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NUMERICAL EXPERIMENT OF COMPRESSIBLE FLOW USING PRESSURE-BASED CALCULATION METHOD AND ADAPTIVE MESH REFINEMENT

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Abstract. *This paper presents the mathematical modeling and numerical simulations of compressible flow using pressure-based calculation method. All the implementations and simulations are carried out using an in-house computational code named MFSim (Multiphysic Simulator), which allows to solve the Navier-Stokes equations in the transient three-dimensional form using block-structured mesh with local adaptability. Consistent qualitative results are obtained and corresponding quantitative results compare well with the analytical solutions and the references results available.*

Keywords: *Compressible flow, All-Mach, Adaptive mesh refinement*

1. INTRODUCTION

Several industrial processes involve both compressible and incompressible flows, among which we can mention: the process of atomization of droplets and the transport of liquids and gases in the same pipe. Even the high-speed flows of the aeronautical industry show the incompressible behavior in regions where the local velocity approaches zero, such as inside boundary layers and near points of stagnation. Other situations that occur both flows is when there is a leak of steam from a vessel containing pressurized water or in cavitation phenomena, ie, vaporization of a liquid by reducing pressure during its movement. Thus, methods capable of simulation both flows simultaneously becomes essential to fulfill this demand.

Various methods and techniques have been developed over the years to deal with each of these flows separately. For compressible flows, the basic methodology of numerical methods is the consideration that the specific mass varies strongly with the pressure. One way to treat this kind of flow is by calculating the specific mass through the mass balance equation and the pressure through the state equation. Note that the formulation for compressible flows can not be applied to incompressible flows, because in these cases the pressure is not a thermodynamic property and therefore can not be calculated by a state equation. On the other hand, for the formulation of incompressible flows, the basic methodology of numerical methods is the assumption that the specific mass is constant or determined only as a function of temperature. Consequently, it is not possible to solve, for example, a supersonic flow where the shock waves are present and can cause a sudden change in the specific mass.

According to Maliska (1995), there are currently two lines of research seeking to extend the methodologies for flows to any Mach. The first line, denominated methods based on specific mass, has as numerical basis the formulation for compressible flows and tries to extend to incompressible flows. The second line of research, called methods based on pressure-velocity coupling, has as numerical basis the formulation for incompressible flows and extends to compressible flows. In the present work the second line of research is adopted.

One of the greatest challenges that is found in the area of computational experimentation is the efficiency of computational tools. The use of an adaptive grid is a powerful way to save mesh refinement and, consequently, save processing time. This method of discretizing the equations allows the mesh to adapt dynamically to the physical or geometric requirements of a given problem. For example, a more refined mesh is required near a wall or on a turbulent wake. Several works have been developed employing adaptive mesh, with block-structured mesh (Berger and Colella, 1989; Bell *et al.*, 1994; Berger and LeVeque, 1998; Baeza and Mulet, 2006; George and LeVeque, 2006). This approach was selected to be implemented in the present work.

All the implementations and simulations are carried out using an in-house computational code named MFSim (Multiphysic Simulator), which allows to solve the Navier-Stokes equations in the transient three-dimensional form using block-structured mesh with local adaptability.

2. MATHEMATICAL MODEL

In this section, the partial differential equations that model the problem along with the boundary conditions and initial conditions are presented, when applicable. In all simulated cases, compressible flows of Newtonian fluids are considered. The equation of the mass balance for the case of compressible flow in Cartesian coordinates, using the index notation is given by Eq. (1).

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0, \quad j = 1, 2, 3, \tag{1}$$

where ρ is the specific mass, t the time variable, u_j is the fluid velocity component in j direction and x_j are the Cartesian coordinates directions x, y and z, respectively. Equation (2) represents the balance of the momentum, written in divergent form, in Cartesian coordinates and in indicial notation.

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\mu\left(\frac{\partial u_k}{\partial x_k}\right)\delta_{i,j}\right], \tag{2}$$

where $i, j = 1, 2, 3$, p is the pressure, t is the time, and δ defined as the Kronecker operator.

