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## **OpenFoam Assignment | The Mach 3 Step**

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### **Abstract**

—SAMPLE ABSTRACT—

*Keywords:* computational fluid dynamics, CFD, incompressible, Paraview, R, Python, coe347, spring 2022.

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### **1. Motivation**

The flow over a Mach 3 step is a well-studied problem in CFD (computational fluid dynamics), making it a good choice for convergence and performance studies. A simple set of studies are undertaken here.

### **2. Implementation**

We implement all simulation with OpenFoam, analysis with Paraview and Python3, and documentation code in R [Xie, Dervieux, and Riederer \(2020\)](#).

### **3. Theory : Governing Equations**

## Part 4: Governing Equations

## Problem Statement

The governing equations for this problem are the two-dimensional Euler equations, complemented with the equation of state for an ideal gas with  $\gamma = 1.4$ .

In your report:

- Write down the governing equations in vector form. Identify clearly the state vector  $\mathbf{U}$ , the  $x$  and  $y$  components of the flux ( $\mathbf{F}$  and  $\mathbf{G}$ , respectively), and any additional equation that relates the variables together, e.g. the equation of state.
- Include working definitions of the local Mach number of the flow and the local sound speed. You will need those definitions when plotting quantities.
- Apply basic normal shock and isentropic flow relations to estimate the pressure at the stagnation point on the surface of the step at  $(x, y) = (0.6, 0)$  for free stream conditions of  $M = 3$  and  $p = 1$  Pa.

## **Solutions**

## 4) Governing Equations

### Development of Governing Equations in Vector Form

Let us begin with the differential form of the momentum equation:

$$\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u \otimes u) = -\nabla p + \nabla \cdot \tau + \rho b. \quad (1)$$

Given that the governing equations for the problem are the two-dimensional Euler equations, combined with the equation of state for an ideal gas with  $\gamma = 1.4$ , we can take the inviscid (Euler) flow limit of the equation neglecting viscous stresses and body forces.

$$\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u \otimes u) = -\nabla p + \rho b + \rho f. \quad (2)$$

The differential form of the continuity equation can be expressed as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \quad (3)$$

The differential form of the energy equation can be expressed as

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho E u) = \nabla \cdot (\lambda \nabla T) + \nabla \cdot (\sigma \cdot u) + s + \rho b \cdot u \quad (4)$$

Maintaining the equation by substituting for "σ" gives,

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho E u) = \nabla \cdot (\lambda \nabla T) + \nabla \cdot (\tau \cdot u) + s + \rho b \cdot u \quad (5)$$

Taking the inviscid (Euler) flow limit of the equation neglecting viscous stresses and assuming that there are no body forces or heat addition in the flow,  $b=0$ ,  $Q=s+\rho b \cdot u=0$ , and  $\nabla T=0$ , and  $\tau=0$  gives

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho E u) = 0 \quad \text{or} \quad s = 0 \quad (6)$$

$$\text{Here, } H = E + \frac{P}{\rho} = h + \frac{u^2}{2} \quad (7)$$

Let us return to the momentum equation (2) and expand the LHS of the expression giving,

$$\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u \otimes u) = \rho \left\{ \frac{\partial u}{\partial t} + u \cdot \nabla u \right\} + u \left\{ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) \right\} \quad \begin{matrix} \text{(from continuity)} \\ \cancel{\text{Equation (3)}} \end{matrix}$$

$$\Rightarrow \frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u \otimes u) = \rho \left\{ \frac{\partial u}{\partial t} + u \cdot \nabla u \right\} \quad (8)$$

Substituting the RHS of equation (8) into the LHS of equation (2) gives

$$\rho \left\{ \frac{\partial u}{\partial t} + u \cdot \nabla u \right\} = -\nabla p \quad (9)$$

w  
local acceleration    convective acceleration

But,  $\frac{\partial u}{\partial t} + u \cdot \nabla u = \frac{D u}{D t}$  giving,

$$\rho \frac{D u}{D t} = -\nabla p \quad (10)$$

Dividing equation (10) by " $\rho$ " gives

$$\frac{D u}{D t} = -\frac{\nabla p}{\rho}$$

Then, since the rescaled (normalized) pressure,  $\pi = \frac{p}{\rho}$ , we have,

$$\frac{D u}{D t} = -\nabla \pi \quad (11)$$

Separating equation (11) using the identities for the total acceleration and rescaled pressure according to  $x$  and  $y$  components gives,

$$x: \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{2(\frac{\rho}{\rho})}{2x} \quad (12)$$

$$y: \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = -\frac{2(\frac{\rho}{\rho})}{2y} \quad (13)$$

Let us now return to the Continuity Equation (3) and expand the LHS of the expression given,

$$\frac{\partial \rho}{\partial t} + \left[ \left( \frac{\partial}{\partial x}, \frac{\partial}{\partial y} \right) \cdot (\rho u, \rho v) \right] = 0$$

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} = 0 \quad (14)$$

Lastly, let us return to the Energy equation (6) and expand the LHS of the expression given,

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho H u) = 0 \quad (\text{where } H = E + \frac{P}{\rho})$$

$$\Rightarrow \frac{\partial \rho E}{\partial t} + \nabla \cdot \left( \rho \left( E + \frac{P}{\rho} \right) u \right) = 0$$

$$\Rightarrow \frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho E u + \rho u) = 0$$

$$\Rightarrow \frac{\partial \rho E}{\partial t} + \left( \frac{\partial}{\partial x}, \frac{\partial}{\partial y} \right) \cdot \left( \rho E \begin{bmatrix} u \\ v \end{bmatrix} + \rho \begin{bmatrix} u \\ v \end{bmatrix} \right) = 0$$

$$\Rightarrow \frac{\partial \rho E}{\partial t} + \left( \frac{\partial}{\partial x}, \frac{\partial}{\partial y} \right) \cdot (\rho E u + \rho u, \rho E v + \rho v) = 0$$

$$\Rightarrow \frac{\partial \rho E}{\partial t} + \frac{\partial}{\partial x} (\rho E u + \rho u) + \frac{\partial}{\partial y} (\rho E v + \rho v) = 0 \quad (15)$$

Now, the governing equations can be expressed in vector form with a single vector equation that can be interpreted as a conservation equation for the far field. Simplified N=5 equations broken down into a vector with time-dependent terms, and two vectors with space-dependent terms as,

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} = 0 \quad (16)$$

(where  $\mathbf{U}$  is the state vector,  $\mathbf{F}$  is the  $x$ -constant of the flux  ~~$\mathbf{U}$~~ , and  $\mathbf{G}$  is the  $y$ -component of the flux).

The state vector, "U" contains the time gradient terms from each of the four variables.

$$\text{Continuity: } \rho$$

$$x\text{-momentum: } \rho u$$

$$y\text{-momentum: } \rho v$$

$$\text{Energy: } \rho e$$

$$\Rightarrow U = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ E \end{bmatrix}$$

the flux vector, "F", contains the x-gradient terms,

$$\text{Continuity: } \rho u$$

$$x\text{-momentum: } \rho u^2 + p$$

$$y\text{-momentum: } \rho uv + p$$

$$\text{Energy: } \rho ut + p$$

$$\Rightarrow F(u) = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv + p \\ \rho ut + p \end{bmatrix}$$

the flux vector, "G", contains the y-gradient terms,

$$\text{Continuity: } \rho v$$

$$x\text{-momentum: } \rho uv + p$$

$$y\text{-momentum: } \rho v^2 + p \Rightarrow G(v)$$

$$\text{Energy: } \rho vt + p$$

$$\begin{bmatrix} \rho v \\ \rho uv + p \\ \rho v^2 + p \\ \rho vt + p \end{bmatrix}$$

The Equation of State for an ideal, calorically perfect gas is expressed as,

$$\underline{PRT = P} \quad (17)$$

(where "R" is the gas constant in  $\text{J kg}^{-1}\text{K}^{-1}$ , "T" is the temperature in K, and "P" is the pressure in  $\text{N m}^{-2}$ ).

The gas constant is expressed as,

$$\underline{R = \frac{R}{w}} \quad (18)$$

(where "R" is the universal gas constant,  $\text{J mol}^{-1}\text{K}^{-1}$ , and "w" is the molar mass of the gas in  $\text{kg mol}^{-1}$ ).

The universal gas constant, "R" equals,

$$R = 8314 \text{ J mol}^{-1}\text{K}^{-1}$$

Again, for an ideal, calorically perfect gas,

$$\underline{e = \frac{P}{\rho} \frac{1}{\gamma-1} = \frac{R}{\gamma-1} T = C_p T} \quad (19)$$

where  $\gamma = \frac{C_p}{C_v}$ ,  $C_p = \frac{R}{\gamma-1}$ , and  $C_v = C_p - R$

The Speed of sound can be expressed as:

$$\underline{a = \sqrt{\gamma RT} = \sqrt{\frac{\gamma P}{\rho}}} \quad (20)$$

Now, we can recover pressure from the state vector by rearranging equation (19)

$$\underline{P = (\gamma-1)Pe = (\gamma-1)(E - \rho U^2/2)} \quad (21)$$

The local mach Number of the flow is quantified according to:

$$\boxed{\underline{Ma = \frac{|U|}{a}}} \rightarrow \begin{array}{l} \text{(magnitude of local velocity)} \\ \text{local sound speed} \end{array} \quad (22)$$

Estimation of pressure at stagnation point on surface of step at  $(x, y) = (0.6, 0)$

Given free-stream conditions,  $Ma = 3$ ,  $P = 1$ ,  $\gamma = 1.4$   
and that density equals

$$\rho = \frac{\gamma P}{a^2} = \gamma = 1.4$$

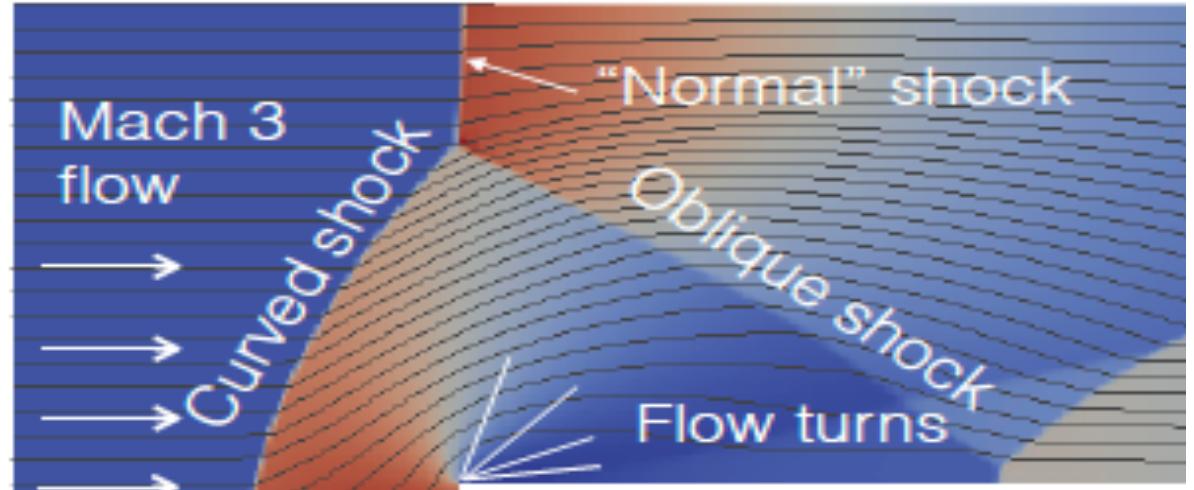
Equation (20) can be used to obtain the speed of sound

$$a = \sqrt{\frac{\gamma P}{\rho}} = \sqrt{\frac{(1.4)(1 \text{ Pa})}{1.4 \text{ kg/m}^3}} = 1 \text{ m/s}$$

Substitution of  $a = 1 \text{ m/s}$  and  $Ma = 3$  into equation (20) gives  
the magnitude of local velocity in the free-stream,

$$|U| = Ma \cdot a = (3)(1 \text{ m/s}) = 3 \text{ m/s}$$

In referencing the flow streamlines over the computational grid in the slide "Flow Streamlines" in lecture16.pdf, it is shown that expected behavior contains a shock wave generated normal to the streamlines between the free stream and the stagnation point over  $(x, y) = (0, 0)$  to  $(x, y) = (0.6, 0)$ . This region is highlighted in the figure below.



Free Stream  
Point with  $P = 1$   
 $P_a, Ma = 3$

1      2      3

**Stagnation point**

**Leading shock**

Point Downstream  
of Normal Shock  
Wave

According to NASA documentation on Normal Shock wave properties in compressible flow, "For compressible flows with little or small flow turning, the flow process is reversible and the entropy is constant, the change in flow properties are then given by the isentropic relations. The region in the freestream that is compressible flow with little flow turning is then compatible with this definition. The documentation then proceeds to state the following regarding Shock waves, "If the shock wave is perpendicular to the flow direction it is called normal shock." Again, referring to the illustration above, it can be assumed for simplicity that the behavior of the flow at the streamlines intersecting the bottom of the curved shock field and the stagnation point exhibits normal shock since the streamline is normal to the shock region along this line. Operating off of this assumption, equations 23) and 24) below are used describe the change in flow properties across a normal shock wave :

$$M_{a2}^2 = \frac{(\gamma - 1) M_{a1}^2 + 2}{2 \gamma M_{a1}^2 - (\gamma - 1)} \quad (23)$$

(where "M<sub>a2</sub>" is the Mach number to the right of the Normal shock wave  
 "M<sub>a1</sub>" is the Mach Number of the free stream)  
 (downstream)

$$\frac{P_2}{P_1} = \frac{2\gamma M_{a1}^2 - (\gamma - 1)}{\gamma + 1} \quad (24)$$

(where "P<sub>2</sub>" is the Static pressure downstream Normal shock wave region, "P<sub>1</sub>" is the static pressure in the freestream).

Substitution of  $\gamma = 1.4$ ,  $M_{\infty} = 3$  into equation (23) and solving for "M<sub>2</sub>" gives,

$$M_{2} = \sqrt{\frac{(1.4-1)(3)^2 + 2}{2(1.4)(3)^2 - (1.4-1)}} \approx 0.4752$$

Rearranging equation (24) and solving for the static pressures,

$$\begin{aligned} P_2 &= P_1 \left( \frac{2\gamma M_{\infty}^2 - (\gamma-1)}{\gamma+1} \right) \\ &= (1 \text{ Pa}) \left( \frac{2(1.4)(5^2) - (1.4-1)}{1.4+1} \right) \\ &\approx 10.3333 \text{ Pa} \end{aligned}$$

Now, the region of the streamline between points 2 (downstream of shock wave) and 3 (stagnation point) is isentropic, meaning that the change in flow variables is small and gradual. In referencing NASA's article on "Isentropic flow" whose citation is provided at the end of the report, equation 25) below depicts the ratio of pressure change between two points in an isentropic flow region,

$$\frac{P_2}{P_t} = \left( 1 + \frac{\gamma-1}{2} M_{2}^2 \right)^{-\frac{\gamma}{\gamma-1}} \quad (25)$$

where " $P_2^{ll}$ " is the static pressure downstream in isentropic flow and " $P_t$ " is the total pressure at isentropic flow region (and at stagnation point).

