Computational Fluid Dynamics: Project 3

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1. Problem Statement

Fluid Flow through Converging-Diverging Rocket Nozzles

Governing Equations

1. *The Continuity Equation:*

$$\frac{\partial(\rho A)}{\partial t} + \frac{\partial(\rho A V)}{\partial x} = 0 \tag{1}$$

   Where ρ is the density, A is the cross-sectional area and V is the velocity.

2. *The Momentum Equation:*

$$\frac{\partial(\rho A V)}{\partial t} + \frac{\partial(\rho A V^2)}{\partial x} = -A\frac{\partial P}{\partial x} \tag{2}$$

   Where P is the pressure, V is the velocity, A is the cross-sectional area and ρ is the density.

3. *The equation for Total Energy:*

$$\frac{\partial}{\partial t}\left[\rho A\left(e + \frac{V^2}{2}\right)\right] + \frac{\partial}{\partial x}\left[\rho A V\left(e + \frac{V^2}{2}\right)\right] = -\frac{\partial(PAV)}{\partial x} \tag{3}$$

   Where e is the internal energy, P is the pressure, V is the velocity, A is the cross-sectional area and ρ is the density.

4. *Ideal Gas Equation:*

$$P = \rho R T \tag{4}$$

   Where P is the pressure, ρ is the density, T is the temperature and R is the specific gas constant.

Also, the the geometry of the nozzle is described by the area function given below:

$$A = 1 + 2.2(x - 1.5)^2 \quad \text{for} \quad 0 \leq x \leq 3 \tag{5}$$

Simulation Requirements

- Utilise only the conservative form of the governing equations as mentioned above, and express them in the form $\frac{\partial Q}{\partial t} + \frac{\partial F}{\partial x} = S$, where Q is the vector of conserved variables, F is the flux vector and S is the source term.
- Utilise the finite difference method (FDM) for discretisation of the governing equations.
- Utilise MacCormack's scheme for obtaining the discretised equations to ensure second order accuracy in both space and time.
- Ensure that the Courant Number is sufficiently small since an explicit scheme is being applied.
- Plot the variation of the following quantities with the axial coordinate and compare the results with the analytical solution:
  1. Pressure (P/P_0)
  2. Density (ρ/ρ_0)
  3. Temperature (T/T_0)
  4. Mach Number (M)

There are three simulation cases:

1. **Part 1:** Isentropic Subsonic Flow
2. **Part 2:** Isentropic Subsonic-Supersonic Flow
3. *Part 3 (optional):* Non-Isentropic Flow with Shock Waves

Analytical Solutions for Isentropic Flow

$$\frac{P}{P_0} = \left(1 + \frac{1-\gamma}{2}M^2\right)^{-\frac{\gamma}{\gamma-1}} \tag{6}$$

$$\frac{\rho}{\rho_0} = \left(1 + \frac{1-\gamma}{2}M^2\right)^{-\frac{\gamma}{\gamma-1}} \tag{7}$$

$$\frac{T}{T_0} = \left(1 + \frac{1-\gamma}{2}M^2\right)^{-1} \tag{8}$$

$$\frac{A}{A^*} = \frac{1}{M}\left[\frac{2}{\gamma+1}\left(1 + \frac{\gamma-1}{2}M^2\right)\right]^{\frac{\gamma+1}{2(\gamma-1)}} \tag{9}$$

$$C = \sqrt{\gamma R T} \tag{10}$$

Where P_0, ρ_0 and T_0 are the stagnation pressure, density and temperature respectively, A^* is the throat area and C is the speed of sound.

2. Mesh Details and Discretisation Approach

2.1. Mesh Details

For this simulation, there is not a specific mesh that is used since it is a one dimensional problem.
The central axis was divided into a certain number of grid points for which the explicit MacCormack's method was applied iteratively to obtain the solution of the equations.

