Week 1:
Procedure to Numerical Analysis

CONTENT

- Governing Equations
- Discretization Techniques
- Solution Methods:
  i. Steady State Iterative Methods
  ii. Transient Iterative Methods
- Code for Assignment Problems
- Modelling Droplet Impact on Mesh

Governing Equations

I. Governing Equations $\longrightarrow$ Partial Differential Equation

Mass Conservation
Momentum Conservation] Fluid Flow

Energy Conservation] Heat Transfer
Scalar Transport Eqn $\rightarrow$ T, Concentration, Species Fraction

Continuity: $\frac{\partial \rho}{\partial t} + \nabla(\rho \bar{V}) = 0$

N.S. Eqn: $\frac{\partial(\rho \bar{V})}{\partial t} + \nabla \rho(\bar{V} \otimes \bar{V}) = -\nabla P + \mu \nabla^2 \bar{V} + \rho \bar{g}$

Energy Eqn: $\frac{\partial(\rho E)}{\partial t} + \nabla(\rho \bar{V} E) = -\nabla \cdot q + \nabla \cdot (\tau \cdot \bar{V}) + \rho \dot{q}$

$q = -k \nabla T$

General Transport Eqn : $\frac{\partial(\rho \phi)}{\partial t} + \nabla(\rho \bar{V} \phi) = \nabla \cdot (\Gamma \nabla \phi) + S$

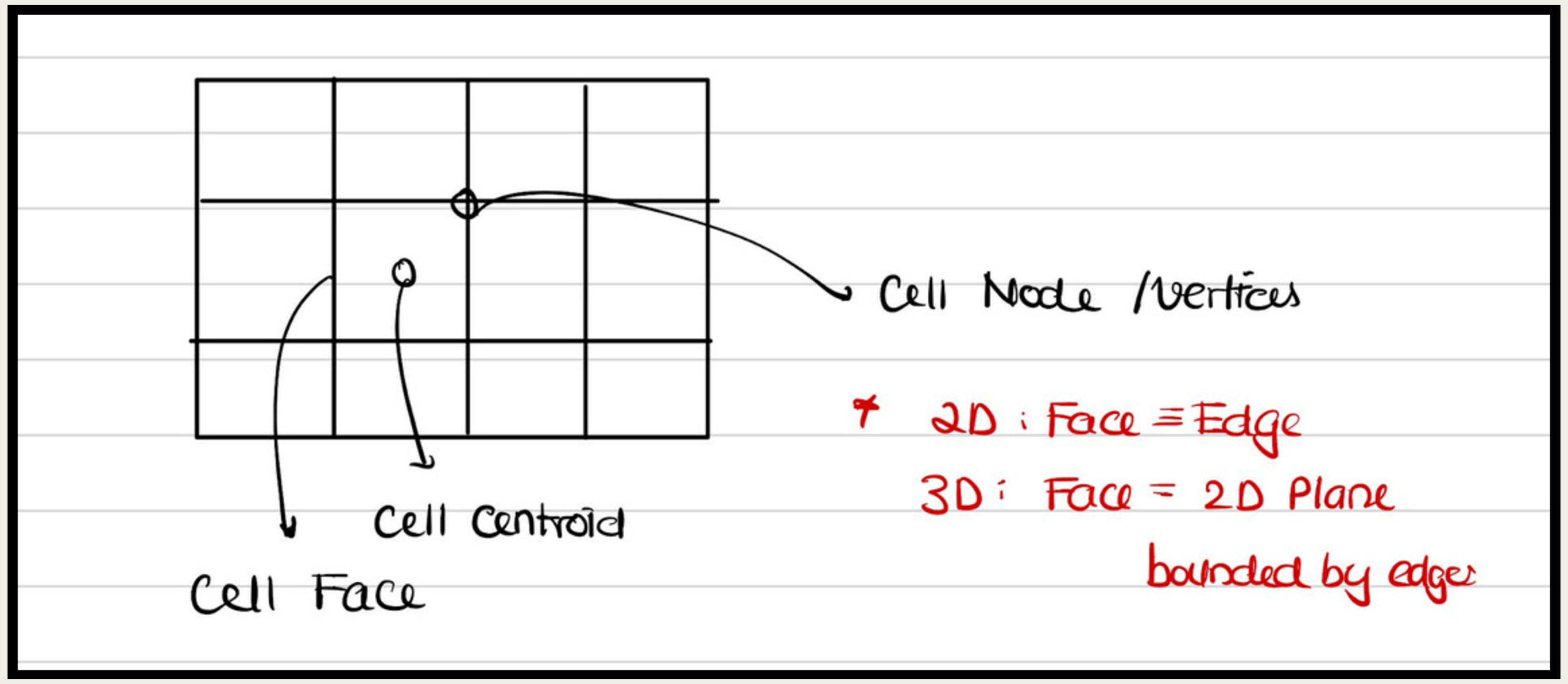
The governing equations are generally in the form of Nonlinear PDEs

- Apply Discretisation
- Obtain approximate Alegbraic Equations
- Combine knowledge of Boundary Condn
- Apply Solution Methods

Discretisation Methods

A. Discretization of Domain

Transform the continuous 1,2,3 Dimensional Space into set of discrete grid points between the domain boundaries. **[Meshing]**



B. Discretization of PDE

Transform the Differential Eqns into Solvable/Iterable Algebraic Eqns.

i. Finite Difference Method

ii. Finite Element Method

iii. Finite Volume Method

Eg. Taylor Truncation Method
Weighted Residual Method — Spatial Discretisation
Galerkin Method
Implicit and Explicit Schemes — Temporal Discretisation

Solution Methods

Solve the Algerbraic Eqns. The method used depends on the type of PDE.

i. Direct Method: Apply the method of Matrix Elimination to obtain solution

ii. Iterative Method:

A. For Steady Solution + Linear: We just need to achieve spatial convergence

Eg: Jacobi, Gauss-Siedel, SOR

ii. Iterative Method:

B. For Transient Solution, Non Linear: We just need to achieve spatial convergence as well as temporal convergence

Eg: Euler Method, Crank-Nicholson Method, Projection Method, Newton Raphson Method

Assignment Problems

Question 1:

b. $u=1 \quad \tau = 0.1 \quad Q=0.$

$$\Rightarrow \frac{\partial \phi}{\partial x} = 0.1\,\frac{\partial^2 \phi}{\partial x^2}$$

$$\Rightarrow \frac{\phi_{i+1}-\phi_{i-1}}{2h} = 0.1\left(\frac{\phi_{i+1}+\phi_{i-1}-2\phi_i}{h^2}\right)$$

$$\Rightarrow \phi_{i+1}\left(\frac{0.1}{h^2}-\frac{1}{2h}\right) + \phi_i\left(-\frac{2}{h^2}\right) + \phi_{i-1}\left(\frac{0.1}{h^2}+\frac{1}{2h}\right)$$

$i:\ 1 \to n-1$

$$a\phi_{i+1} + b\phi_i + c\phi_{i-1} = 0$$

$i=1 \quad a\phi_2 + b\phi_1 + c\phi_0 = 0 \Rightarrow a\phi_2 + b\phi_1 = -c\phi_0$

$i=2 \quad a\phi_3 + b\phi_2 + c\phi_1 = 0$

$i=3 \quad a\phi_4 + b\phi_3 + c\phi_2 = 0$

$\vdots$

$i=n-2 \quad a\phi_{n-1} + b\phi_{n-2} + c\phi_{n-3} = 0$

$i=n-1 \quad a\phi_n + b\phi_{n-1} + c\phi_{n-2} = 0 \Rightarrow b\phi_{n-1} + c\phi_{n-2} = -a\phi_n$