Rearranging the equation to solve for the stagnation pressure gives,

$$\frac{P_2}{P_3} = \left( 1 + \frac{\gamma-1}{2} M_{2}^2 \right)^{-\frac{\gamma}{\gamma-1}}$$

$$P_3 = \left[ \left( 1 + \frac{\gamma-1}{2} M_{2}^2 \right)^{-\frac{\gamma}{\gamma-1}} \right] P_2 \approx \left[ \left( 1 + \frac{1.4-1}{2} (0.4752)^2 \right)^{\frac{1.4-1}{1.4-1}} \right] (10.333 \text{ Pa}) \approx 12.06 \text{ Pa}$$

(total)  
Therefore, the pressure at the stagnation point on the surface of the  
step at  $(x, y) = (0.6, 0)$  for free stream conditions of  $M = 3$   
and  $P = 1$  Pa is approximately 12.06 Pa.

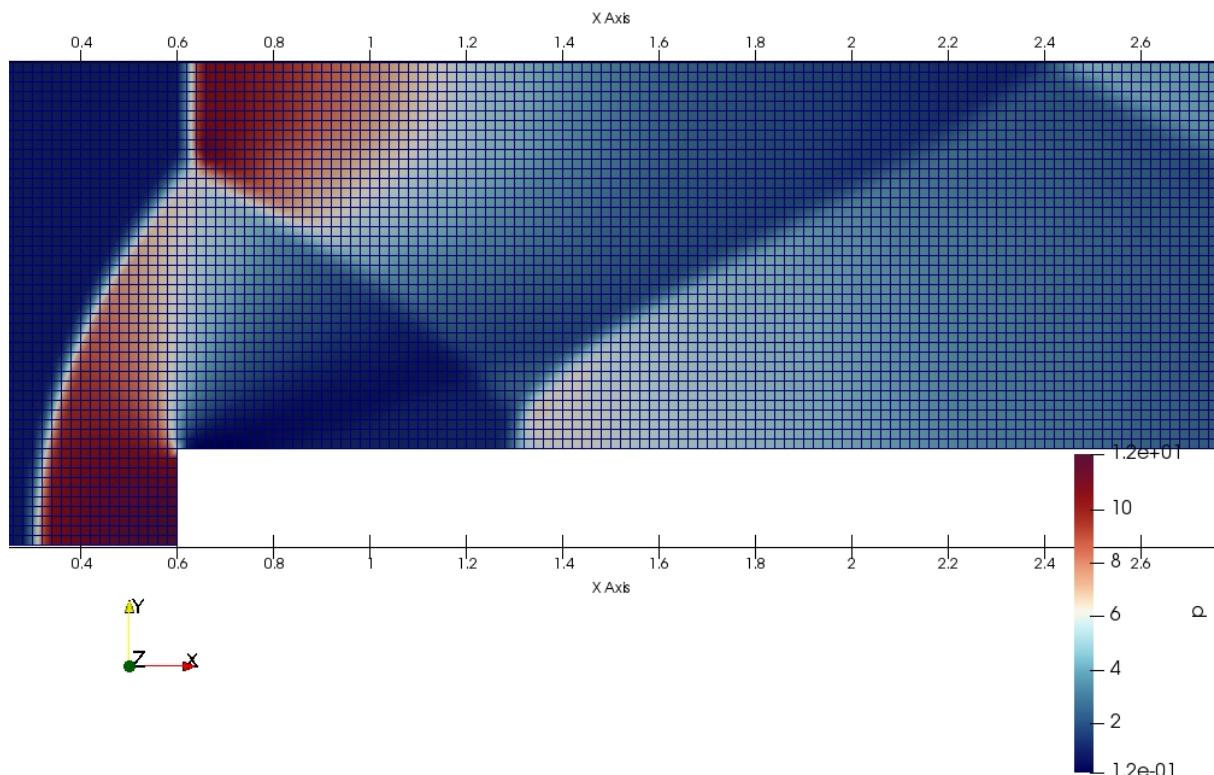
## **References**

- 1) "Normal Shock Wave Equations." Edited by Nancy Editor, *NASA*, NASA,  
<https://www.grc.nasa.gov/WWW/k-12/airplane/normal.html>.
- 2) "Isentropic Flow Equations." Edited by Nancy Hall, *NASA*, NASA,  
<https://www.grc.nasa.gov/WWW/K-12/airplane/isentrop.html>.

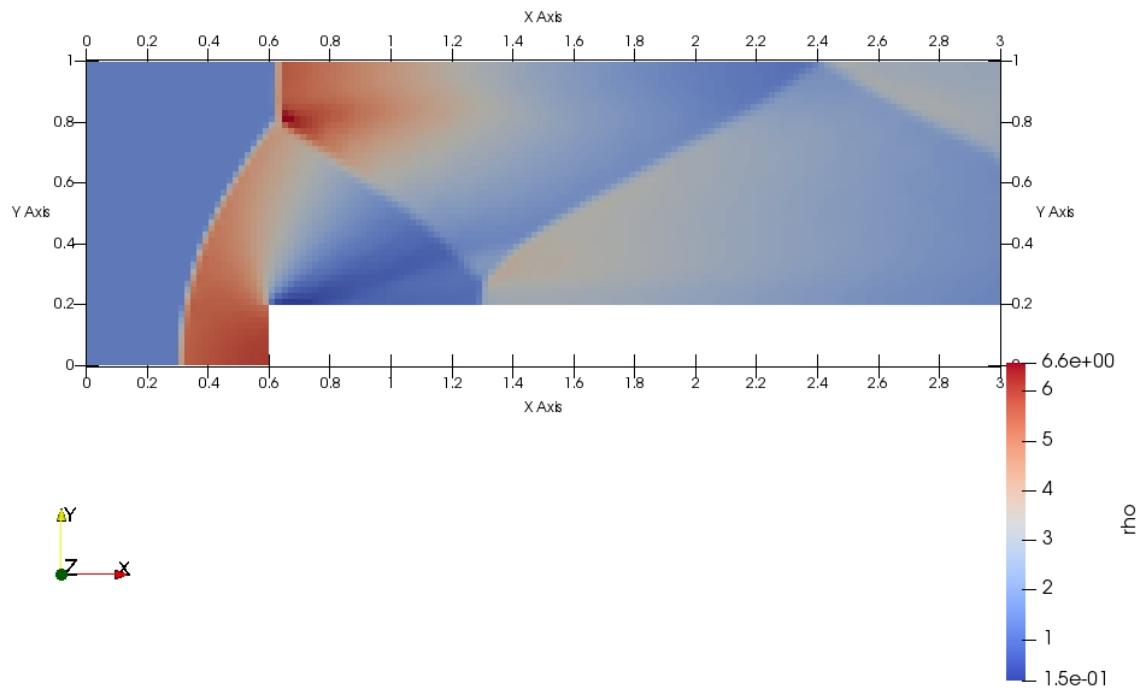
## 4. Mesh Assembly : Preliminaries

We assemble a preliminary solution at  $T = 4s$  with 6300 cells, for the following inlet conditions:  $M = 3, p = 1Pa, T = 1K, \rho = \gamma \frac{kg}{m^3}$  with  $\gamma = 1.4$ . All results have been non-dimensionalized: velocity, pressure, density and temperature are all measured with respect to inlet conditions.

