^{sgs}$$

$$\widetilde{V_{i,k}} = -\frac{D_k}{\widetilde{Y_k}}\frac{\partial \widetilde{Y_k}}{\partial x_i}$$

$$\tau_{ij}^{sgs} = -2\overline{\rho}\nu_t\left(\widetilde{\dot{\varepsilon}_{ij}} - \frac{1}{3}\widetilde{\dot{\varepsilon}_{kk}}\delta_{ij}\right) + \frac{2}{3}k^{sgs}\delta_{ij}$$

$$H_i^{sgs} + \sigma_i^{sgs} = -\left(\overline{\rho}\nu_t + \mu\right)\frac{\partial k^{sgs}}{\partial x_i} - \frac{\overline{\rho}\nu_t c_p}{Pr_t}\frac{\partial \widetilde{T}}{\partial x_i} + \widetilde{u_j}\tau_{ij}^{sgs}$$

$$Y_{i,k}^{sgs} = -\frac{\overline{\rho}\nu_t}{Sc_t}\frac{\partial \widetilde{Y_k}}{\partial x_i}$$

$$\theta_{i,k}^{sgs} = \overline{\rho}\left(\widetilde{V_{i,k}Y_k} - \widetilde{V_{i,k}}\widetilde{Y_k}\right)$$

$$q_{i,k}^{sgs} = \overline{\rho}\left(h_k\widetilde{Y_k}V_{i,k} - \widetilde{h_k}\widetilde{Y_k}\widetilde{V_{i,k}}\right)$$

$$T^{sgs} = \sum_{k=1}^{N_s}\frac{\left(\widetilde{Y_k T} - \widetilde{Y_k}\widetilde{T}\right)}{MW_k}$$

$$E_k^{sgs} = Y_k\widetilde{e_k}(T) - \widetilde{Y_k}e_k(\widetilde{T})$$

According to Smagorinsky the turbulent viscosity, ν_t, is modeled as [44]

$$\nu_t \ = \ C_\nu \overline{\Delta}^2 |\bar{\bar{\varepsilon}}| \tag{5}$$

Thus, the conditions of high Reynolds number, isotropic flow and considering that $\overline{\Delta}/\eta >> 1$, where the cutoff wavenumber - κ_c - is defined by $\kappa_c \ = \ \pi/\overline{\Delta}$ [45], result in $\kappa_c \eta << 1$. In this way, since the exponential of the spectral distribution of the flow can be ignored,

$$E^*(\kappa) \ = \ \alpha \epsilon^{\frac{2}{3}} \kappa^{-\frac{5}{3}} \tag{6}$$

The turbulent viscosity can be obtained by applying the closed spectral theory of Kraichnan [46] applied to isotropic flows:

$$\nu_t \ = \ 0.441 \alpha^{\frac{3}{2}} \sqrt{\frac{E^*(\kappa_c)}{\kappa_c}} \tag{7}$$

where α is Kolmogorov constant ($\alpha \approx 1.5$).

The dissipation can be approximated by $\epsilon^{sgs} \ \approx \ \epsilon \ = \ 0.931 \frac{(k^{sgs})^{3/2}}{\overline{\Delta}}$ [47]. Therefore, equalling equations 5 and 7 the subgrid kinetic energy becomes

$$\kappa^{sgs} \ = \ 22.5523 |\bar{\bar{\varepsilon}}|^2 C_\nu^2 \overline{\Delta}^2 \tag{8}$$

This novel model of the subgrid kinetic energy proposed in this work differs from the method presented by Génin [47], Lin [48] and Pope [45] with the purpose of avoiding the addition of one more transport equation, this way reducing the computational cost and the complexity of the system of equations.

The application of the LES methodology implies directly a very refined mesh for convergence. Thus, one way to verify this refining is by applying the concept of spectral distribution, which is addressed in Figure 1 and explained in Pope [45]. As shown in Figure 1, LES modeling requires refined meshes to reproduce the behavior of the small vortices and the viscous subgrid effects.

