CFD Project 3

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1 Problem Statement

Nozzles are essential devices used to accelerate fluid flow, which is crucial for various applications, including rocket propulsion. In this context, a converging-diverging nozzle is used to increase the velocity of combustion products to supersonic speeds, generating thrust. This project focuses on the computational analysis of fluid flow through a Converging-Diverging nozzle using the time-dependent Euler equations in their conservative form. The study assumes quasi one-dimensional, inviscid, compressible, and unsteady flow under adiabatic conditions. The goal is to compute steady-state solutions for different flow regimes by solving the Euler equations using numerical methods.

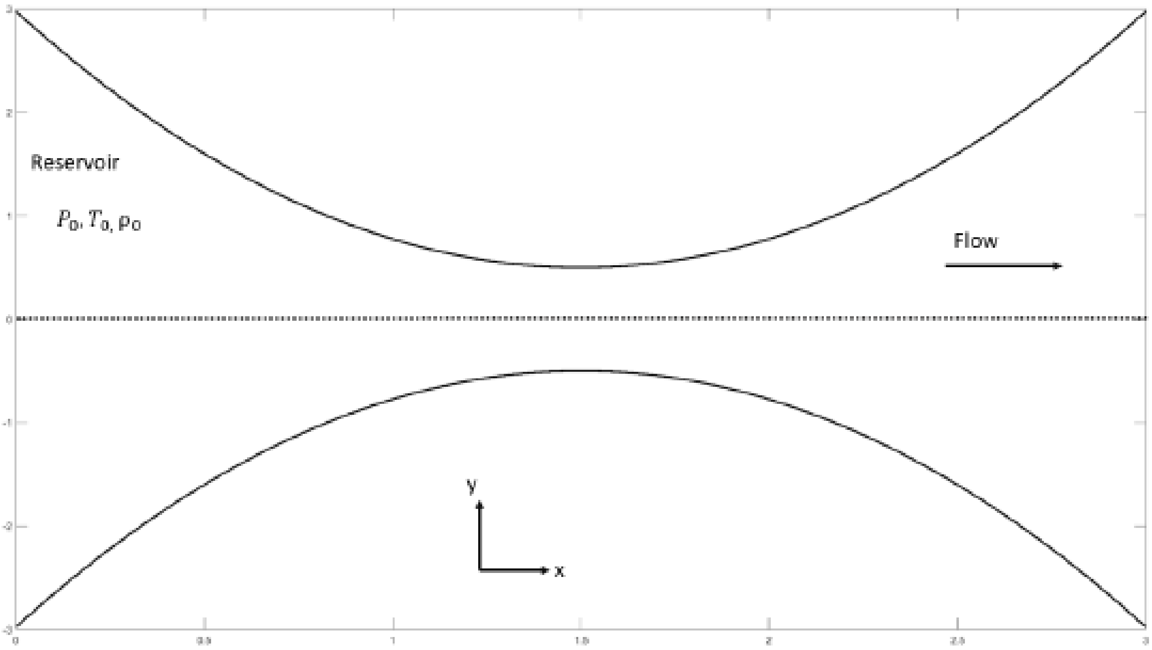

Figure 1: Converging-Diverging nozzle

1.1 Assumptions and Geometry

The following assumptions are made to simplify the problem:

- The flow is quasi one-dimensional, implying uniform properties across the nozzle's cross-sectional area, varying only along the axial direction.
- The flow is inviscid, as the objective is not to study wall effects on the flow.
- The flow is unsteady, compressible, and laminar.
- The nozzle wall is adiabatic, neglecting heat transfer.

The nozzle geometry is represented by the following area function:

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

1.2 Governing Equations

The governing equations for mass, momentum, and energy conservation are derived from the Euler equations for compressible flow. The equations are presented in conservative form as follows:

1.2.1 Continuity Equation

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

1.2.2 Momentum Equation

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

1.2.3 Energy Equation

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

Here, ρ is the fluid density, V is the velocity, P is the pressure, and e is the internal energy. These equations are discretized using the finite difference method with MacCormack's scheme for second-order accuracy in space and time.

1.3 Numerical Approach and Cases Studied

The numerical approach involves solving the time-dependent Euler equations until a steady-state solution is obtained. The study involves two flow regimes, characterized by different back pressure conditions:

- **Isentropic Subsonic Flow:** The back pressure is slightly lower than the stagnation pressure, resulting in subsonic flow throughout the nozzle.
- **Isentropic Subsonic-Supersonic Flow:** The back pressure is sufficiently low for the flow to accelerate to supersonic speeds in the diverging section after reaching sonic speed at the throat.

1.4 Boundary and Initial Conditions

Boundary conditions are imposed based on the characteristics of the flow at the nozzle's inlet and outlet. At the inlet, stagnation conditions are assumed, while at the outlet, different back pressures are specified for the respective flow regimes. Initial conditions are chosen creatively to ensure fast convergence to the steady-state solution.

2 Discretization

The computational domain for the converging-diverging nozzle is discretized using a uniform mesh with 101 nodes. The nozzle length is divided evenly, ensuring that each node represents a fixed interval along the axial direction. This uniform grid ensures a consistent spatial resolution throughout the domain, providing a straightforward implementation of the finite difference scheme.

2.1 Spatial and Temporal Discretization

The spatial discretization is performed using the finite difference method (FDM). Given the uniform nature of the mesh, the spatial derivative of a variable $f(x)$ at the i-th node is approximated using central differences for interior nodes as follows:

$$\left.\frac{\partial f}{\partial x}\right|_i \approx \frac{f_{i+1} - f_{i-1}}{2dx}$$

where dx is the uniform grid spacing, calculated as:

$$dx = \frac{x_{\text{end}} - x_{\text{start}}}{N - 1}$$

Here, $N = 201$ is the number of nodes, $x_{\text{start}} = 0$, and $x_{\text{end}} = 3$, corresponding to the nozzle length.

2.2 System Analysis and Eigenvalue Derivation

2.2.1 Quasi-Linear Form

To analyze the system characteristics, we first express the conservation equations in quasi-linear form:

$$\frac{\partial Q}{\partial t} + A(Q)\frac{\partial Q}{\partial x} = S$$

where $A(Q)$ is the Jacobian matrix:

$$A(Q) = \frac{\partial F}{\partial Q}$$

2.2.2 Jacobian Matrix

The Jacobian matrix components are derived as:

$$A(Q) = \begin{bmatrix} 0 & 1 & 0 \\ -\frac{Q_2^2}{Q_1^2} + \frac{\gamma-1}{2}\frac{Q_2^2}{Q_1^2} & 2\frac{Q_2}{Q_1} - (\gamma-1)\frac{Q_2}{Q_1} & \gamma - 1 \\ -\frac{Q_2 Q_3}{Q_1^2} + (\gamma-1)\frac{Q_2^3}{Q_1^3} & \frac{Q_3}{Q_1} - \frac{3(\gamma-1)}{2}\frac{Q_2^2}{Q_1^2} & \gamma\frac{Q_2}{Q_1} \end{bmatrix}$$

2.2.3 Eigenvalue Analysis

The eigenvalues of the system are obtained by solving:

$$|A(Q) - \lambda I| = 0$$

This yields three eigenvalues:

$$\lambda_1 = V - c, \quad \lambda_2 = V, \quad \lambda_3 = V + c$$

where $c = \sqrt{\gamma RT}$ is the local speed of sound, and $V = \frac{Q_2}{Q_1}$ is the local velocity.