Equation (3) represents the thermal energy balance for a Newtonian fluid, written in divergent form, in Cartesian coordinates and in indicial notation.

$$\frac{\partial(\rho c_p T)}{\partial t} + \frac{\partial\left(\rho c_p T u_i\right)}{\partial x_i} = \frac{\partial}{\partial x_i}\left(k\frac{\partial T}{\partial x_i}\right) + \Phi + \lambda \tag{3}$$

where i, j and $k = 1, 2, 3$, c_p is the specific heat at constant pressure and Φ and λ are given by Eqs. (4) and (5), respectively.

$$\Phi = \mu\left[\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)^2 + \left(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i}\right)^2 + \left(\frac{\partial u_j}{\partial x_k} + \frac{\partial u_k}{\partial x_j}\right)^2 + 2\left(\frac{\partial u_i}{\partial x_i}\right)^2\right] - \frac{2}{3}\mu\left(\frac{\partial u_i}{\partial x_i}\right)^2 \tag{4}$$

$$\lambda = \frac{\partial p}{\partial t} + u_i\frac{\partial p}{\partial x_i} \tag{5}$$

In the present work, the SIMPLE (Semi-Implicit Method for Pressure Linked Equations) method developed by Patankar and Spalding (1983) was used in a Cartesian and staggered grid. In this method the equations for the correction of velocities are obtained by from the momentum equations and mass balance equation. For more details, see Ferziger and Peric (2012).

The time steps are calculated based on constraints associated with advective and diffusive terms. Equations (6) to (9) have these restrictions and the calculation of the time step. Constants are used to control constraints and must be adjusted between 0 and 1 to obtain numerical stability in different simulated cases.

$$\Delta t_1 = min\left(t_f - t, h\right) \tag{6}$$

$$\Delta t_{adv} = C_{adv} \cdot \left(\frac{|u|_{max}}{\Delta x} + \frac{|v|_{max}}{\Delta y} + \frac{|w|_{max}}{\Delta z}\right)^{-1} \tag{7}$$

$$\Delta t_{dif} = C_{dif} \cdot min\left(\frac{\Delta x^2}{\nu} + \frac{\Delta y^2}{\nu} + \frac{\Delta z^2}{\nu}\right) \tag{8}$$

$$\Delta t = min\left(\Delta t_1, \Delta t_{adv}, \Delta t_{dif}\right) \tag{9}$$

where Δx, Δy and Δz denote, respectively, the size of the discretization cells in the directions x, y and z at the thinnest level, $|u|_{max}$, $|v|_{max}$ and $|w|_{max}$ are the maximum absolute velocity value in the three coordinate directions, ν is the kinematic viscosity, t_f is the final simulation time, h is the minimum spacing defined at the finest mesh and t is the current time.

3. RESULTS

3.1 Shock tube

The first case simulated for validation against cases available in the literature was the classic case of the shock tube (Sod, 1978). In this problem we have the same fluid with different thermodynamic properties in two distinct regions of the computational domain. The information on the physical properties of the fluid is shown in Fig. 1.

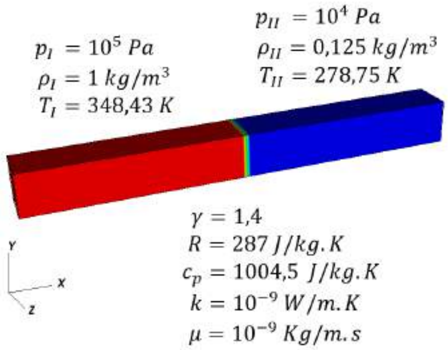


Figure 1. Physical properties of the fluid.

The domain is a parallelepiped whose dimensions are given by 10 m $\times$ 1 m $\times$ 1 m, with the wave propagating toward the x-axis, and a base mesh of 200 volumes in the x-direction, 20 volumes in the y-direction, and 20 volumes in the z-direction. Dirichlet condition was adopted in the walls $x = 0$ m and $x = 10$ m, modeling a closed tube, and slip condition in the other walls. For the temporal discretization is used the totally implicit method. The SIMPLE method was applied in the velocity and pressure coupling and the final simulation time is $t = 0.0061$ s. Fixed the temporal scheme, the advective scheme was varied: first order upwind (Upwind1O), MinMod and SUPERBEE. In Figure 2 the analytical solutions of the shock tube problem are compared with the pressure profiles, specific mass, u component of the velocity and Mach number obtained from the numerical simulations.