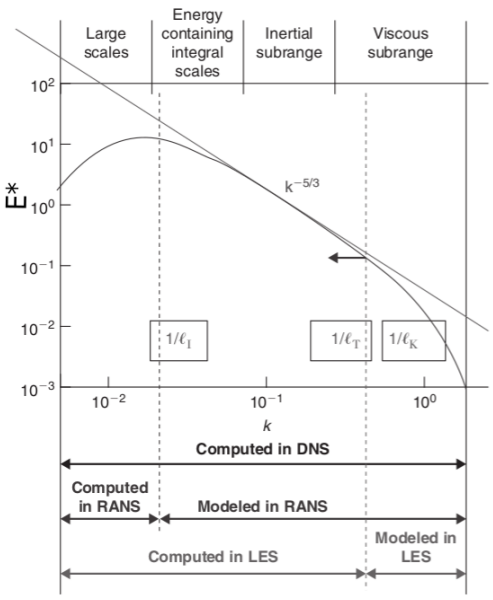


Figure 1. Comparated small scale analised by differents methodologies. Source: Adapted by the author from Hirsch [49].

Analyzing from the point of view of combustion, laminar combustion generates a stable and well defined flame front, in contrast the effects of turbulence generate perturbations in this fire flame front as a flame brush as shown in Figure 2.

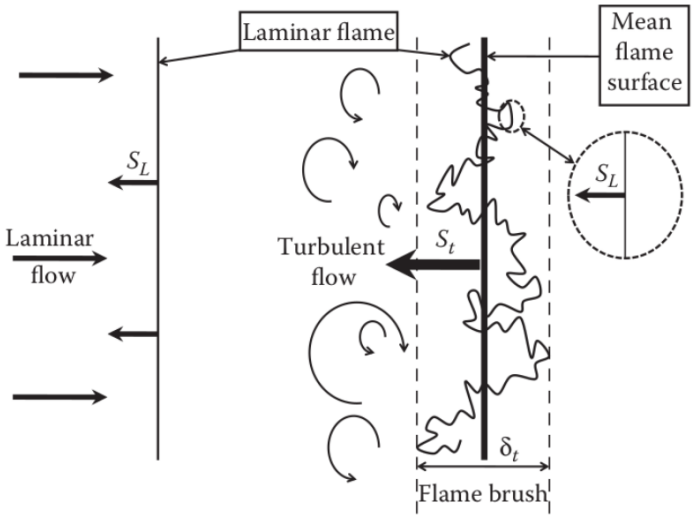


Figure 2. Scheme of laminar (left) and turbulent (right) premixed flames. Source: Lipatnikov [50].

For the characterization of the turbulent premixed flame front the Flamelet/ Progress Variable model, was presented in detail in [51]. With this, as shown by Cecere et al. [36], the proposal of this method is the additional resolution of two transport equations for the non-normalized progress variable $\widetilde{\mathbb{G}_\zeta}$ and for the square of variable $\widetilde{\mathbb{G}_\zeta}^2$. Thus, the variance of the progress variable is given by $\widetilde{\mathbb{G}}_{\zeta_v} = \widetilde{\mathbb{G}_\zeta^2} - \widetilde{\mathbb{G}_\zeta}^2$.

Cecere et al. [36] suggests that the progress variable may be any scalar that characterizes the flame (mass fraction of the species, temperature, etc.), but this must be a monotonic function of the coordinates of space. It is still suggested in that work that, for a methane/oxygen mixture, the progress variable be a combination of the CO_2 and CO species. This way, the mass fraction will be used as a progress variable with the following correlation

$$\mathbb{G} = \widetilde{Y}_{CO_2} + \widetilde{Y}_{CO} \tag{9}$$

Consequently, the normalization of the progress function is given by

$$\zeta = \frac{\mathbb{G}(\vec{x}) - \mathbb{G}^u(\vec{x})}{\mathbb{G}^b(\vec{x}) - \mathbb{G}^u(\vec{x})} \tag{10}$$

where $\square^u$ represents the unburnt gases, similarly, $\square^b$ the flared gases.