These eigenvalues determine the characteristic directions of information propagation and are crucial for:

- Determining the boundary condition requirements
- Establishing the CFL condition
- Analyzing the hyperbolic nature of the system

2.3 Governing Equations in Conservative Form

The governing equations for quasi-one-dimensional, inviscid, compressible flow are expressed as:

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

2.3.1 Conservative Variables

The conservative variables Q are:

$$Q = \begin{pmatrix} \rho A \\ \rho A V \\ \rho A \left(e + \frac{V^2}{2}\right) \end{pmatrix} = \begin{pmatrix} Q_1 \\ Q_2 \\ Q_3 \end{pmatrix}$$

where:

- ρ is the density
- V is the velocity
- $e = \frac{RT}{\gamma - 1}$ is the internal energy
- A is the cross-sectional area
- T is the temperature
- R is the gas constant
- γ is the specific heat ratio

2.3.2 State Variables Recovery

From the conservative variables, we can recover the physical variables:

$$\rho = \frac{Q_1}{A}$$
$$V = \frac{Q_2}{Q_1}$$
$$T = \frac{\gamma - 1}{R}\left(\frac{Q_3}{Q_1} - \frac{1}{2}\left(\frac{Q_2}{Q_1}\right)^2\right)$$
$$P = \rho RT = (\gamma - 1)\left(Q_3 - \frac{Q_2^2}{2Q_1}\right)$$

2.4 Flux Vector Derivation

The flux vector F represents the physical fluxes of mass, momentum, and energy:

$$F = \begin{pmatrix} \rho AV \\ \rho AV^2 + AP \\ \left(\rho Ae + \frac{1}{2}\rho AV^2 + AP\right) V \end{pmatrix}$$

Expressing in terms of conservative variables:

$$F = \begin{pmatrix} Q_2 \\ \frac{Q_2^2}{Q_1} + A(\gamma - 1)\left(Q_3 - \frac{Q_2^2}{2Q_1}\right) \\ \frac{Q_2 Q_3}{Q_1} + A(\gamma - 1)\left(Q_3 - \frac{Q_2^2}{2Q_1}\right)\frac{Q_2}{Q_1} \end{pmatrix}$$

2.5 Source Term Analysis

The source term accounts for the geometric variations in the nozzle:

$$S = \begin{pmatrix} 0 \\ -(\gamma - 1)\left(Q_3 - \frac{Q_2^2}{2Q_1}\right)\frac{dA}{dx} \\ 0 \end{pmatrix}$$

where $\frac{dA}{dx}$ represents the rate of change of cross-sectional area along the nozzle.

2.6 Stability Analysis

The time step Δt must satisfy the CFL condition based on the maximum eigenvalue:

$$\Delta t \leq \text{CFL} \times \frac{\Delta x}{\max(|V \pm c|)}$$

where the maximum is taken over all grid points. This ensures that numerical waves do not propagate faster than physical waves in the system.

For stability, we require:

- CFL ≤ 1 for explicit schemes
- Smaller CFL numbers near discontinuities
- Additional considerations for source term effects

3 MacCormack Scheme

The MacCormack scheme is a widely used predictor-corrector method for solving hyperbolic partial differential equations, such as the Euler equations that govern fluid flow. It is an explicit, second-order accurate scheme in both time and space, and is particularly well-suited for problems involving shock waves and flow discontinuities.

3.1 Predictor Step

In the first step of the MacCormack scheme, we compute the predicted values of the conservative variables at the next time step using forward differencing in space. The predictor step is expressed as:

$$Q_i^{\text{pred}} = Q_i^n - \frac{\Delta t}{\Delta x}\left(F_{i+1}^n - F_i^n\right)$$

Here, Q_i^n represents the conserved variables at the i-th node at time step n, and F_i^n is the flux at node i. The forward spatial differencing is applied between nodes i and $i+1$. This step provides an estimate of the solution but is not yet accurate enough.

3.2 Corrector Step

In the second step, the predicted solution is corrected using backward differencing in space. The corrector step refines the prediction to obtain the solution at the next time level:

$$Q_i^{n+1} = \frac{1}{2}\left(Q_i^n + Q_i^{\text{pred}} - \frac{\Delta t}{\Delta x}\left(F_i^{\text{pred}} - F_{i-1}^{\text{pred}}\right)\right)$$

The backward differencing is applied between nodes i and $i-1$, using the fluxes calculated based on the predicted values. This corrector step improves the accuracy of the solution, ensuring second-order accuracy in both space and time.

3.3 Stability Considerations: CFL Condition

To maintain numerical stability, the MacCormack scheme must adhere to the Courant-Friedrichs-Lewy (CFL) condition. The time step Δt must satisfy:

$$\Delta t = \text{CFL} \times \frac{\Delta x}{\max(\lambda)}$$

where λ is the maximum eigenvalue of the system, representing the highest wave speed in the flow. The CFL number is typically chosen to be less than 1, often around 0.5, to ensure stability.