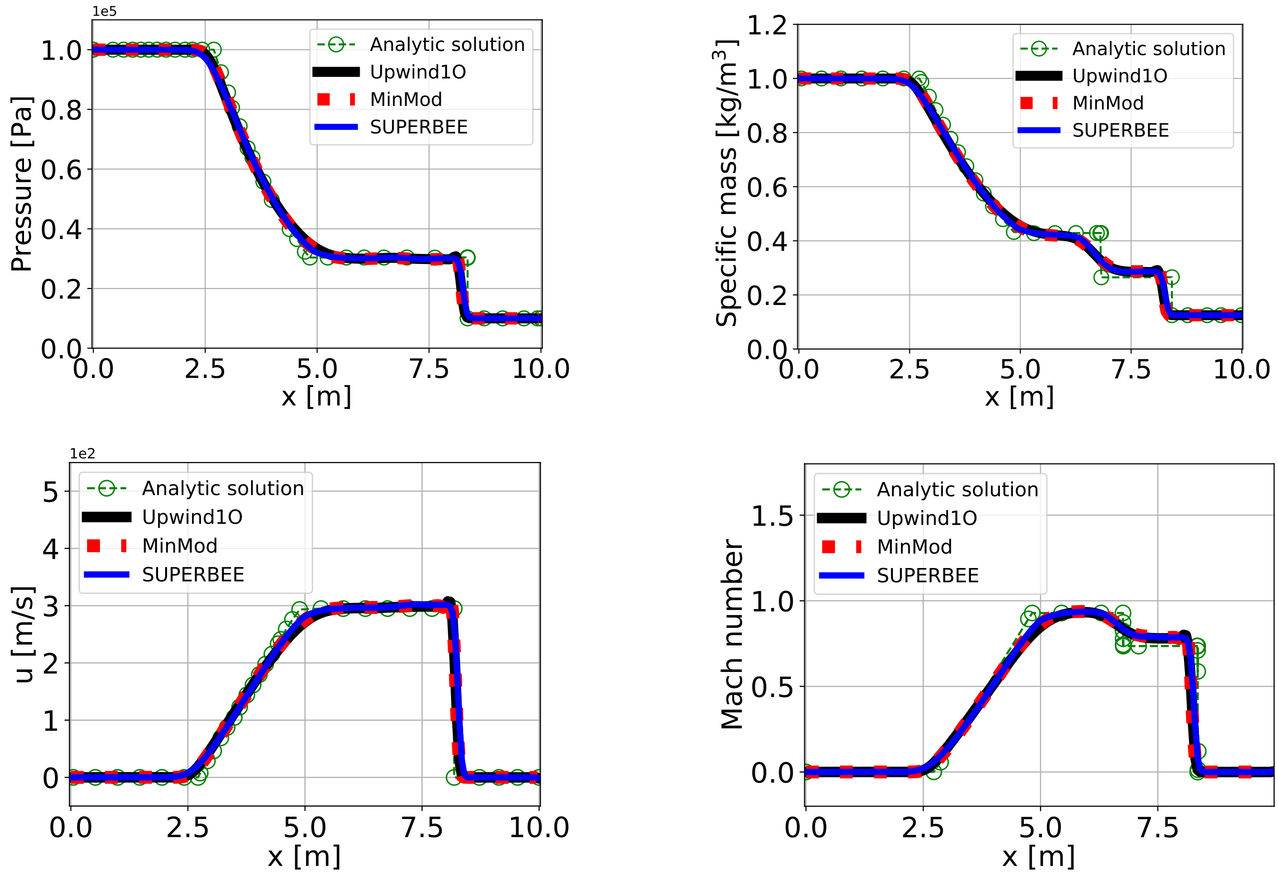


Figure 2. Comparison of the numerical solution with the analytical solution of the shock tube for different advective schemes.

Note that the MinMod and Upwind1O schemes display a small oscillation near the shock wave. Therefore, for this case the best choice for the advective scheme is SUPERBEE. In order to obtain grid independence, a detailed mesh refinement study is carried out by employing three uniformly spaced grids consisting of 200 cells, 1000 cells and 6400 cells toward the x-axis. The simulation results for pressure, specific mass, u component of the velocity and Mach number are shown in Fig. 3. For all the evaluated variables there was a convergence of the results, and also an approximation of the result obtained with the analytical solutions.