Thus the, additional non-normalized transport equations are

$$\frac{\partial \bar{\rho}\widetilde{\mathbb{G}}_\zeta}{\partial t} + \frac{\partial}{\partial x_j}\left(\bar{\rho}\widetilde{u_j}\widetilde{\mathbb{G}}_\zeta\right) = \frac{\partial}{\partial x_k}\left(\bar{\rho}\alpha_{\mathbb{G}_\zeta}\frac{\partial \widetilde{\mathbb{G}}_\zeta}{\partial x_k}\right) + \bar{\rho}\widetilde{\omega}_{\mathbb{G}_\zeta} + \frac{\partial f_{\zeta k}}{\partial x_k} \tag{11}$$

and

$$\frac{\partial \bar{\rho}\widetilde{\mathbb{G}^2}_\zeta}{\partial t} + \frac{\partial}{\partial x_j}\left(\bar{\rho}\widetilde{u_j}\widetilde{\mathbb{G}}_\zeta^2\right) = \frac{\partial}{\partial x_k}\left(\bar{\rho}\alpha_{\mathbb{G}_\zeta}\widetilde{\mathbb{G}^2}_\zeta\right) + \frac{\partial f_{\zeta_k}^2}{\partial x_k} - 2\bar{\rho}\widetilde{X}_{\mathbb{G}_\zeta} + 2\bar{\rho}\widetilde{\omega_{\mathbb{G}_\zeta}\mathbb{G}_\zeta} \tag{12}$$

where

$$f_{\zeta k} = \bar{\rho}\alpha^t_{\mathbb{G}_\zeta}\frac{\partial \widetilde{\mathbb{G}_\zeta}}{\partial x_k}$$

and

$$\alpha^t_{\mathbb{G}_\zeta} = C_{\mathbb{G}_\zeta}\overline{\Delta}^2|\bar{\bar{\varepsilon}}|\bar{\bar{\varepsilon}}$$

For the value of the constant $C_{\mathbb{G}_\zeta}$ Germano et al. [52] proposes a dynamic produce, but for the present work it is proposed that the calculation be performed taking into account the subgrid kinetic energy, for further details see [46, 50, 53].

$$C_{\mathbb{G}_\zeta}(x,t) \;=\; -0.4655\frac{k^{sgs}{}^{\frac{3}{2}}}{\bar{\Delta}^3|\bar{\dot{\varepsilon}}|\dot{\varepsilon}^2} \tag{13}$$

The proposal of the equations 8 and 13 aims to reduce the turbulence control parameters, so the only external parameter to be controlled is the Smagorinsky constant, together with the analytical closure of the transport equations.

The closure of balance equation of progress variable is given by

$$f_{\zeta^2 k} \;=\; \bar{\rho}\alpha^t_{\mathbb{G}^2_\zeta}\frac{\partial\widetilde{\mathbb{G}^2_\zeta}}{\partial x_k}$$

$$\bar{\rho}\widetilde{X}_{\mathbb{G}_\zeta} \;=\; \bar{\rho}D|\nabla\widetilde{\mathbb{G}_\zeta}|^2 \;+\; \bar{s}_{X\mathbb{G}_\zeta}$$

According to Veynante and Vervisch [54] if a linear relaxation of the fluctuations generated by micromixing is postulated result

$$\bar{s}_{X\mathbb{G}_\zeta} \;=\; \frac{\bar{\rho}\widetilde{\mathbb{G}_{\zeta_v}}}{\tau_t}$$

and following Domingo et al. [22] the turbulent Schmidt number assumed 0.7.

5 Programming Aspect

In the present work a numerical solution of a high complexity problem, with tenths of transport equation and many millions of elements, was to be developed and that would demand a great computation power. So, in the case of mulitcore CPUs and GPUs by themselves local homogeneous parallel programming was employed, whereas heterogeneous parallel programming was necessary for the communication with the GPUs.

Regarding the CPUs, thread control, with the Python *threading* library, was deployed, allied to the concept of processes control, with the *multiprocessing* library. For CPUs and GPUs communication, the C-based OpenCL language was selected, for higher processing speed, since the language is robust enough to be applied to different hardware devices and architectures, unlike the popular CUDA, which is only applied to NVIDIA®.

