INDIAN INSTITUTE OF TECHNOLOGY BOMBAY

DEPARTMENT OF AEROSPACE ENGINEERING

SIMULATION OF COMPRESSIBLE FLOWS USING SU2

SUPERVISED LEARNING PROJECT

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Abstract

The prime objective of this Supervised Learning Project is to get an overview of high speed flow simulations using the CFD software SU2. Firstly it delves into the features used in SU2 through a simple inviscid simulation, various numerical methods used in SU2 and finally we look at the simulation of flow through optimum expanded, under-expanded and over-expanded nozzle. Then the Method of Characteristics is used to design a minimum length nozzle.

1 Introduction

1.1 Fundamentals of SU2

SU2 is an open source software built using C++ and Python for largely solving problems pertaining to Computational Fluid Dynamics and also other domains such as electrodynamics, elasticity etc. SU2 makes use of the Finite Volume Solver for most of the fluid flow problems. In this report the flow is assumed to be Euler to reduce complexity.

1.1.1 Markers & Boundary Conditions

Farfield: If a marker is assigned as Farfield no specific value is imposed on the marker and the governing equations are solved to arrive at the values of the flow variables. Generally inlet is defined as farfield for external flow problems and the free-stream values are assigned for the flow variables at the inlet. **Free-stream** values are also used as **initial conditions**, so it is necessary to define free-stream values

Total Conditions: Total Conditions is primarily used at the inlet to define the total temperature, total pressure, unity velocity vector to define the flow direction. A typical example of Total Condition
MARKER_INLET = ($Inlet_1$, T_0 , P_0, $\hat{v_x}$, $\hat{v_y}$, $\hat{v_z}$)

Pressure Outlet: Defines the exit static pressure at the outlet
MARKER_OUTLET = (Outlet, P)

The biggest disadvantage is that SU2 doesn't provide a velocity inlet option for compressible flows

1.1.2 Convergence Criteria

Steady-State Residual: If the convergence criteria is a residual, the solver stops once the computed residual is smaller than the value set by the user.

Steady-State Coefficient: If the convergence criteria is a coefficient, a cauchy series approach is used for which a cauchy element is defined as the difference between coefficients of consecutive iterations. When the average over a certain number of elements is below the value set by the user the solver stops iterating.

Maximum Iteration: The user can also define the maximum number of iterations, if the solver encounters this limit then it automatically quits the iteration even if the residuals are not converged.

1.2 Convective Schemes

JST: The Jameson-Schmidt-Turkel scheme is a second order accurate central scheme.

ROE: ROE is a second order accurate unpwind scheme, for the linear advection equation the information travels in the direction of the characteristic speed. If $a \geq 0$ then the information travels from the i^{th} to the $(i+1)^{th}$ coordinate in the stencil

HLLC: HLLC is also an upwind second order scheme

1.2.1 Other Features

Multigrid: The *multigrid algorithm* is used for accelerated convergence, it automatically agglomerates the original mesh into a series of coarser representation and smoothing iterations are performed on all mesh levels with each non-linear solver iteration in order to provide a better residual update. A multigrid with X levels implies there are X coarser mesh levels and 1 level for the original mesh. W_CYCLE provides better convergence rates though it is more computationally intensive.

Windowing Functions for Unsteady Flows:

$$C_D = 1/M \int_0^M w(t/M) C_D(t) dt \tag{1}$$

A windowing function is zero on boundaries and has an integral value of 1. "WINDOW_START_ITER" must start once the transient phase of flow begins. Su2 offers several window functions with which the time-averaged value converges faster

WINDOW_FUNCTION	CONVERGENCE ORDER
SQUARE	1
HANN	3
HANN_SQUARE	5
BUMP	Exponential

Table 1: Windowing Functions

CFL Adaptive: The CFL adaptive feature can be turned ON or OFF. It controls the multiplicative factors to increase or decrease the CFL with each iteration (depending on the success of each nonlinear iteration). CFL_i is given by $CFL_{i-1}(Residual_{i-1}/Residual_i)^n$

2 Comparing Various Numerical Schemes

2.1 Grid Independence Test

Firstly a Grid Independent Test was carried out to find the approximate number of cells to run an economical simulation and finally the mesh with 15000 number of cells was chosen.

M_∞	2.0
P_∞	10^5
T_∞	300

Table 2: Free-stream Value

M_2	1.64052
P_2	170658 Pa
T_2	351.045 K
Shock angle	39.3134

Table 3: Theoretical Values from Oblique Shock relation

Solver	Euler
Num_Method_Grad	Weighted_Least_Squares
Conv_Num_Method_Flow	**HLLC**
CFL	5
Time_Diecre_Flow	Euler_Implicit
Conv_Field	RMS_Density
Conv_Residual_Minval	-13 ($\log_{10}$)
Conv_Cauchy_Eps	1E-10 (last 100 elements)

Table 4: Setup

Mesh Cells	M_2	P_2	T_2
90000	1.6431X	17073X	351.09X
30000	1.6431X	17073X	351.09X
15000	1.6431X	17073X	351.09X
7500	1.643XX	1707XX	351.0XX
1900	1.64XXX	1707XX	351.0XX