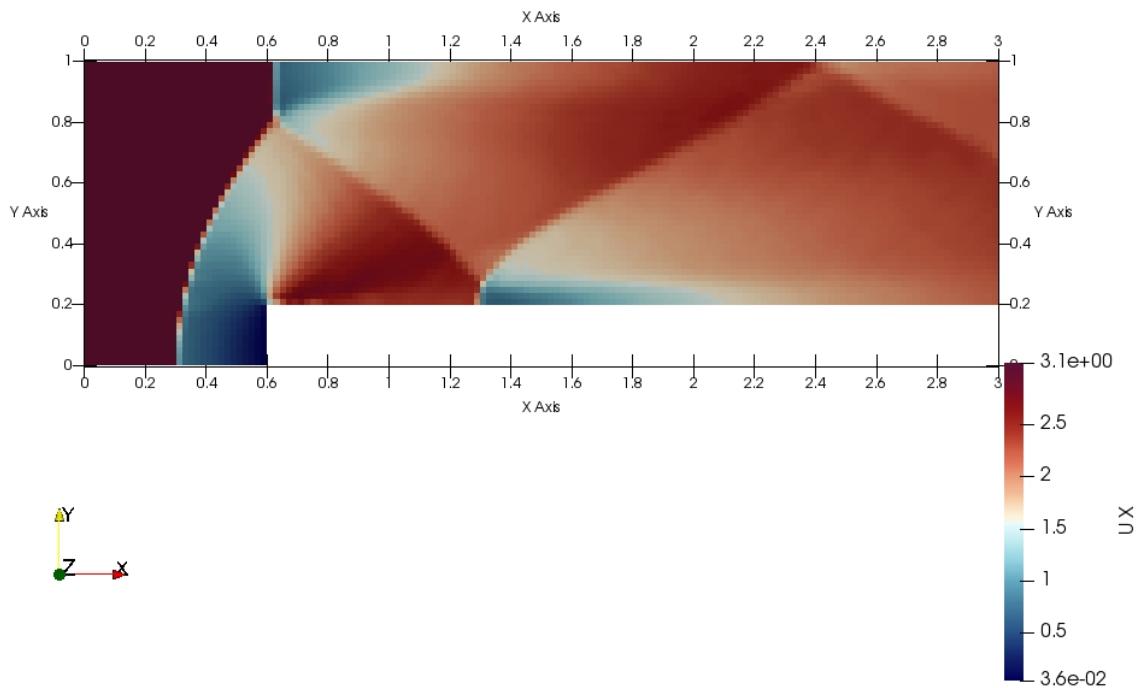
### 4.1. Mesh

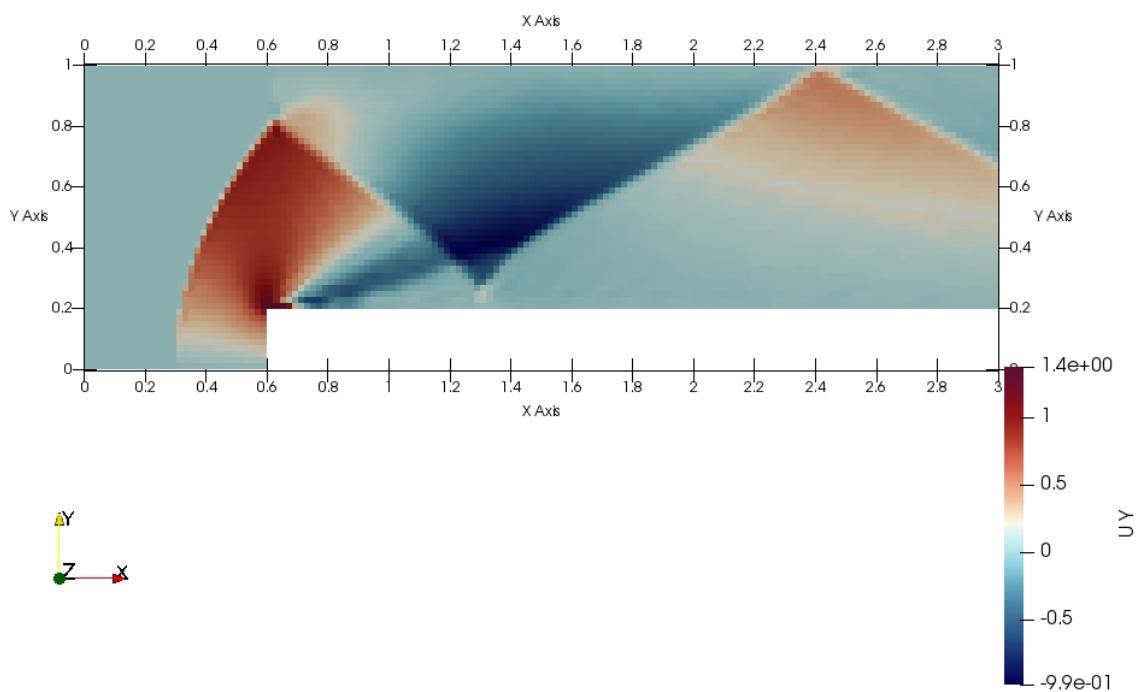


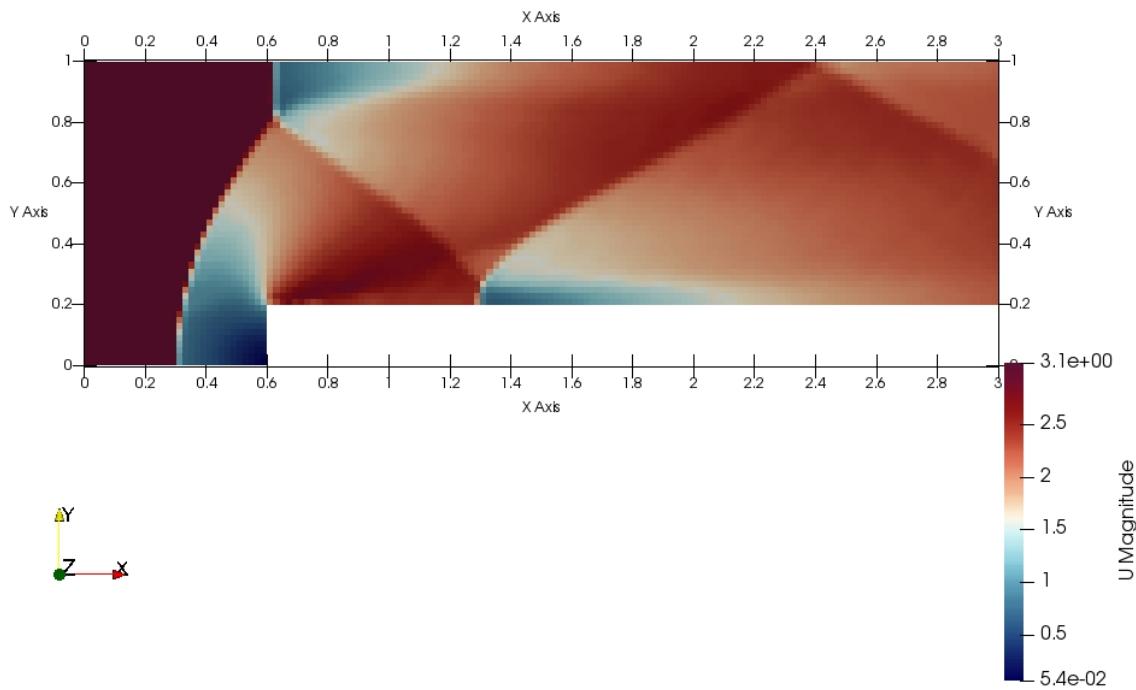
### 4.2. Density



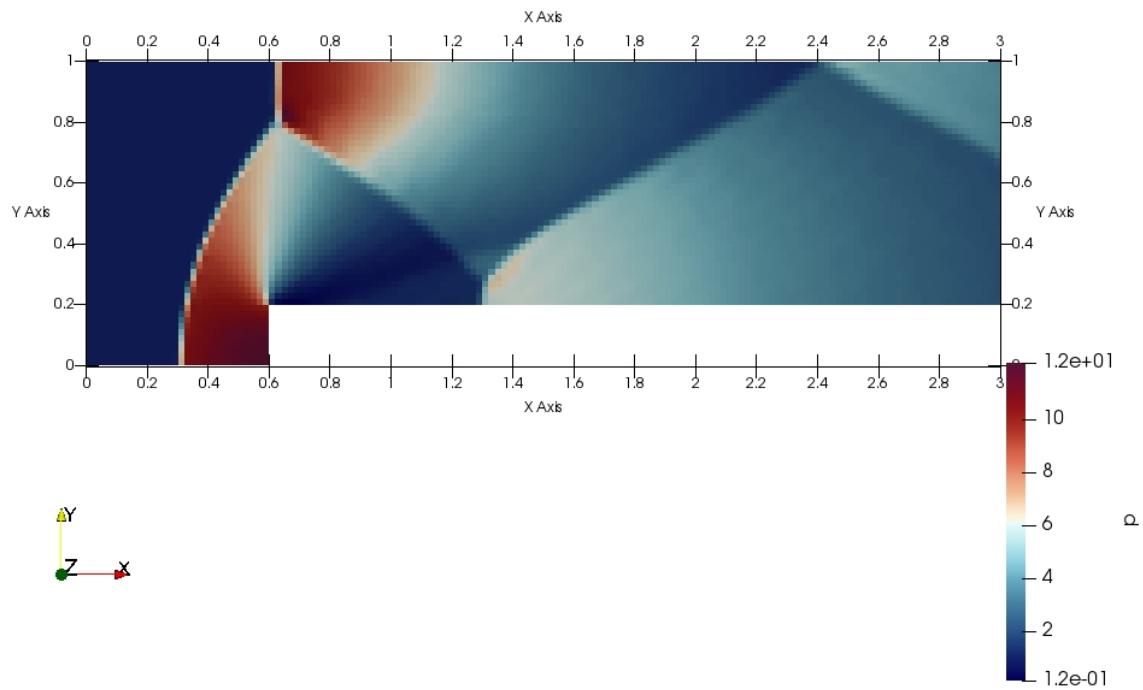
#### 4.3. Velocity X, Y, Magnitude



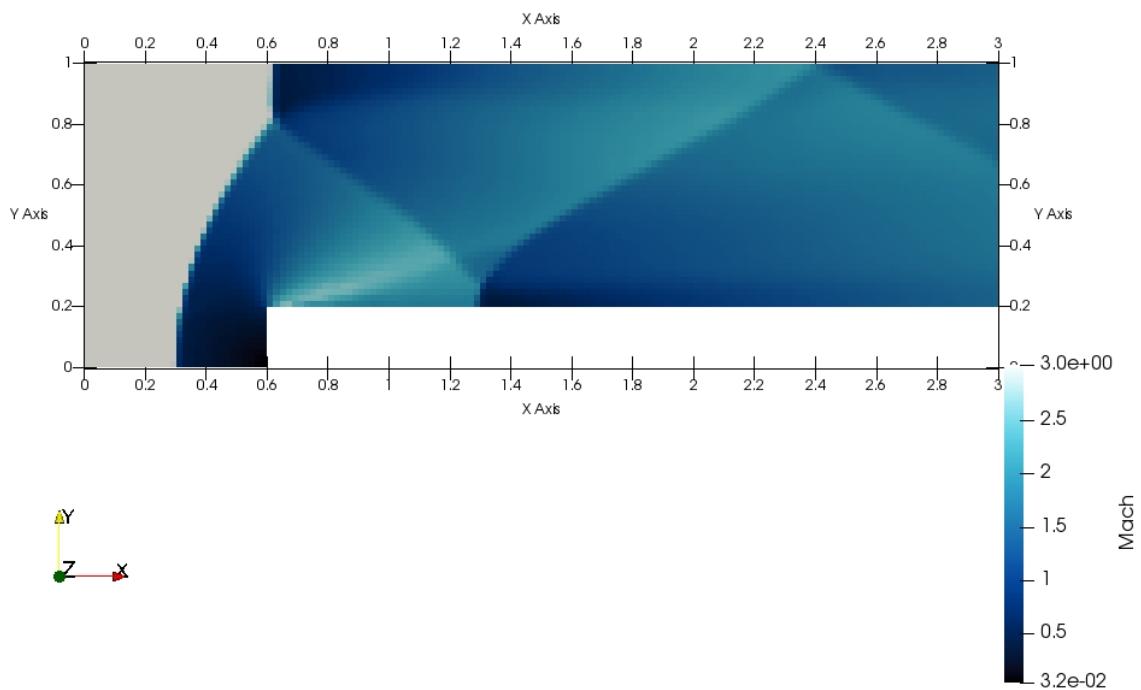




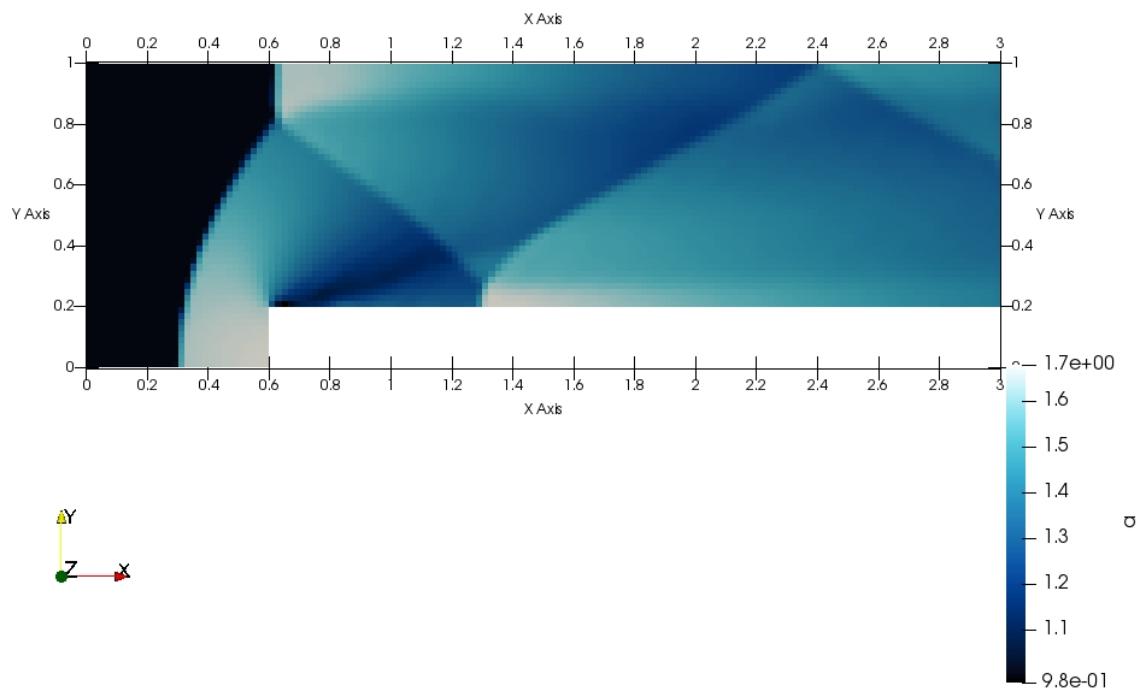
#### 4.4. Pressure



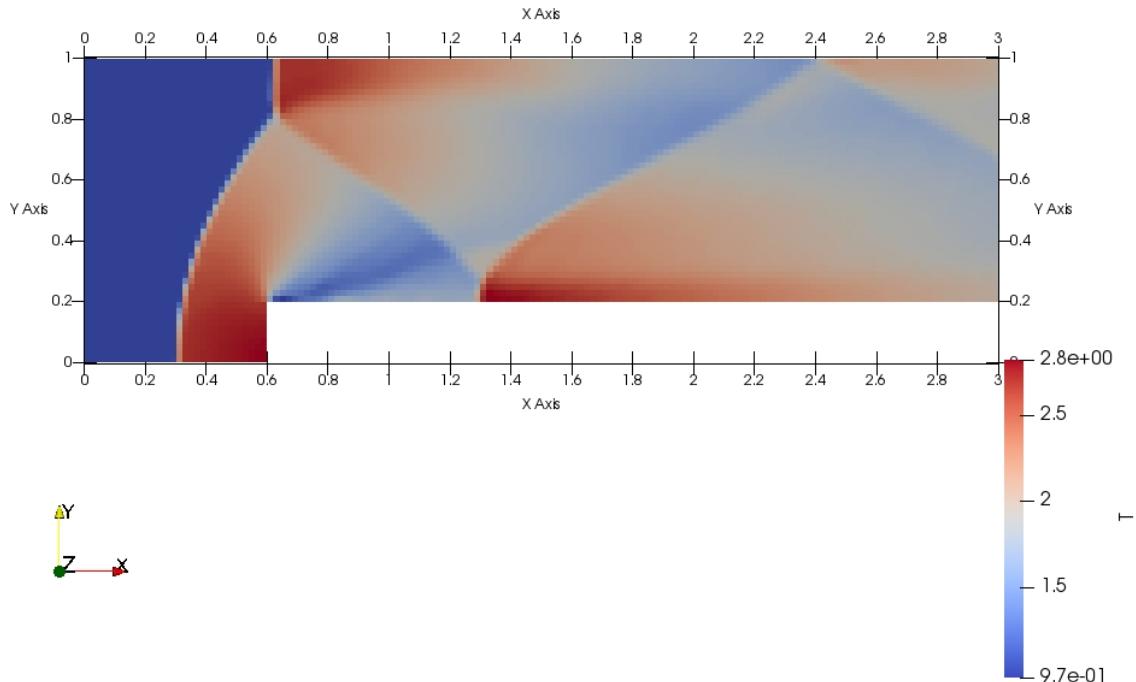
#### 4.5. Mach Number



#### 4.6. Speed of Sound



#### 4.7. Temperature



## 5. Convergence

Three meshes were used, with increasing numbers of cells and smaller timesteps, as follows: (note the timesteps are approximate as the solver, RhoCentralFoam, adjusts timesteps as necessary to maintain a maximum Courant number of 0.2).

Run\_10\_64 : 6300 cells,  $dx = 0.04000$ ,  $dt = 0.00110$

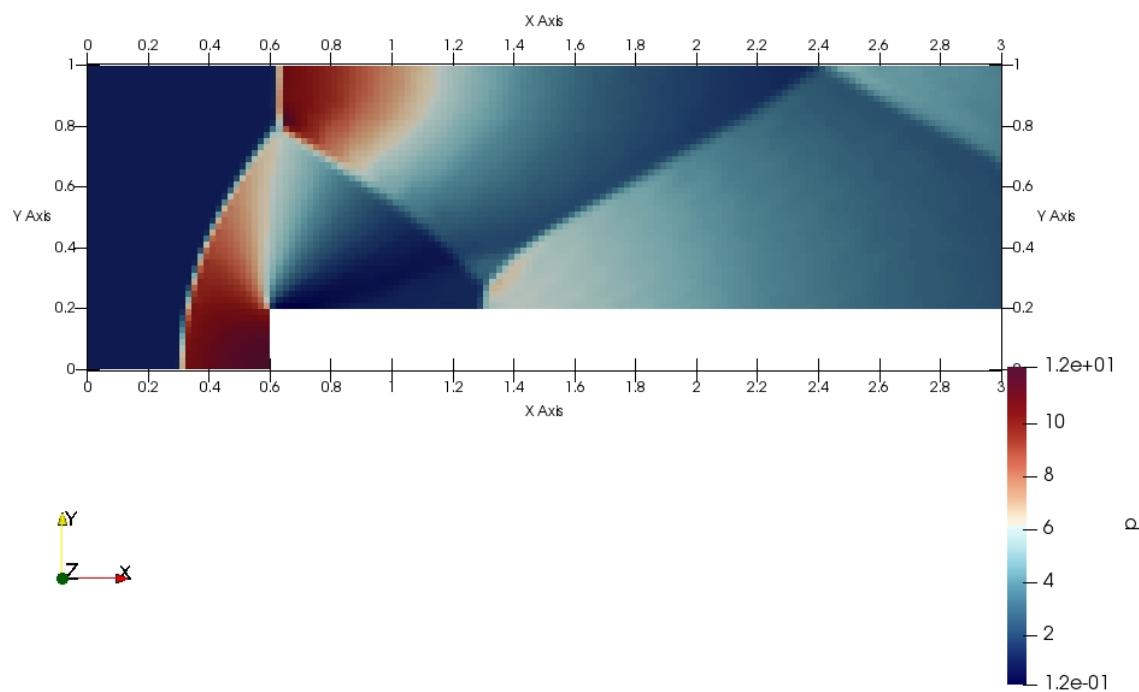
Run\_20\_64 : 25200 cells,  $dx = 0.02000$ ,  $dt = 0.00056$

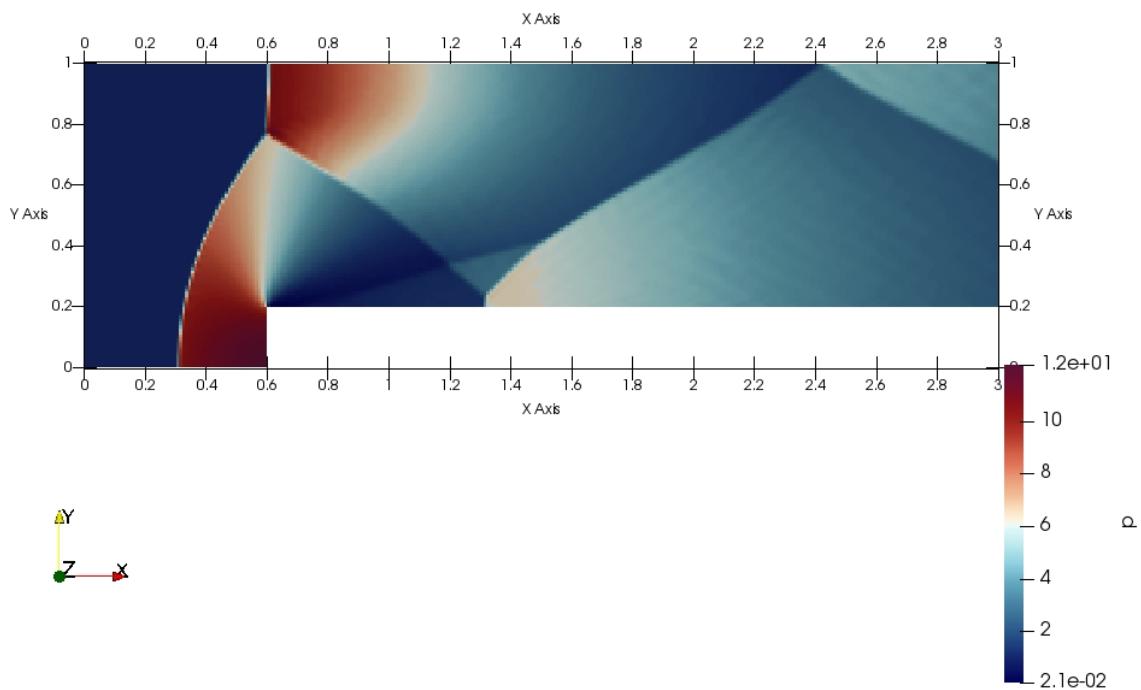
Run\_32\_64 : 64512 cells,  $dx = 0.00625$ ,  $dt = 0.00034$

