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Cold Gas Flow Simulation in a Rocket Nozzle Using a Density Based Solver

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Resumo. Open source softwares to solve different kinds of mathematical problems are becoming very popular research tools, particularly in the field of fluid dynamics. However, these tools are still viewed as unfriendly and the commom lack of detailed documentation and test cases available support this idea. Here, an application using three of these tools was performed, namely, the simulation of the high speed viscous compressible flow inside an optimized thrust rocket nozzle with high pressure rate. A computational mesh, with a prysmatic boundary layer is constructed using Gmsh and Engrid mesh generators and the flow computations were performed using OpenFoam finite volume density solver rhoCentralFoam. The computations were numerically stable and the results obtained were physically consistent, showing the capability of these tools to handle the simulations of the high pressure rate optimized thrust nozzle.

Palavras-chave. Nozzle flow, finite volume, computational fluid dynamics, open source software.

1 Introduction

Open source computational softwares are widely used nowadays as a research tool and more recently, industrial apllications using such softwares has becoming more popular. Among these, computational fluid dynamics (CFD) pre-processing, solvers and post-processing tools are being used for whole different applications from low Reynolds number microfluidics to high speed flows around or inside aerospace devices.

In this context, CFD applications, particularly in the realm of compressible high speed flow, imposes challenging tests for these open source tools because of the ocurrence of complex physical phenomena like, for example, shock wave formation, compressible boundary layers, strong momentum dissipation and high rates of heat transfer due to the strong variation in physical flow parameters.

Paricularly, here, a numerical simulation of the compressible high speed flow inside an optimized rocket nozzle in cold flow conditions was performed. The computational mesh was generated using the *Gmsh*[3] and *Engrid*[4] open source softwares, while the simulations were done using the *OpenFoam* [5] package, that consists of a collection of

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numerical toolboxes written in $C++$, with pre and post processing utilities for the solution of partial differential equations of continuum mechanics using a tensorial approach. Inside *OpenFoam*, the *rhoCentralFoam* package was used for the simulation of the compressible viscous flow inside the nozzle. This case was chosen because research on the internal flow dynamics inside rocket nozzles is still an important theme in the field of aerospace engineering and the proper characterization of the flow inside these devices is a difficult task due to the variety of conditions that take place during its different operation stages [1], [2], such as shock-boundary layer interactions, shock wave formation and boundary layer detachments causing side loads, among others.

The development and calibration of Computational Fluid Dynamics (CFD) based tools capable of simulating the flow inside these nozzles is an indispensable step for obtaining new reults and insights due to the difficulty in performing experimental measurements inside real rocket nozzles. Furthermore, the continuous application of open source tools in different problems is essential to create an ensemble of results that are necessary for users to correct code issues, as well as implementing new functionalities in these open source softwares. Although open source softwares are frequently viewed as unfriendly tools, the possibility of using a fully customizable and adaptable numerical code is of great interest for research institutes working on the development of new technologies.

2 The rhoCentralFoam solver

The *rhoCentralFoam* [6] is a unsteady, density based compressible flow solver, based on central upwind schemes proposed by [7]. According to [6], it is implemented as a finite volume discretization using semi-discrete, non-staggered central schemes for collocated variables. Here, a briefly description of the *rhoCentralFoam* solver is given. Details of the solver implementaion can be found in [6]

The Navier-Stokes solution strategy for the *rhoCentralFoam* is implemented using the operator-splitting approach, as follows. Taking ρ as the fluid density, u_i, as the fluid velocity in the *ith* direction and E as the energy contained in the flow, first the continuity equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0, \tag{1}$$

is solved providing a new value for ρ. After this step an Euler equation

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} + \frac{\partial p}{\partial x_i} = 0. \tag{2}$$

is solved explicitly providing a value for ρu_i. This new primitive updated velocity is used to compute the diffusive part of the solution through equation 3

$$\left(\frac{\partial \rho u_i}{\partial t}\right)_{viscous} - \frac{\partial}{\partial x_j}\left(\frac{\mu \partial u_i}{\partial x_j}\right) - \frac{\partial \tau}{\partial x_j} = 0. \tag{3}$$

where τ represents the stress tensor terms, that are treated explicitly. Following Boussinesq assumption, τ is written as