Table 5: Comparison

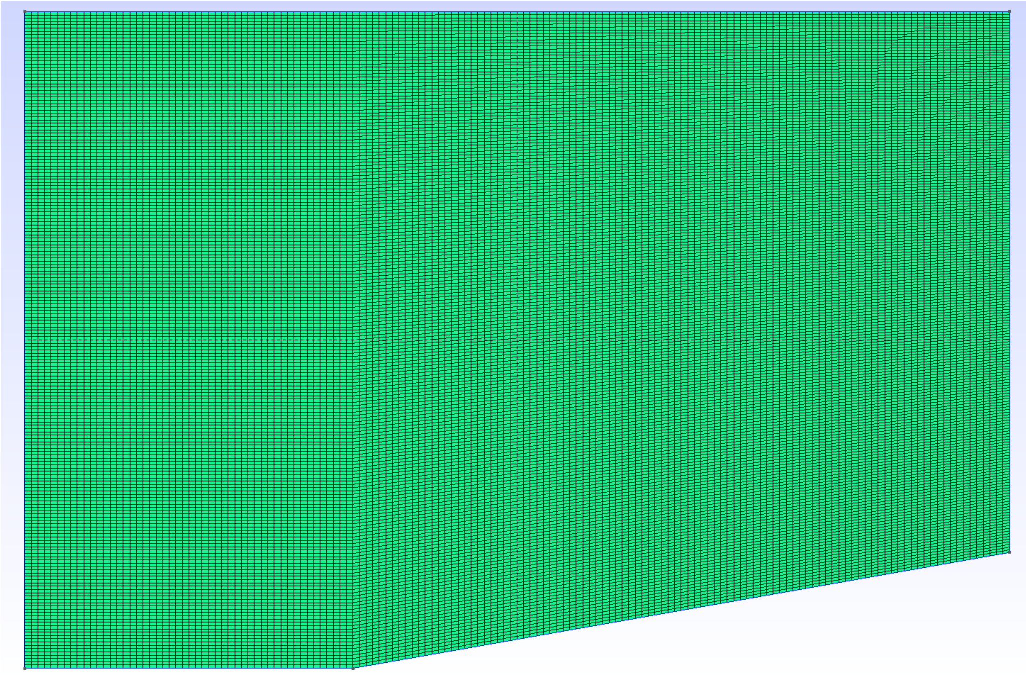


Figure 1: Mesh: 30,000 Cells | Generated in Gmsh

Figure 2: Mach Contour

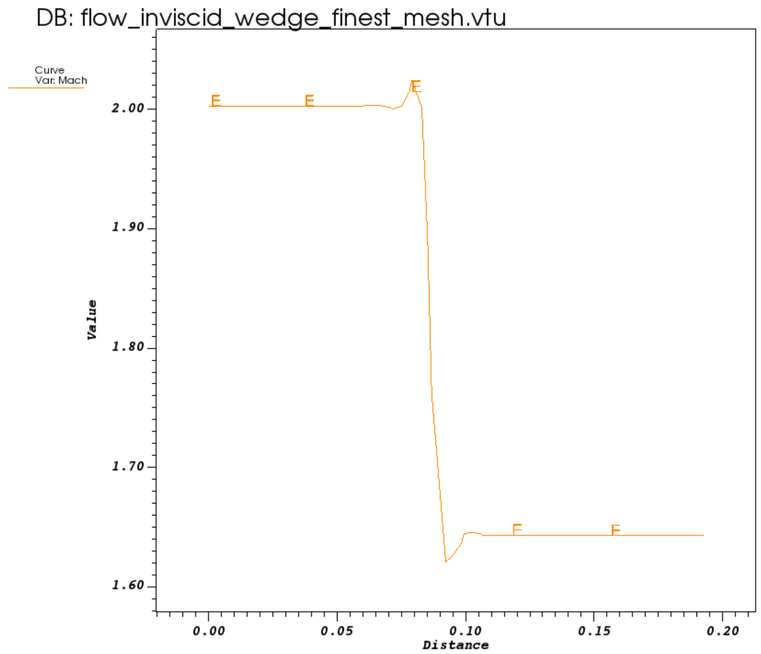


Figure 3: HLLC - Mach vs. X

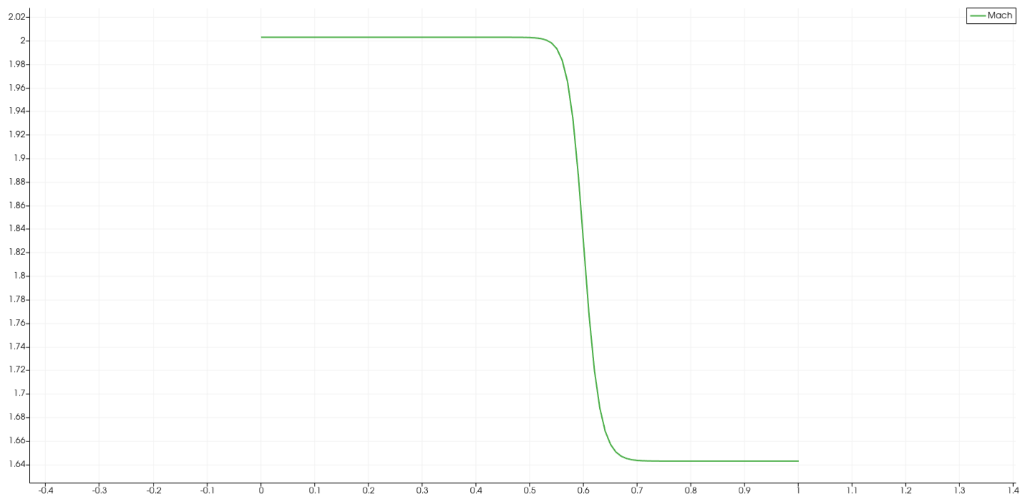


Figure 4: Lax-Friedrich - Mach vs. X

Post-Processing: The theoretical value of shock angle is 39.314^0, but the value from the simulation is 40.019^0. This was found using the density gradient, where the maximum value of the gradient was calculated at the shock, since the maximum gradient has to be perpendicular to the shock, 90^0 was added to the gradient angle to find the shock angle. The shock angle was averaged over four such values calculated from five different horizontal lines passing through the shock with a spacing of 0.005 units along the y-axis. The error in shock angle is 1.80%.

$$\nabla \rho = \frac{d\rho}{dx}\hat{\imath} + \frac{d\rho}{dy}\hat{\jmath}$$
$$|\nabla \rho| = \sqrt{(\frac{d\rho}{dx})^2 + (\frac{d\rho}{dy})^2}$$
$$\theta_{shock} = \frac{\pi}{2} + \arctan\left(\frac{d\rho/dy}{d\rho/dx}\right) \text{ at } |\nabla \rho|_{max}$$