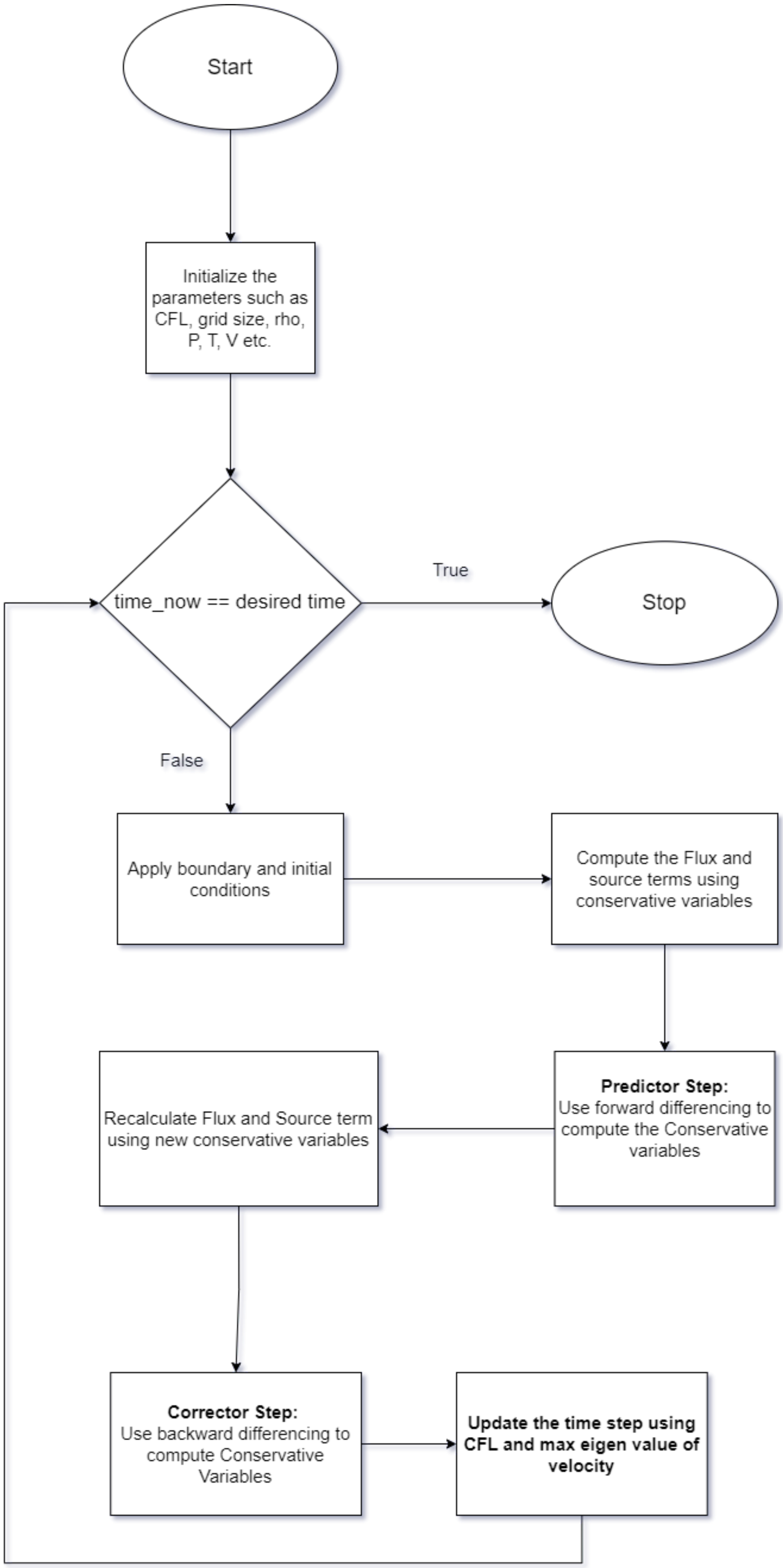

Figure 2: Mac Cormac Algorithm

4 Isentropic Subsonic Flow Regime

In the isentropic subsonic flow regime, the flow remains subsonic throughout the nozzle ($M < 1$). The flow accelerates through the converging section and decelerates in the diverging section. This regime is smooth and isentropic, meaning there are no shock waves or entropy changes.

4.1 Characteristics and Boundary Conditions

For subsonic flow, the boundary conditions are based on the characteristics (eigenvalues) of the system, which indicate the direction of information propagation:

$$\lambda_1 = V - c, \quad \lambda_2 = V, \quad \lambda_3 = V + c$$

where V is the velocity, and c is the local speed of sound.

- **Inlet Boundary**: Since the flow is subsonic, two of the eigenvalues are negative (indicating incoming information), and one is positive (indicating outgoing information).
  - **Specified Conditions (incoming)**: Stagnation pressure p_0 and stagnation temperature T_0, representing the reservoir conditions upstream.
  - **Extrapolated Condition (outgoing)**: Velocity V, which propagates information out of the domain, is extrapolated from the interior.
- **Outlet Boundary**: Here, two eigenvalues are positive (outgoing), and one is negative (incoming).
  - **Specified Condition (incoming)**: Static pressure p_{out} is imposed to control the flow at the outlet.
  - **Extrapolated Conditions (outgoing)**: Density ρ and velocity V are extrapolated from the interior to maintain smooth subsonic flow.

4.2 Implementation of Boundary Conditions

- **Inlet**:
  - Set p_0 and T_0 directly as specified by the inlet conditions.
  - Extrapolate V from the neighboring interior points to allow for outgoing information.
- **Outlet**:
  - Set p_{back} directly to impose the desired static pressure at the outlet.
  - Extrapolate ρ and V from the neighboring interior points to ensure a stable subsonic outflow.

This characteristics-based approach ensures accurate boundary condition implementation, maintaining stability and proper flow behavior for the isentropic subsonic flow regime.

4.3 Results and Observations

The simulations conducted for the isentropic subsonic flow regime were intended to yield smooth, shock-free flow profiles across the converging-diverging nozzle. However, an unexpected shock wave consistently appears in the solution, as observed in the plots of pressure, density, and velocity profiles. Various combinations of parameters, including mesh resolution, time step, and Courant-Friedrichs-Lewy (CFL) number, were tested to address this issue, but the shock feature remains.

- **Pressure Profile**: The pressure distribution shows a sudden jump at a certain point within the diverging section, indicating the presence of a shock. This is atypical for the isentropic subsonic regime, where the pressure is expected to decrease smoothly.