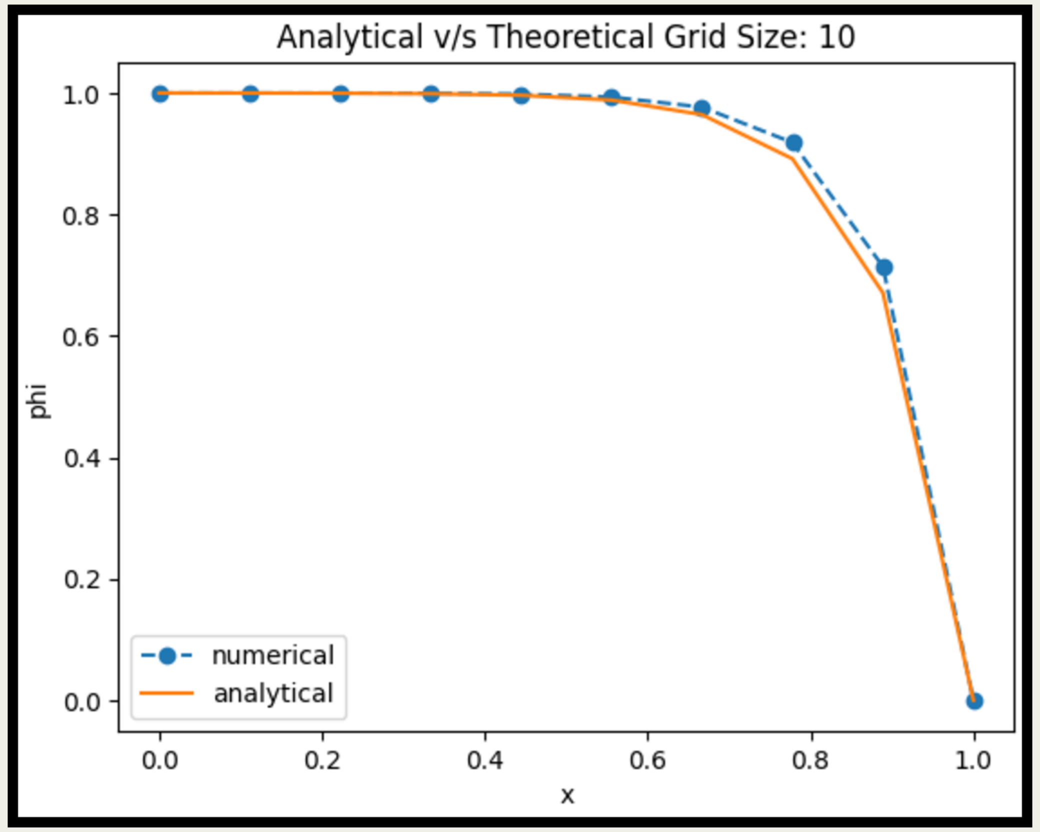
$$\underbrace{\begin{bmatrix} b & a & 0 & 0 & 0 \\ c & b & a & 0 & 0 \\ 0 & c & b & a & 0 \\ 0 & 0 & \vdots & \vdots & \vdots \\ 0 & 0 & c & b & a \\ 0 & 0 & 0 & c & b \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \vdots \\ \phi_{n-2} \\ \phi_{n-1} \end{bmatrix}}_{\phi} = \underbrace{\begin{bmatrix} -c\phi_0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ -a\phi_n \end{bmatrix}}_{B}$$

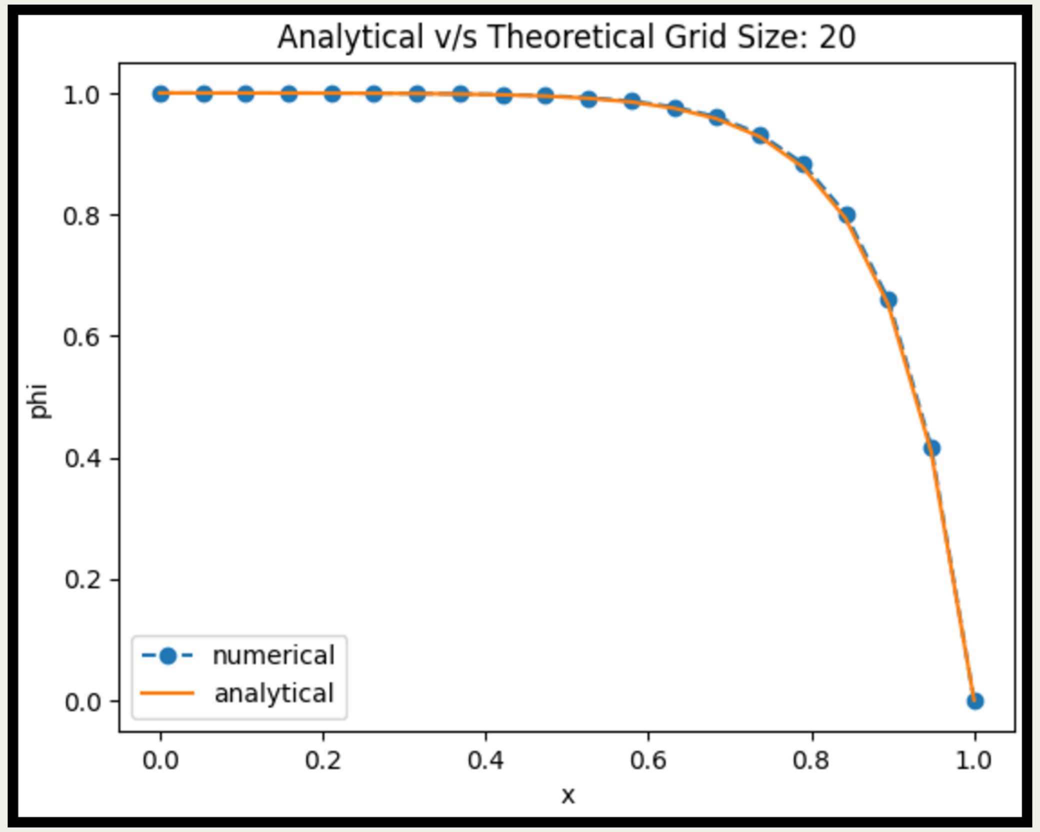
Use the TDMA to solve this Question.