The data from the numerical schemes were extracted and plotted for comparison

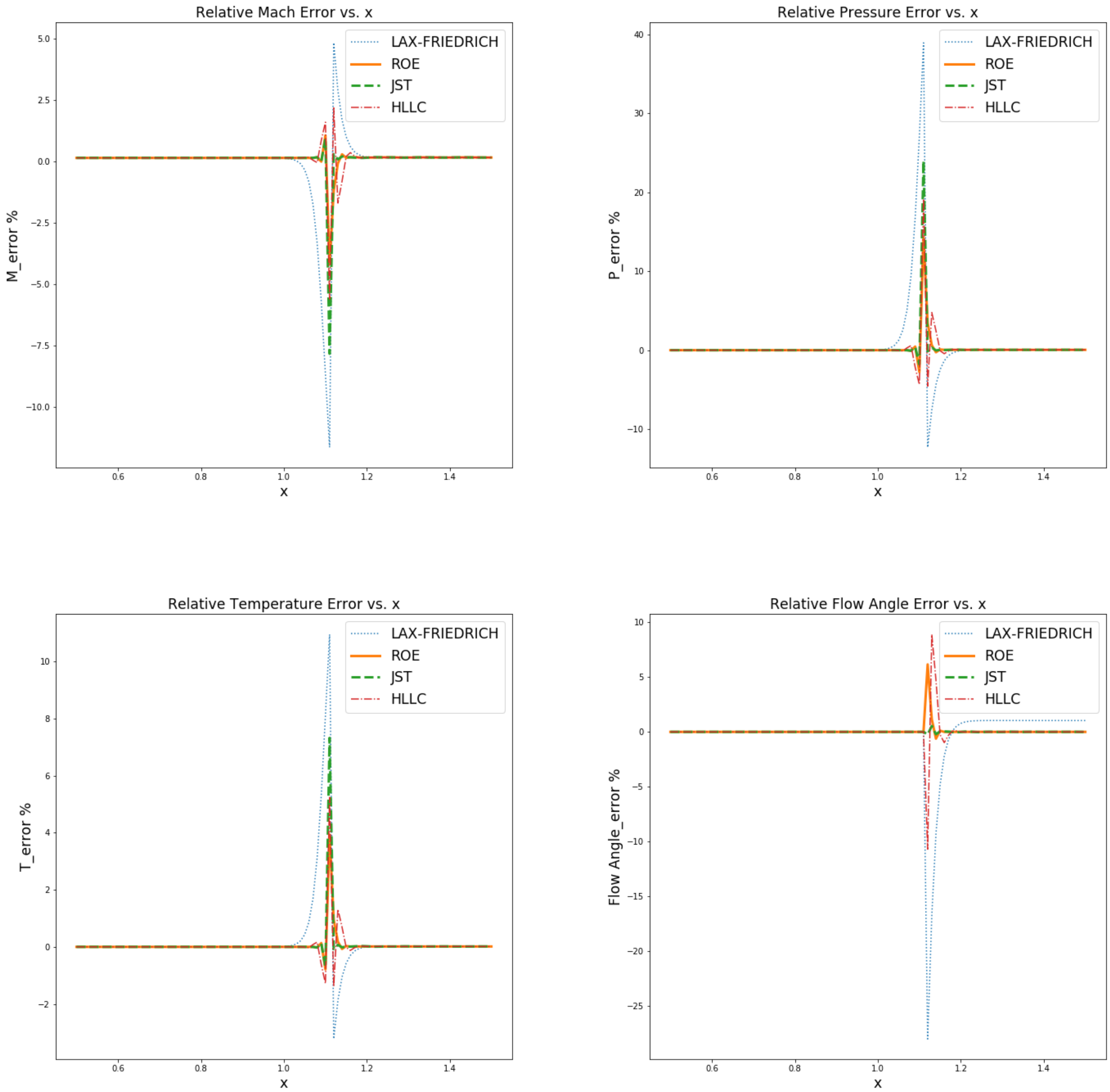


Figure 5: Errors associated with the Numerical Scheme

From the plots shown above the ROE scheme seems to have the least error, followed by the HLLC scheme, but it is computationally expensive, so the HLLC scheme was chosen for its faster convergence and accurate results

Convective NM	M_2	P_2	T_2	Time(sec)
JST	1.643XX	1707XX	351.0XX	644.16
LAX_FRIEDRICH	1.642XX	17075X	351.XXX	197.6
HLLC	1.6431X	17073X	351.09X	106.75
ROE	1.6431X	17073X	351.09X	553.2

Table 6: Comparison between Convective NM

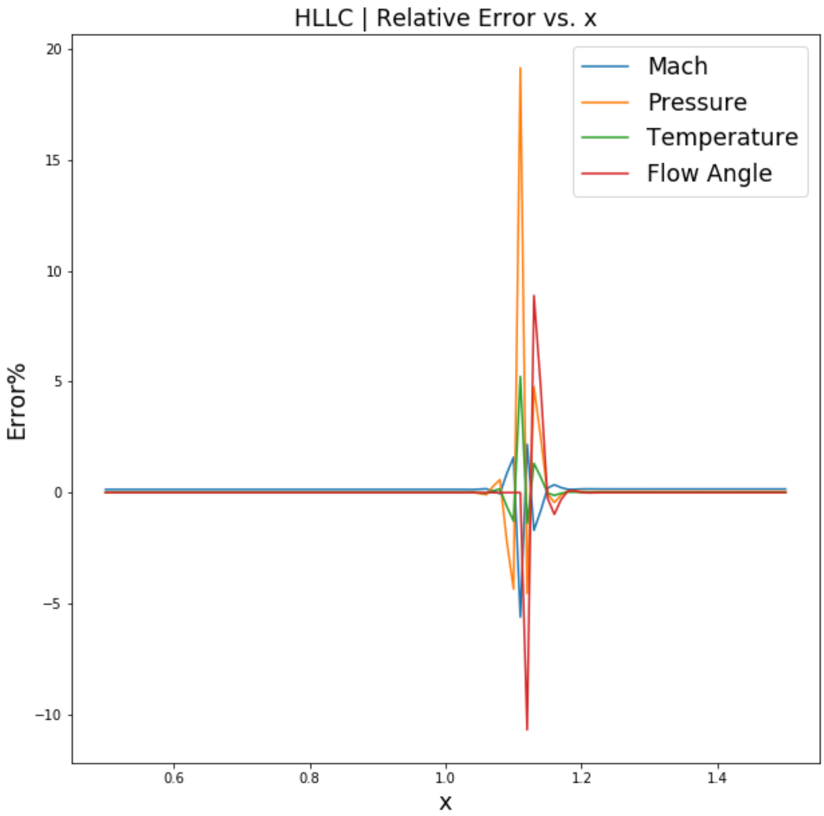
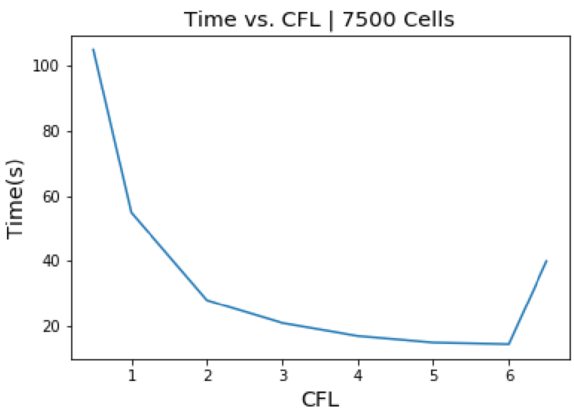
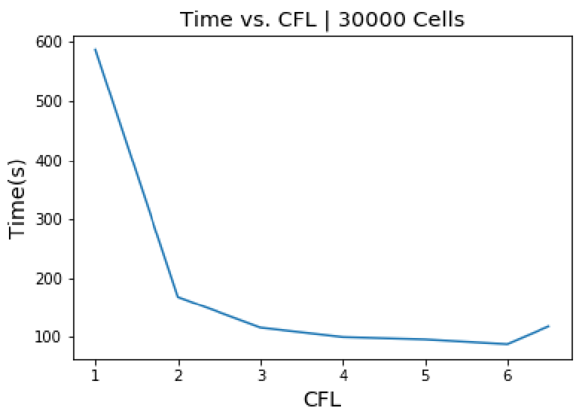


Figure 6: Relative Error in flow variables

2.2 Time vs. CFL

In this section, for a constant number of cells, the optimum CFL number is found by plotting Time vs. CFL number, which has the minimum computational cost. And then the number of mesh cells is quadrupled to test if the same trend continues.





For CFL values lesser than 1, the convergence is so slow that even after 10000 iterations the residual were far from the convergence criteria. For CFL values greater than 7, the residual initially oscillates around and then later diverges.