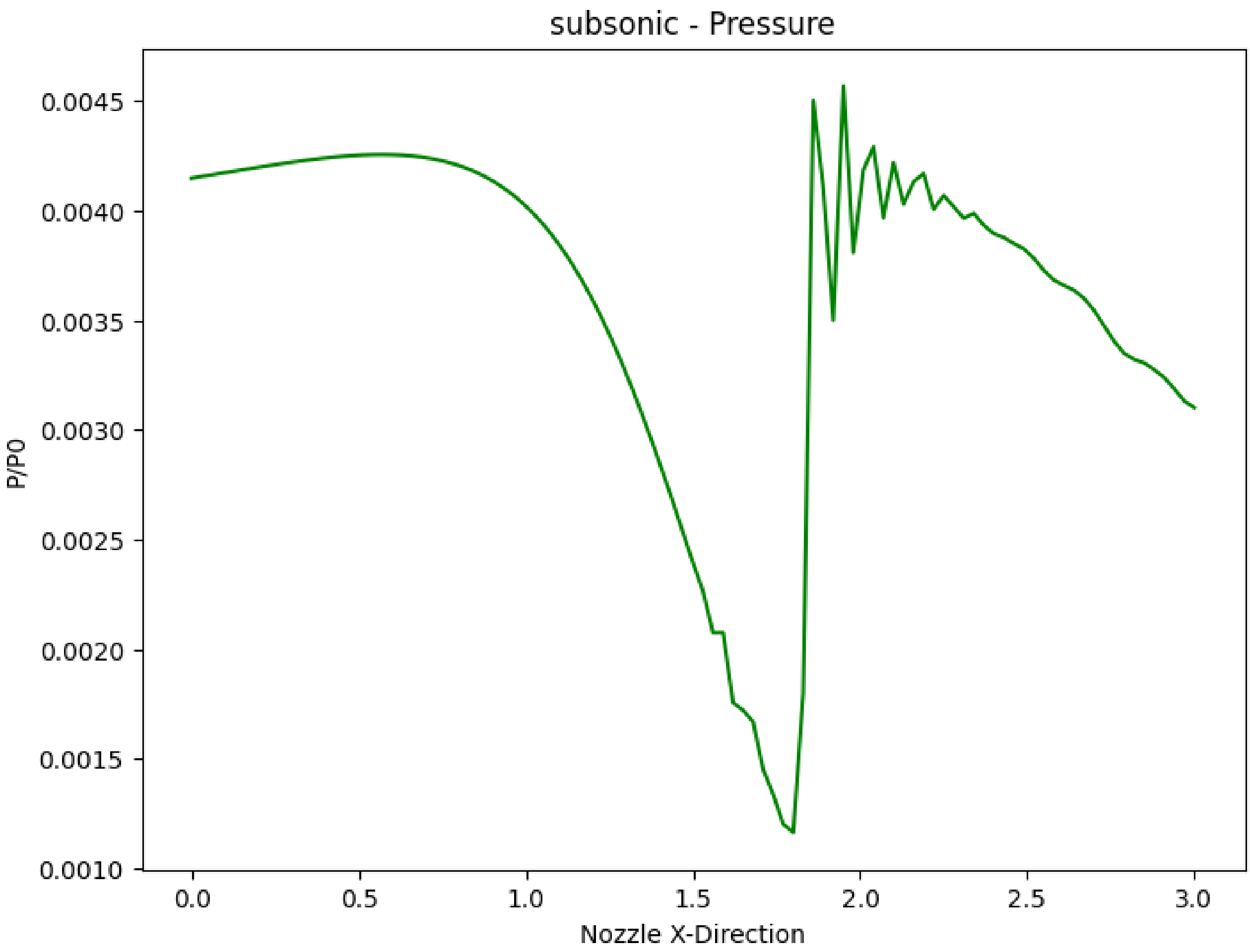

Figure 3: Pressure Variation in Nozzle

- **Density Profile**: The density profile similarly exhibits an abrupt change at the same location as the pressure jump. This behavior is characteristic of a shock wave, causing a discontinuity in the density distribution.

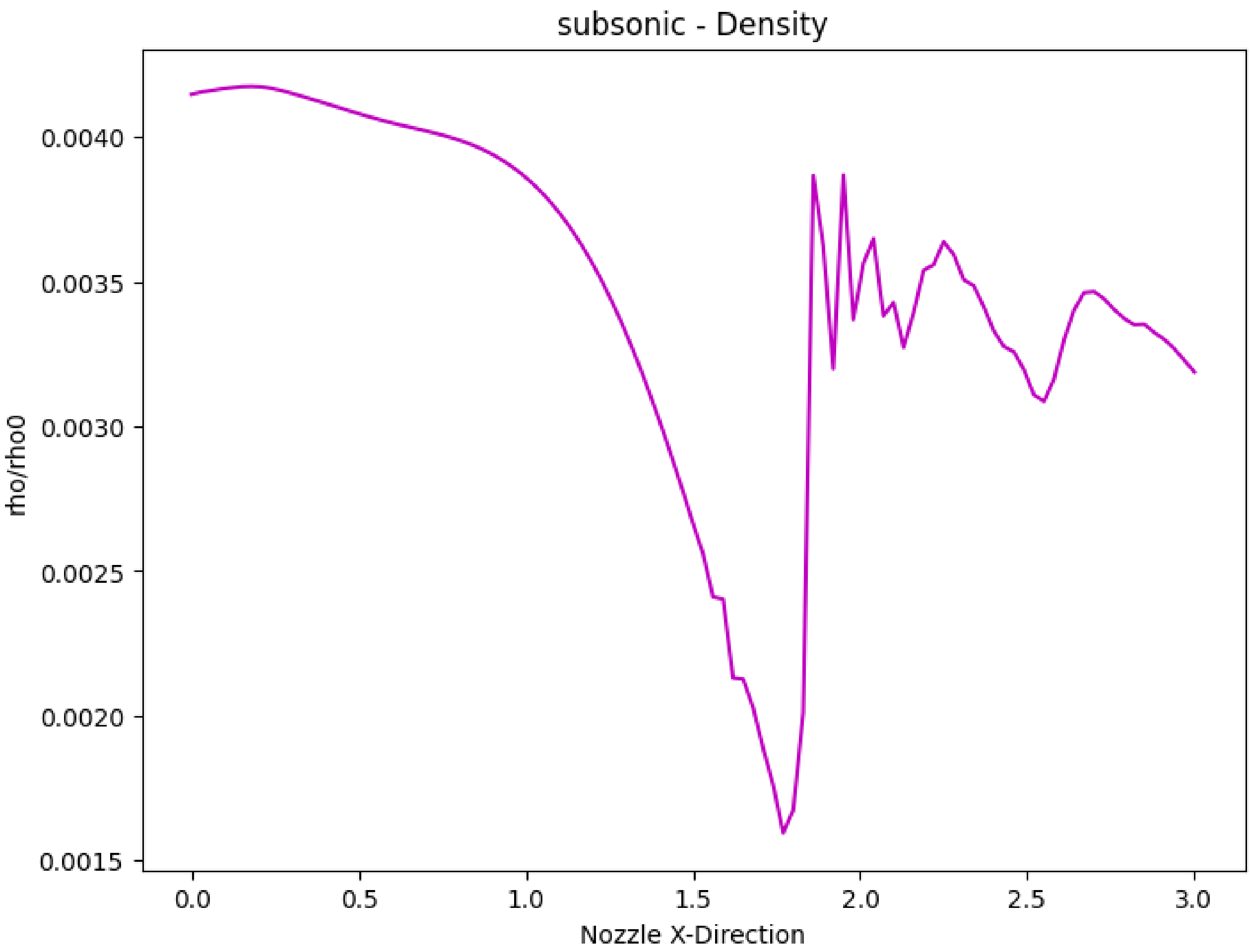

Figure 4: Density Variation in Nozzle

- **Velocity Profile**: The velocity plot reveals a rapid deceleration at the shock location, further confirming the presence of a shock. In a true isentropic subsonic flow, velocity should smoothly vary without abrupt drops.