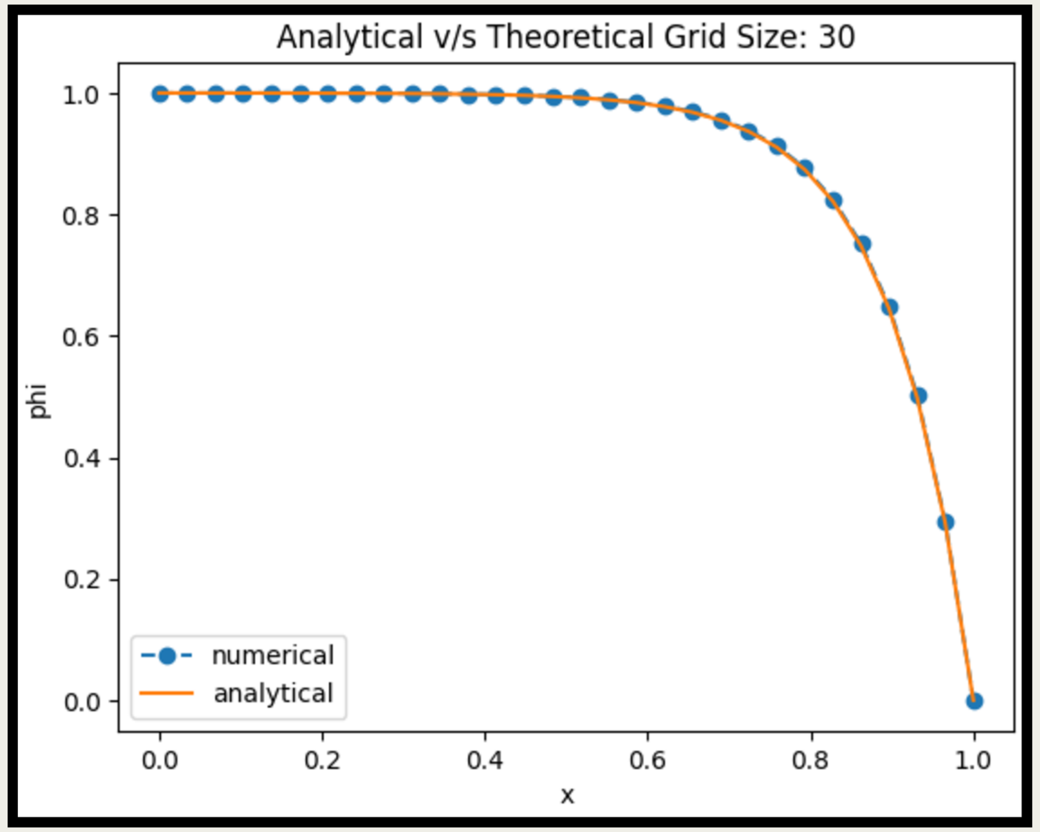
Apply Direct Method

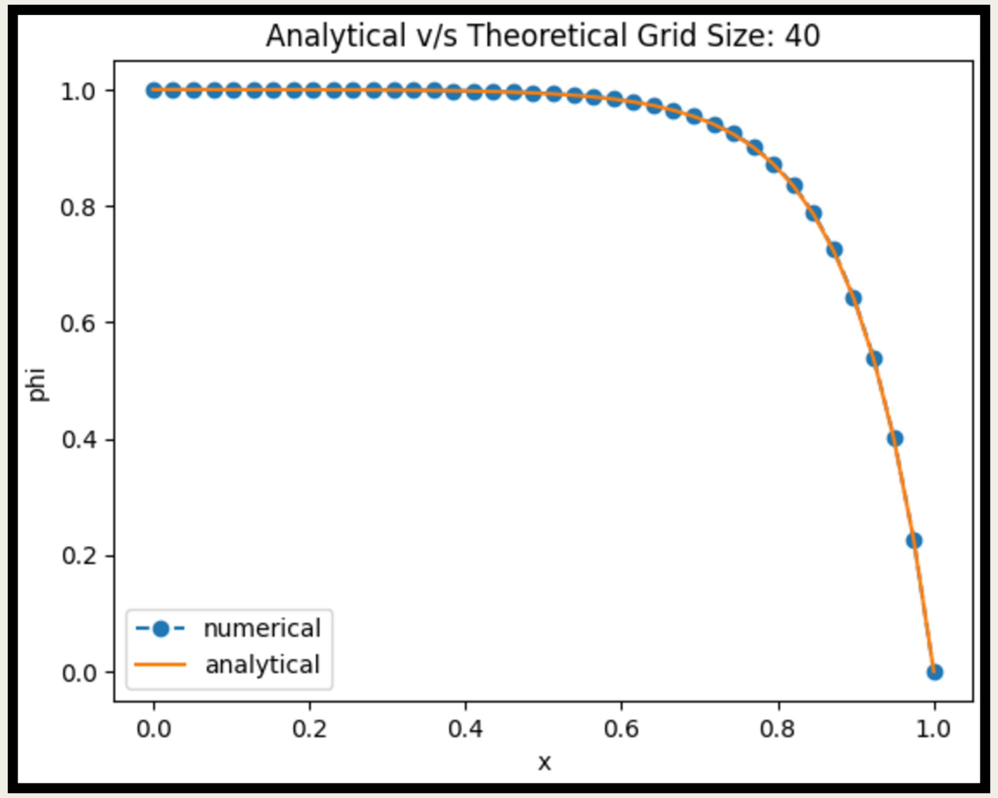
The accuracy of the solution at a point is decided solely by the discretisation method used

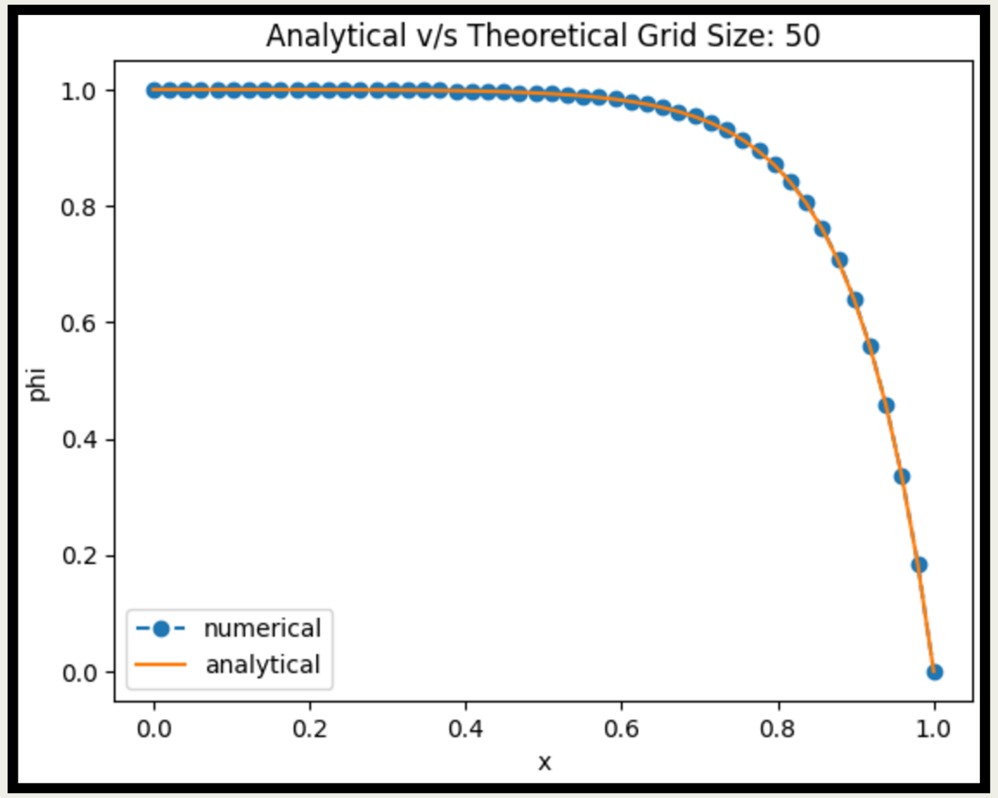
Question 1:


Analytical v/s Theoretical Grid Size: 10
phi
x
numerical
analytical

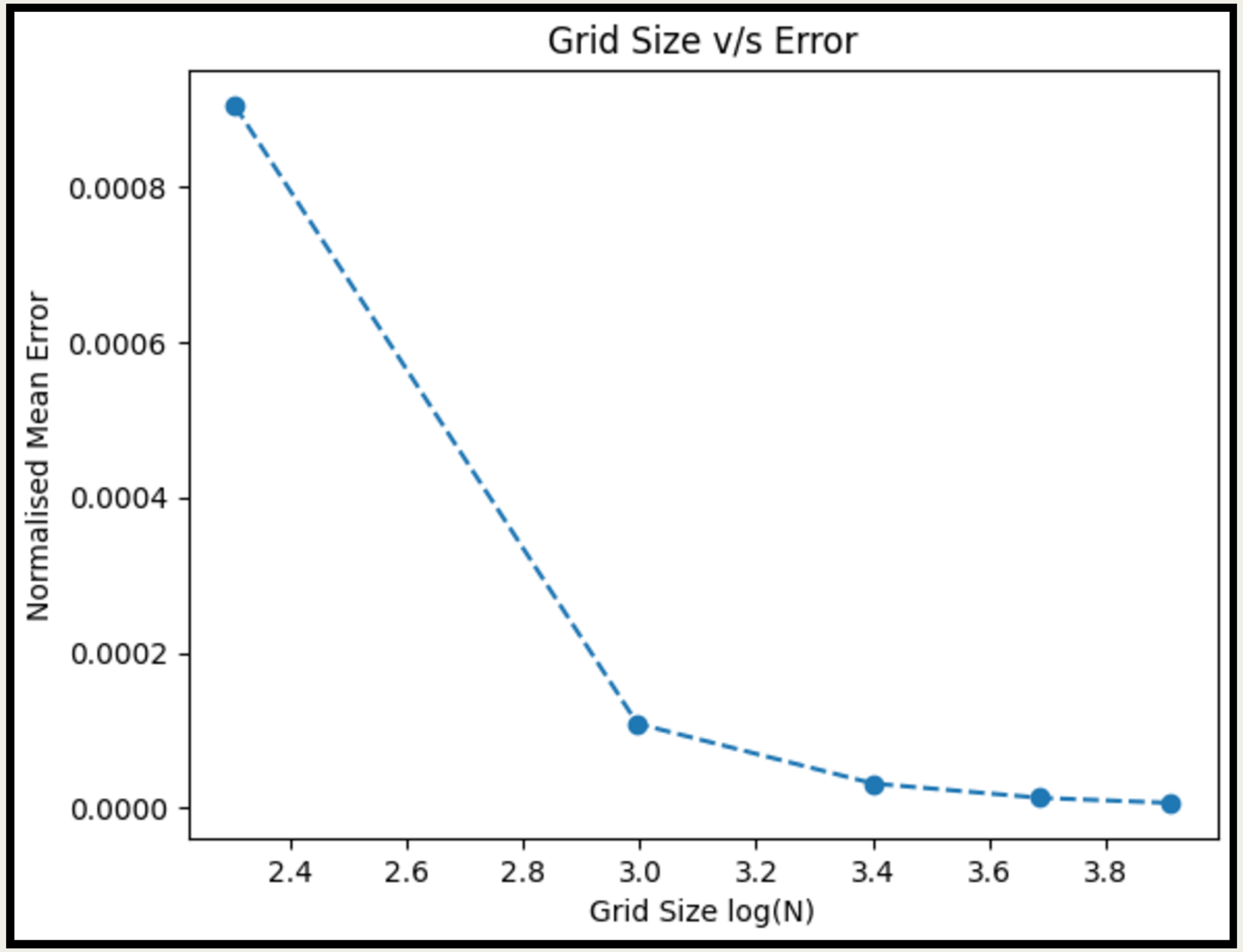

Analytical v/s Theoretical Grid Size: 20
phi
x
numerical
analytical

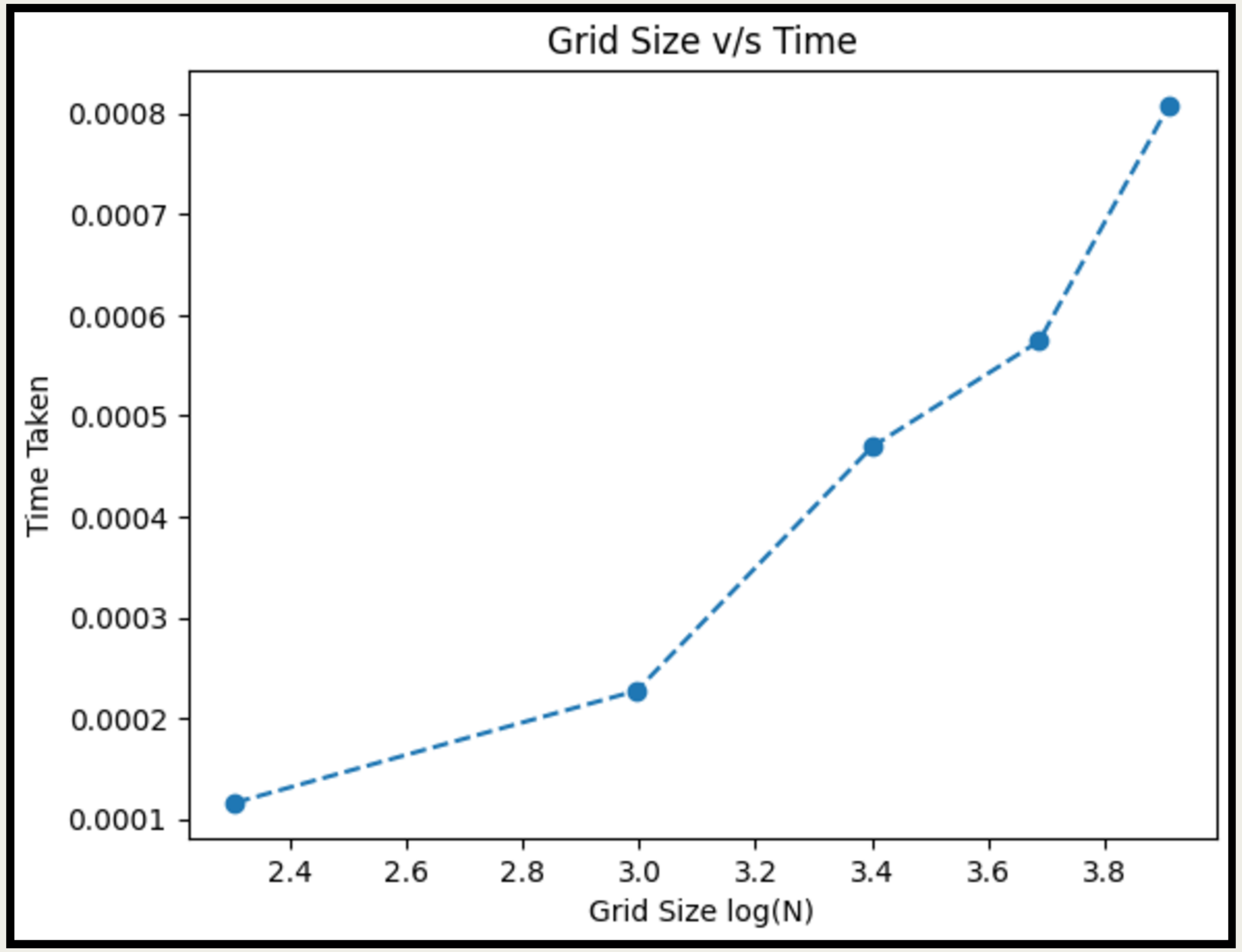

Analytical v/s Theoretical Grid Size: 30
phi
x
numerical
analytical


Analytical v/s Theoretical Grid Size: 40
phi
x
numerical
analytical


Analytical v/s Theoretical Grid Size: 50
phi
x
numerical
analytical

Question 1:



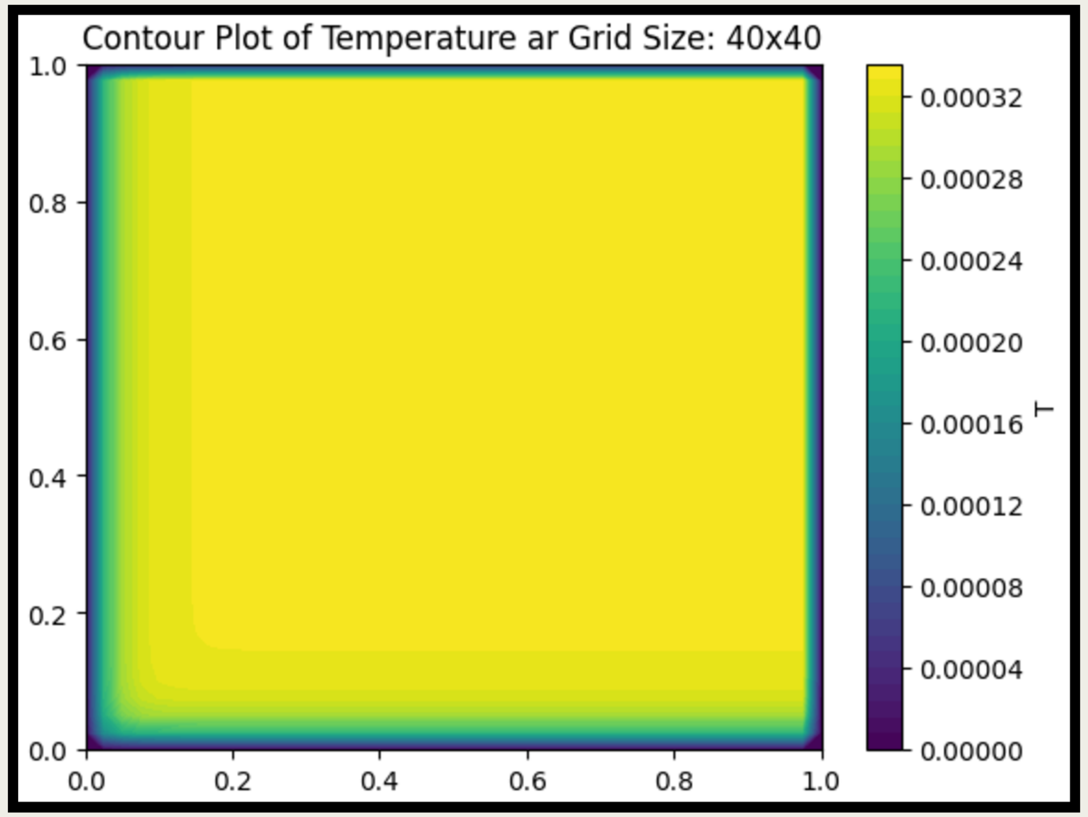


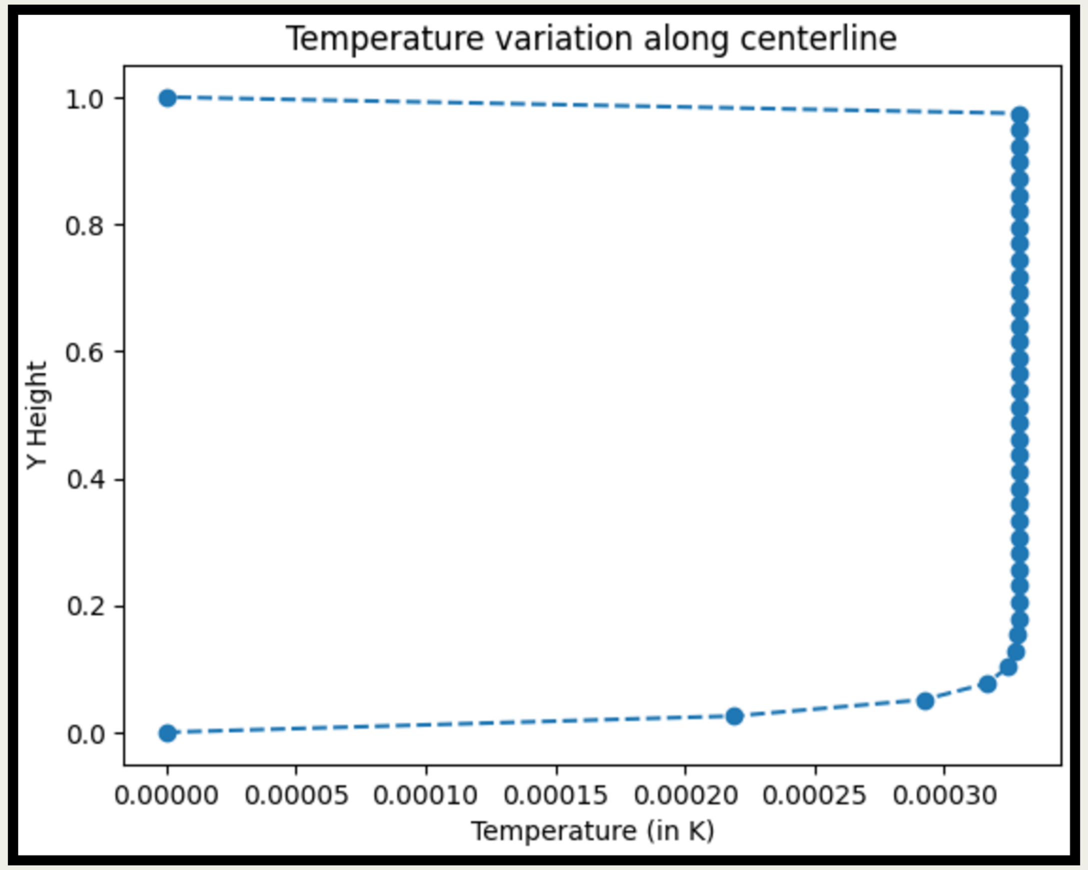
N = 10	20	30	40	50
$O(n^{0.97})$	$O(n^{1.27})$	$O(n^{1.34})$	$O(n^{1.06})$	$O(n^{1.53})$

Assignment Problems

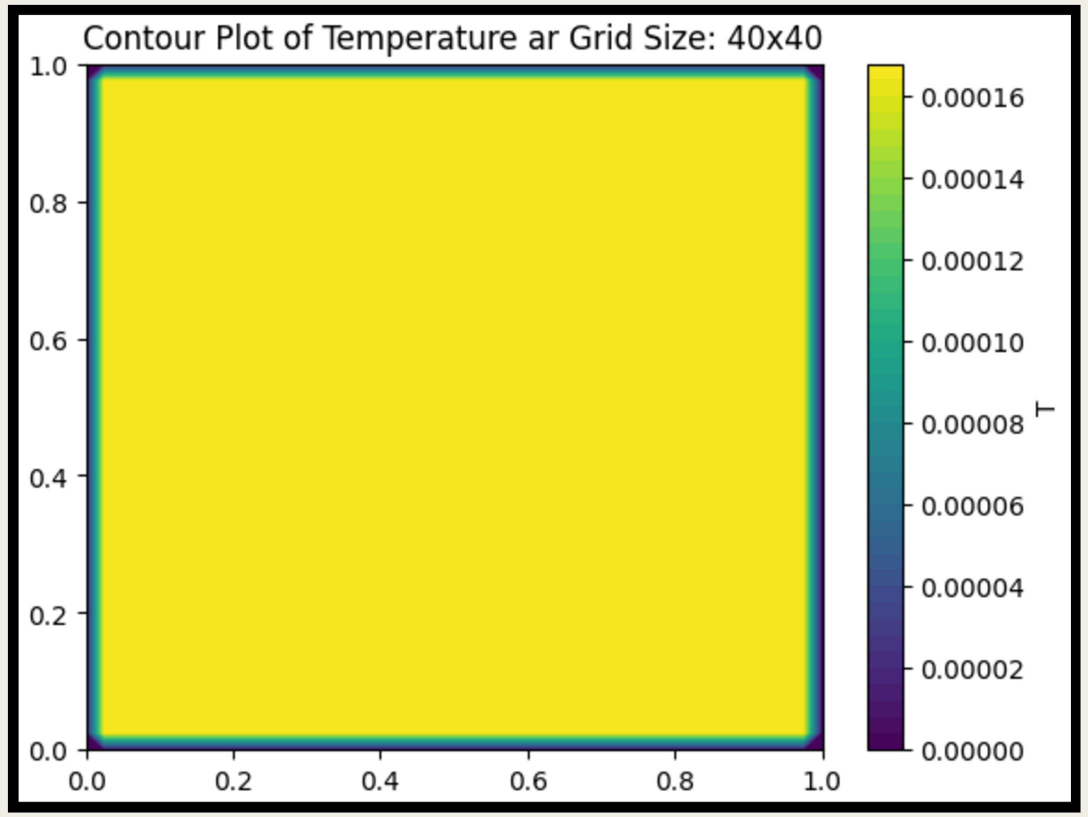
Question 2:

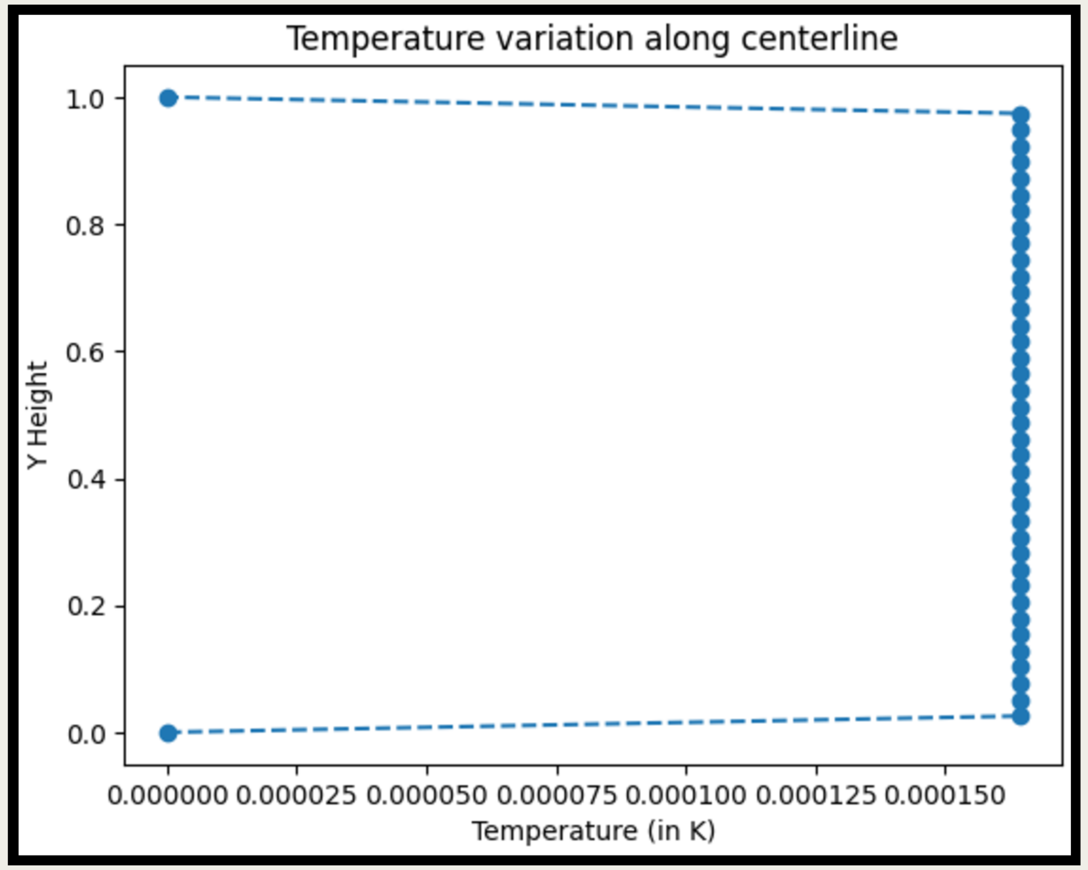
Gauss Siedel



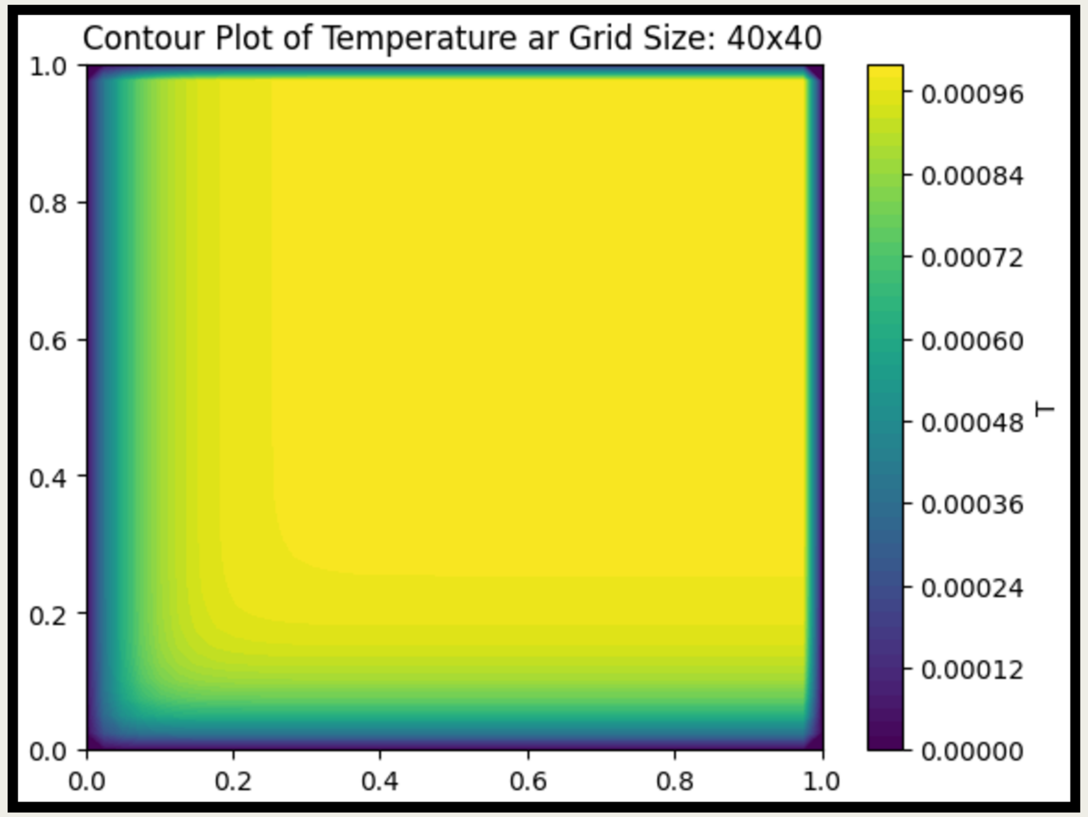


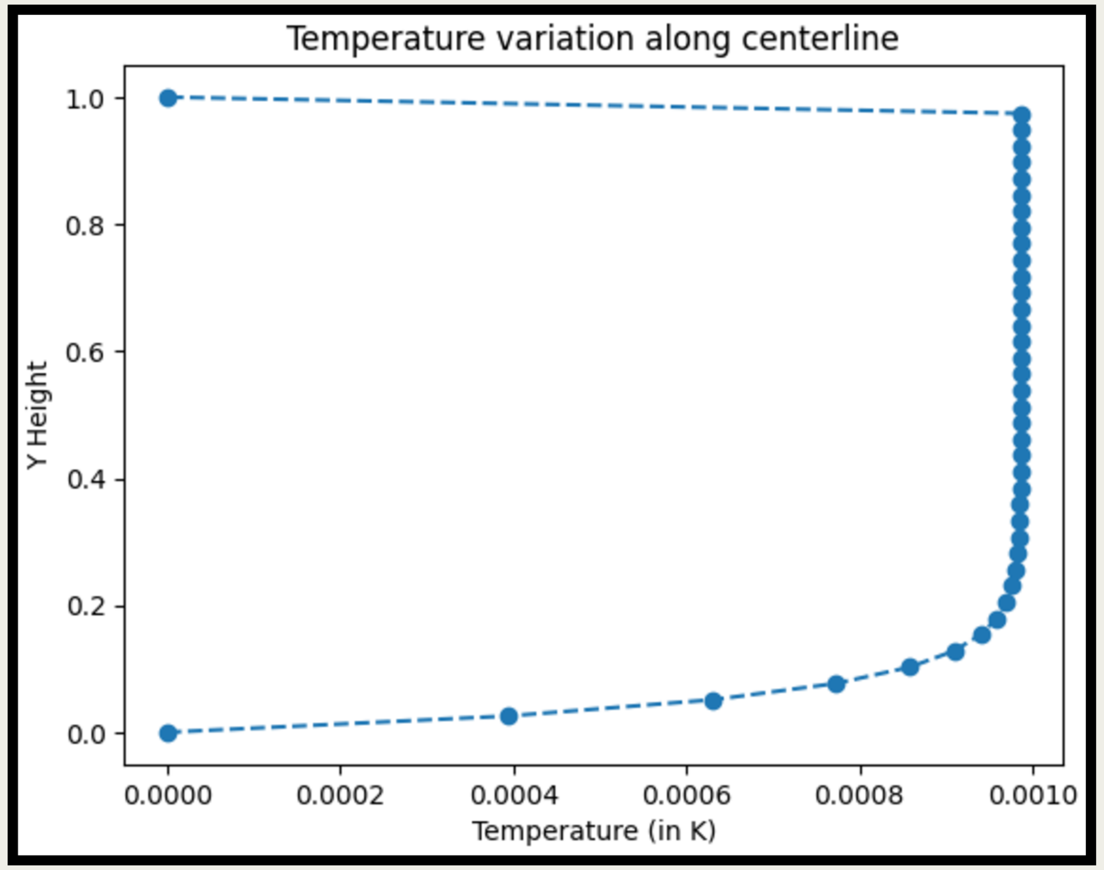
Jacobi



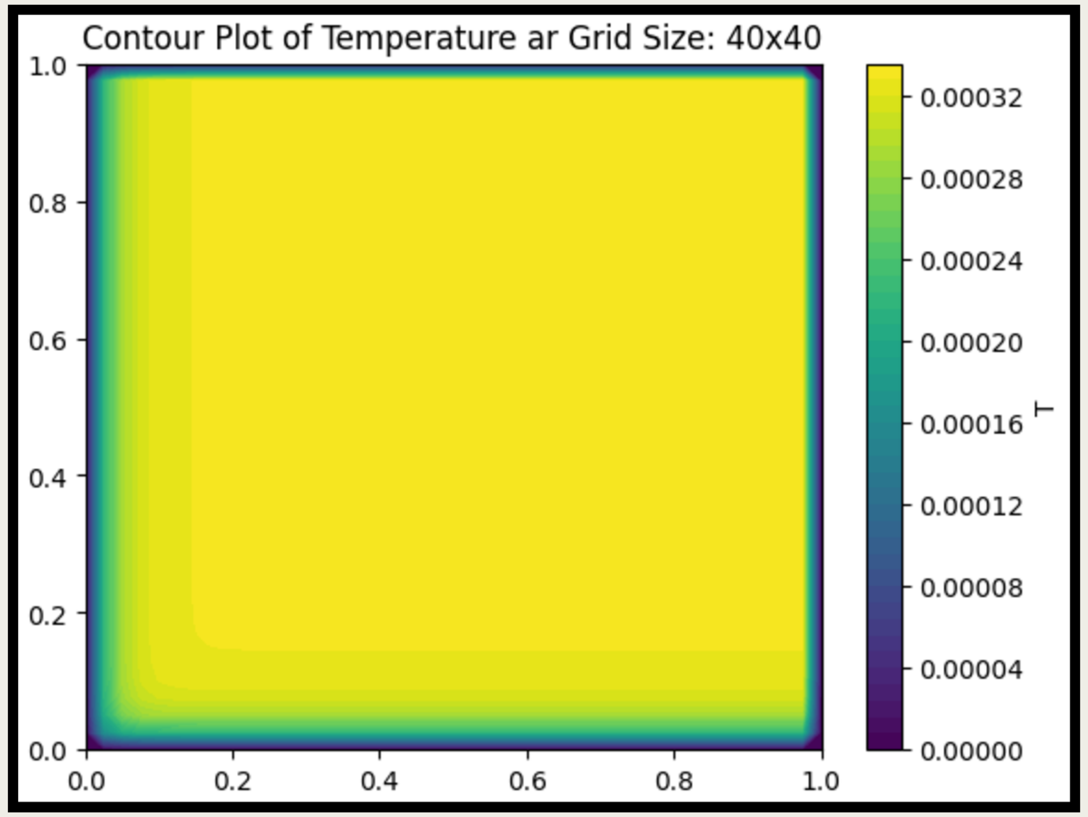


SOR

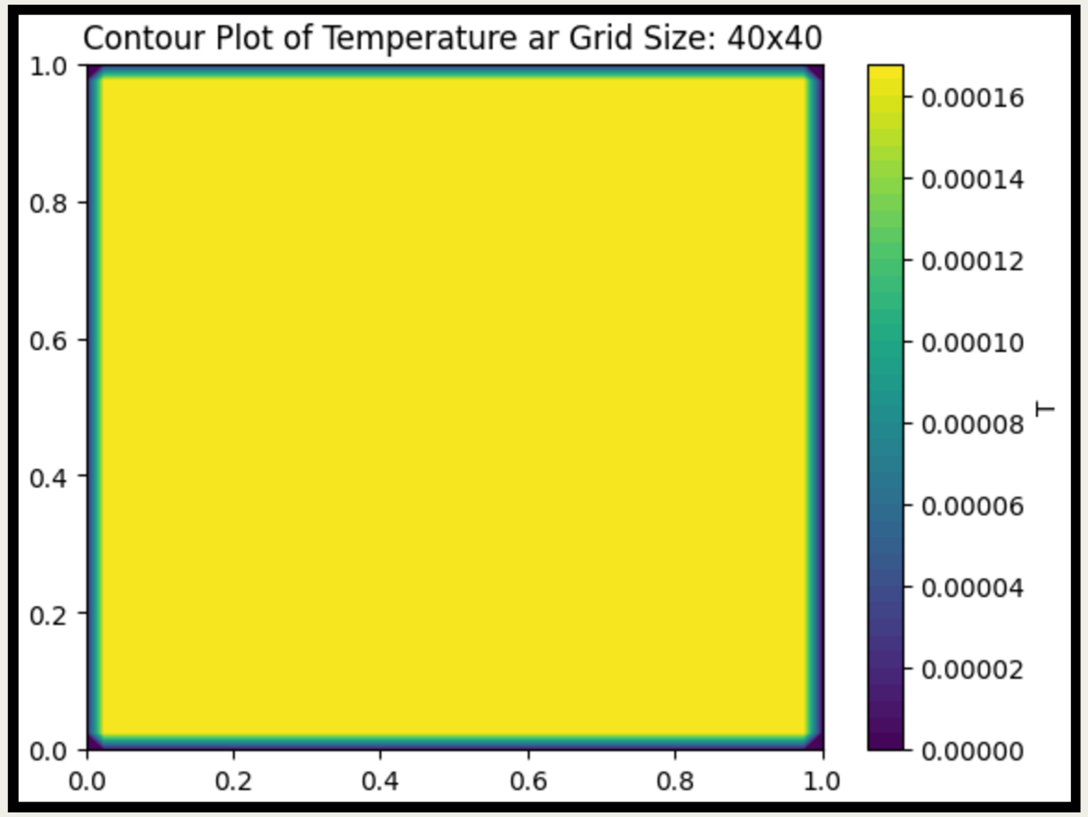