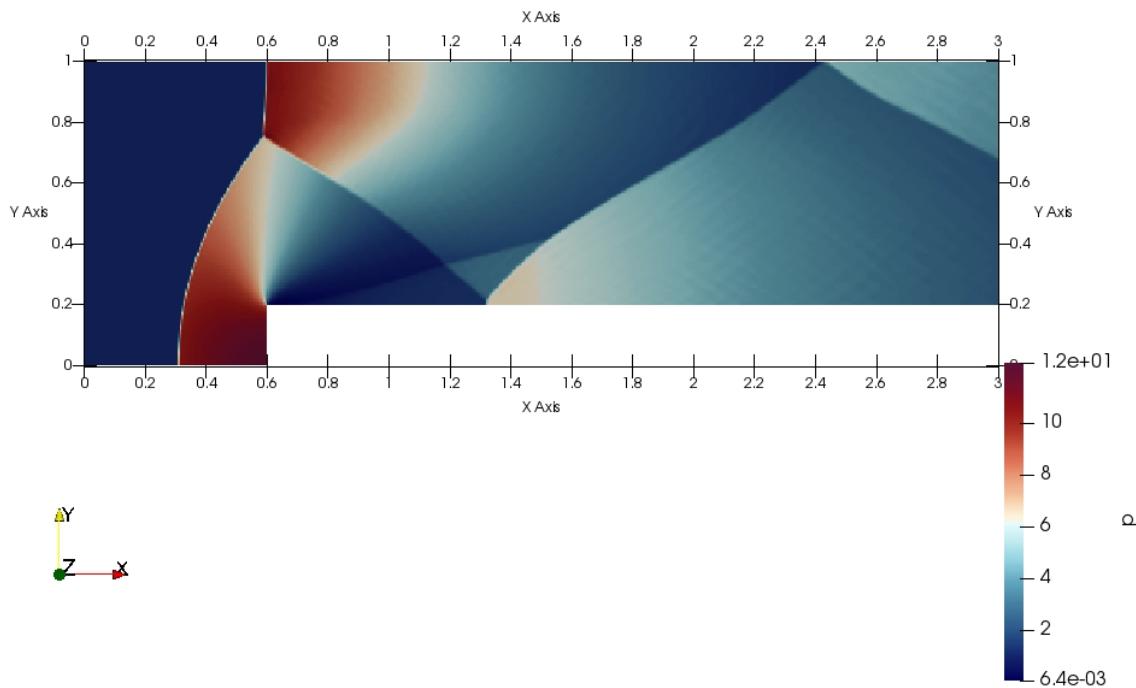
### 5.8. Improvements in Pressure, Density, and Y-Velocity with increasing resolution:

Note the upper shock turbulent features (the small waves), and how they resolve much more appropriately with higher resolution meshes.