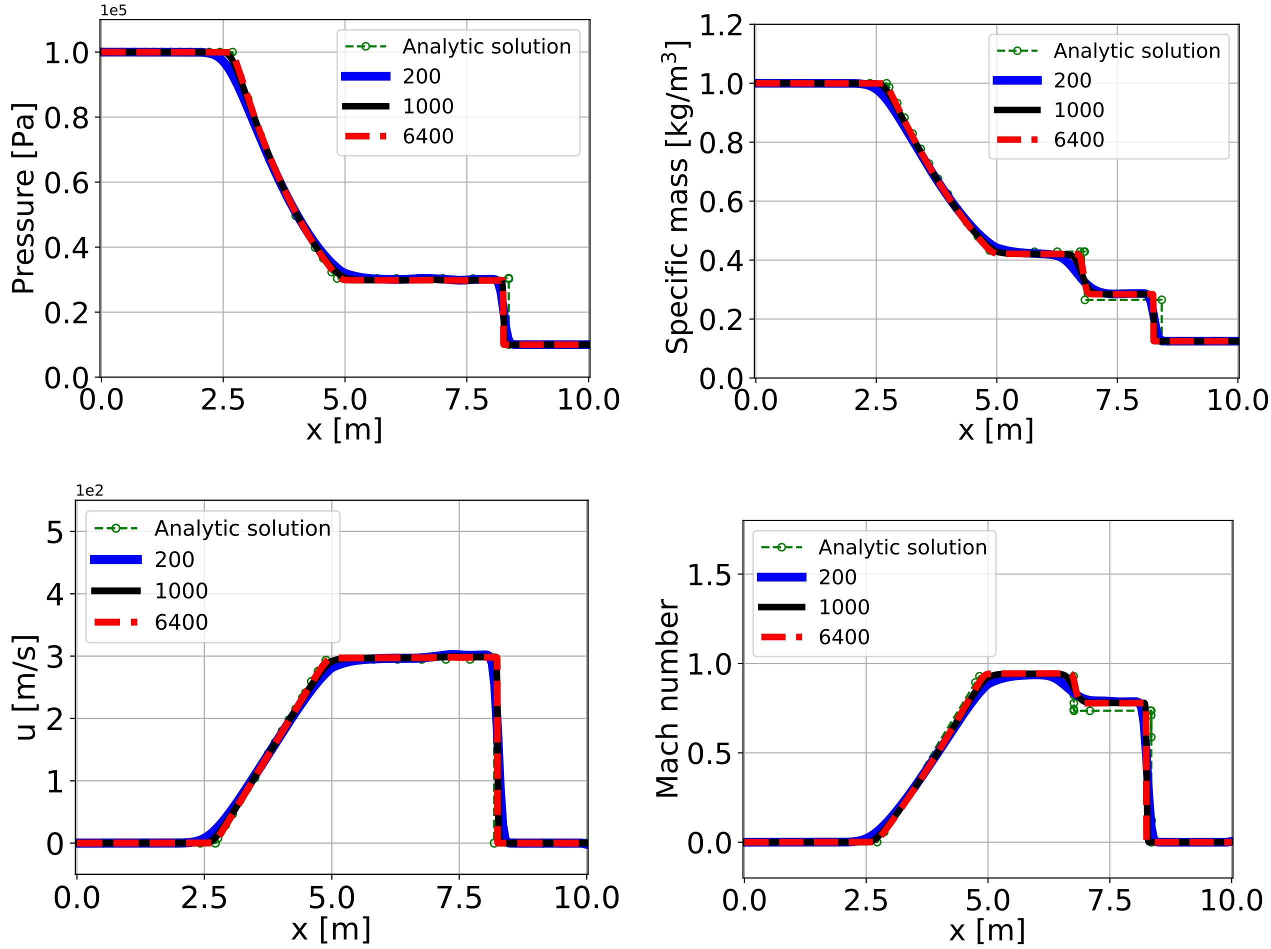


Figure 3. Comparison of the numerical solution with the analytical solution of the shock tube for different mesh refinement.

3.2 Mach 3 test case

In the shock tube problem the flow remains subsonic throughout the simulation. In order to study a case with supersonic flow, the initial data considered are presented in Fig. 4.

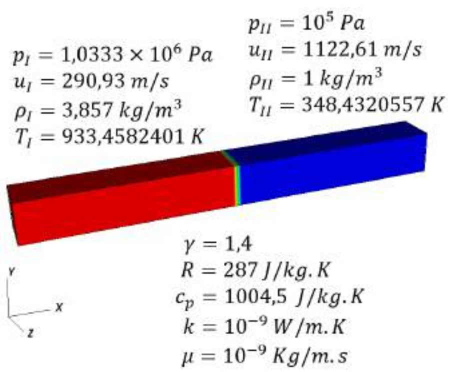


Figure 4. Physical properties of the fluid.

