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Computational Techniques for Thermochemical Propulsion

Report: Assignement 2

Incompressible fluid solver

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1 Introduction

1.1 Physics

The previous incompressible fluid analysis will be considered as a baseline to study the contribution from compressibility in a flow. In this report only the main modifications with respect to the baseline will be described. Four cases will be studied in which the flow velocity and the temperature at the wall interface will be varied. In the first two the velocity at the inputs is kept constant and unchanged from the previous assignment, while the temperatures at the wall are changed. In the third and fourth cases the velocity at the inlets is increased.

The primary difference between this problem and incompressible fluid flow case is that the density is not assumed to be constant; instead, it varies as a function of pressure and temperature. Consequently, it becomes necessary to solve an nonlinear set of equations for enthalpy transport, or internal energy transport. This additional step is done between the solution of the intermediate velocity and the equation for correction of pressure and its purpose is to extract the temperature field, which is connected to density and pressure by means of the compressibility factor. The relationship between temperature and enthalpy, or internal energy, is established through the specific heat capacity at constant pressure or volume respectively, which is typically estimated using 7th or 9th order polynomial functions of temperature from thermodynamic datasets. These polynomial approximations are valid only within certain temperature ranges. Finally, as in the incompressible fluid solver, the viscosity is updated in order to estimate the viscous stress term in the next outer iteration.

1.2 Quantities of interest

The three main variables for this problem are velocity, pressure and enthalpy. Temperature and density can be retrieved as a next step. The pressure is explicitely solved as the thermodynamic quantity because the assumption of constant pressure does not hold.

Both `k` and ϵ are still needed to evaluate the turbulent contribution of viscosity and a similar process must be done for the characterization of diffusion inside the energy equation, which is the overlapping of molecular term and the additional diffusive contribution due to the turbulence. As in the previous assignement the $k-\epsilon$ turbulence model will be used to estimate the second quantity.

2 Setup of the problem

2.1 Boundary conditions and initial conditions

The files in the 0 folder that were used in the previous assignments are mostly unchanged, with the following small exceptions. Additionally new quantities must be introduced.

2.1.1 p field

The units of measurement must be set to Pa and a different type of boundary condition, the `waveTransmissive`, is preferred at the outlet. This type of boundary handles in better way the transmission of eventual shockwaves that are exiting the domain, by avoiding undesired reflections towards the domain. The initial pressure field is changed from zero in all the domain to a uniform atmospheric condition.

2.1.2 U field

The settings for the boundary conditions of the velocity field are identical for the the first two test cases and correspond to the ones from the incompressible baseline. For the last two test cases of this assignment the velocity values in the y direction at the two inlets need to be changed to 95 and 120 m/s respectively at the `inlet` and `fuel_inlet`.

2.1.3 T field

The field must be generated in the 0 folder, with `K` as unit of measurement. The boundary conditions are imposed as follows:

- test case 1 and 3: the BCs at the `inlet` and `fuel_inlet` are set to uniform and equal to 300 and 350 K respectively. All the walls are adiabatic, meaning that `zeroGradient` option is set as BC.
- test case 2 and 4: the BCs at the `inlet` ,`fuel_inlet` and all the walls are set to uniform and equal to respectively 700, 900 and 850 K.

In all the simulations the initial condition for temperature is set to uniform and equal to the value at the `inlet`, thus 300 or 700 K.

2.2 `alphat` field

This is another field which needs to be introduced inside the simulation. As for the `nut` quantity, it is a variable which is function of only ϵ and k, thus the required BC condition is `computed` in all the boundaries except for the walls, in which the `compressible::alphatWallFunction` type of BC is imposed. The unit of measurement for this quantity is $\frac{kg}{ms}$.

2.3 physicalProperties

The thermodynamic properties of the flow need to be specified for the transport of energy and for the link with temperature. For this the `physicalProperties` from the pitzDaily fluid OpenFOAM tutorial is used as a reference. However some modifications need to be done to adapt the input file to this problem.

The problem under examination deals with a single species perfect gas. Differently from the pitzDaily tutorial the specific enthalpy is solved inside the energy equation, therefor the c_p needs to be defined instead of c_v. For this case it is constant with respect to temperature and equal to 1004 $[J/kgK]$. Also the other thermodynamic properties needed for the transport, such as molecular viscosity, Prandtl number and molecular weight, are kept constant.