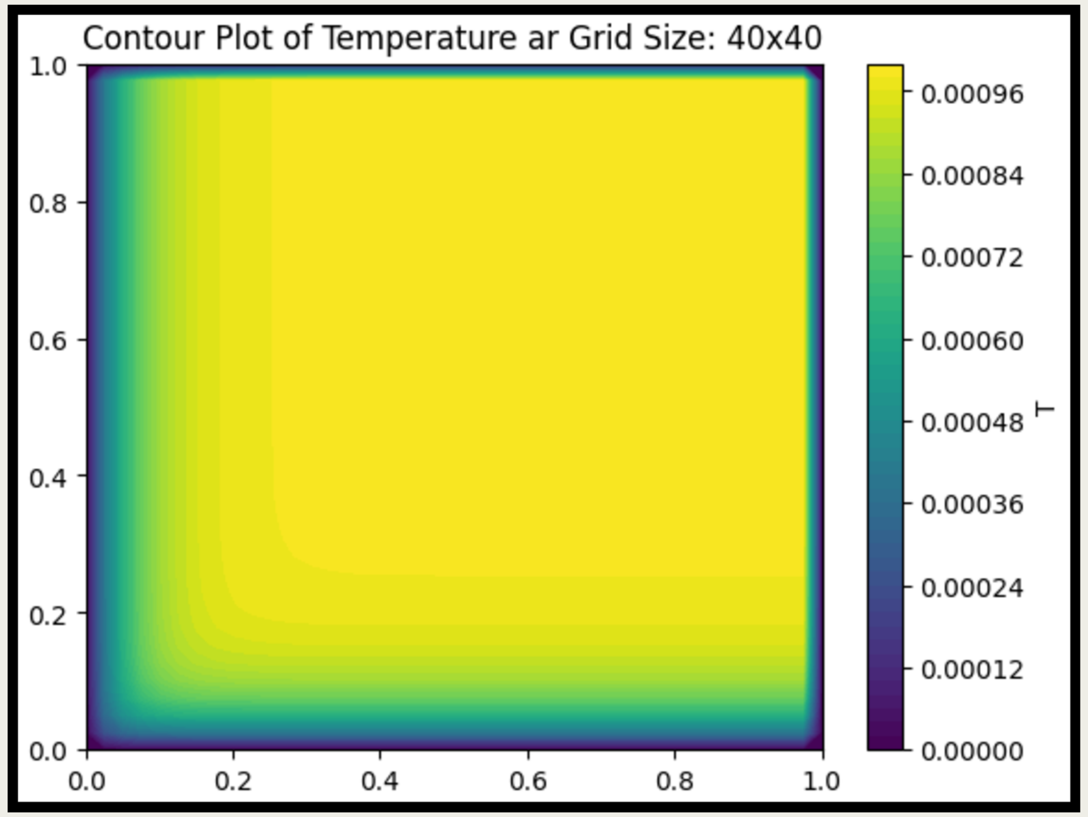
Gauss Siedel

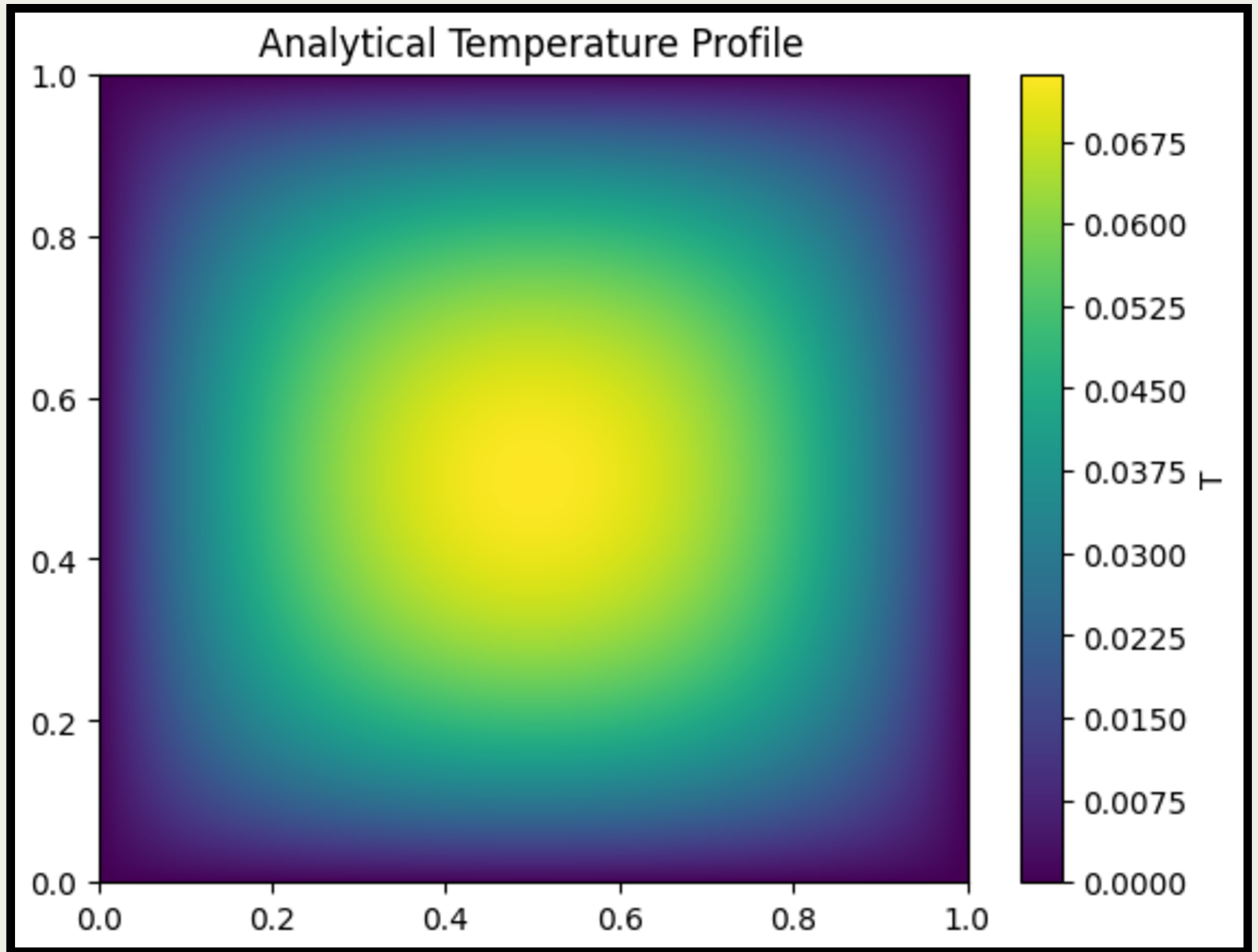


Jacobi



SOR





Gauss Siedel

Average Error:

Grid = 10: 0.002588

Grid = 20: 0.0132875

Grid = 30: 0.032249

Grid = 40: 0.033068