3 Nozzle Simulations

3.1 Optimum Nozzle Expansion

Quasi 1-D Theory: The quasi 1-D theory is used for verification purposes, which assumes that all the variables are only a function of x, the below equation can be derived from invoking mass conservation and isentropic conditions

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

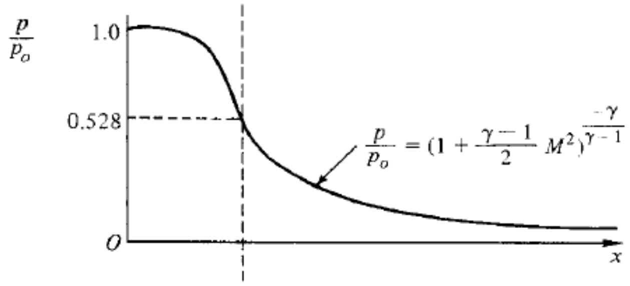


Figure 7: Pressure ratio vs. Center-line (Source [1])

T_o	3600
P_o	7 Mpa
P_e/P_{th}	0.0473
A_e/A_{th}	3
M_{th}	1
M_e	2.63741
P_e	331090.842
T_e	1505.525

Table 7: Parameters

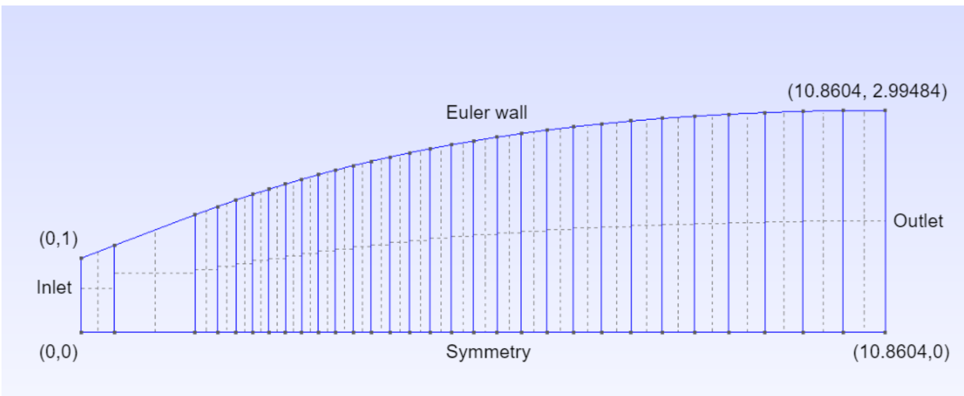


Figure 8: Geometry

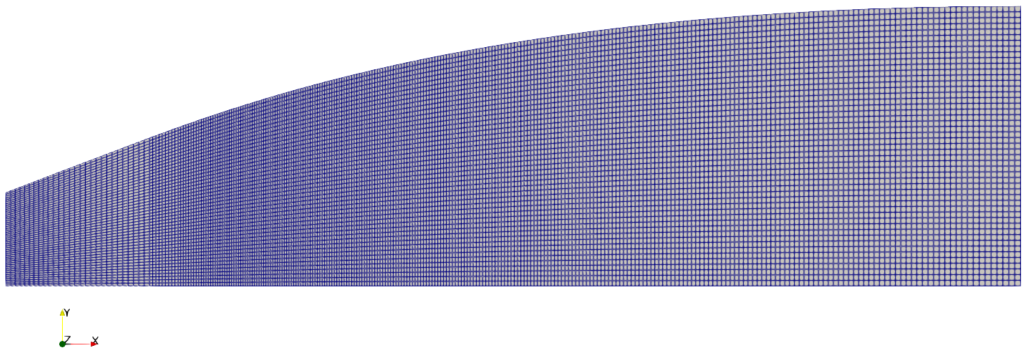


Figure 9: Mesh

Set-Up

Solver	Euler
Num_Method_Grad	Weighted_Least_Squares
Conv_Num_Method_Flow	**JST**
CFL	5
Time_Diecre_Flow	Euler_Implicit
Conv_Field	RMS_Density
Conv_Residual_Minval	-12 ($\log_{10}$)
Conv_Cauchy_Eps	1E-10 (last 100 elements)

Initial Condition
Mach$_{free-stream}$ = 1 also serves as the initial condition. In this case, this is valid as the mach number inside the nozzle is always greater than 1.

Solver & Convective Numerical Scheme
Euler solver is used with JST convective numerical scheme. Other than JST and Lax-Friedrich scheme only ROE scheme showed convergence with high multigrid option. Other schemes either diverged or didn't converge. The cauchy convergence criteria is used, the average of the last 100 $\log_{10}$(density residual) is set less than -12 for convergence.

Grid Independent Test

No of Elements	M_e	P_e	T_e	M_{error}	P_{error}	T_{error}	Time
73755(S)	2.63818	330742	1505.02	0.045	0.106	0.034	580s
13720(S)	2.63973	330060	1504.03	0.104	0.311	0.100	53s
7630(S)	2.64024	329909	1503.73	0.123	0.357	0.120	25s
26324(US)	2.63607	331749	1506.42	0.051	0.2	0.120	75s
7053(US)	2.63435	332671	1507.56	0.116	0.478	0.135	10s

Table 8: S is Structured and US is Unstructured Grid

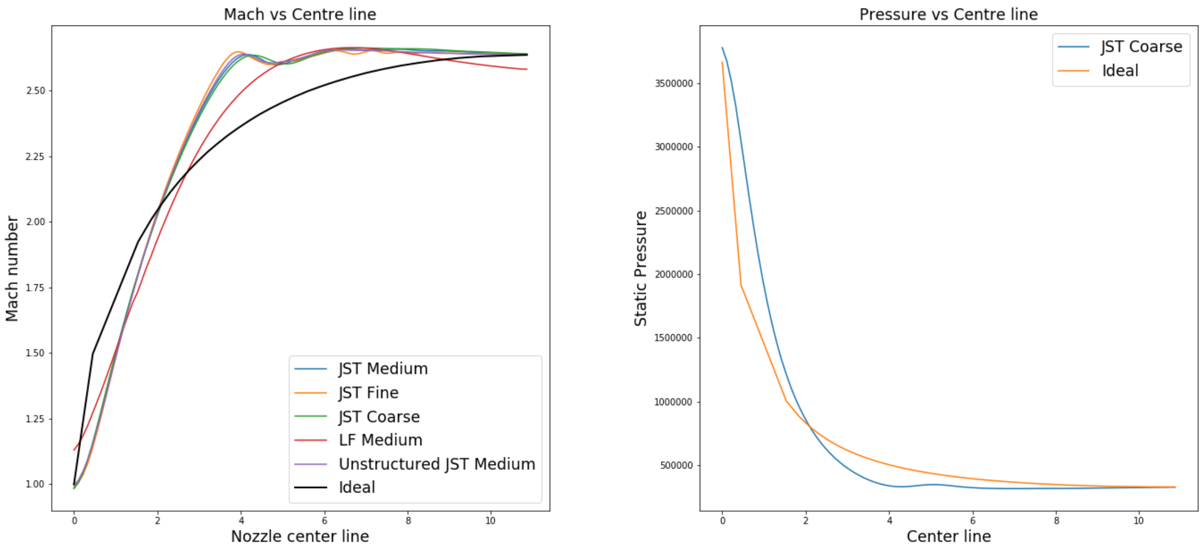


Figure 10: Error along Center line

Conclusion

Even though the exit parameters from the simulation are close enough to the values calculated from the quasi 1-D theory, the values in between the inlet and outlet show considerable deviation.