Finally the computation of the pressure derivative in time cannot be omitted in the energy equation solved for the enthalpy, since the problem is gaseous and highly compressible. Therefor it needs to be enabled by means of the setting `dpdt`.

All four test cases share the same settings in the `physicalProperties` file.

2.4 fvSchemes

Since the energy equation is introduced and needs to be solved by means of a linear system, all the new terms inside of it need to be discretized. Thus inside the `fvSchemes` input file the discretization methods for the convection of enthalpy and kinetic energy and for the expression of the compressible stress tensor are specified.

2.5 fvSolution

The original settings coming from the previous assignment for the solution of the linear systems remain the same. Also the PIMPLE algorithm with 100 maximum outer iterations and an `outerCorrectorResidualControl` of 1e-04 is mantained.

However the solver and the tolerance for the new variable h need to be imposed and they are set equal to the ones of the velocity, ϵ and k fields, both for the final iteration and for the ones needed to reach the convergence inside the outer loop.

The same needs to be done for the evaluation of density throgh the pressure and the temperature. However in this case the process is more direct because the linear matrix is perfectly diagonal and its solution does not require complex iterative algorithms which require its factorization. Therefor a stricter tolerance, equal to 1e-09, is imposed to take advantage of the simplicity of the process and to obtain an accurate solution with relatively low computational effort.

The same `relaxationFactors` of k and ϵ are applied to the enthalpy.

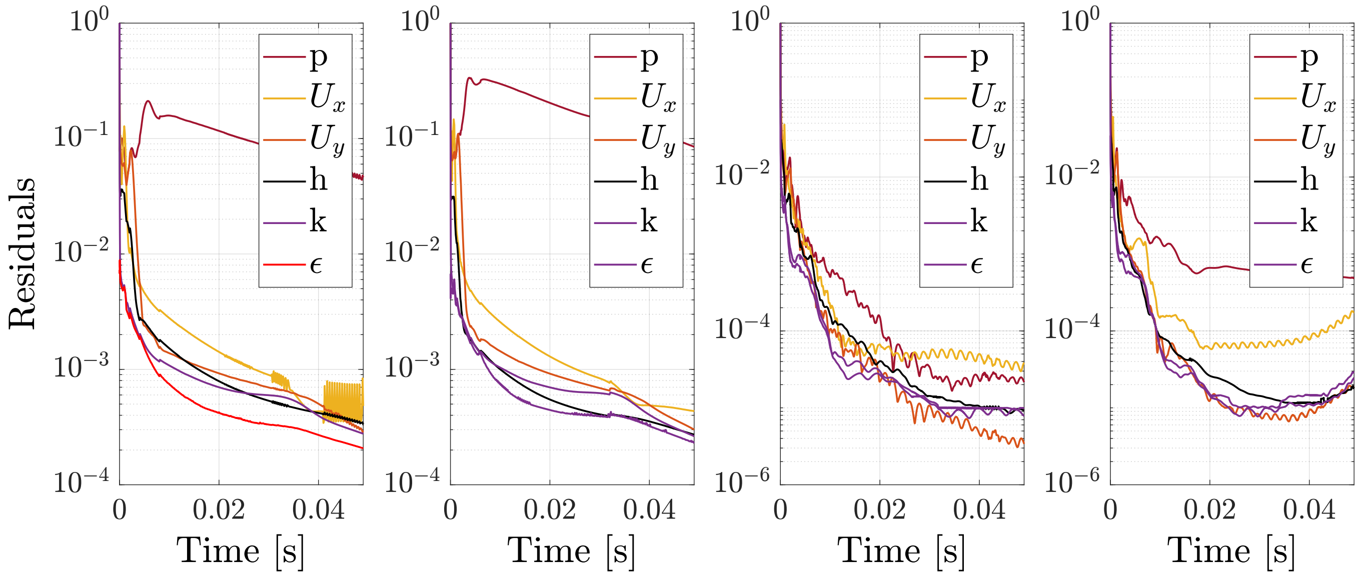
2.5.1 controlDict

For this assignment it is required to simulate the flow for only for 0.05 seconds and a maximum Courant number equal to 5 is imposed. An additional modification which is done inside the `controlDict` file is the implementation of the post-process for the Mach number field by means of the functionObjects. The field is computed as first through the thermodynamic quantities and then it is saved in a VTK format contour in the postProcessing folder. The second output required, the velocity field, will be directly extracted in Paraview.

3 Results

3.1 Convergence

As for the previous assignment two kinds of residuals are analysed for the convergence of the solution.