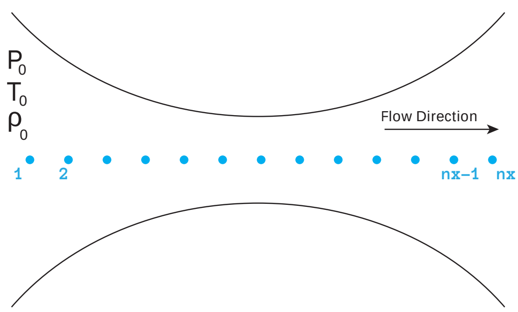

Figure 1. *Schematic of the discretised axial line and the nozzle*

2.2. Boundary Conditions

Based on the conservative form of the governing equations (equation 14), there are three parameters we can potentially set at the inlet and outlet. They are: Pressure (P), Density (ρ) and Velocity (V).

1. **For Part 1:** This is the subsonic isentropic flow case. For this case, we need to specify two boundary conditions and extrapolate the third, and specify one boundary condition at the outlet and extrapolate the other two. For this simulation, I have chosen to specify the pressure at the outlet.

Boundary Condition	Location	Value
Density (ρ)	Inlet	1.0
Temperature (T)	Inlet	1.0

Table 1. *Subsonic flow: Boundary Conditions (non-dimensionalised values)*

2. **For Part 2:** This is the subsonic-supersonic flow case. For this case, we need to specify two boundary conditions at the inlet and extrapolate the third. Also, all the boundary conditions at the outlet have to be extrapolated.
   For this simulation, I have chosen to specify the density and the temperature at the inlet. Velocity at the inlet will be indirectly extrapolated.

Boundary Condition	Location	Value
Density (ρ)	Inlet	1.0
Temperature (T)	Inlet	1.0
Pressure (P)	Outlet	0.99

Table 2. *Subsonic-Supersonic flow: Boundary Conditions (non-dimensionalised values)*

For the extrapolation of the velocity and all three of the outlet boundary conditions, a simple linear extrapolation was used as shown:

$$x_i = 2x_{i+1} - x_{i+2}$$

It is important to note that the velocity was not directly extrapolated, and rather Q_2 was extrapolated (from equation18) from which the velocity was obtained.

2.3. Variables and Constants Utilised

Adiabatic Ratio (γ)	1.4 (for air)
Specific Gas Constant (R)	240.7734 J/K (for air)

2.4. Approach for discretising the equations

MacCormack's scheme [2] needs to be utilised for discretising the equations. MacCormack's scheme is a variation of the Lax-Wendroff scheme. It involves two steps:

1. **Predictor Step:** A forward difference scheme in space is applied.

2. **Corrector Step:** A backward difference scheme in space is applied. The two steps ensure that MacCormack's method remains second order accurate in both space and time even though the partial differential equation is solved explicitly, which means the solution at level $n+1$ is calculated using the values at level n.

Consider the following hyperbolic PDE:

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0 \tag{11}$$

Consider value of the solution at level $n+1$ to be denoted by a superscript '*', and i refers to the grid point of calculation.

Predictor Step: In this step, we take the time step to be Δt.

$$u_i^* = u_i^n - a\frac{\Delta t}{\Delta x}(u_{i+1}^n - u_i^n) \tag{12}$$

Corrector Step: In this step, we take the time step to be $\Delta t/2$ and calculate the solution at level $n+1/2$, that is then replaced by the average of the solutions at levels n and $n+1$.

$$\left(\frac{\partial u}{\partial t}\right)^{n+1} = -a\left(\frac{u_i^* - u_{i-1}^*}{\Delta x}\right)$$

When we replace the derivative, we get:

$$\frac{u_i^{n+1} - u_i^{n+1/2}}{\Delta x/2} a\left(\frac{u_i^* - u_{i-1}^*}{\Delta x}\right)$$

Simplifying this equations and replacing $u_i^{n+1/2}$ with $\frac{u_i^n + u_i^*}{2}$, we get:

$$u_i^{n+1} = \frac{u_i^n + u_i^*}{2} - a\frac{\Delta t}{2\Delta x}(u_i^* - u_{i-1}^*) \tag{13}$$