Element-by-Element FEM

Traditionally, CFD[10] programs have been based on the assembly techniques. The Element-by-Element technique was introduced by Smith et al. [55], with the goal of minimizing the computational cost by turning unnecessary the construction of the large and sparse assembly arrays.

In oder to exemplify the application of de EbE[11] method, the solution of the transient compressible Navier-Stokes equations was structured as following. Considering the element system and applying *Split B* in fully explicity form, the steps 1 and 2 become:

Step 1

$$\underbrace{M_u}_{LHS}\Delta\widetilde{U}^*_i \;=\; \underbrace{\Delta t\left[(C_u\widetilde{U} \;+\; K_\tau\widetilde{u} \;+\; G^T\widetilde{p} \;-\; f) \;-\; \Delta t\left(K_u\widetilde{U} \;+\; f_s \;+\; \frac{1}{2}P\widetilde{p}\right)\right]^n}_{RHS} \tag{14}$$

[10]Computer Fluid Dynamics

[11]Element-by-Element

Step 2

$$\underbrace{M_\rho}_{LHS}\,\Delta\widetilde{\rho} \;=\; \underbrace{\Delta t\left[G\widetilde{U}^n \;+\; \theta_1 G\Delta\widetilde{U}^* \;-\; f_\rho\right]^n}_{RHS} \tag{15}$$

The EbE is an iterative technique whereby the linear system for each element is solved, and the residues are dealt with methods such as Conjugate Gradient Method (CGM) or BiConjugate Gradient Method (BiCGM). Therefore, system of equations 14 and 15, should be interpreted as LHS[12] and RHS[13] of the linear systems.

For the present work the EbE technique with the BiCGM method was employed, using heterogeneous parallel programming with OpenCL.

For further details regarding the complete construction of the CBS method see Zienkiewicz et al. [20].

OpenCL in EbE FEM

Open Computing Language (OpenCL) is an open standard for heterogeneous system parallel programming.

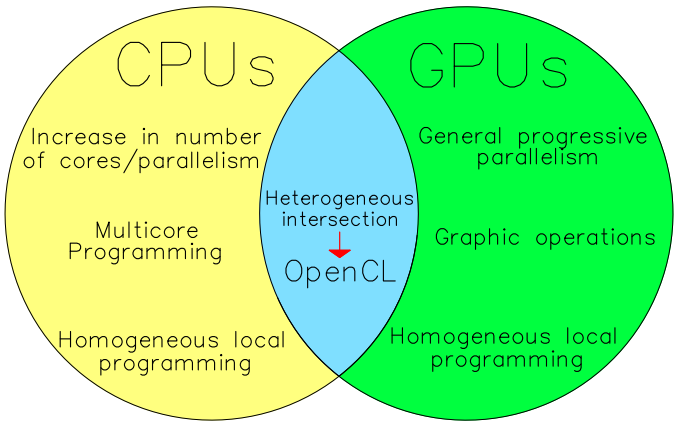


Figure 3. Integration between CPUs and GPUs with OpenCL. Source: Prepared by the author.

The OpenCL concept is based on one or more base programs, called hosts, which perform one or more kernel tasks, and these executed templates – kernels – are identified globally and locally by IDs. The Figure 4 simply presents the concept of these processes.

The generation of these global and local IDs are divided into N-dimensional processes, divided into NDRanges, in the analyzed dimensions. The Figure 5 represents the concept of a N-dimensional mesh mapping for a two-dimensional (matrix) work, 2DRange.

Control of the information shared by kernels is given through the memory model, so there are several types of models, Figure 6. Global memories have large sizes and good accessibility for jobs, private memories are restricted to one job item, while constant memories are read by immutable objects and can be shared by all job items.

According to Tay [56], memory mapping in OpenCL allows a region of memory space to be evaluated to perform the operation and these memories can be locked or unblocked to perform some task. A *Context* defines a collection of *Devices*, which one uses to run the kernels. A complete OpenCL approach is presented by Scarpino [57] in his work.

With the basic concepts of OpenCL with the EbE technique, the present work proposes the BiCLGM method in EbE with OpenCL, based on CUDA's Kiss et al. [58] work, but suggesting some changes of its pseudocode that contained some inconsistencies in their symbology.