(a) testCase1 (b) testCase2 (c) testCase3 (d) testCase4

Figure 1: Outer Loop initial residual evolution.

In Fig. 1 it can be seen that the traces for the first initial residual at each timestep are not characterized by the ascending behavior at the end of the simulation. This is because only 0.05 seconds are simulated and there is no time for the aerodynamic instability to take place. It can also be noted that the third and fourth test cases are characterized by lower residuals thanks to the smaller timestep, which is a consequence of the higher velocity and the Courant number which is fixed. However also compressibility plays an important factor on this: more compressible flows are characterized by pressure changes which propagate at relatively lower speeds, and this could be a second reason for which the solvers, and in particular the one for the pressure, start iterating in each timestep from a condition which is closer to the solution, with respect to the low Mach number test cases.

Again the plot of the initial residual at the final outer iteration can confirm that the solution satisfies the coupling between pressure and velocity at each timestep. This time, for testCase4, the residual trace of the U_y quantity is plotted in Fig. 2, because pressure was not chosen as one of the discriminating variables in the `outerCorrectorsResidualControl`. It is clear that the solution is satisfying the requirement for the coupling, given by the residual control of 1e-04, in every single timestep.

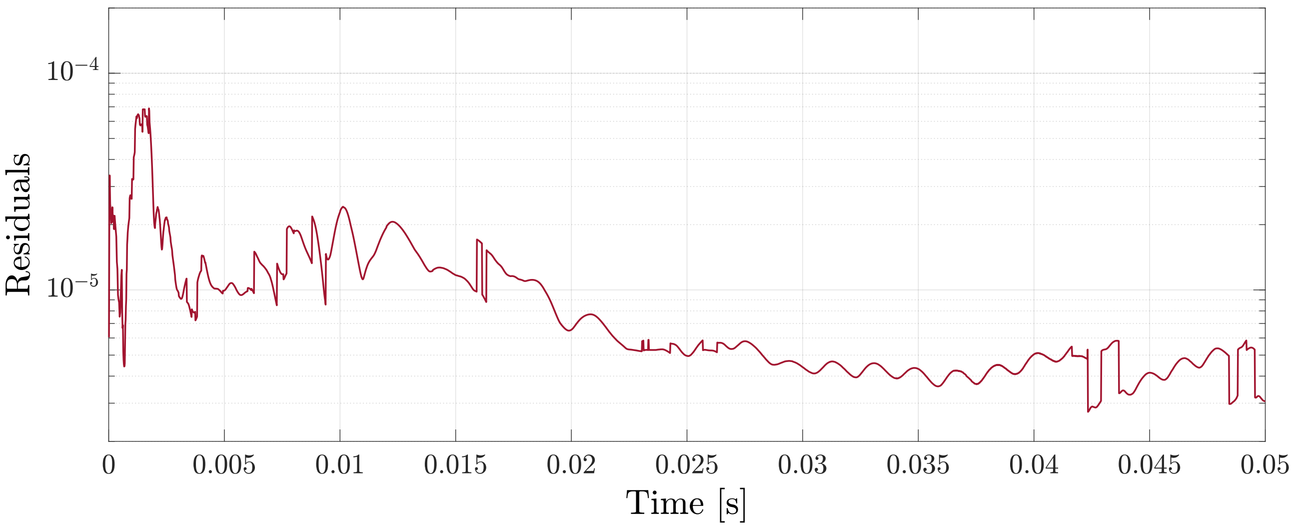


Figure 2: Initial residuals of U_y for the final iteration in the outer loop for the testCase4.