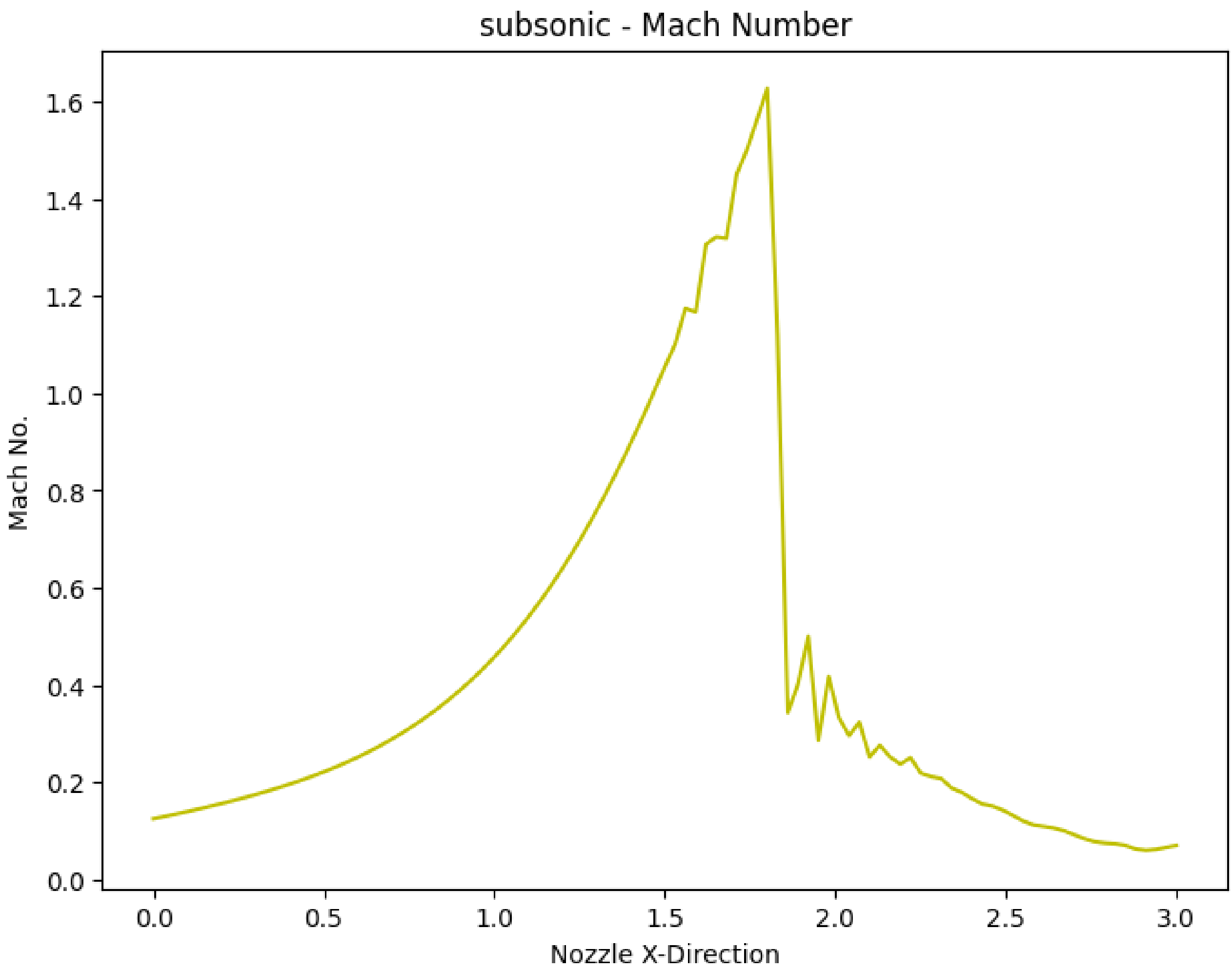

Figure 5: Mach Number Variation in Nozzle

- **Density Profile**: The temperature profile similarly exhibits an abrupt change at the same location as the pressure jump. This behavior is characteristic of a shock wave, causing a discontinuity in the temperature distribution.