[12]Left Hand Side
[13]Right Hand Side

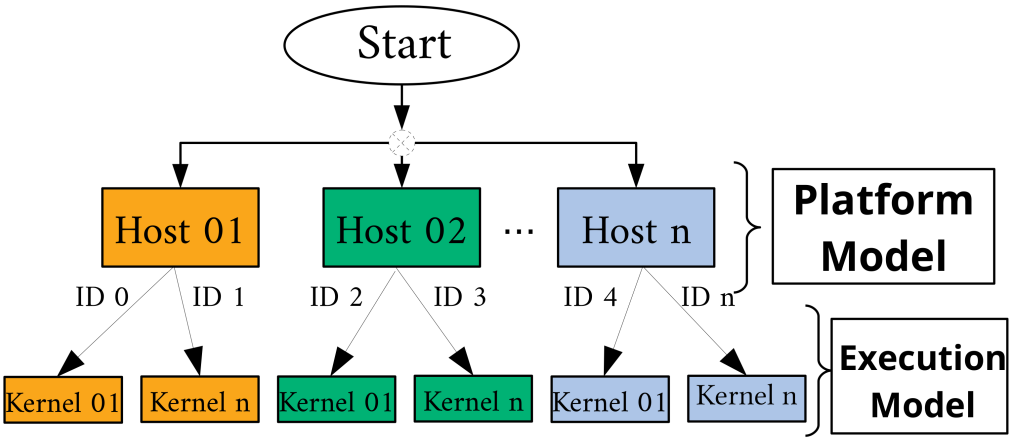
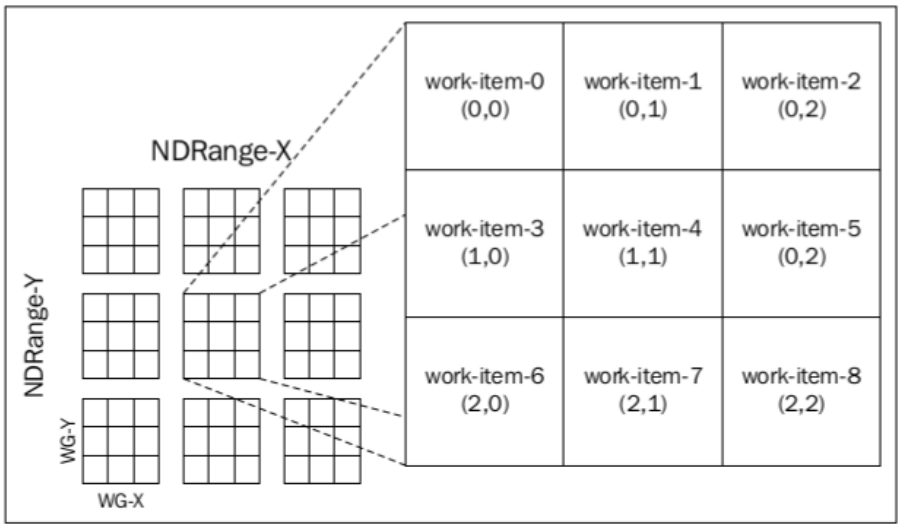


Figure 4. Scheme of concept parallelism with OpenCL. Source: Prepared by the author.



*WG-X and WG-Y, denotes the lenght in row and columns for particular work group.

Figure 5. Mapping ID works to mesh 2D. Source: Tay [56].

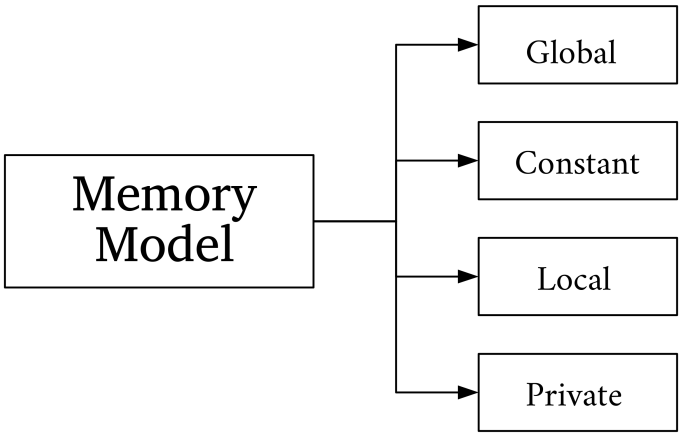


Figure 6. Memory model in OpenCL. Source: Prepared by author.