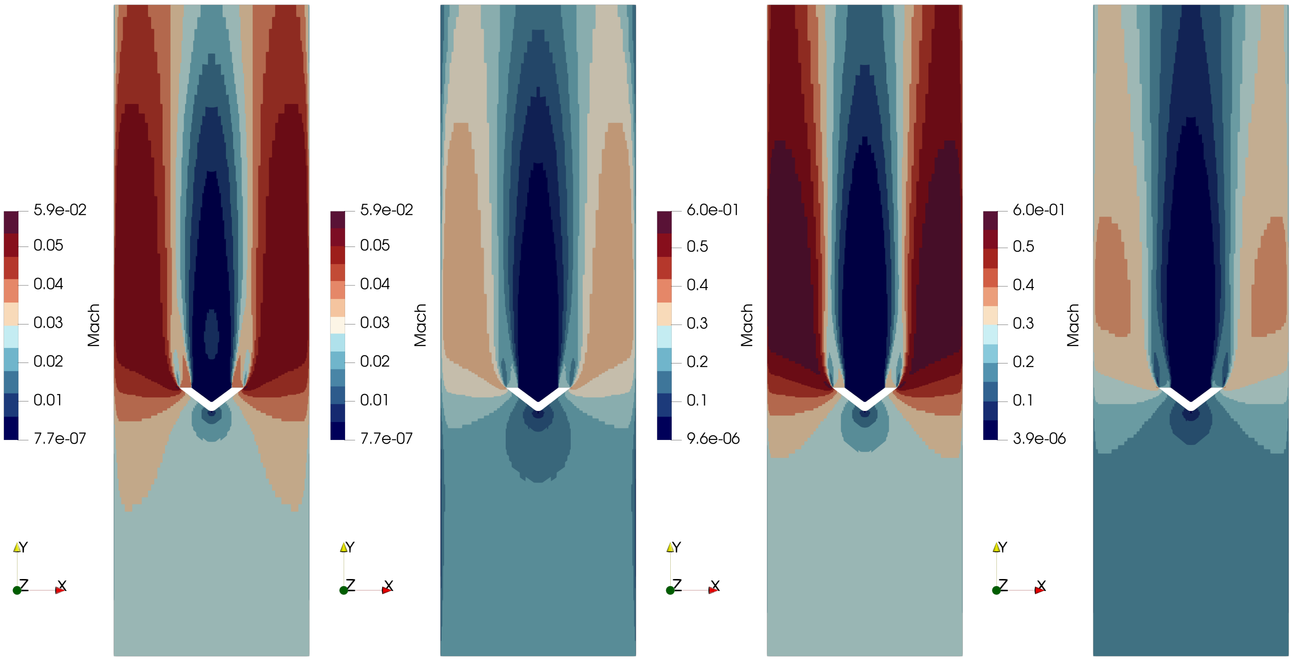
3.2 Post processing

The contours for the Mach number and density are shown in Figs. 3 and 4. To easily compare the results the same color scale is kept between test cases 1 and 2 and between 3 and 4.

As it was expected both the velocity and the temperature boundary conditions are higly influencing the mach number, which increases for higher velocities but decreases for higher temperatures. For this reason test cases 2 and 4 are characterized by lower Mach number fields than respectively test cases 1 and 3.

By looking at the density contours it can be noted that density variation due to the stagnation in front of the splitter is more pronounced for the two cases with higher Mach number, indicating that in the test cases 1 and 2 the flow is behaving more as an incompressible fluid.

Finally the velocity profiles over the line y = 0.1 m at the final timetep (0.05 seconds) are shown in Fig. 5.



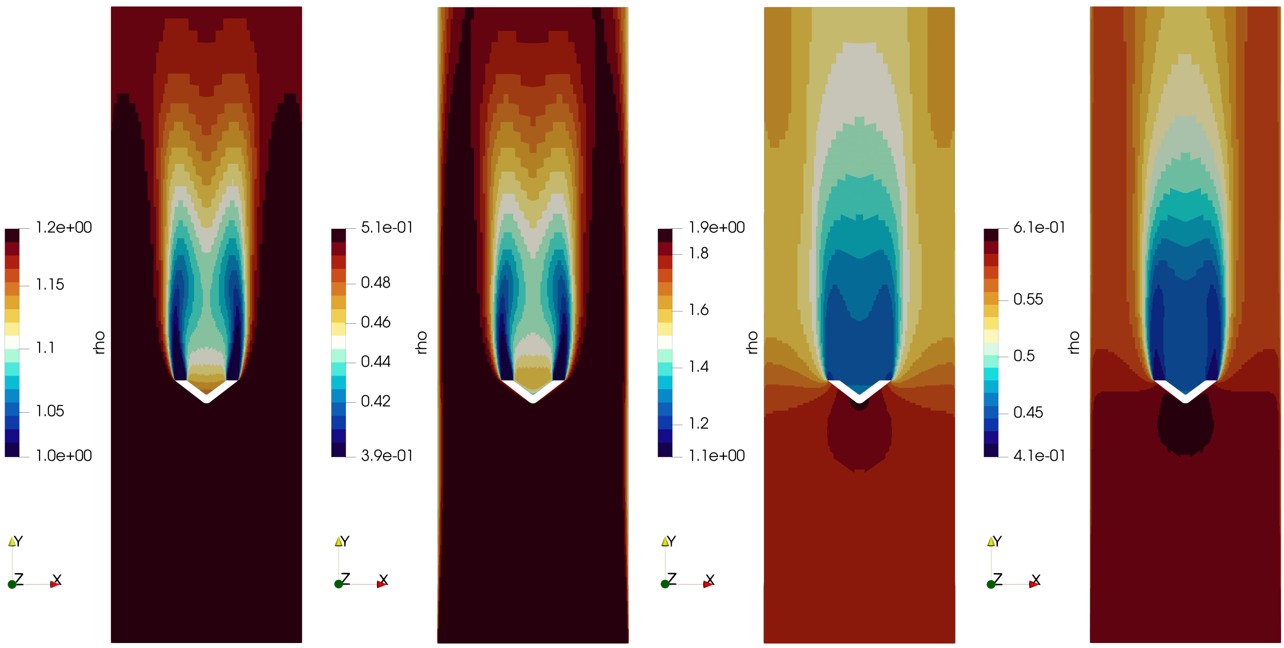
(a) testCase1 low velocity, low temperature