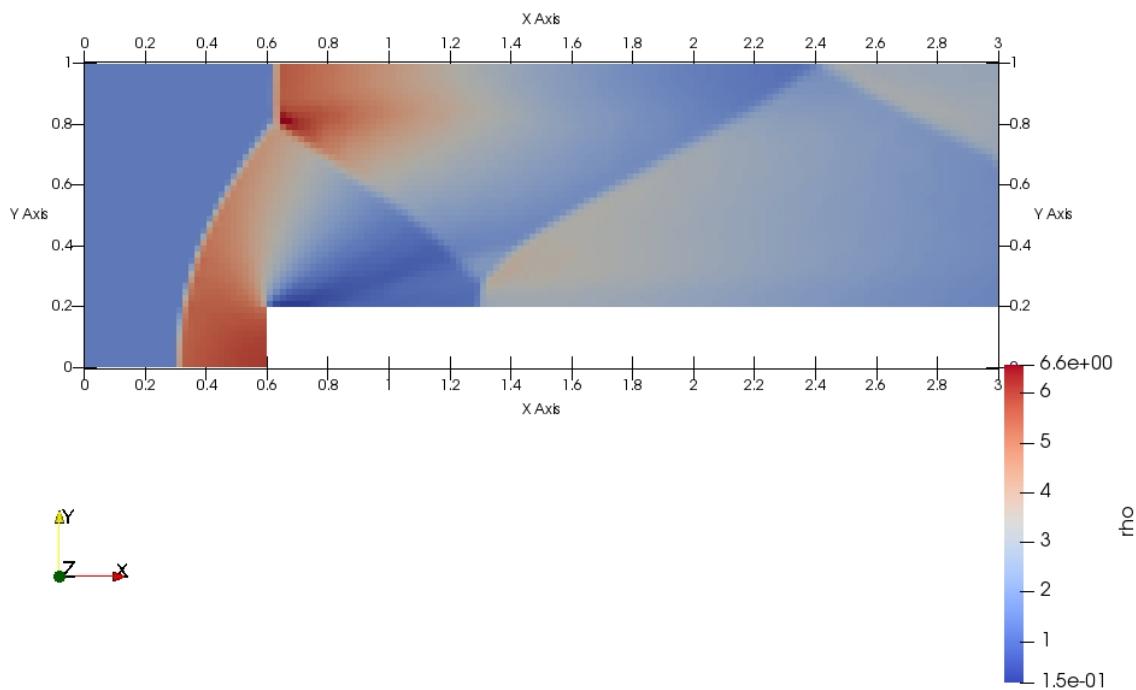
**Pressure (from Run\_10 to Run\_32):**

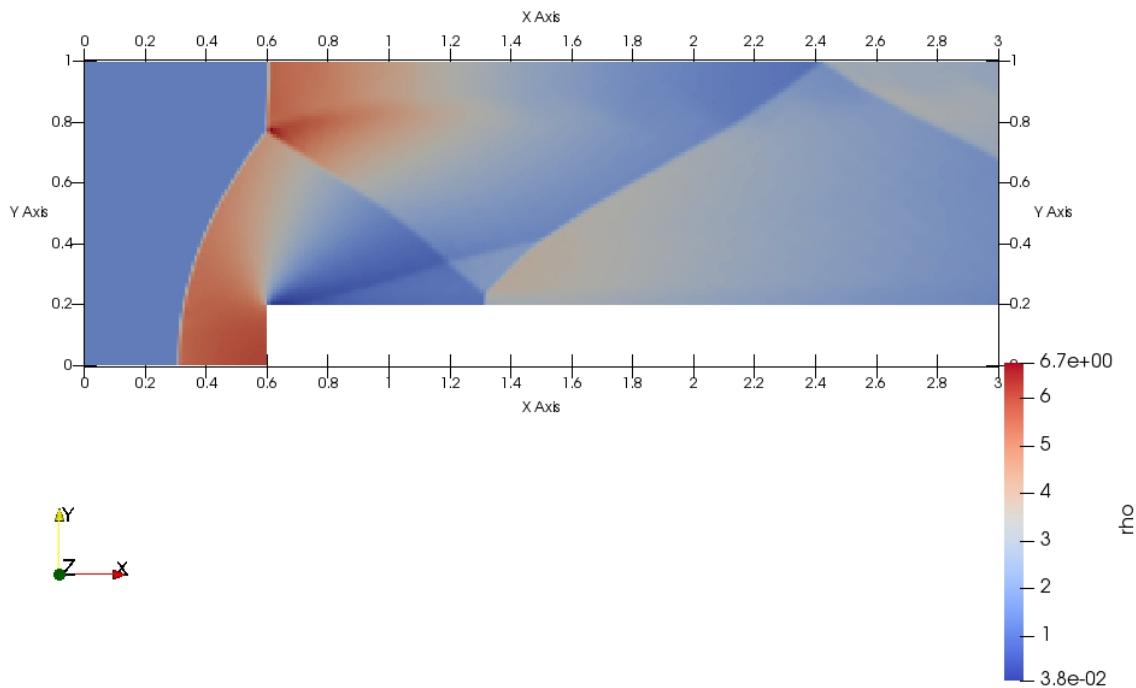


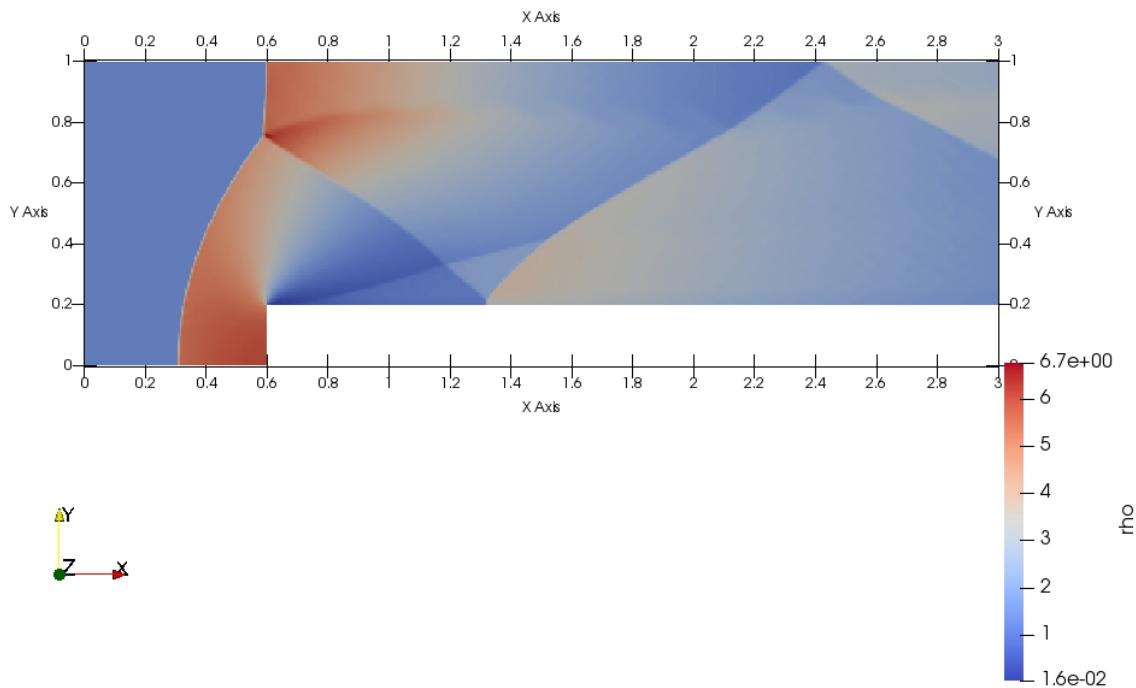




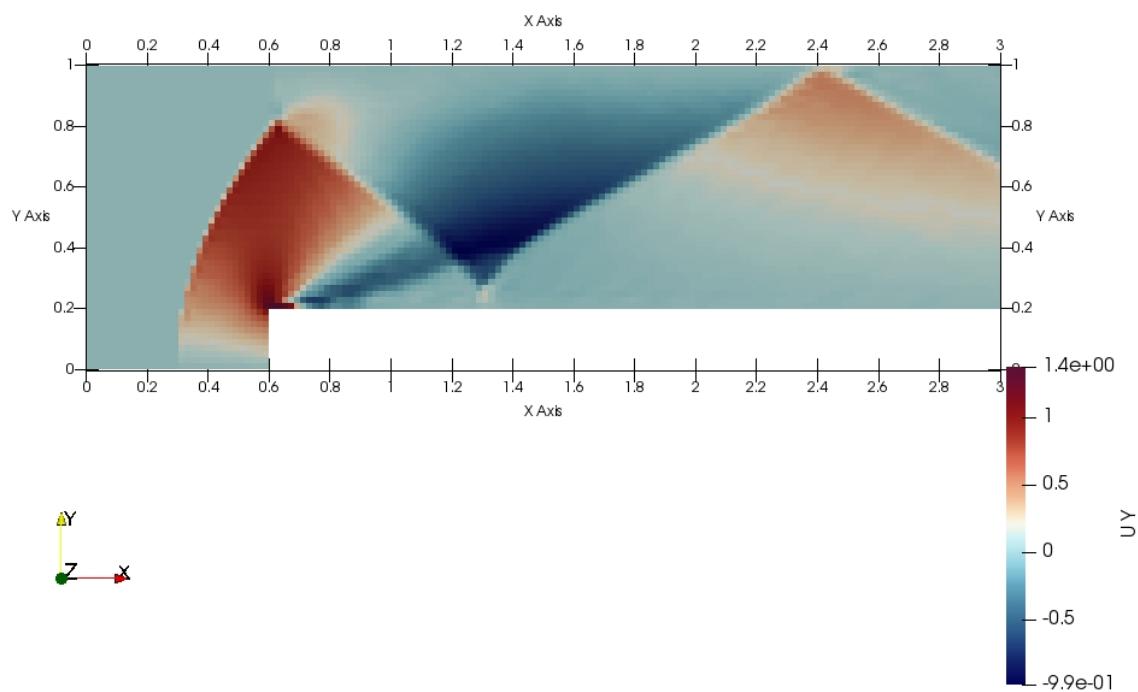
**Density:**

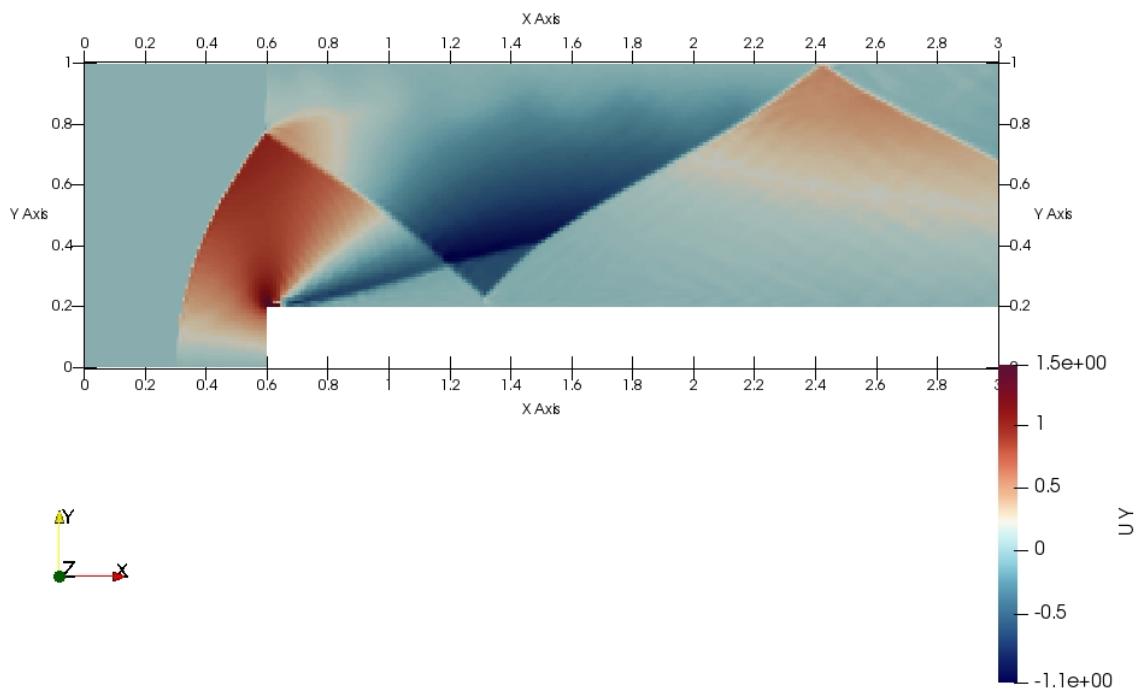


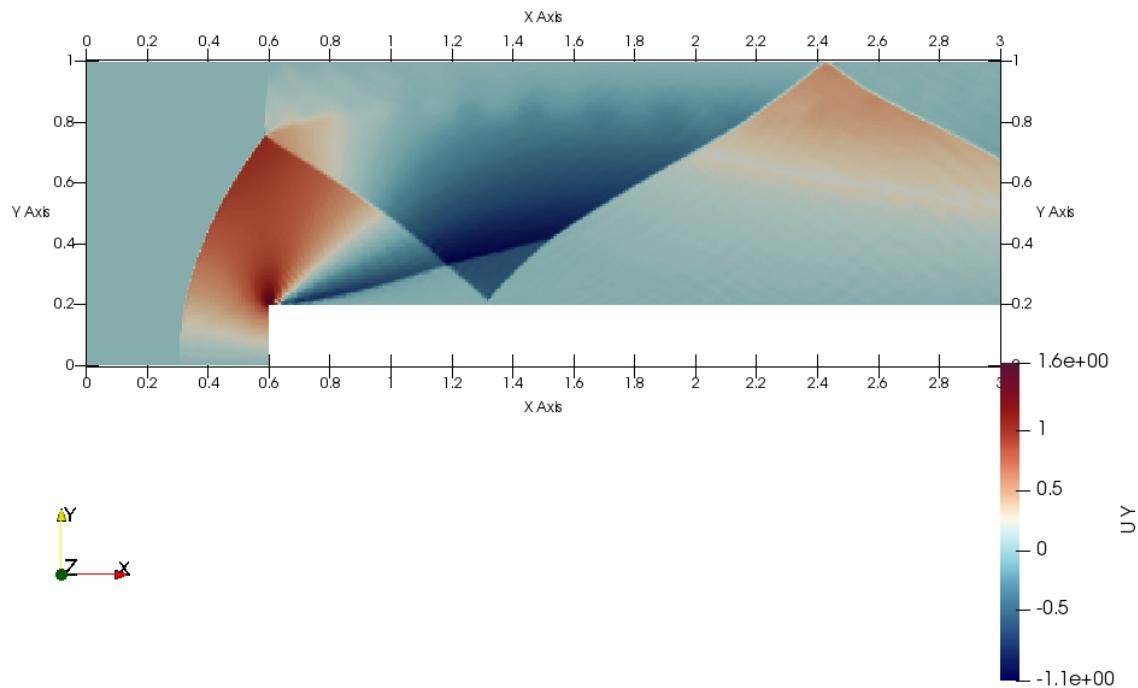




**Y-velocity:**





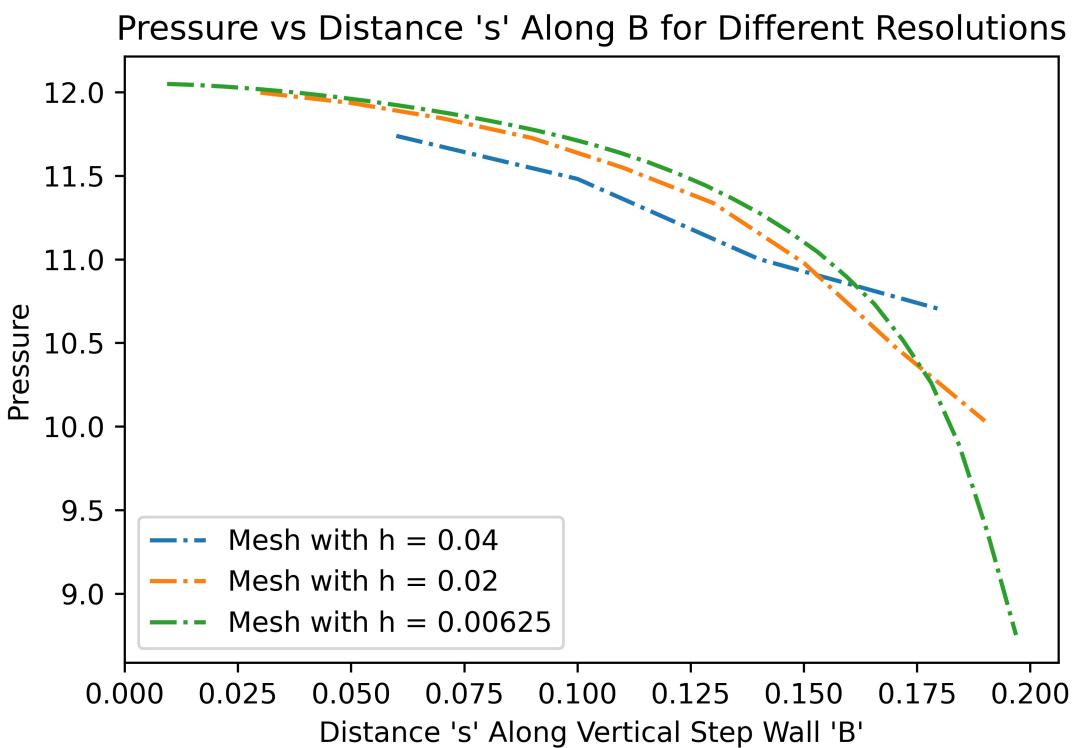
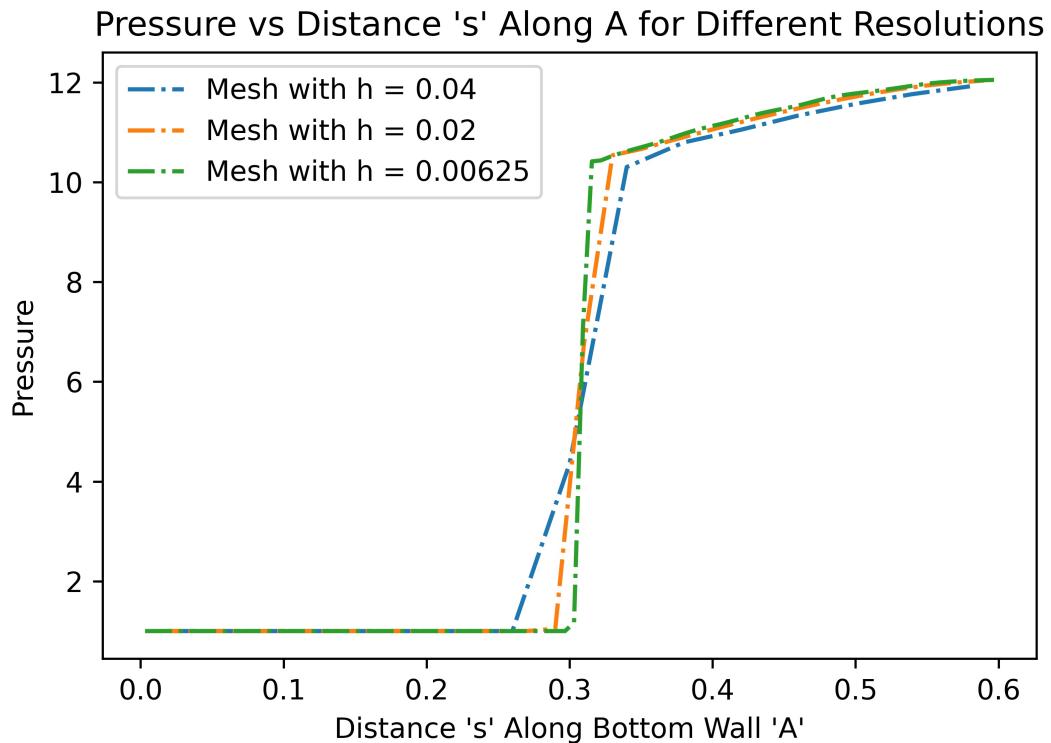


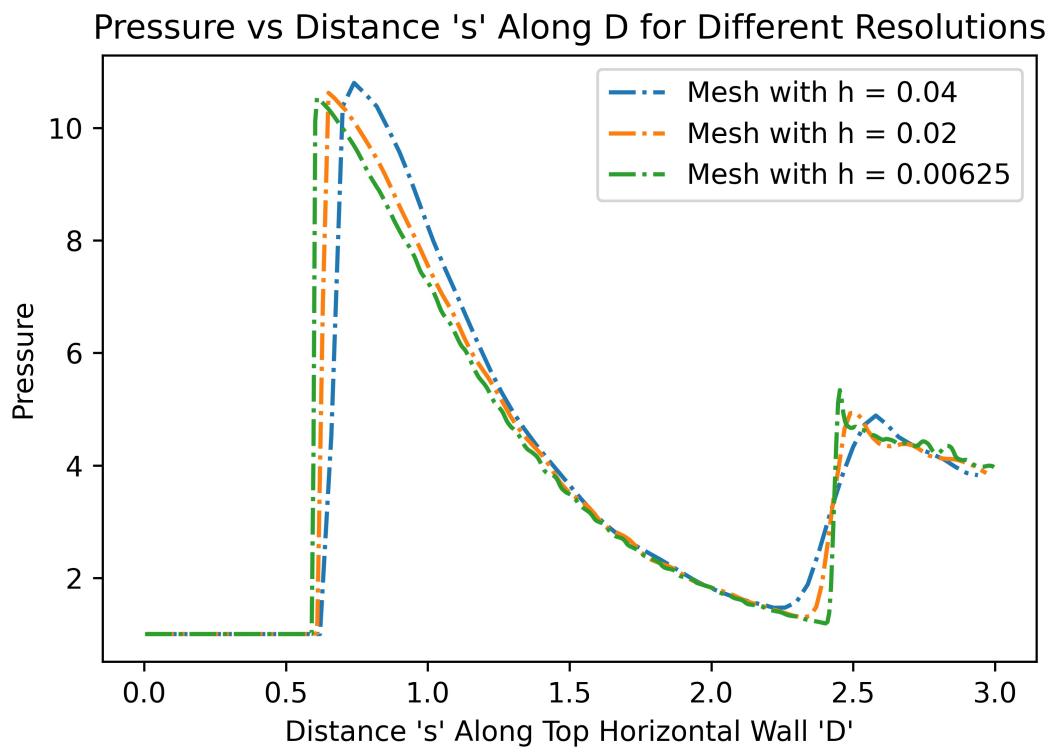
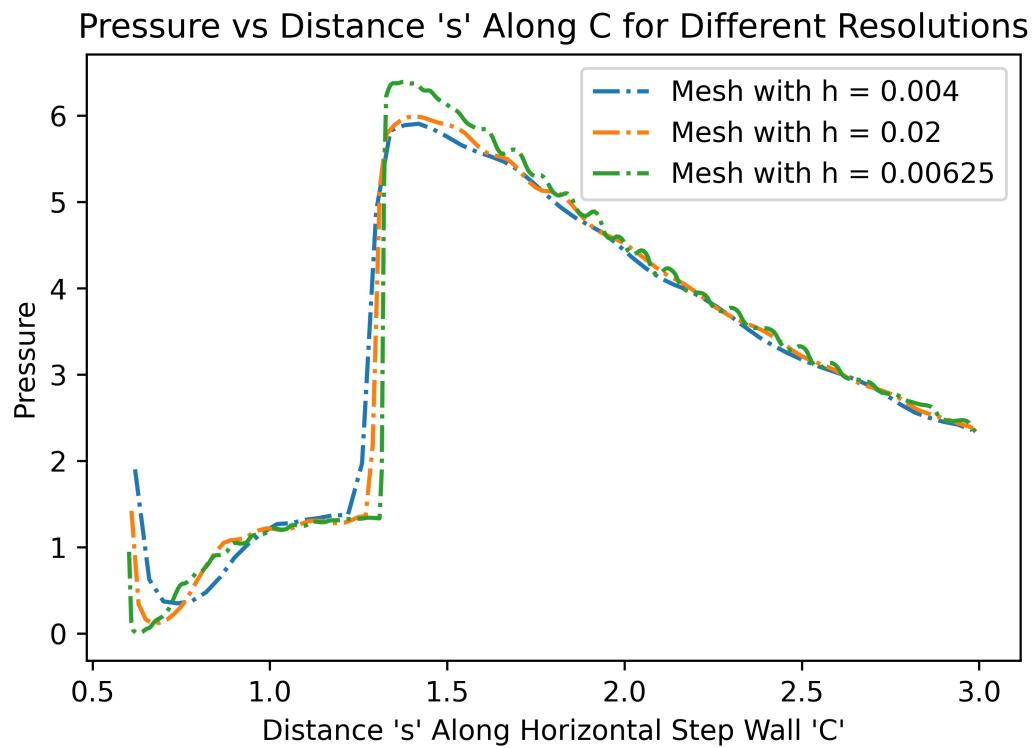
### 5.9. Wall Distributions w.r.t Resolution Levels:

Pressure, density, x-velocity, y-velocity, and temperature are reported in that order. Note that the walls are traversed from left to right, first the horizontal wall prior to the step, then the vertical step wall (traversing upward), then the horizontal wall (the step itself), and finally the upper horizontal wall.