The computational domain is a parallelepiped of 20 m length, 1 m width, 1 m height and the final simulation time is $t = 0.006$ s. The pressure-velocity coupling in the flow is solved by using SIMPLE scheme, totally implicit time discretization are used and Neumann boundary conditions are imposed for all flow variables at the inlet and outlet. Similar to previous numerical simulation, the temporal scheme was fixed and the advective scheme varied. The results from these simulation can be seen in Fig. 5.

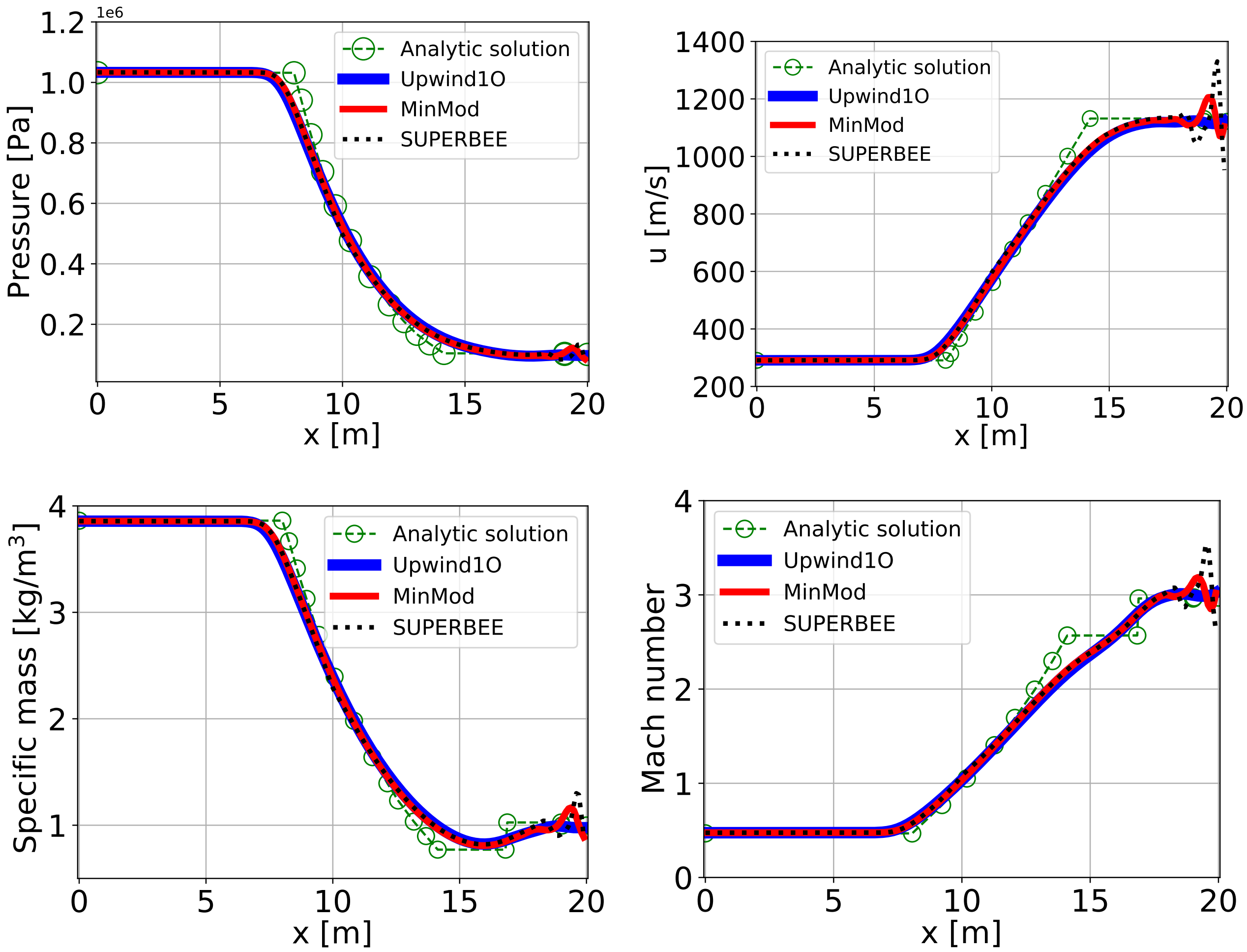


Figure 5. Comparison of the numerical solution with the analytical solution of the supersonic shock tube.