(b) testCase2 low velocity, high temperature

(c) testCase3 high velocity, low temperature

(d) testCase4 high velocity, high temperature

Figure 3: Contour of Mach number at the last iteration. The contour of testCase1 is scaled with respect to testCase1. The contour of testCase4 is scaled with respect to testCase3.



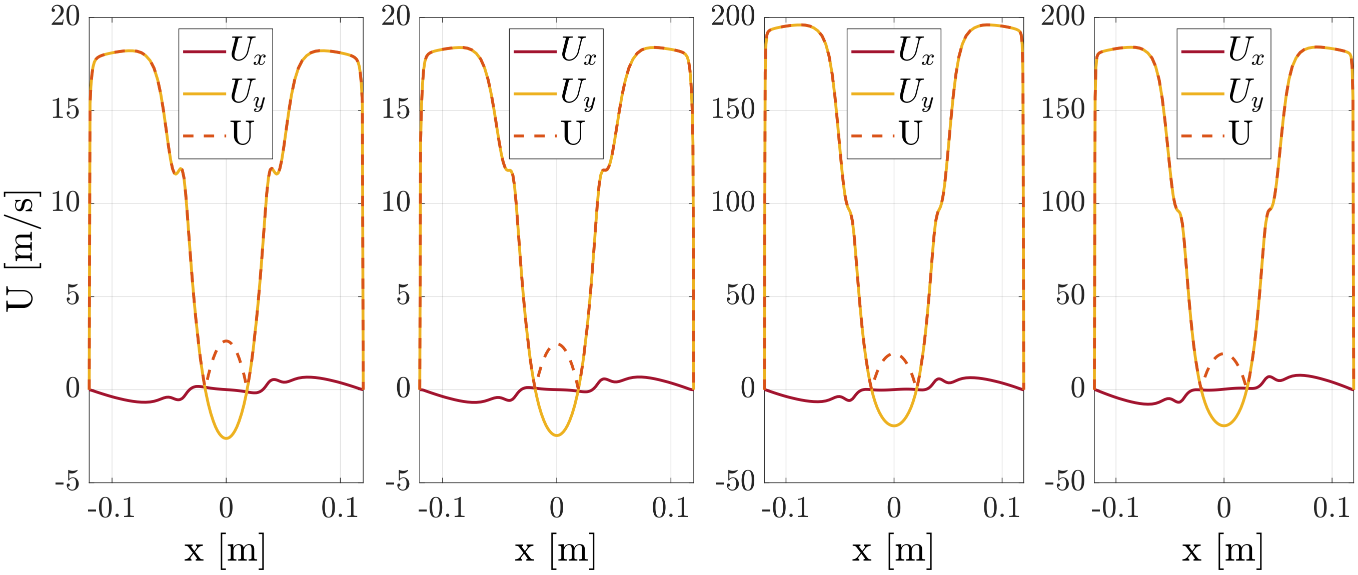
(a) testCase1 low velocity, low temperature

(b) testCase2 low velocity, high temperature

(c) testCase3 high velocity, low temperature

(d) testCase4 high velocity, high temperature

Figure 4: Contour of density at the last iteration.



(a) testCase1 (b) testCase2 (c) testCase3 (d) testCase4

Figure 5: Velocity contour at last iteration, t = 0.5s.