3. Discretised Equations

We have to express equations 1, 2, 3 in the following format as vectors [1]:

$$\frac{\partial Q}{\partial t} + \frac{\partial F}{\partial x} = S \tag{14}$$

We first non-dimensionalise the governing equations, and we obtain the following form of the governing equations:

Continuity

$$\frac{\partial(\rho' A')}{\partial t'} + \frac{\partial(\rho' A' V')}{\partial x'} = 0 \tag{15}$$

Momentum

$$\frac{\partial(\rho' A' V')}{\partial t'} + \frac{\partial(\rho' A' V'^2 + \frac{1}{\gamma}P' A')}{\partial x'} = \frac{1}{\gamma}P'\frac{\partial A'}{\partial x'} \tag{16}$$

Total Energy

$$\frac{\partial\left[\rho' A'\left(\frac{e'}{\gamma-1} + \frac{\gamma}{2}V'^2\right)\right]}{\partial t'} + \frac{\partial'\left[\rho\left(\frac{e'}{\gamma-1} + \frac{\gamma}{2}V'^2\right)V'A' + P'A'V'\right]}{\partial x'} = 0 \tag{17}$$

Expressing Q, F and S in matrix form, we get:

$$\begin{bmatrix} \rho' A' \\ \rho' A' V' \\ \rho' A'\left(\frac{e'}{\gamma-1} + \frac{\gamma}{2}V'^2\right) \end{bmatrix} = 0 \tag{18}$$

$$\begin{bmatrix} \rho' A' V' \\ \rho' A' V'^2 + \frac{1}{\gamma} P' A' \\ \rho' \left(\frac{e'}{\gamma - 1} + \frac{\gamma}{2} V'^2 \right) V' A' + P' A' V' \end{bmatrix} = 0 \tag{19}$$

$$\begin{bmatrix} 0 \\ \frac{1}{\gamma} P' \frac{\partial A'}{\partial x'} \\ 0 \end{bmatrix} \tag{20}$$

The scales for the variables are given below:

$$\begin{aligned} \rho &\rightarrow \rho_0 \\ P &\rightarrow P_0 \\ A &\rightarrow A^* \\ V &\rightarrow a_0 \\ x &\rightarrow L \\ t &\rightarrow L/a_0 \\ e &\rightarrow e_0 \end{aligned}$$

Since $e = c_v T$ and $e_0 = c_v T_0$, we can conclude that the non-dimensionalised energy term $e' = e/e_0$ is equal to the non-dimensionalised temperature term $T' = T/T_0$.
Since we need to solve for Q, the solution to the problem becomes easier if we express F and S in terms of the elements of Q.

$$F_1 = Q_2 \tag{21}$$

$$F_2 = \frac{Q_2^2}{Q_1} + \frac{\gamma - 1}{\gamma} \left(Q_3 - \frac{\gamma}{2} \frac{Q_2}{Q_1} \right) \tag{22}$$

$$F_3 = \gamma \frac{Q_2 Q_3}{Q_1} - \frac{\gamma(\gamma - 1)}{2} \frac{Q_2^3}{Q_1^2} \tag{23}$$

The governing equations now become:

$$\frac{\partial Q_1}{\partial t'} = -\frac{\partial F_1}{\partial x'} \tag{24}$$

$$\frac{\partial Q_2}{\partial t'} = -\frac{\partial F_2}{\partial x'} + S_2 \tag{25}$$

$$\frac{\partial Q_3}{\partial t'} = -\frac{\partial F_3}{\partial x'} \tag{26}$$

We now discretise the above equations using the MacCormack Scheme.
For the continuity and total energy equations, the following discretisation will be used since they are of the same form, and Q, F will be replaced by Q_1, F_1 and Q_3, F_3 for the continuity and total energy equations respectively.