The upwind scheme presented a better result than the other advective schemes tested in the case of the supersonic shock tube. A new test was performed using a thinner mesh and the simulation results for pressure, velocity, specific mass and Mach number for two different mesh resolutions and it results are shown in Fig. 6 and Fig. 7. As expected, the result after refinement of the mesh was better than that of the coarse mesh.

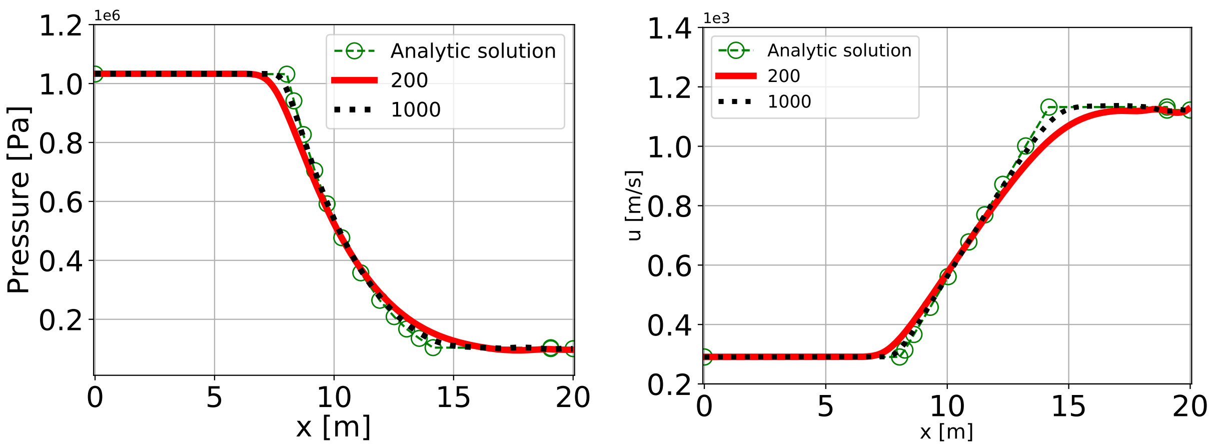


Figure 6. Comparison of the numerical solution with the analytical solution of the supersonic shock tube.

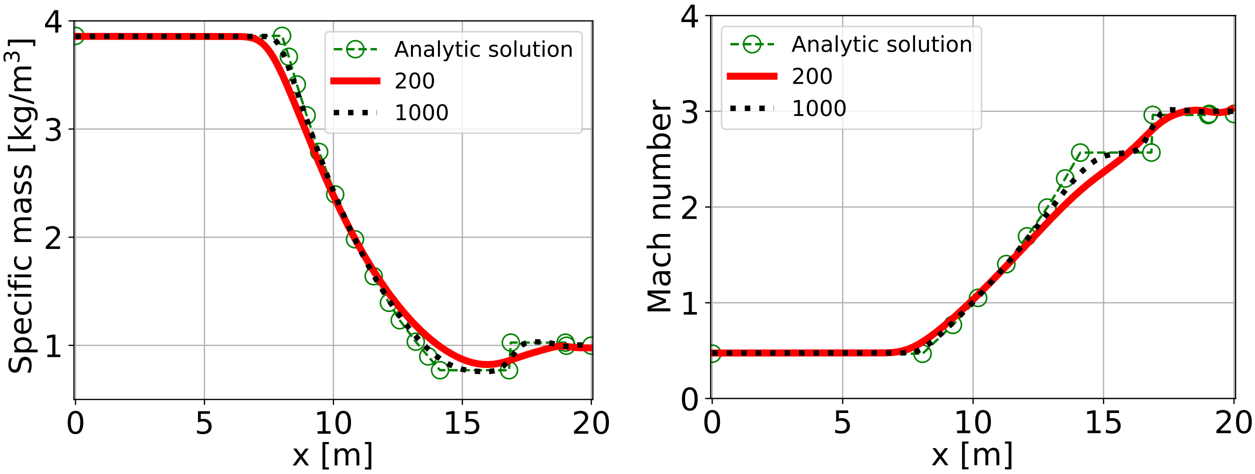


Figure 7. Comparison of the numerical solution with the analytical solution of the supersonic shock tube.

3.3 Riemann's two-dimensional problem

The case tested is Riemann's two-dimensional problem. The domain of the simulation is a parallelepiped of dimensions 1 m $\times$ 1 m $\times$ 0.05 m. As a boundary condition Neumann was adopted for all velocity components, pressure and temperature. For the solution of the Navier-Stokes equations the totally implicit formulation was used with the discretization of the temporal term made with the BDF2 method and the second order upwind method for the discretization of the advective term. The diffusive term is discretized using the centered differences method and the SIMPLE method was adopted for pressure-velocity coupling.