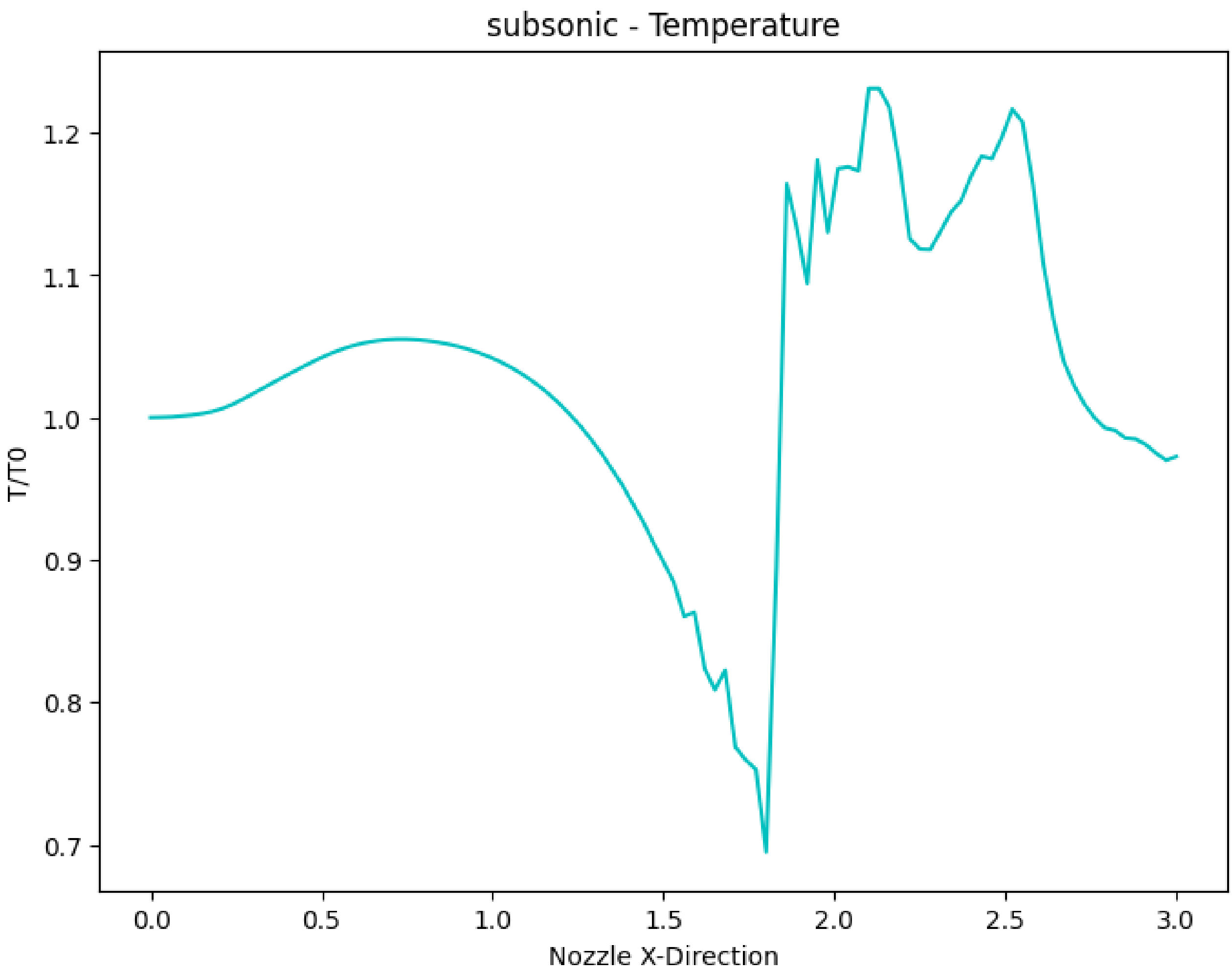

Figure 6: Temperature Variation in Nozzle

5 Isentropic Supersonic Flow Regime

In the isentropic supersonic flow regime, the flow accelerates from subsonic speeds at the inlet to supersonic speeds in the diverging section after passing through the throat. This regime is achieved by lowering the back pressure sufficiently, allowing the flow to reach and exceed Mach 1 in the diverging section. In this regime, flow properties vary smoothly, and the flow remains isentropic, with no shock waves or entropy changes.

5.1 Characteristics and Boundary Conditions

For the supersonic regime, boundary conditions are based on the eigenvalues of the system, which represent the characteristic speeds and directions of information propagation:

$$\lambda_1 = V - c, \quad \lambda_2 = V, \quad \lambda_3 = V + c$$

where V is the velocity, and c is the local speed of sound.

In supersonic flow, all eigenvalues are positive, indicating that information primarily propagates downstream. This impacts boundary condition selection at the inlet and outlet:

- **Inlet Boundary**: Since one eigenvalue is negative (indicating incoming information), one condition is specified at the inlet, while the remaining two conditions are extrapolated.
  - **Specified Condition (incoming)**: Stagnation pressure p_0, representing the total pressure at the inlet.
  - **Extrapolated Conditions (outgoing)**: Density ρ and velocity V are extrapolated from interior points to allow for smooth downstream propagation of information.
- **Outlet Boundary**: In supersonic flow, all characteristics propagate information out of the domain. Thus, no conditions are explicitly set at the outlet.
  - **Extrapolated Conditions**: Pressure p, density ρ, and velocity V are extrapolated from the last interior points to maintain the smooth flow profile typical of supersonic outflow.

5.2 Implementation of Boundary Conditions

- **Inlet**:
  - Specify p_0 directly.
  - Extrapolate ρ and V from the neighboring interior points.
- **Outlet**:
  - Extrapolate p, ρ, and V from the neighboring interior points without specifying any conditions directly, allowing free supersonic outflow.

5.3 Results and Observations

The simulation results for the isentropic supersonic regime are consistent with theoretical predictions, exhibiting smooth, continuous profiles across the nozzle. Importantly, no shock waves were observed in the flow, confirming the isentropic nature of the solution. The plots of pressure, density, velocity, and temperature reflect expected supersonic behavior.

- **Pressure Profile**: The pressure decreases smoothly in the diverging section, consistent with supersonic expansion, where pressure drops as velocity increases.

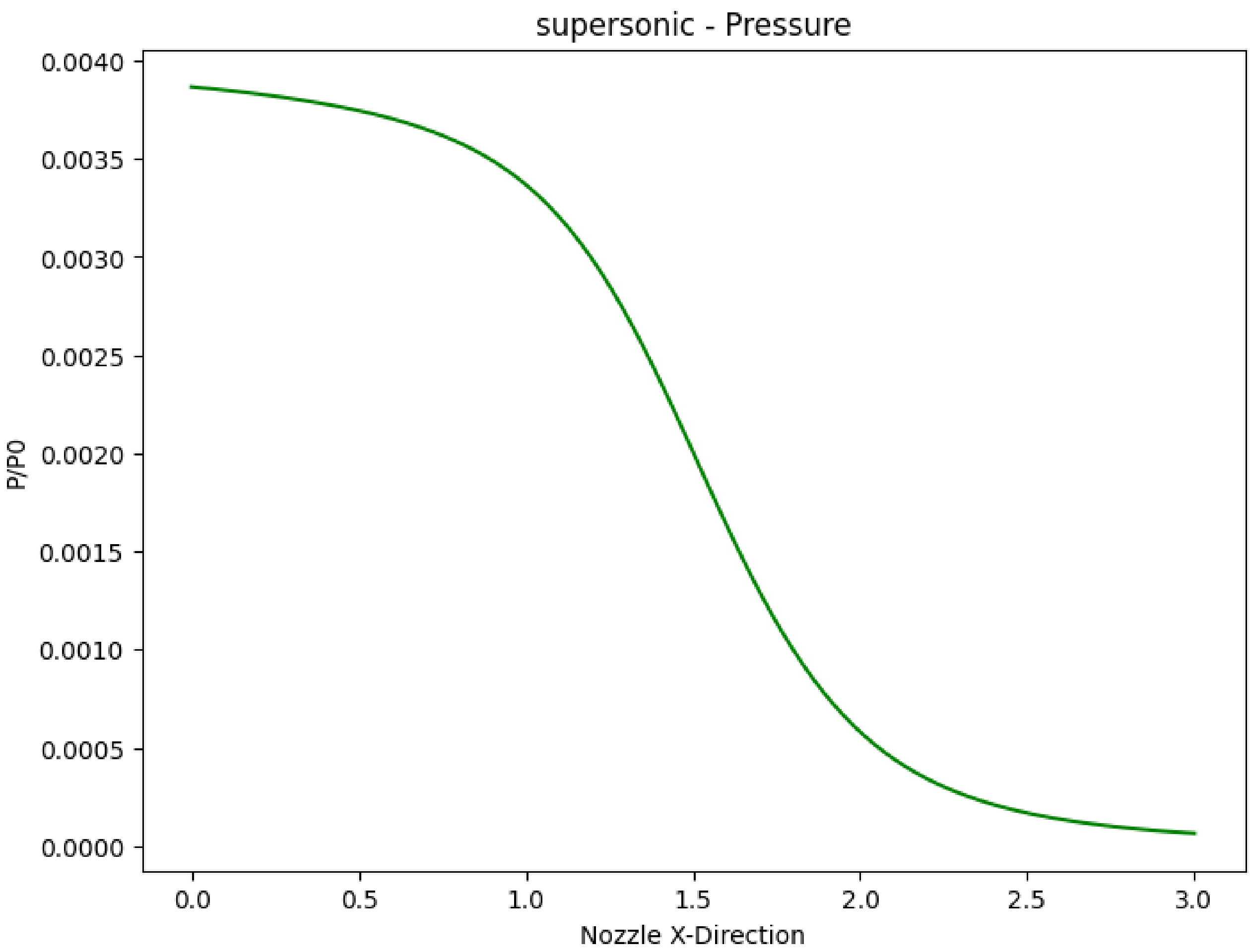

Figure 7: Pressure variation in Nozzle

- **Density Profile**: The density shows a gradual decrease through the nozzle, aligning with isentropic expansion relations for supersonic flow.