Thus, taking into account the general linear system:

$$M\Delta\phi = F \tag{16}$$

The following pseudocode demonstrates the parallelism methodology applied in the EbE technique:

INIT
for u ∈ DoF **do** #Dof Interation
  $r_{(u)} \leftarrow 0$
  $D_{(u)} \leftarrow 0$
Multiprocessing in OpenCL on GPU
for c in 0 to *colors* **do** #Serial loop
  for e ∈ $\Xi^{(c)}$ **do** #EbE iteration
    $\#\Xi^{(c)} \rightarrow$ Elements slice for each color
    $r_e \leftarrow r_e + F_e - M_e \Delta\phi_e$
    $D_e \leftarrow D_e + diag(M_e)$
for u ∈ DoF **do** #Dof Interation
  $D_{(u)} \leftarrow 1/D_{(u)}$
  $\bar{r}^{(u)} \leftarrow r^{(u)}$
  $d^{(u)} \leftarrow D^{(u)} \cdot r^{(u)}$
  $\bar{d}^{(u)} \leftarrow D^{(u)} \cdot \bar{r}^{(u)}$
  $q^{(u)} \leftarrow 0$
  $\bar{q}^{(u)} \leftarrow 0$
$\delta \leftarrow 0$ $\#Error$
for u ∈ DoF **do** #Dof Interation
  $\delta \leftarrow \delta + r^{(u)} \cdot d^{(u)}$ #Global error DoF
while δ ¿ *tolerancy* **do** #host loop
  for c **in** 0 **to***colors* **do**
    #Slice Elements for GPU
    ...
    for $e \in \Xi^{(c)}$ **do** $\#EbE\ iteration$
      $q_e \leftarrow q_e + M_e \cdot d_e$
      $\bar{q}_e \leftarrow \bar{q}_e + M_e \cdot \bar{d}_e$
  $\alpha \leftarrow 0$
  for $u \in DoF$ **do** $\#Dof\ Interation$
    $\alpha \leftarrow \alpha + \bar{d}^{(u)} \cdot q^{(u)}$
  for $u \in DoF$ **do** $\#Dof\ Interation$
    $\Delta\phi^{(u)} \leftarrow \Delta\phi^{(u)} + \delta/\alpha \cdot d^{(u)}$
    $r^{(u)} \leftarrow r^{(u)} - \delta/\alpha \cdot q^{(u)}$
    $\bar{r}^{(u)} \leftarrow \bar{r}^{(u)} - \delta/\alpha \cdot \bar{q}^{(u)}$
  #Update iteration
  $\bar{\delta} \leftarrow \delta$; $\delta \leftarrow 0$
  for $u \in DoF$ **do** $\#Dof\ Interation$
    $\delta \leftarrow \delta + r^{(u)} \cdot D^{(u)} \cdot \bar{r}^{(u)}$
  $\alpha \leftarrow \delta/\bar{\delta}$
  for $u \in DoF$ **do** $\#Dof\ Interation$
    $d^{(u)} \leftarrow D^{(u)} \cdot r^{(u)} + \alpha \cdot d^{(u)}$
    $\bar{d}^{(u)} \leftarrow D^{(u)} \cdot \bar{r}^{(u)} + \alpha \cdot \bar{d}^{(u)}$
    $q^{(u)} \leftarrow 0$
    $\bar{q}^{(u)} \leftarrow 0$

Heterogeneous programming using OpenCL with Python is given through the pyOpenCL library, which works on multiprocesses built in different GPU colors.

The overall construction of the problem is characterized in Figure 7.

As shown in Figure 7, one can verify the separation of the problem in CPU parallelism by applying the concept of multiprocesses, however, for the solution of the elementary systems, GPU parallelism is preferable, due to its large capacity of data processing. This strategy aims to optimize the resolution of the problem without the need for clusters or workstations to solve problems with very refined meshs, characteristic of the application of LES to detect the effects of subgrid.