1. **Predictor Step**
   Using equation 12, we get:

$$Q_i^* = Q_i^n - \frac{\Delta t}{\Delta x}(F_{i+1}^n - F_i^n) \tag{27}$$

2. **Corrector Step**
   Using equation 13, we get:

$$Q_i^{n+1} = \frac{Q_i^n + Q_i^*}{2} - \frac{\Delta t}{2\Delta x}(F_i^* - F_{i-1}^*) \tag{28}$$

For the momentum equation, the following discretisation will be used since it is has a source term on the right hand side. Q, F and S will be replaced by Q_2, F_2 and S_2 respectively and P and A will be replaced by

$$\text{For Predictor Step:} \quad S_i^n = -P_i^n \frac{A_{i+1} - A_i}{\Delta x}$$

$$\text{For Corrector Step:} \quad S_i^* = -P_i^* \frac{A_i - A_{i-1}}{\Delta x}$$

1. **Predictor Step**
   Using equation 12, we get:

$$Q_i^* = Q_i^n - \frac{\Delta t}{\Delta x}(F_{i+1}^n - F_i^n) + \Delta t S_i^n$$

$$Q_i^* = Q_i^n - \frac{\Delta t}{\Delta x}(F_{i+1}^n - F_i^n) - \frac{\Delta t}{\Delta x} P_i^n (A_{i+1} - A_i) \tag{29}$$

2. **Corrector Step**
   Using equation 13, we get:

$$Q_i^{n+1} = \frac{Q_i^n + Q_i^*}{2} - \frac{\Delta t}{2\Delta x}(F_i^* - F_{i-1}^*) + \frac{\Delta t}{2} S_i^*$$

$$Q_i^{n+1} = \frac{Q_i^n + Q_i^*}{2} - \frac{\Delta t}{2\Delta x}(F_i^* - F_{i-1}^*) - \frac{\Delta t}{2\Delta x} P_i^* (A_i - A_{i-1}) \tag{30}$$

4. Solution Methodology

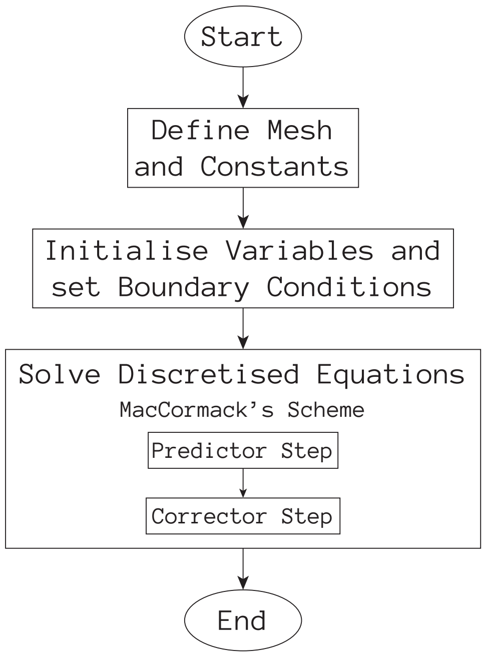

Figure 2. *Program Control Flow*

1. Initialise all the constants and values required for solving the problem.
2. Next, non-dimensionalise the governing equations.
3. Express the non-dimensionalised governing equations in the form of equation 14.

4. Now, discretise the obtained vector equation using MacCormack's scheme, as explained in detail in section 3.

5. Next, write code to solve the discretised equations. Carefully applied the boundary conditions as specified in section 2.2.