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$$\tau = \mu \left(\frac{\partial \hat{u}_i}{\partial x_j} - \frac{2}{3} \frac{\partial \hat{u}_k}{\partial x_k} \delta_{ij} \right) = 0. \tag{4}$$

where $\hat{u}_i = \rho\, u_i$ is the solution of the equation 2. For the energy equation the same procedure is used, so that equation 5 is explicitly solved

$$\left(\frac{\partial \rho E}{\partial t} \right) + \frac{\partial}{\partial x_k} \left[u_k (\rho E + p) \right] - \frac{\partial}{\partial x_i} \mu u_j \left(\frac{\partial u_j}{\partial x_i} + \tau \right) = 0. \tag{5}$$

Using the new ρE, u_i and ρ values the temperature is obtained by the subtraction of the kinetic energy from the total inviscid energy

$$T = \frac{1}{C_v} \left(E - \frac{u_k u_k}{2} \right) \tag{6}$$

where C_v is the specific heat to constant volume. Finally, the heat diffusion is taken into account implicitly by solving the diffusion correction equation

$$\left(\frac{\partial \rho C_v T}{\partial t} \right)_{viscous} - \frac{\partial}{\partial x_k} \left(k \frac{T}{\partial x_k} \right) = 0. \tag{7}$$

With the new values for temperature the thermodynamic parameters $k, /mu$ and p are updated at the end of iteration.

Numerically, the convective fluxes are calculated using the volumetric flux J_f as

$$\int_V \nabla.[\mathbf{\Phi U}] dV \approx \Sigma_f J_f \mathbf{\Phi}_f \,, \tag{8}$$

while Φ_j is obtained through flux splitting in outgoing and incoming directions to the owner cell using

$$\Sigma_f J_f \mathbf{\Phi}_f = \left[\Sigma f \alpha J_{f+} \mathbf{\Phi}_{f+} + (1-\alpha) J_{f-} \mathbf{\Phi}_{f-} + \omega_f (\mathbf{\Phi}_{f+} - \mathbf{\Phi}_{f-}) \right], \tag{9}$$

where $+$ and $-$ represent the outcoming and incoming directions, respectively. If $\alpha = 0,5$ the scheme is called central and if α is biased in the upwind direction the scheme is called central upwind. The volumetric flux ω_f is calculated as given by [6]. Also low and high order schemes are interchanged using flux limiter functions that are TVD and symmetric as, for example Van Leer and Van Albada, among others. Additional flux limiters can also be easily implemented by the user in the code. So, for example, the f_+ interpolation is given in [6] as

$$\mathbf{\Phi}_{f+} = (1 - g_{f+}) \mathbf{\Phi} P + g_{f+} \mathbf{\Phi}_N \tag{10}$$

where P is the owner cell index and N, the neighbor cell index. Gradient schemes are discretized as

$$\int_V \nabla[\mathbf{\Phi}] dV \approx \Sigma \mathbf{S}_f \mathbf{\Phi}_f \,, \tag{11}$$

and the interpolation is done using the central schemes proposed by [7] using

DOI: 10.5540/03.2018.006.01.0336

$$\Sigma_f \mathbf{S}_f \mathbf{\Phi}_f = \left[\Sigma f \alpha \mathbf{S}_f \mathbf{\Phi}_{f+} + (1-\alpha)\mathbf{S}_f \mathbf{\Phi}_{f-}\right], \tag{12}$$

and the f_+ and f_- interpolations use the same previous flux limiter functions.
Finally, the diffusion terms are discretized as

$$\int_V \nabla.(\Gamma \nabla \mathbf{\Phi}) dV \approx \Sigma_f \Gamma_f \mathbf{S}_f.\nabla(\mathbf{\Phi}_f)\,. \tag{13}$$

Generally, the evaluation of the above expression is done spliting the gradient flux into an orthogonal and a non orthogonal component as shown in [6]

$$S_f.\nabla(\mathbf{\Phi}_f) = A(\mathbf{\Phi}_N - \mathbf{\Phi}_P) + \mathbf{a}.(\nabla\mathbf{\Phi})_f] \tag{14}$$

with $A = |\mathbf{S}_f|^2/\mathbf{S}_f.\mathbf{d}$ and $\mathbf{a} = S_f - A\mathbf{d}$, d being the vector connecting the centroids of owner and neighbor cells.

3 Numerical Computations

The numerical computations were performed to simulate cold gas flow inside an optimized thrust rocket nozzle using the Reynolds Average Navier Stokes (RANS) equations with a compressible $k-\omega$ model for turbulence closure, incorporated to the *rhoCentralFoam*. The flow parameters were chosen so that, theorectically, a supersonic Mach 4.5 condition would be estabilished at the nozlle exit and a pressure difference of 40 bar was applied between the inlet and outlet regions.