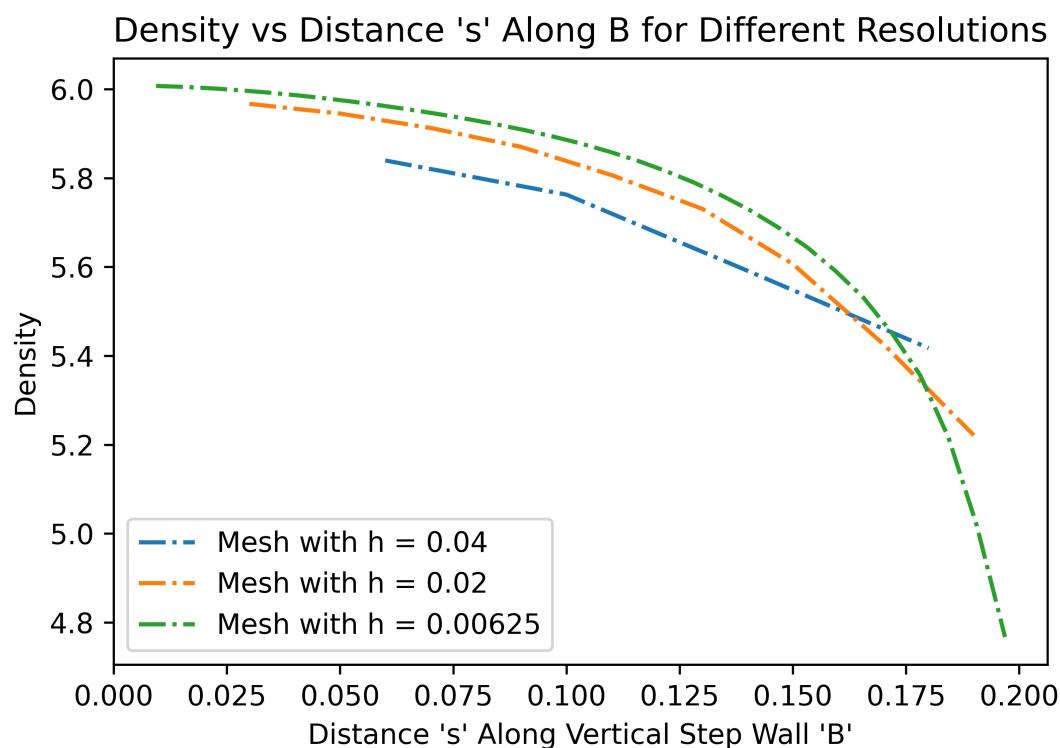
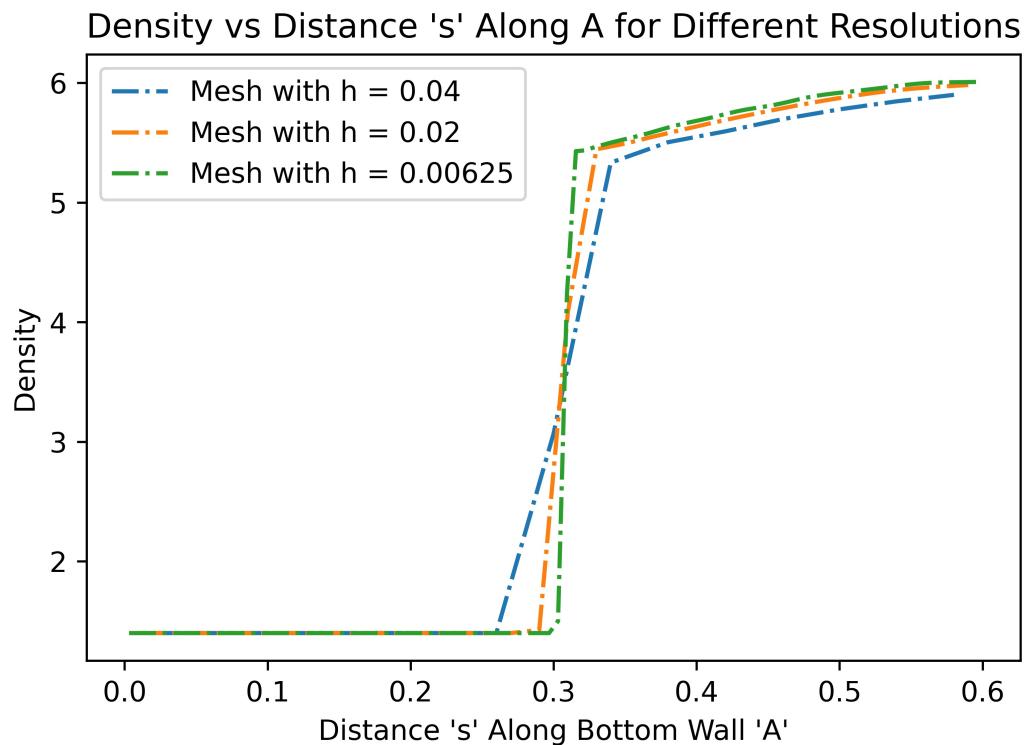
Convergence is shown through decreasing  $h$  (the spatial step-size).

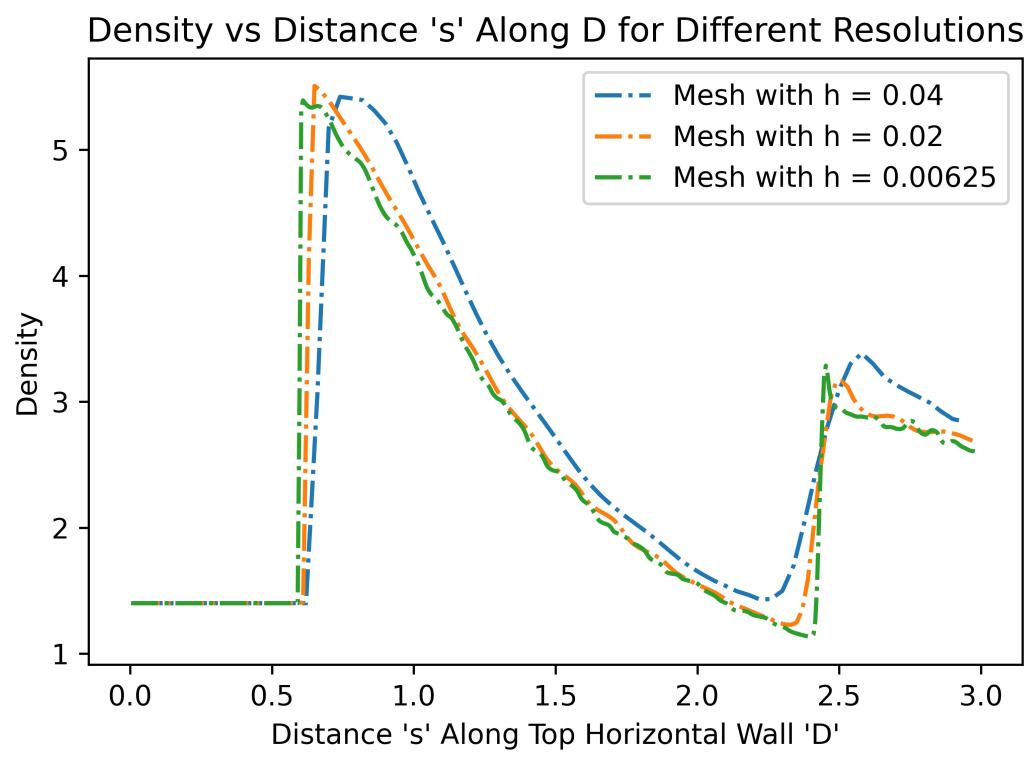
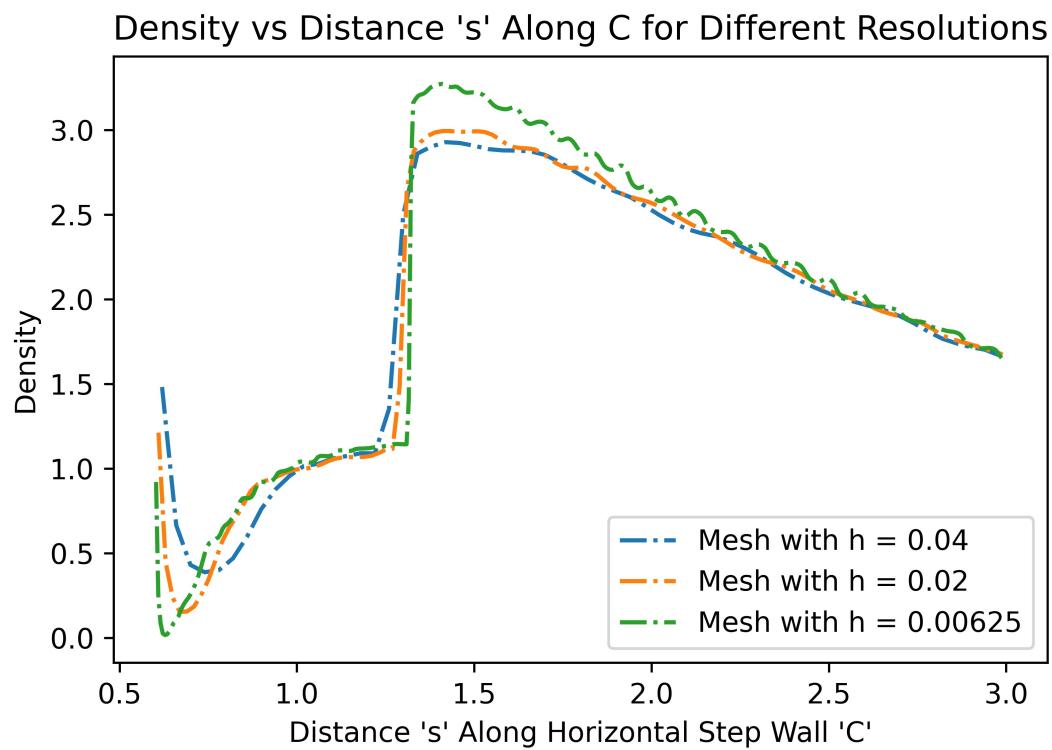
#### Pressure:





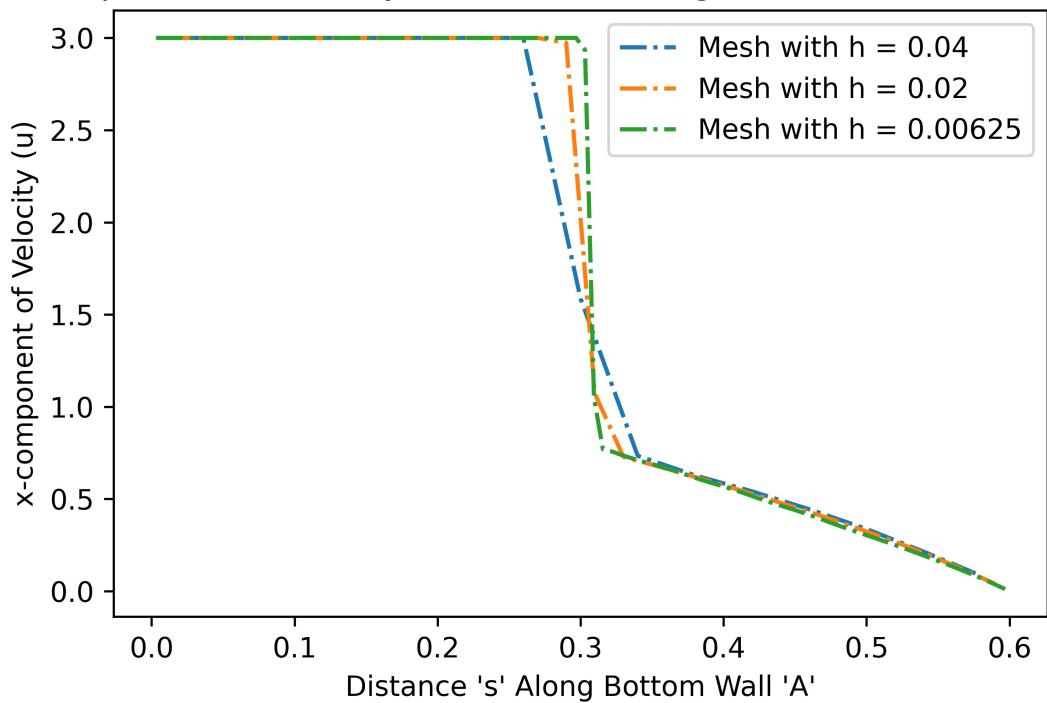
**Density:**



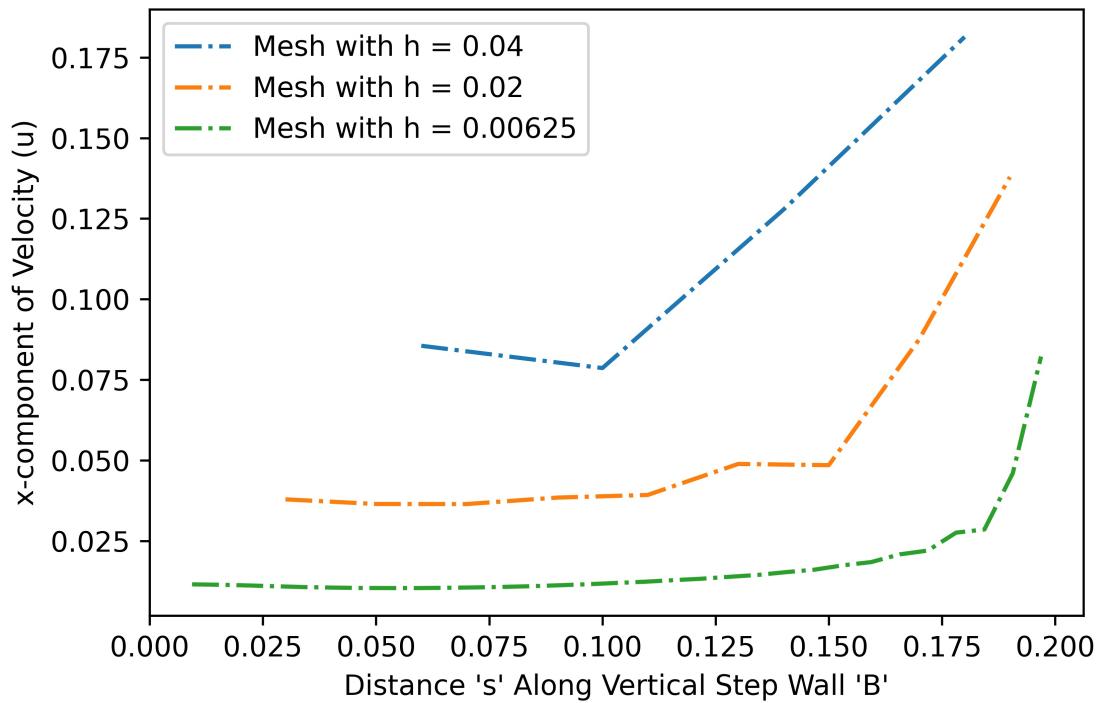


**X-velocity:**

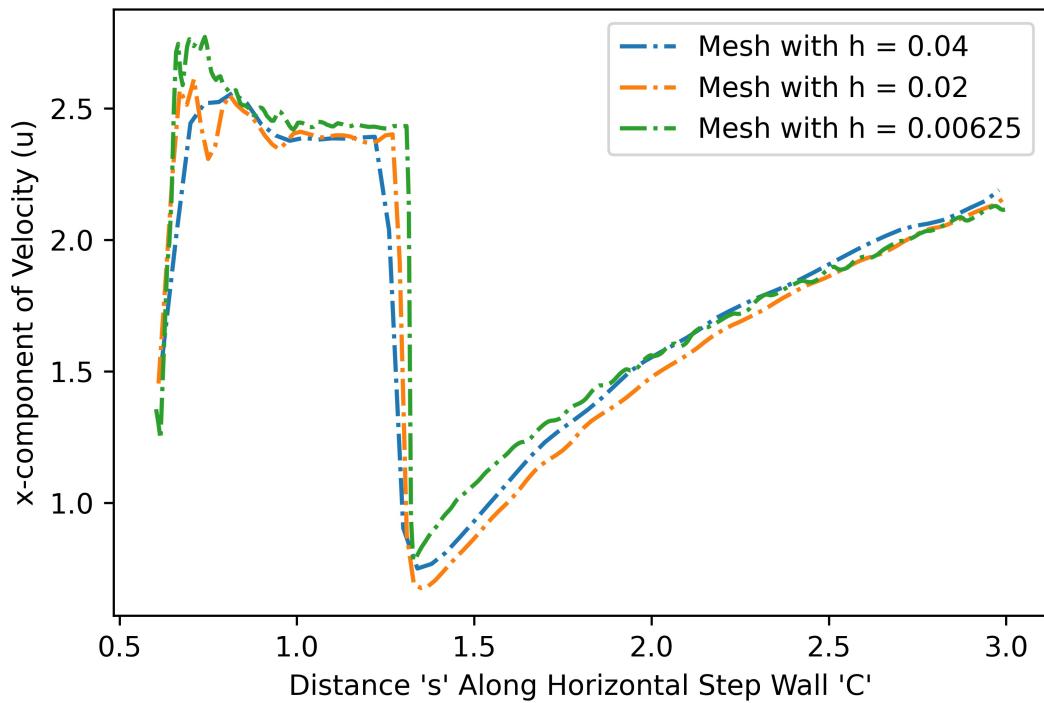
x-component of Velocity vs Distance Along A for Different Resolutions