6. Obtain the results and the required plots and draw inferences.

5. Results and Discussions

Part 1: Isentropic Subsonic Flow

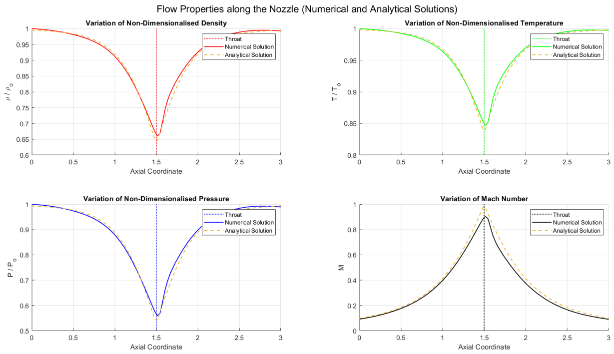

Figure 3. *Comparison of Numerical and Analytical Solutions for Part 1*

Explanation of trends in figure 3:

1. **Variation of $\mathbf{P/P_0}$:** The pressure decreases from the inlet until the throat, after which it increases till the outlet. This is because the cross-sectional area first decreases up until the throat, which causes the flow to speed up and the pressure to decrease. The reverse occurs after the throat since the cross-sectional area increases up until the outlet. The reduction in pressure is governed by the isentropic relations specified in section 1 (equations 6 to 10)

2. **Variation of ρ/ρ_0:** The density decreases along with pressure following the continuity equation for compressible flow. To maintain a constant mass flow rate, the density has to decrease in the converging section since the speed increases, and it has to increase in the diverging section as the speed decreases.

3. **Variation of $\mathbf{T/T_0}$:** The temperature decreases until the throat, and then it increases till the outlet. The reason for the decrease in temperature in the converging section is the first law of thermodynamics, due to which the internal energy of the flow converts to kinetic energy speeding it up. Due to our assumption that the problem is isentropic, the temperature variation is gradual and smooth.

4. **Variation of M:** The Mach number increases till the throat and decreases until the outlet. This behaviour can be explained by the isentropic relations in section 1 (equations 6 to 10), and also the variation of the pressure, density and temperature as explained above. For this simulation, there is a small difference between the numerical and the analytical solution.

- The numerical solution does not reach $M = 1$ at the throat as it should. When the number of iterations are increased, the code begins to show instabilities.
- Selecting an effective breaking point was necessary to avoid instabilities. For this simulation, the breaking point was chosen as 95.5% of the expected Mach number at the throat. This means that the iterative loop would stop executing once the computed Mach number was equal to 0.955, or when the maximum number of specified iterations is reached.