The simulations utilized a nozzle geometry obtained from a previous calculation using the Rao method [8]. The nozzle has a total length of $16,5.10^{-2}$ m, a throat radius of $2,5.10^{-2}$ m and an exit radius of $7,9.10^{-2}$ m and these points of reference were connected by an optimized curve obtained from an equivalent 15^o conical nozzle with the same expansion rate. More details for the nozzle contour calculation can be found in [8].

After the geometrical points of the nozzle contour were calculated a first volumetrical mesh, of one quarter nozzle, was generated using the open source Gmsh software [reference gmsh] through extrusion of the nozzle contour. Ater that, the initial mesh was exported to another open source software, Engrid, where it was refined, optimized and a prismatic boundary layer was inserted in the mesh. The final mesh is shown in Figure 1 and is composed of 56061 cells, with 17408 prismatic cells and 38653 tetrahedric cells. The prismatic boundary layer is contructed such that $y^+ = 100$ in the simulation. At the wall the no slip and zero flux conditions were used for the velocity and thermodynamic fields, respectively, while at the lateral faces of the one quarter nozzle a symmetry condition was applied.

The implementation of the boundary conditions for the inlet and outlet were the main issues to perform the simulations. These conditions were contructed to simulate a stagnant vessel, so that at the inlet a total pressure condtion of $4.10^6 Pa$ was used, while the velocity was allowed to be induced by the pressure. Also, the total temperature was maintained constant at the inlet, with a value of $330K$.

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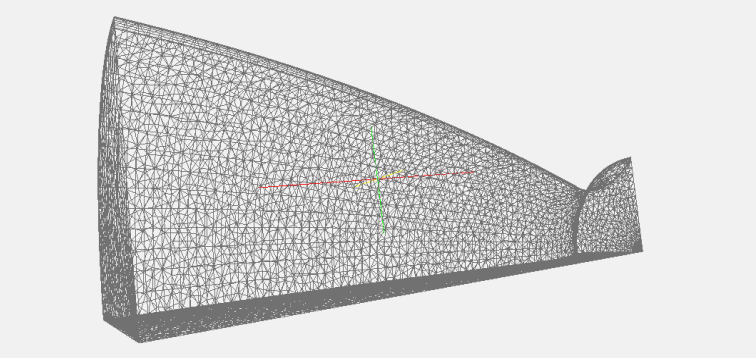

Figure 1: Computational mesh for the simulation of internal nozzle flows.

At the outlet a known value the back pressure of $1.10^5 Pa$ was chosen to simulate atmospheric pressure conditions. For total temperature an outflow zero gradient condition is used, where a user-specified value is applied in the case of reverse flow. As the flow is supersonic at the outlet a non-reflective boundary condition based on [9] was applied to the velocity field. This partially non-reflecting boundary condition has a reflection coefficient that is based on a parameter K, which makes the boundary condition perfectly reflecting if $K = 0$, leading to a zero amplitude of the incoming wave, or partially non-reflecting if $K \neq 0$, what often ensures that mean calculated pressure stays close to the desired pressure.

For the turbulent parameters a turbulent intensity of 1% was used at the inlet and a viscosity ratio of 5 was used to calculate the ω initial conditions. At the walls, wall functions were used for both parameters and at the outlet they were allowed to float. It should be emphasized that a fine setup of the parameters in the boundary conditions is essential for the convergence of the calculations.

The computations were carried for $0,5s$, in order to achive a steady state condition for exit Mach number. The initial timestep was chosen as $2,12.10^{-06} s$ for stability reasons, but it is allowed to float during the computations, with its value limited by maximum local Courant number of $Co = 0.75$.

Figures 2 and 3 show the results for pressure and Mach number distibution, respectively, where 0 is the inlet postion. It can be seen that the pressure boundary conditions perform well, specially at the nozzle outlet where no reflections are observed. Also, the Mach number distribution is to the theoretically expected value from analytical solutions.

Also, the turbulent parameters were calculated using the $k\omega$ closure model and the turbulent viscosity μ_t was computed over the whole domain. Figure 4 shows the values of μ_t along nozzle centreline, where it is observed that the turbulent viscosity reaches a peak and rapidly falls reaching values close to zero at the nozzle exit. This behavior is physically consistent as, theer are no separation or recirculation zones observed, the turbulence signal is expected to decrease significantly away from the walls.