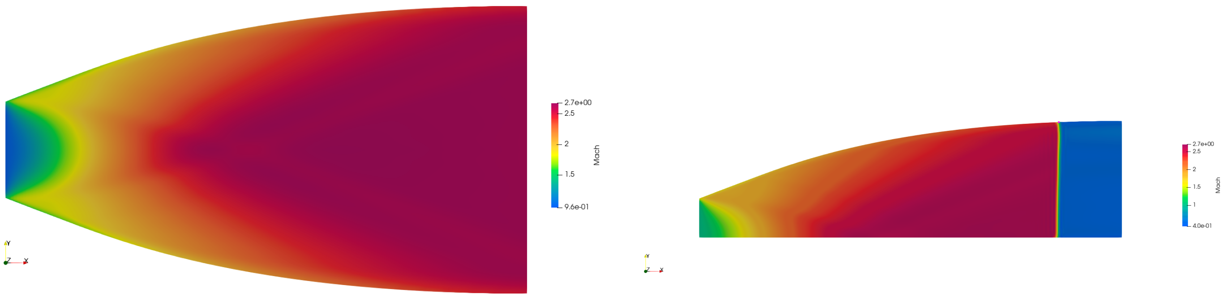


Figure 11: Mach Contour using JST Scheme

3.2 Extended Nozzle Simulations

Theory

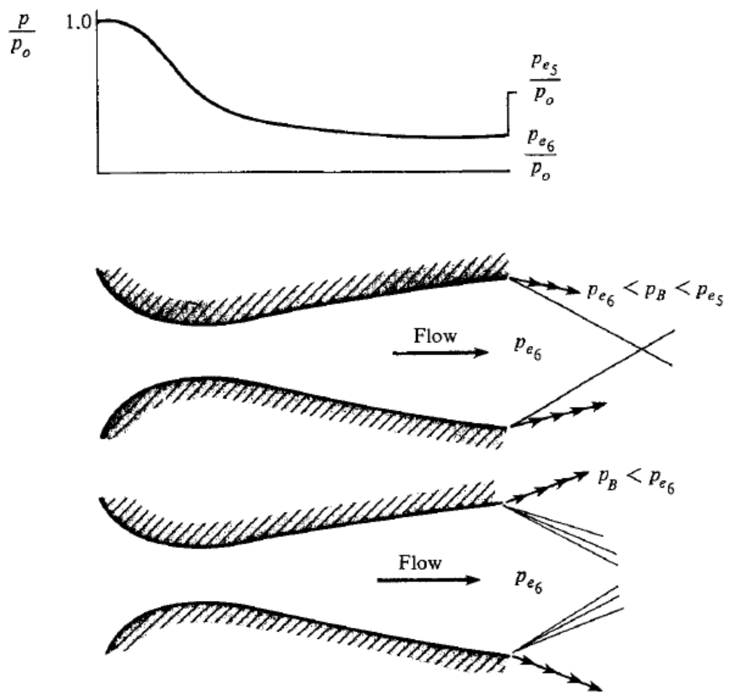


Figure 12: Over-expanded and Under-expanded Nozzle (Source [1])

Geometry

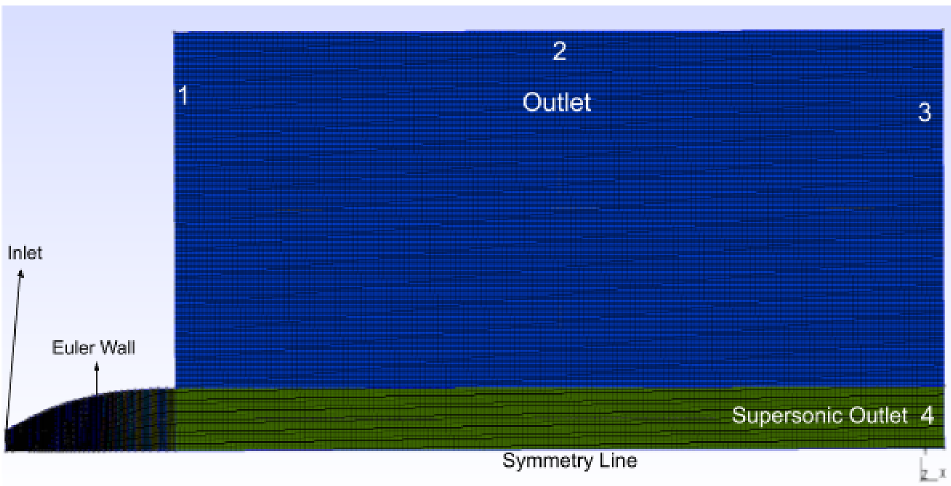


Figure 13: Mesh

Impact of Boundary Conditions & Initial Conditions on the Result

For an optimum expanded nozzle the **Outlet** is assigned a back-pressure that equals P_{e6}. The is a **pressure outlet** boundary condition. Since there is no velocity inlet option for compressible flows, P_0 and T_0 are assigned at the inlet. For a rocket engine that is just about to start the natural initial condition is that the speed is zero everywhere and the pressure is P_{e6} and temperature is same as the atmospheric temperature. There is **NO OPTION** in SU2 to simultaneously assign Mach 1 at the inlet and Mach 0 to the rest of the domain as the initial conditions. This simulation always resulted in divergent issues or the residual oscillates continuously without a proper velocity field. To solve this issue several approaches were tried out.

(A) Supersonic Outlet:The outlet which would have supersonic flow is given outlet supersonic. Other outlets have atmospheric pressure as the BC. The atmospheric pressure is same as the nozzle outlet pressure for optimum expansion of the nozzle.

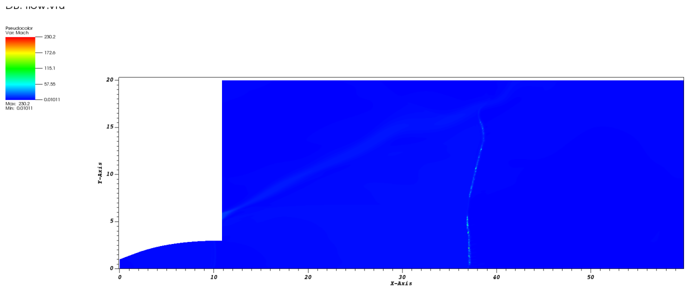


Figure 14: Mach Contour

The simulation resulted in residuals that oscillated continuously. diverged residuals. Different CFL values were used in the simulation, but none yielded the desired results.

(B) Free-stream Conditions: The initial condition throughout the domain is assigned the free-stream values as shown
FREESTREAM_PRESSURE = 3697972.51402 Pa
FREESTREAM_TEMPERATURE = 3000 K

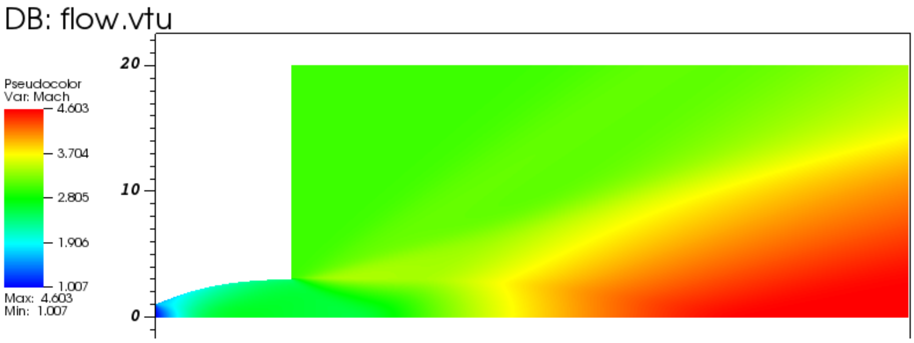


Figure 15: Mach Contour

Though the exit parameters match the required optimum conditions, due to the incorrect initial conditions at the domain outside the nozzle the flow develops expansion fans.