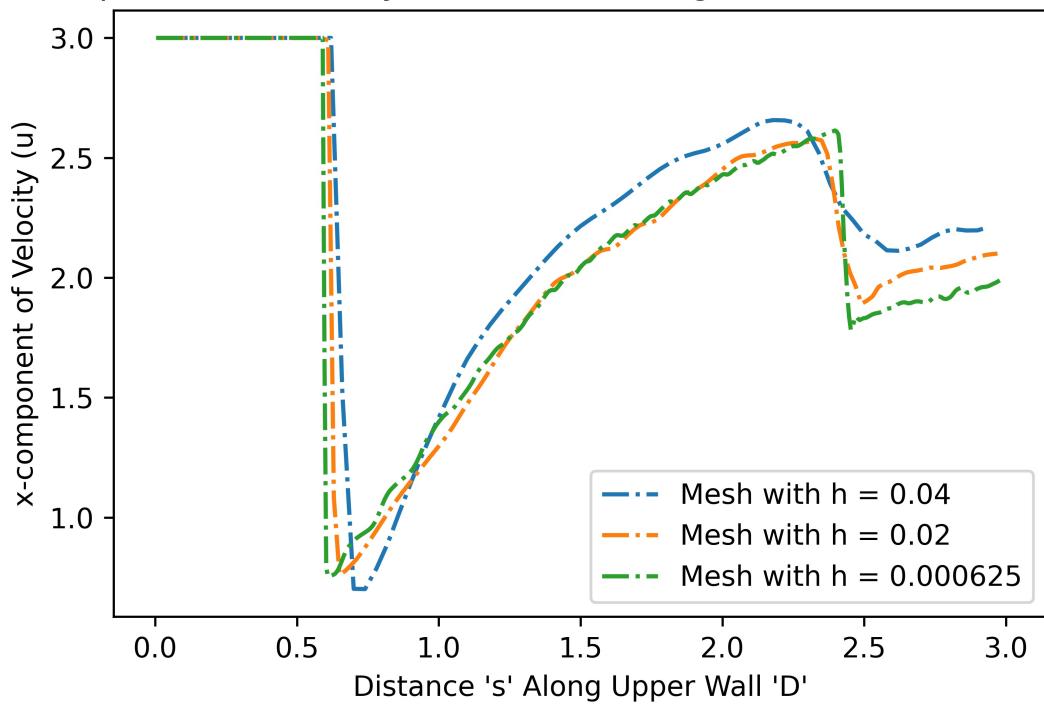
x-component of Velocity vs Distance Along B for Different Resolutions



x-component of Velocity vs Distance Along C for Different Resolutions

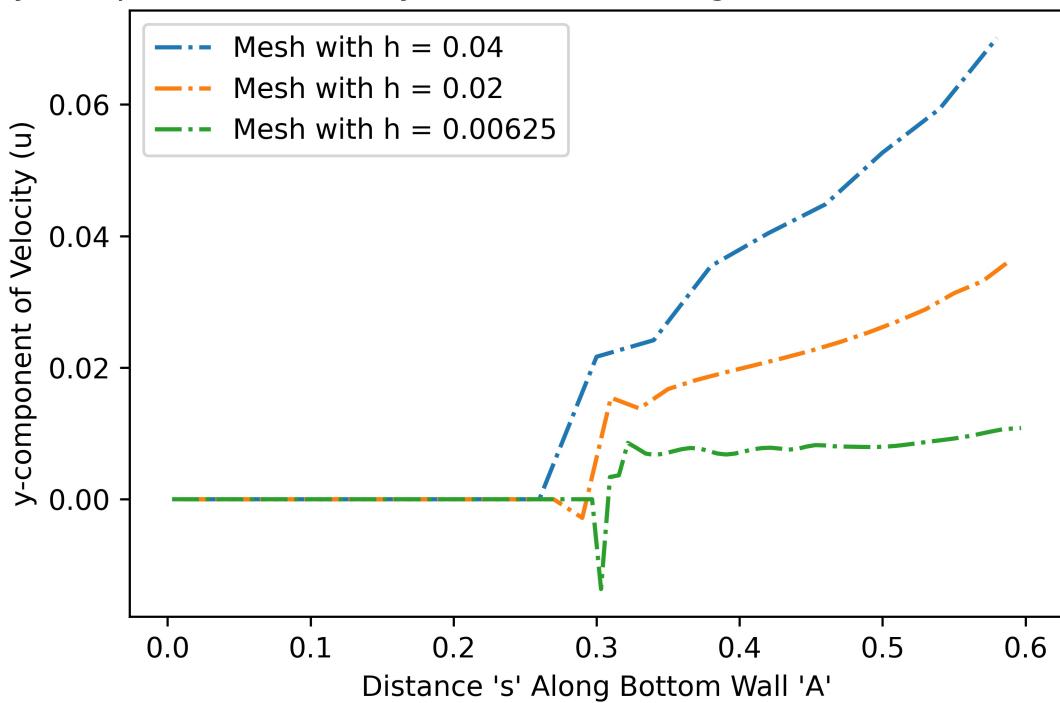


x-component of Velocity vs Distance Along D for Different Resolutions

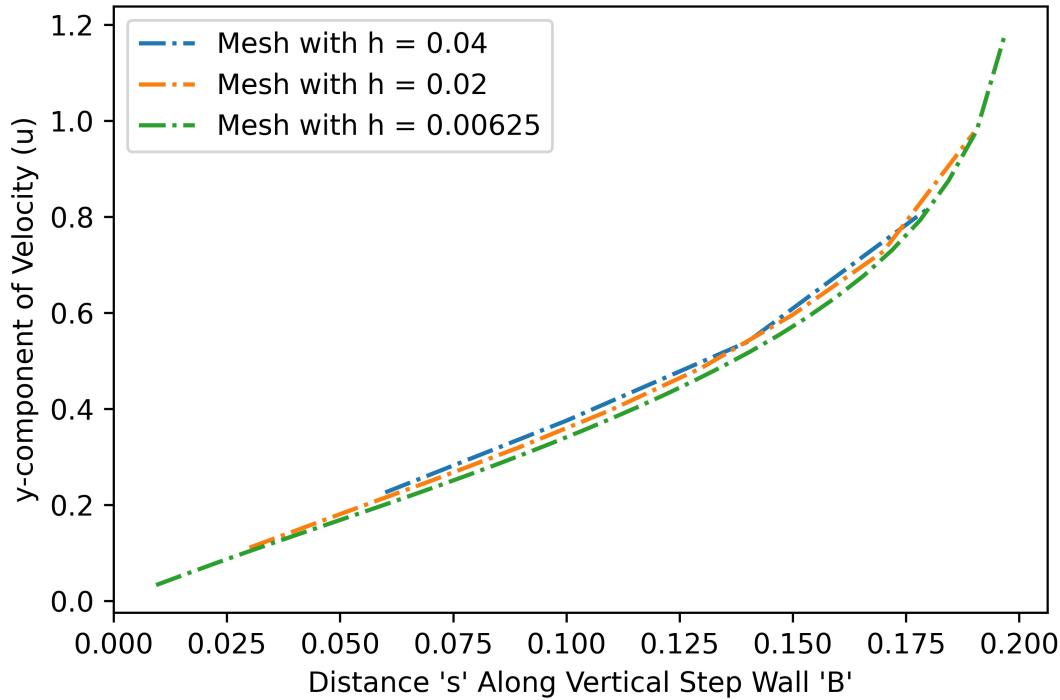


**Y-velocity:**

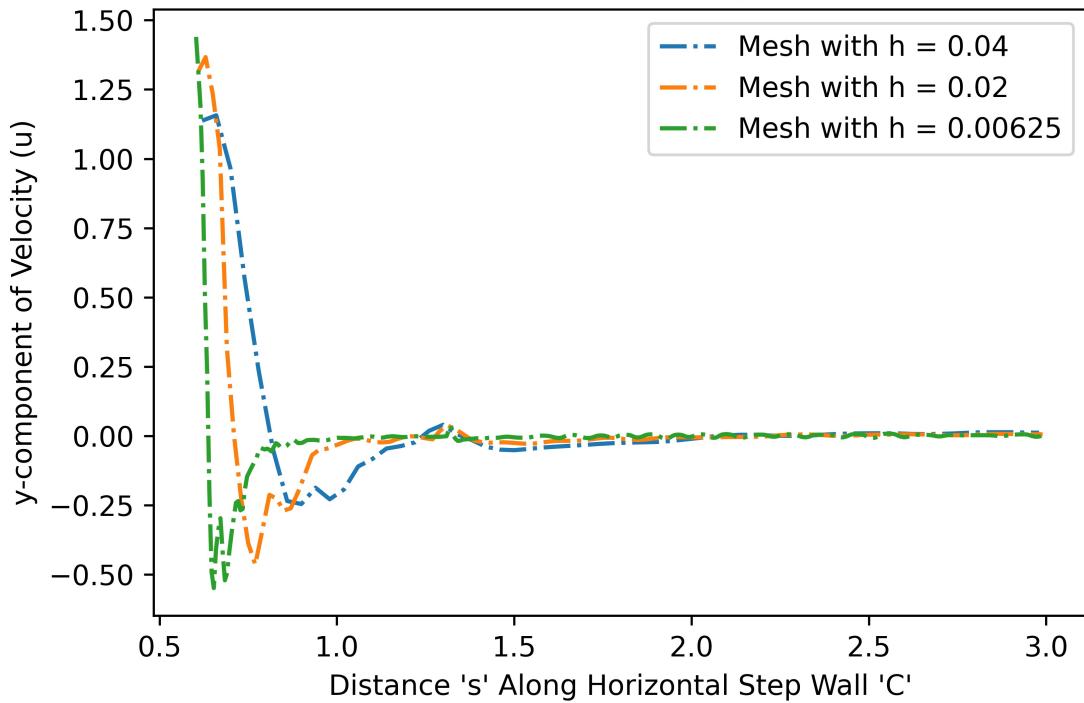
y-component of Velocity vs Distance Along A for Different Resolutions



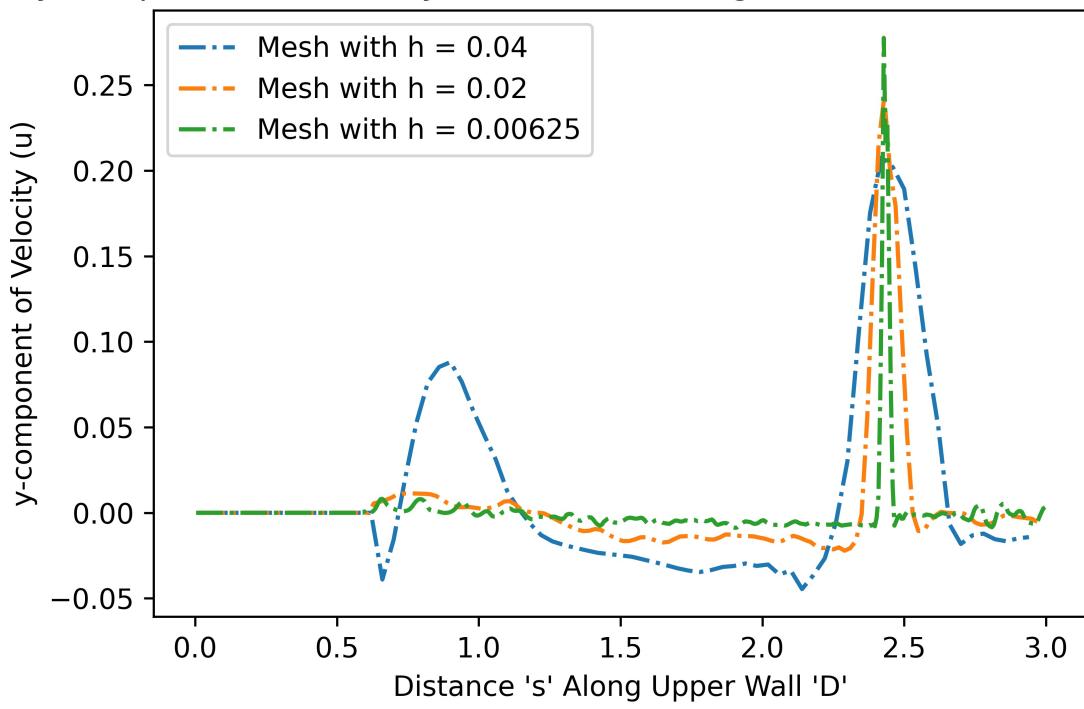
y-component of Velocity vs Distance Along B for Different Resolutions