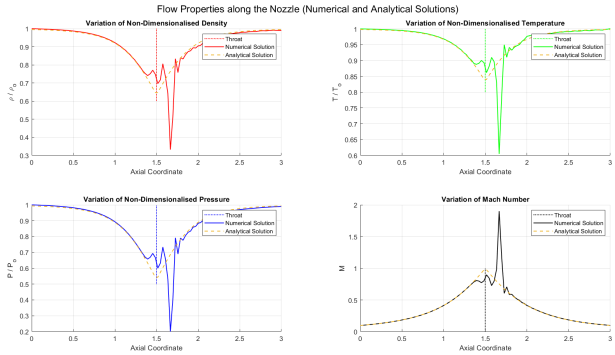

Figure 4. *Instabilities in the Numerical Solution for Part 1*

Part 2: Isentropic Subsonic-Supersonic Flow

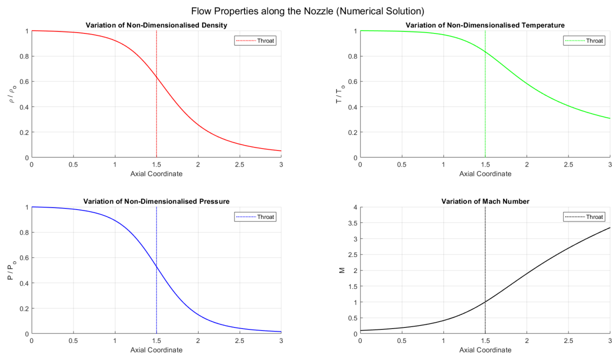

Figure 5. *Numerical Solution for Part 2*

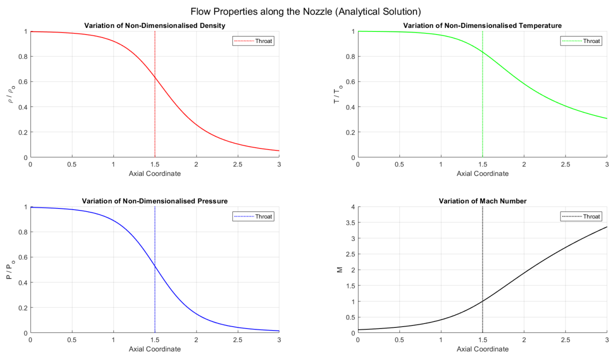

Figure 6. *Analytical Solution for Part 2*

Explanation of trends in figures 5 and 6:

1. **Variation of $\mathbf{P/P_0}$:** Pressure decreases sharply as the flow passes through the throat region into the diverging section, where it further decreases but at a much gradual rate. The speed of the air is faster than the speed of sound at the throat, which make the compressibility effects of the air translate into a pressure decrease and a transfer of energy into the kinetic domain.

2. **Variation of ρ/ρ_0:** Similar to the subsonic case, the trend in density is observed due to the need to maintain continuity or a constant mass flow rate. As per compressible flow theory, lower densities are required to accommodate the higher velocity as the cross-sectional area decreases.

3. **Variation of $\mathbf{T/T_0}$:** Since the compressibility effects of air cause a transfer of energy into the kinetic domain, a substantial decrease in temperature is observed. In simplified terms, the thermal energy of the fluid is transformed into kinetic energy. The gradient of the temperature is quite steep, which indicates that energy conversions in converging-diverging nozzles are efficient.

4. **Variation of M:** At the throat, the Mach number attains a value of 1. Before the flow reaches the throat, the gradient of the Mach number gradually increases, but the gradient becomes much steeper after the throat and the flow attains very high speeds rapidly in the diverging section. This effect is captured by the area-Mach number relation from compressible flow theory, and demonstrates the effect of nozzle geometry on the flow speed.

Comparison of Errors

Parameter	RMSE
ρ/ρ_0	0.0091
T/T_0	0.0042
P/P_0	0.0116
M	0.0348

Table 3. *Root Mean Square Error (RMSE) for Part 1*

Parameter	RMSE
ρ/ρ_0	0.0024
T/T_0	0.0010
P/P_0	0.0032
M	0.0037

Table 4. *Root Mean Square Error (RMSE) for Part 2*

From tables 3 and 4, we can see that the root mean squared errors for the subsonic-supersonic flow case are lesser than those of the subsonic flow case. This may be due to fewer numerical diffusion effects in the high-speed flow region. The subsonic-supersonic flow case is more well-defined and predicatable compared to the subsonic flow case which makes it less susceptible to numerical instabilities.

6. Conclusion

This project resulted in the successful simulations of both the required simulation cases, the isentropic subsonic flow and the isentropic subsonic-supersonic flow. The simulation was performed by discretising the governing equations in conservative vector forms using MacCormack's scheme so that second-order is achieved in space and time.
The obtained numerical results were compared with the analytical solutions for isentropic flow, and the trends were analysed and explained.
Some interesting observations and analyses are listed below:

- The accuracy of MacCormack's scheme was verified by comparing the numerical results to the analytical results for both cases. However, it was observed that the numerical solution was slightly unstable for the subsonic flow case.

- Setting the boundary conditions for both parts of this simulation was the most important part. Even a slight mistake in the boundary conditions would completely destroy the solution. Therefore, it was necessary to carefully implement the boundary conditions.

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References

[1] J. D. Anderson, *Computational Fluid Dynamics: The Basics with Applications*. McGraw-Hill, 1995.

[2] Wikipedia contributors, *MacCormack method — Wikipedia, The Free Encyclopedia*, [Online; accessed 14-October-2024], 2024. [Online]. Available: https://en.wikipedia.org/wiki/MacCormack_method.