(C) Optimum Expanded Nozzle: The **pressure outlet** boundary condition is replaced as **farfield**. The freestream values are P_{e6} and atmospheric temperature 3000 K

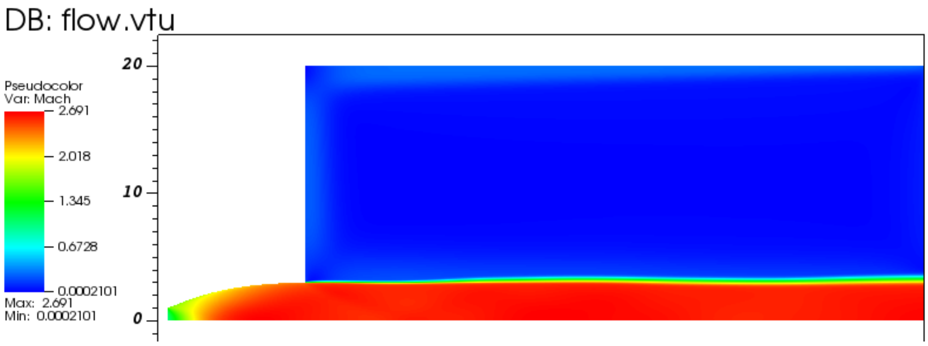


Figure 16: Mach Contour

T_o	3600
P_o	7 Mpa
P_e/P_{th}	0.0473

Table 9: Parameters

(D) Under-Expanded Nozzle: he **pressure outlet** boundary condition is **farfield**. The freestream values are P_{exit} = 1 atm and atmospheric temperature 3000 K

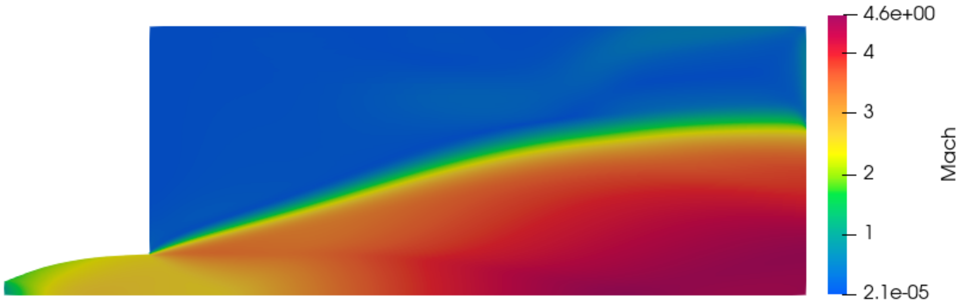


Figure 17: Mach Contour Under-Expanded Nozzle

The initial condition on temperature seems to be the crucial parameter as it produces converging residuals. Altering this value to any other value either gives unsteadiness in the flow or produces viscous like effect.

(E) Under-Expanded Nozzle: he **pressure outlet** boundary condition is **farfield**. The freestream values are P_{exit} = 500000 Pa and atmospheric temperature 3000 K

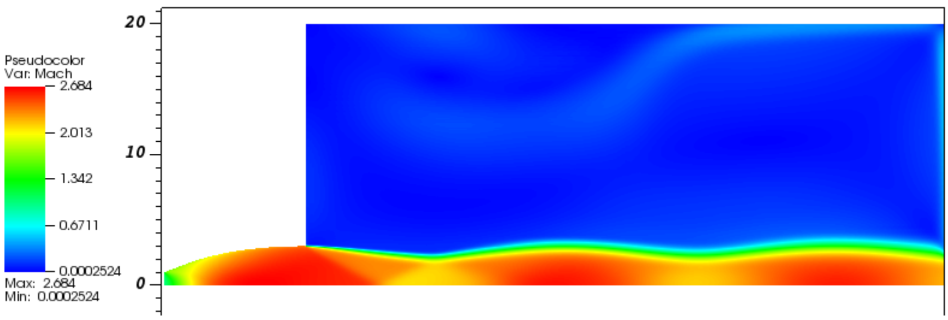


Figure 18: Mach Contour Over-Expanded Nozzle

Results and Analysis

The initial condition for temperature is strictly incorrect for the entire domain that is present outside the nozzle as the temperature outside the nozzle is just 288 kelvin and pressure is P_{e6}. But the prime reason to take this approach is to ensure that the inlet initial condition meets the required mach number, i.e., 1. There is no clear picture to understand how SU2 calculates the inlet mach number with the given boundary conditions and initial condition. One hypothesis is that with the given total conditions SU2 might assume isentropic flow and it evaluates the mach number as 2.64 at the outlet. This value may be used to back calculate the mach number at the inlet. But when the free-stream temperature is assigned 288 K, the residual starts to **oscillate**. One hypothesis could be the Mach number which is calculated from P_{e6} and T_0 must be same for physical consistency.

4 Method Of Characteristics

4.1 Theory of MoC

The key assumptions are the flow is inviscid and irrotational. For such flows the complete velocity governing equation can be written as:

$$(1-\frac{u^2}{a^2})\frac{\partial u}{\partial x}+(1-\frac{v^2}{a^2})\frac{\partial v}{\partial y}-\frac{2uv}{a^2}\frac{\partial du}{\partial dy}=0$$

The velocity of any supersonic flow can be broken down such that one of its two components has speed of sound, from the above equation when u equals a, $\frac{\partial u}{\partial x}$ becomes indeterminate, and it remains indeterminate along the line $\sin\mu=\frac{a}{V}$. Such lines are called characteristic lines, which are also the mach waves. It can be shown that

$$(\frac{dy}{dx})_{char}=\tan(\theta\mp\mu)$$
$$\theta+\nu(M)=K_{-}$$
$$\theta-\nu(M)=K_{+}$$

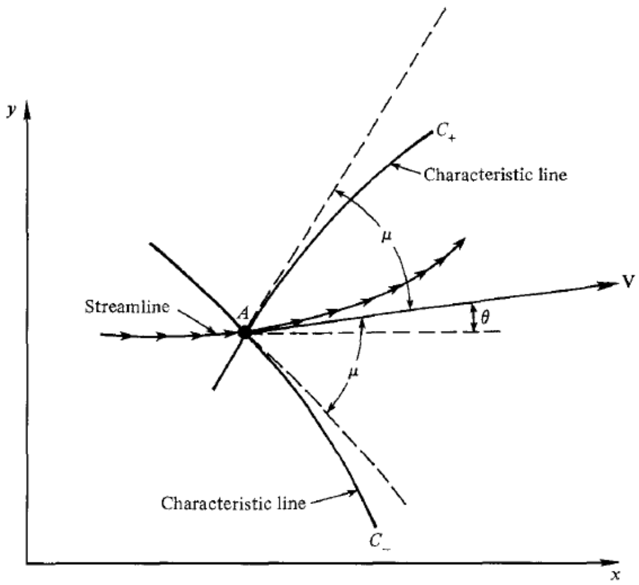


Figure 19: Slope of characteristic line (Source [1])

When two characteristics are intersecting at a point, then the flow angle θ and prandlt meyer function ν can be estimated using

$$\theta_1+\nu(M)_1=K_{-1}=K_{-3}=\theta_3+\nu(M)_3$$
$$\theta_2-\nu(M)_2=K\text{+-}_1=K\text{+-}_3=\theta_3-\nu(M)_3$$