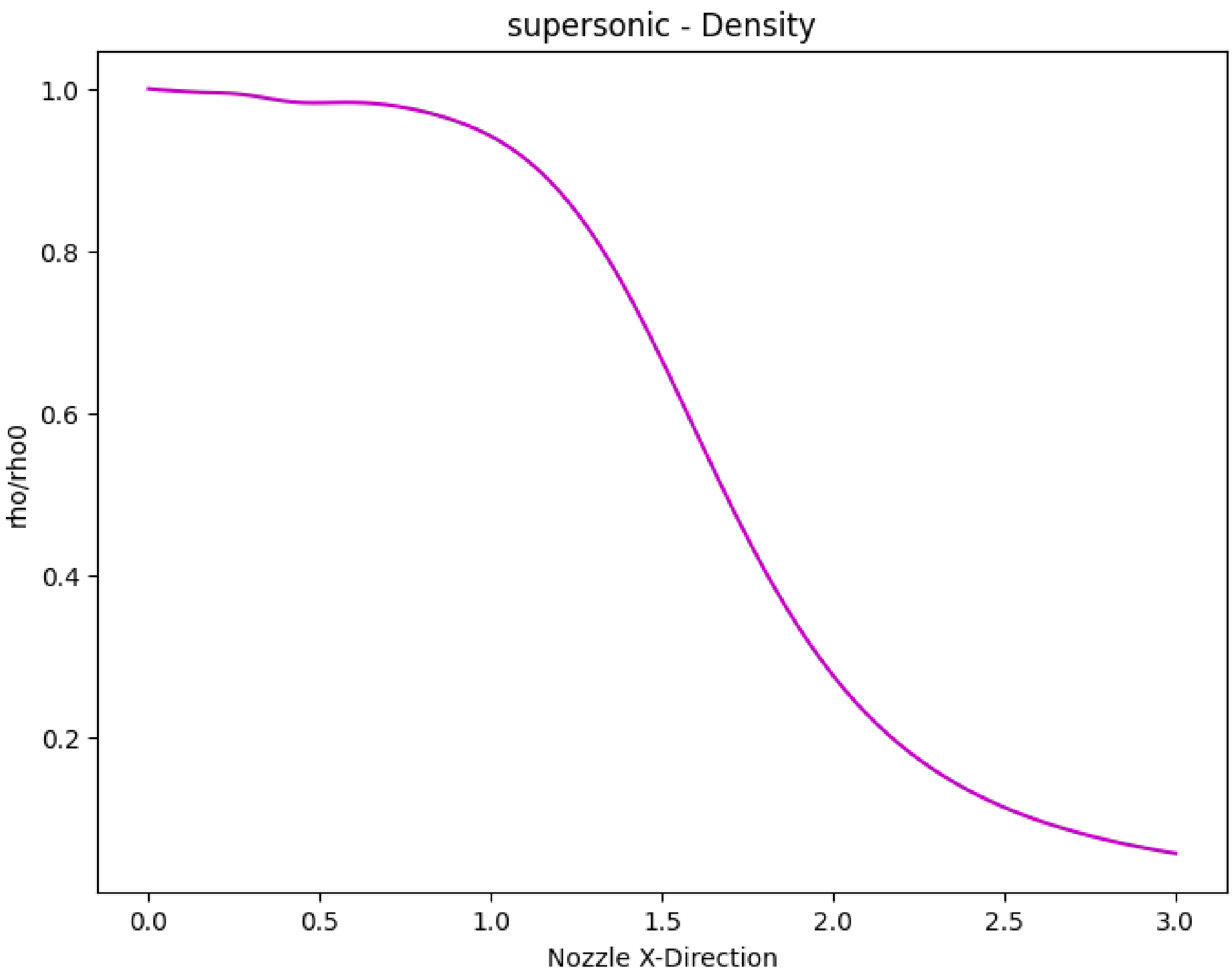

Figure 8: Density variation in Nozzle

- **Velocity Profile**: The velocity increases smoothly from subsonic to supersonic after the throat, without abrupt changes or shocks. This smooth acceleration in the diverging section confirms the supersonic flow regime.