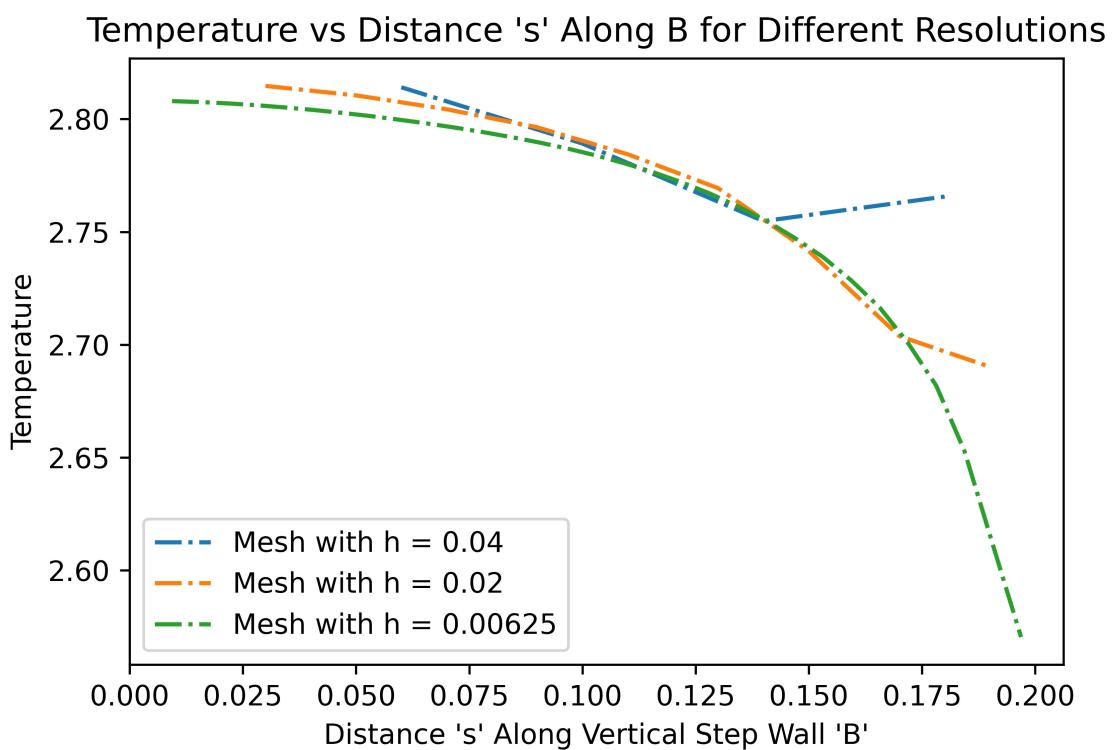
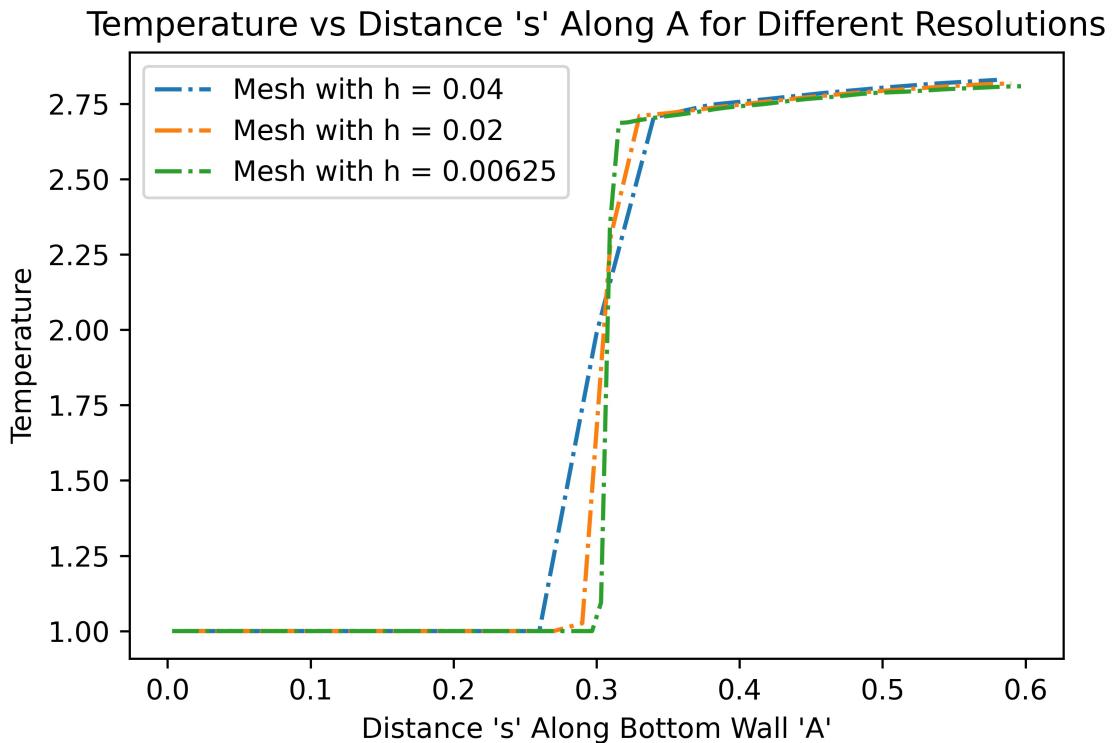
y-component of Velocity vs Distance Along C for Different Resolutions

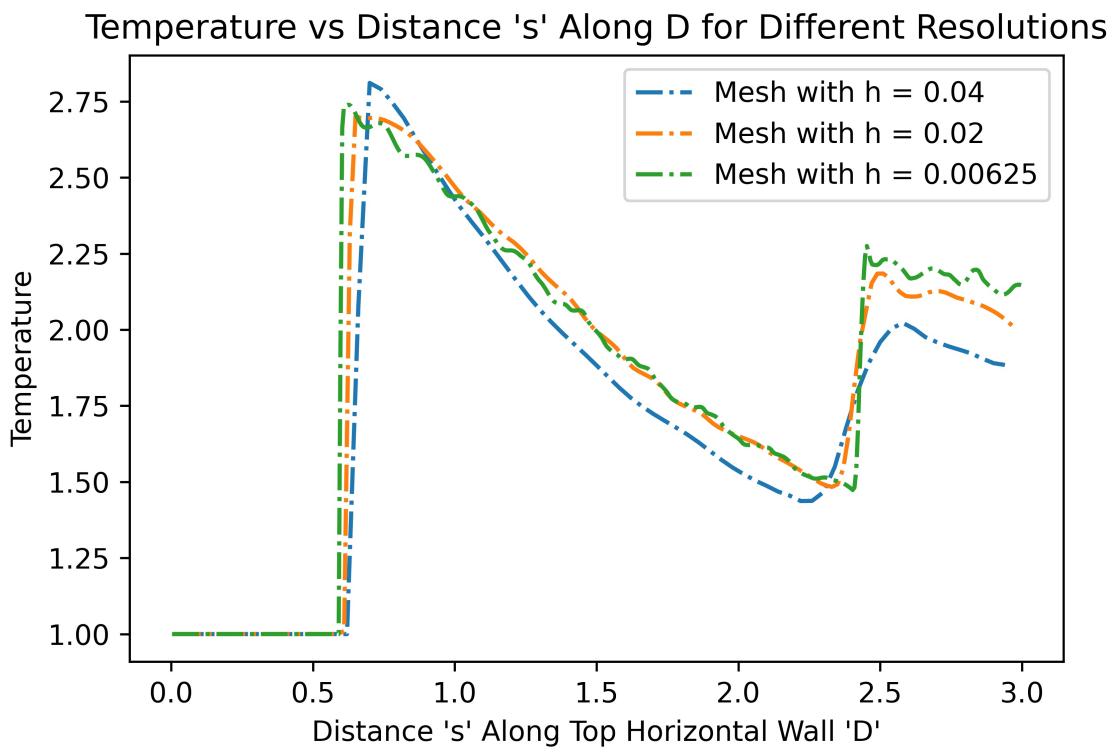
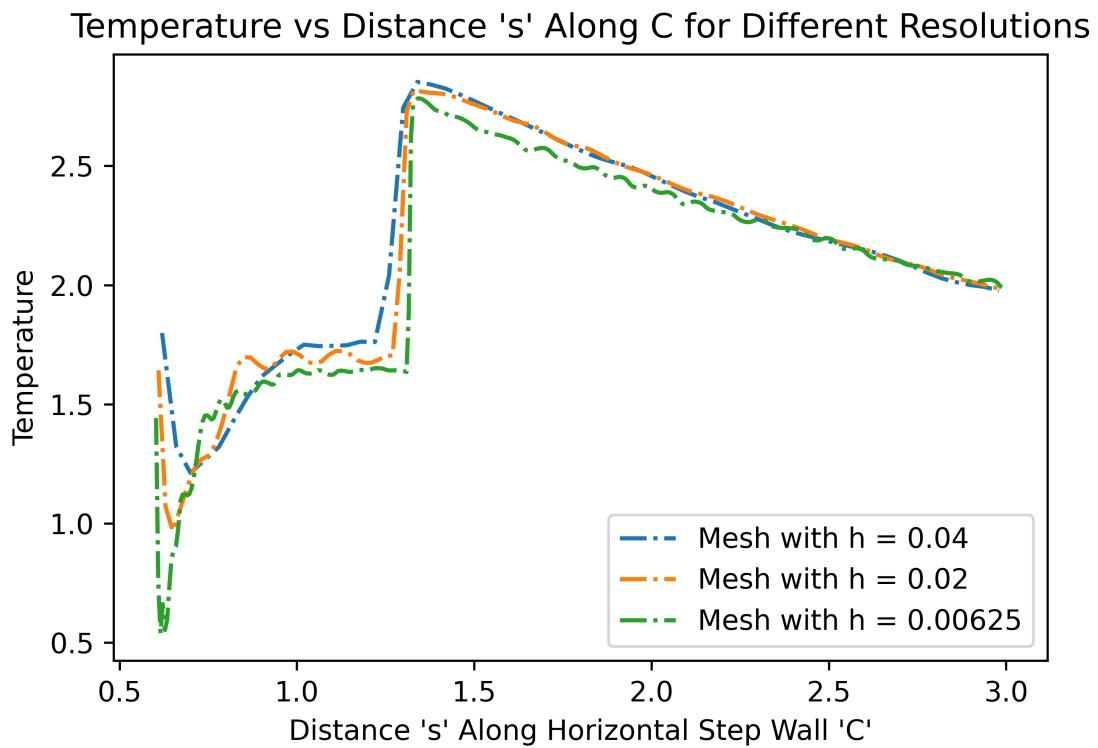


y-component of Velocity vs Distance Along D for Different Resolutions



**Temperature:**





### 5.10. Stagnation Pressure at Step

Note from the first two pressure plots, the pressure at the base of the step is slightly over 12Pa. The simulation measures a value of about 12.05Pa, which is in agreement with the theoretical calculation performed earlier.

## 6. Parallel Performance Improvements

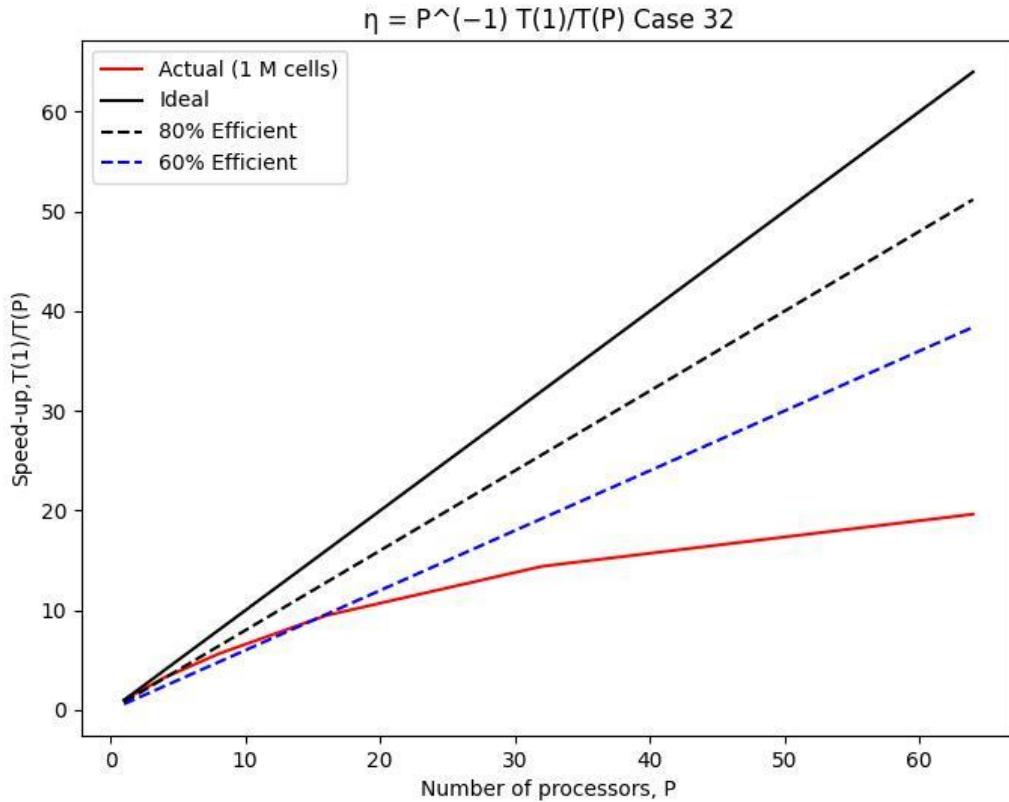
Define the speedup as the time taken for one processor ( $T(1)$ ) divided by the time taken for  $P$  processors ( $T(P)$ ). Similarly, let the parallel efficiency  $\eta$  be the speedup divided by  $P$ .

Note that the tables report the total  $T(P)$ , not that of single steps. The single step  $T(P)$  is used instead for the plots.

On a mesh of 64512 cells, for  $P$  ranging from 1 to 64 in steps of 2, the following scaling is obtained.

$T(P)$  Speedup  $\eta$

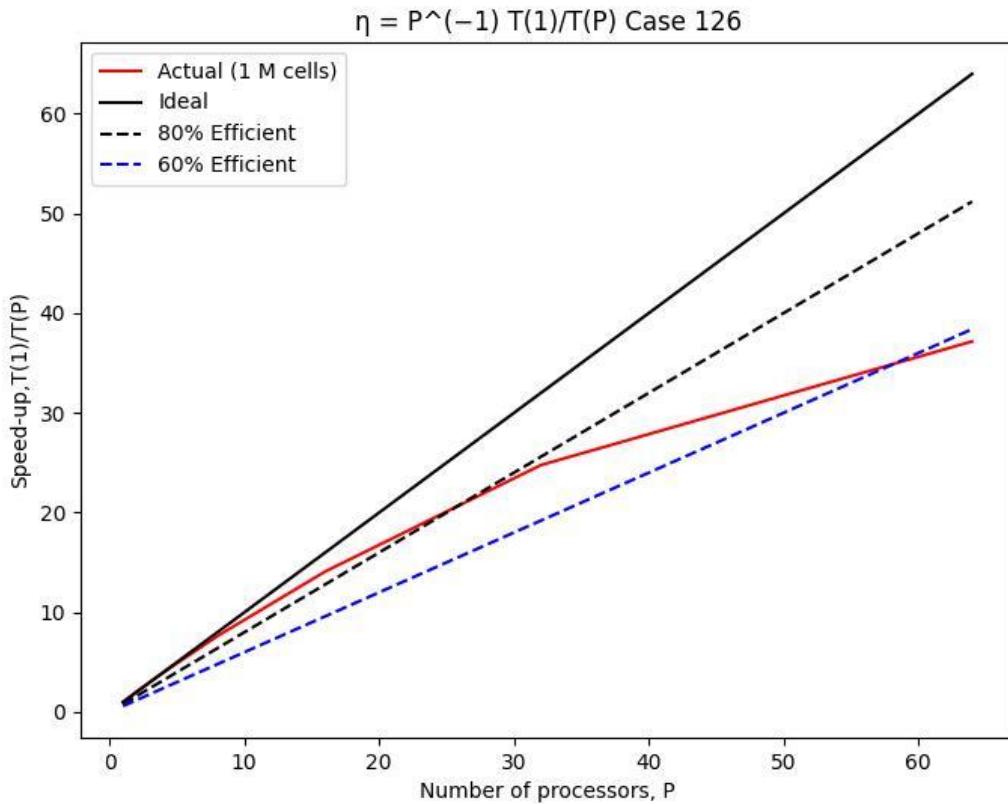
4870.28	1.0000	1.0000
2745.57	1.7738	0.8869
1493.30	3.2614	0.8154
0865.21	5.6290	0.7036
0513.54	9.4837	0.5927
0337.99	14.409	0.4503
0247.94	19.642	0.3069



A slightly improved scaling is obtained for a mesh of 1000188 cells.

$T(P)$  Speedup  $\eta$

270763.66	1.0000	1.0000
034192.10	2.0239	1.0119
034129.40	3.9783	0.9946
039850.40	7.6188	0.9524
021542.00	14.094	0.8808
012256.70	24.765	0.7739
008170.29	37.171	0.5808



Clearly the larger mesh case scales much more nicely, which can be expected due to the more even load distribution.

## 7. References

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## 8. Appendix

Thank you so much for reading this work!

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