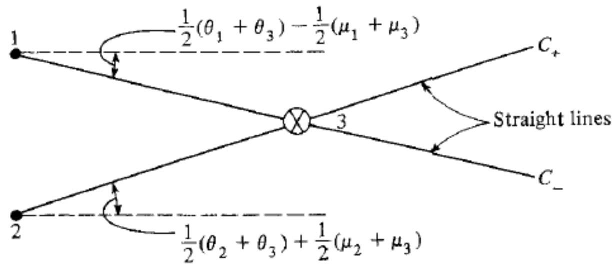


Figure 20: Intersection of Characteristics (Source [1])

Assuming the slope angle of mach lines is the average of the slope angles, the coordinates of the third point can be calculated from

$$\frac{y_3-y_2}{x_3-x_2} = \tan(0.5(\theta_3+\theta_2)+0.5(\nu_3+\nu_2))$$
$$\frac{y_3-y_1}{x_3-x_1} = \tan(0.5(\theta_3+\theta_1)-0.5(\nu_3+\nu_1))$$

4.2 Nozzle Design

Key assumptions

1. Inviscid and Irrotational
2. Characteristics are only slightly curved

The diverging section of the nozzle generally consists of expansion section and straightening section. The slope of the nozzle contour at the expansion fan is continuously increasing, or in other words the function of the nozzle contour at the expansion section is monotonously increasing hence it generates expansion waves and as well as reflects the incident expansion waves. The slope of the nozzle contour at the straightening section is monotonously decreasing, hence it terminates all the expansion waves incident on it. So the junction of expansion and straightening section has the highest slope(θ_{max}) in the nozzle wall contour. For a minimum length nozzle there is only a straightening section, as expansion section would just add on to excess mass. Henceforth the word nozzle is used instead of minimum length nozzle. At the throat there is a discontinuity in the slope of the nozzle contour. At this junction expansion fan emanates, which consists of series of expansion waves. At point 'A'

θ_{exp} = $\nu(M_2)$ - $\nu(M_1)$
θ_{max} = ν_A | Since 'A' is a sonic point, $\nu(M=1)=0$, hence K_+ = 0
θ_{max} + ν_A = $(K_-)_A$
$(K_-)_A$ = θ_{exit} + ν_{exit} as both the points lie on the same characteristic
θ_{exit} = 0 | Imposing the condition that the flow has to emerge parallel to the center at the exit line
θ_{max} = ν_A = ν_{exit}/2

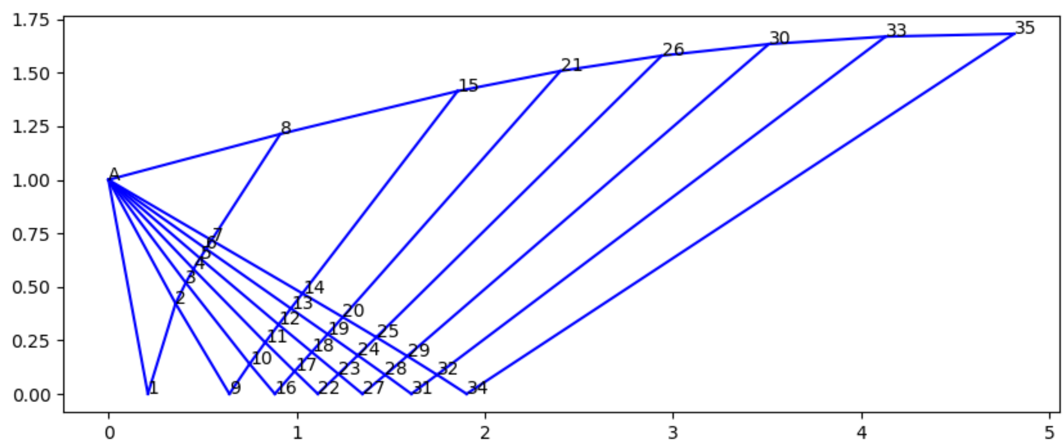


Figure 21: Minimum Length Nozzle

So to design a nozzle, the first requirement is the exit mach number. And the slope at the throat corner point is decided by the prandlt meyer function at the exit point. All the points on the centerline has θ as zero, hence the mach number at the last point lying on the centerline has the same mach number as the design exit mach number. For the supersonic nozzle design, the algorithm to find the nozzle contour is as follows:

1. Design the exit mach number and evaluate θ_{max}
2. Decide the number of characteristics required, say N
3. At point 1, we assume† θ_1 a finite non-zero value, say 0.01^0, since K$_+ = 0, \theta_1 = \nu_1$ for all the points 1, 2... N, N+1
4. We assume† that for points 2,3...N flow angle θ is $\Delta\theta = \theta_{max}/(N-1)$ inclined with θ_1
5. Assume the first set of characteristics are straight lines
6. There are two approaches to find the slope:
   (a) Assuming the angle between the characteristics is also $\Delta\theta$
      i. $\frac{x_i - x_a}{y_a - y_i} = \tan(\theta_i + \theta_1)$ for all i $\in 2...N$
   (b) Assuming the slope angle of the line has contribution only from the points 1,2...N
      i. $\frac{y_i - y_a}{x_i - x_a} = \tan(\theta_i - \nu_i)$ for all i $\in 1, 2...N$
7. For contour points $0.5(\theta_a + \theta_i)$ is the slope angle