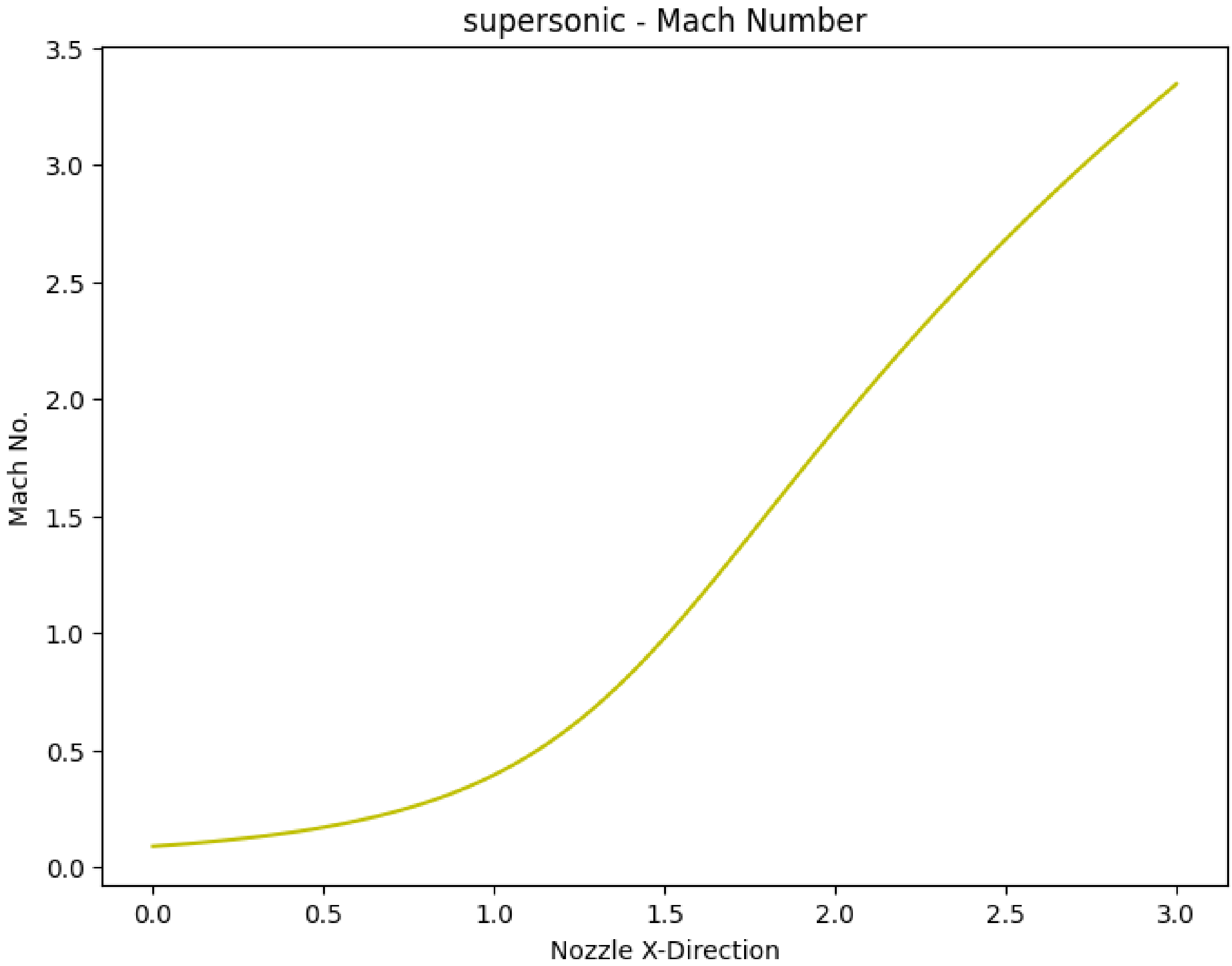

Figure 9: Mach number variation in Nozzle

- **Temperature Profile**: The temperature decreases steadily along the diverging section, in line with isentropic expansion, where temperature drops as kinetic energy increases. This smooth temperature profile further confirms that the flow is expanding supersonically without entropy changes or shocks.

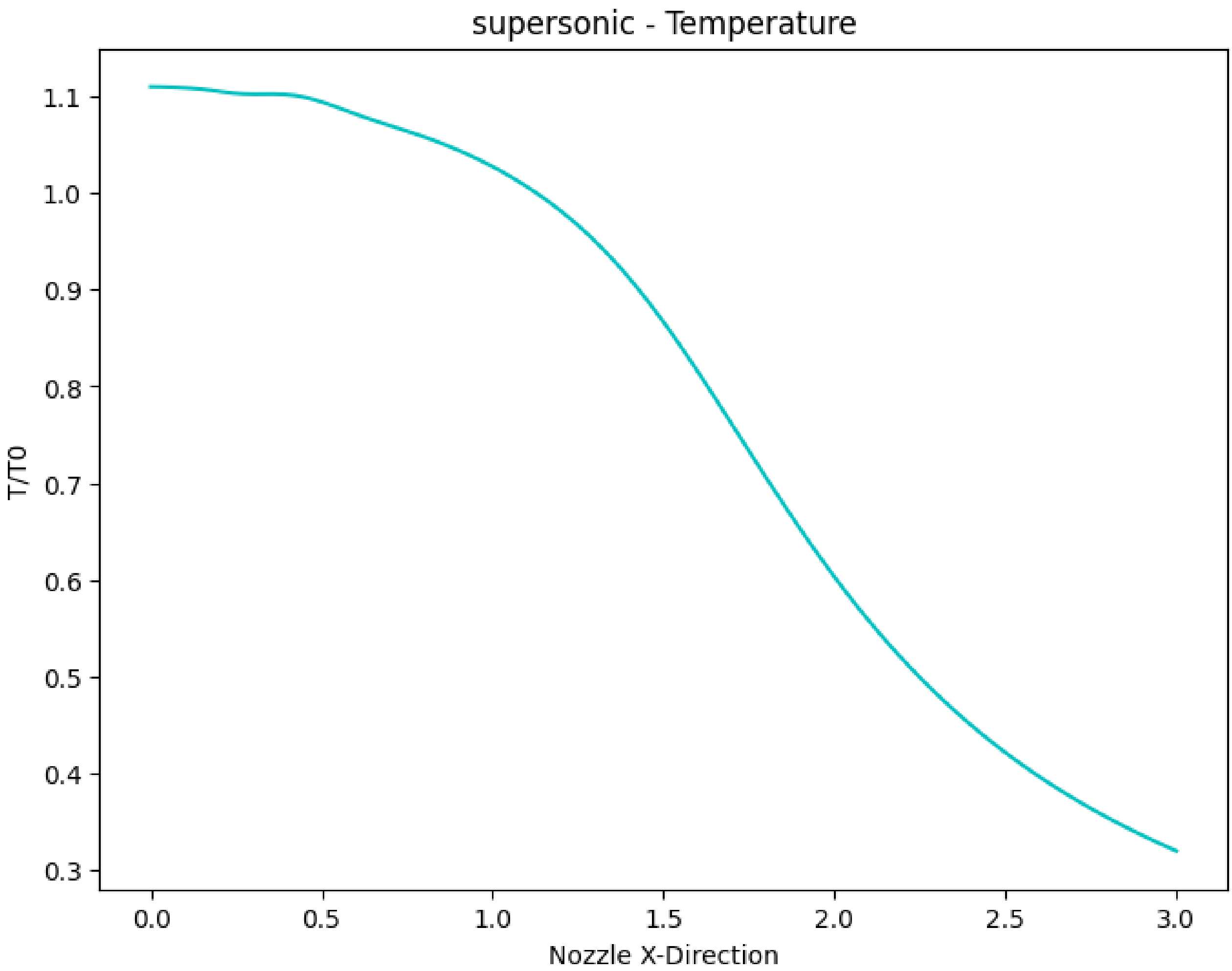

Figure 10: Temperature variation in Nozzle

6 Conclusion

This computational study of fluid flow through a converging-diverging nozzle using time-dependent Euler equations has yielded several significant findings. The investigation employed MacCormack's scheme, a second-order accurate method in both space and time, to analyze two distinct flow regimes under quasi one-dimensional, inviscid, and compressible flow conditions.

For the isentropic subsonic flow regime, the numerical results revealed unexpected behavior. Despite theoretical predictions of smooth, continuous flow, the solution consistently exhibited a shock wave in the diverging section. This phenomenon persisted across various numerical parameters, including different mesh resolutions and CFL numbers, suggesting either a fundamental limitation in the numerical scheme or possibly incorrect boundary condition implementation for this regime.

In contrast, the isentropic supersonic flow regime demonstrated excellent agreement with theoretical predictions. The results showed:

- Smooth acceleration from subsonic to supersonic velocities after the throat
- Continuous decrease in pressure and density through the diverging section
- Consistent temperature reduction along the nozzle length
- No shock waves or discontinuities in the flow field

The MacCormack scheme proved to be particularly effective for the supersonic case, capturing the flow physics accurately while maintaining numerical stability. The implementation of characteristic-based boundary conditions was crucial for achieving physically meaningful results, especially in handling the transition from subsonic to supersonic flow.

The project demonstrates both the capabilities and limitations of computational methods in analyzing complex fluid flow problems, while providing valuable insights into the numerical modeling of nozzle flows.