The first simulation was performed using a uniform mesh of 200 $\times$ 200 $\times$ 10 volumes, parallel processing and the domain was divided into sixteen processes. Four different configurations were simulated for the initial conditions, as shown in Fig. 8 and Fig. 9.

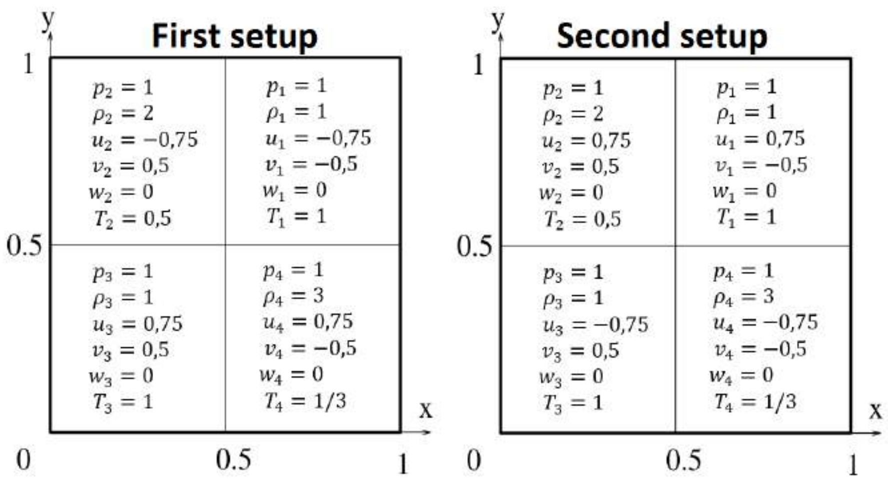


Figure 8. Initial conditions.

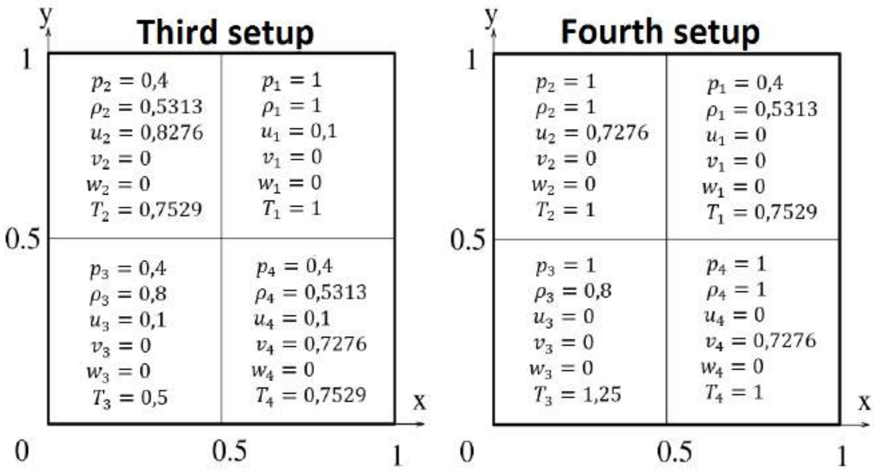
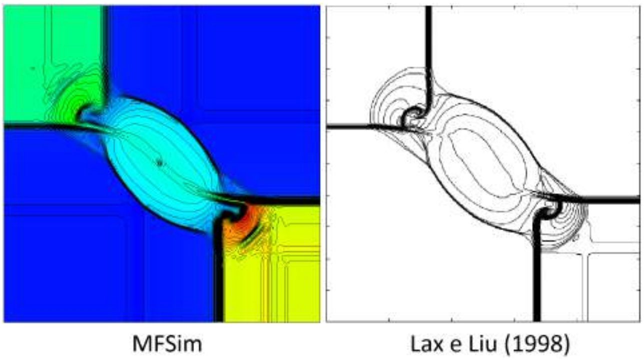
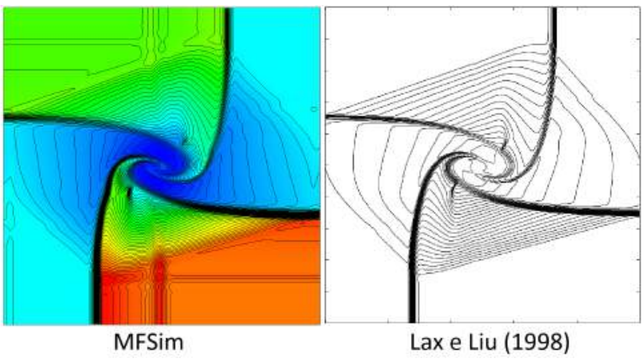


Figure 9. Initial conditions.