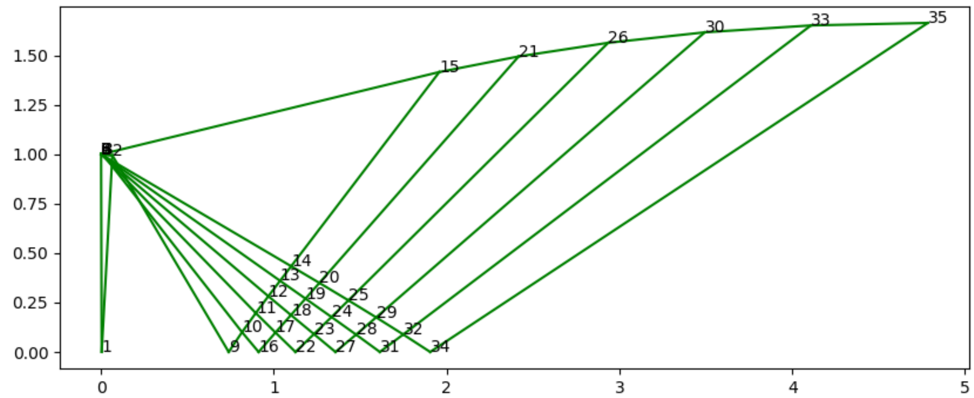


Figure 22: MOC Method I

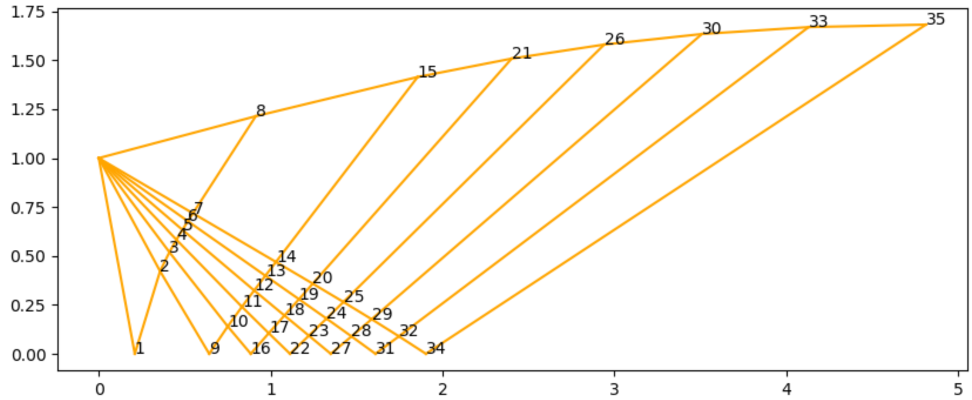
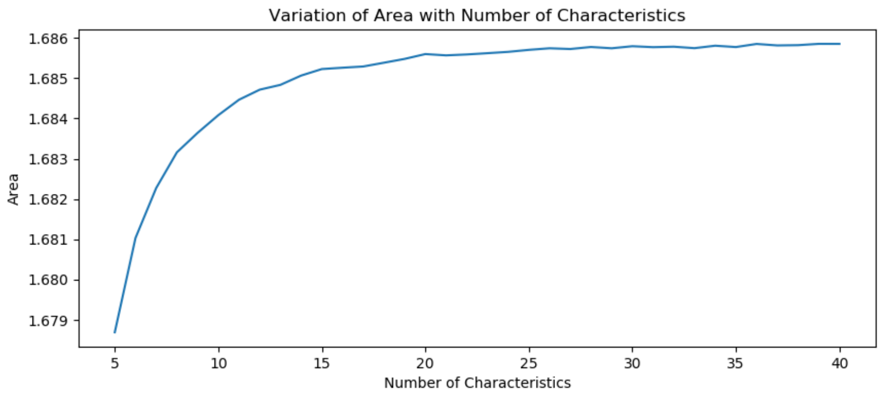
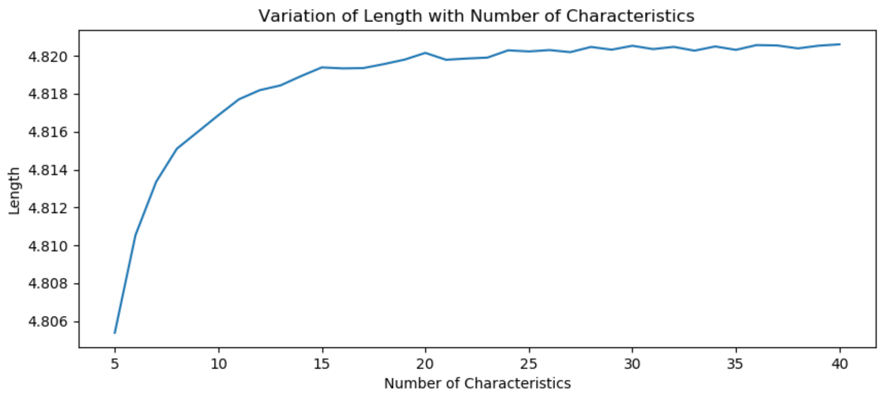


Figure 23: MOC Method II

Convergence

The values of Area ratio and length of the Nozzle converges when Number of Characteristics is about 30. But the variation is small even at lower number of characteristics.





Future Work

The mathematics aspect of the numerical schemes are yet to be explored. In the subsequent week the simulation of the 2-D nozzle using Time Marching MacCormack's technique will be performed.

MacCormack Technique
Let's say the Initial Conditions are known on a vertical line, and there are no source terms

- $\frac{\partial F}{\partial x} = -\frac{\partial G}{\partial y}$
- $F_{i+1} = F_i + \frac{\partial F}{\partial x}_{avg}\Delta x$
- $\frac{\partial F}{\partial x}_{avg} = 0.5 * (\frac{\partial F}{\partial x}_{i,j} + \frac{\partial F}{\partial x}_{i+1,j})$

- First F_{i+1} is evaluated using $\overline{F_{i+1}} = F_i + \frac{\partial F}{\partial x}_{i,j}\Delta x$
- Predictor Step: $\frac{\partial F}{\partial x}_{i,j}$ is obtained from $\frac{\partial G}{\partial y}_{i,j}$ using a forward difference $\hat{j}$
- $\overline{F}_{i+1}$ is used to evaluate $\overline{G}_{i+1}$
- Corrector Step: $\frac{\partial F}{\partial x}_{i+1,j}$ is obtained from $\frac{\partial \overline{G}}{\partial y}_{i+1,j}$ using a rearward difference along $\hat{j}$
- Even though each of the predictor and corrector step are first order, the overall scheme is second order as in the $\frac{\partial F}{\partial x}_{avg}$ the Δx terms cancel due to averaging

The same technique can be applied with a small modification by adding the unsteady term, and initial condition is known at the sonic line at the throat of the nozzle. The rest of the initial conditions are assumed arbitrarily in some fashion.

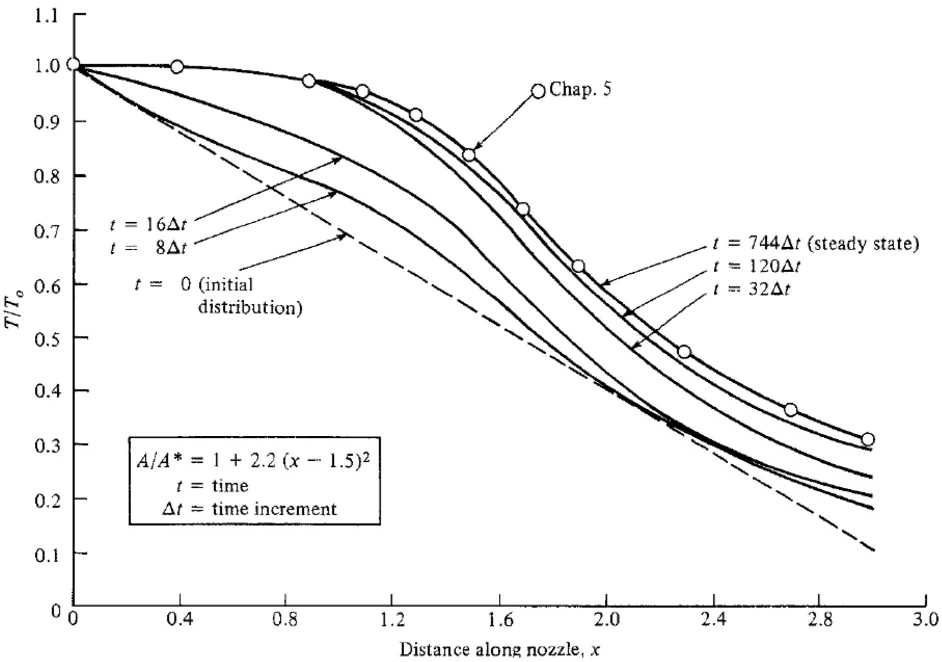


Figure 24: Time Marching

References

[1] Modern Compressible Flows by John D. Anderson, Jr
[2] SU2 Official Documentation https://su2code.github.io/docs_v7/
[3] CFD Discussion Forum https://www.cfd-online.com/Forums/su2/
[4] CFD Blog http://www.joshtheengineer.com/2018/02/28/how-to-run-su2-start-to-finish/