6 Conclusion

The presented methodology aims at several new aspects for analysis of turbulent compressible reactive flows applied in rocket engines. Two guidelines presented were the analytical models, suggested by the author, of closing the turbulence equations and turbulence-combustion integration. However, for the present work, the focus is on the advanced programming strategies that were employed to solve the proposed problem. The methods presented were chosen due to the practicality of use in the Python language, which provides great versatility when it comes to homogeneous or hetherogeneous parallelism, coupled with the large data handing for the I/O of the results.

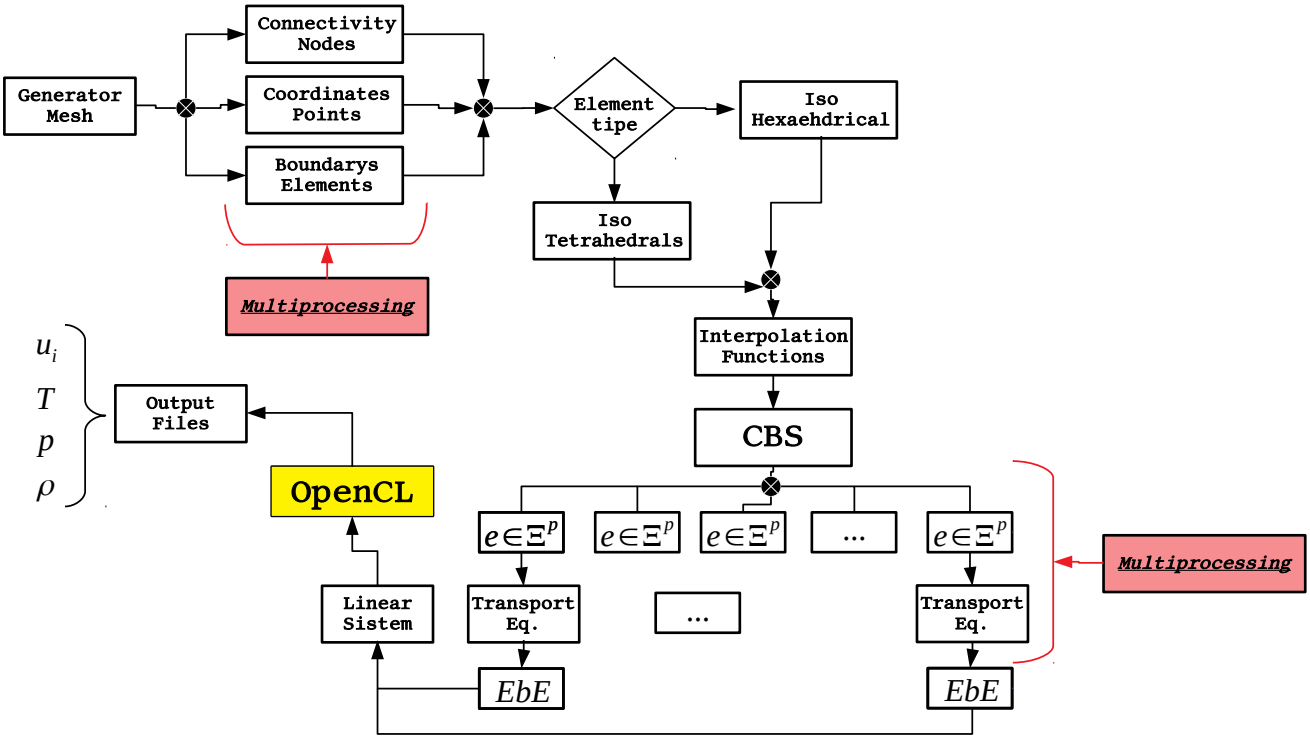


Figure 7. Global scheme of parallelism methodology for CBS method in flow. Source: Prepared by the author.

Acknowledgements

The authors are grateful for the financial support from the PPGEM – UNESP/FEIS, from the National Council of Technological and Scientific Development of Brazil (CNPq grant number 458702/2014-5).

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