The results of the numerical simulation were compared with Lax and Liu (1998), as shown in Fig. 10 and Fig. 11. In these figures, the contours of the specific mass are represented. It is observed a good agreement between the data of the literature and the present numerical simulation.



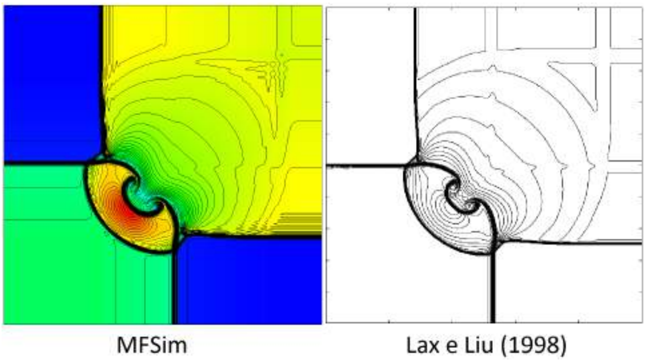
(a) First setup



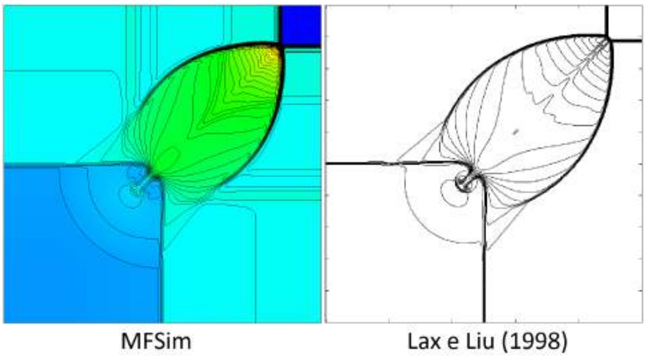
(b) Second setup

Figure 10. Density contours, compared with Lax and Liu (1998).

And for the second configuration we also used an adaptive mesh with two refining levels and base mesh $120 \times 120 \times 6$ volumes. The result of this simulation is shown in Fig. 12 and the fine mesh is represented by the semi-transparent white blocks. In Figure 13 we can see a larger reflation where there is the presence of the discontinuity.



(a) Third setup



(b) Fourth setup

Figure 11. Density contours, compared with Lax and Liu (1998).

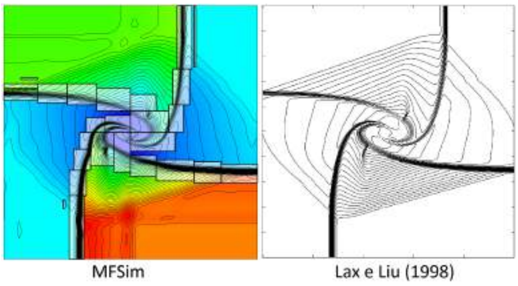


Figure 12. Simulation of the second configuration with adaptive mesh.

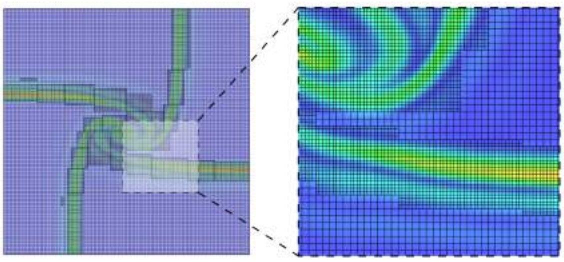


Figure 13. Refinement in the discontinuity region.

4. CONCLUSION

In the present work the results obtained by the extension of the SIMPLE method for compressible flows were presented, with the implementation of the All-Mach technique. Satisfactory results were obtained for the benchmark test cases, showing a good efficiency of the applied technique. To reduce the computational cost, the adaptive mesh technique was used, refining only in the region of interest. As a perspective, the all-mach solver will be used together with the VOF technique already implemented in MFSim in order to identify the phases of the flow and allow the simulation of two-phase flows.

5. ACKNOWLEDGEMENTS

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