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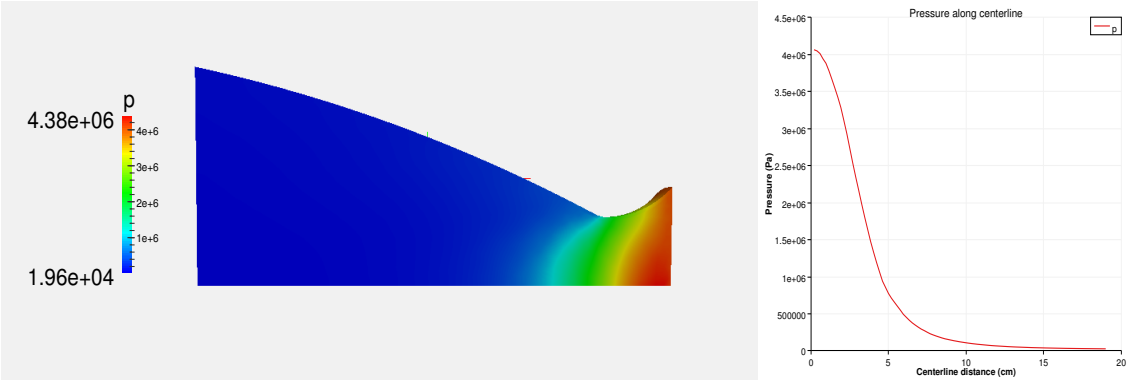

Figure 2: Nozzle pressure distribution at final timestep(left) and pressure along centreline (right). Position 0 corresponds to the inlet.

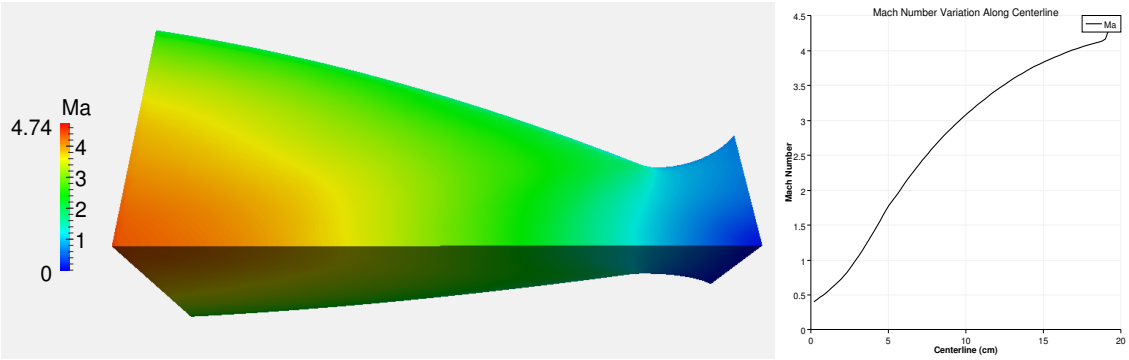

Figure 3: Nozzle Mach number distribution at final timestep(left) and Mach number along centreline (right).Position 0 corresponds to the inlet.

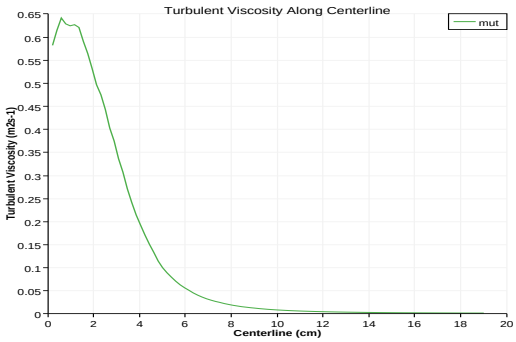

Figure 4: Nozzle Mach number distribution at final timestep(left) and Mach number along centreline (right).

4 Conclusions

The computations performed, even though are not compared with experimental results or numerical benchmarks show the capability of *rhoCentralFoam* to provide stable

numerical solutions, free of oscilations, for the simulation of nozzle flows with high pressure rates, wich is widely known to be a difficult numerical task in compressible CFD caalculations. The dynamic and thermodynamic fields agrees with analytical calculations and indicate that the solver, used together with open source mesh generation tools *Gmsh* and *Engrid*, can be a valuable tool for the numerical investigation of flow behavior inside nozzles operating at high pressure rates. Future research will be done on the unsteady flow dynamics inside these thrust optimized nozzles to analyze the ability of these open source tools to handle complex phenomena as, for example, flow separation, reatachment and shock boundary-layer interactions.

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