Grid = 80: 0.034182

Jacobi

Average Error:

Grid = 10: 0.005165

Grid = 20: 0.030951

Grid = 30: 0.03249

Grid = 40: 0.033209

Grid = 80: 0.034219

SOR

Average Error:

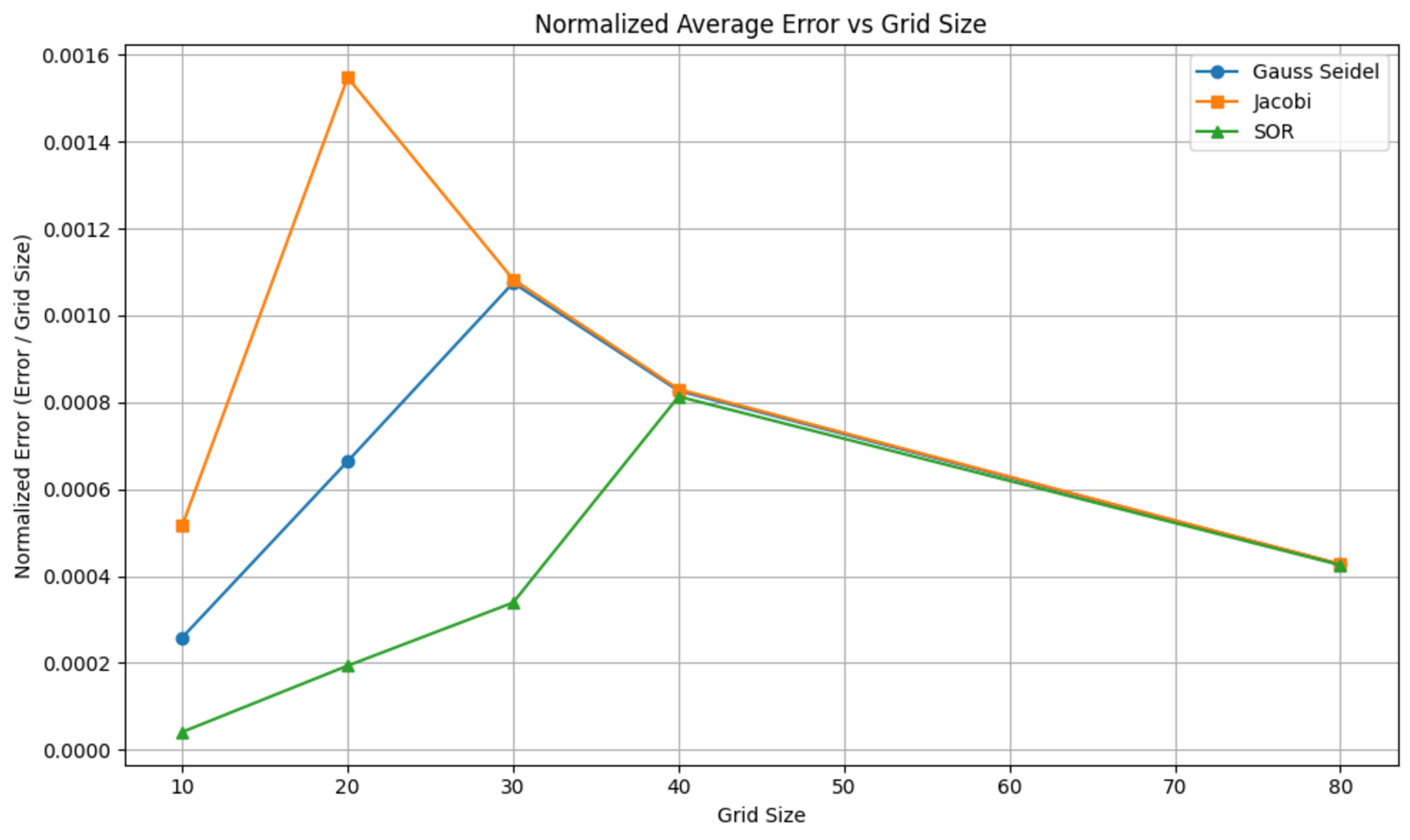
Grid = 10: 0.0004126

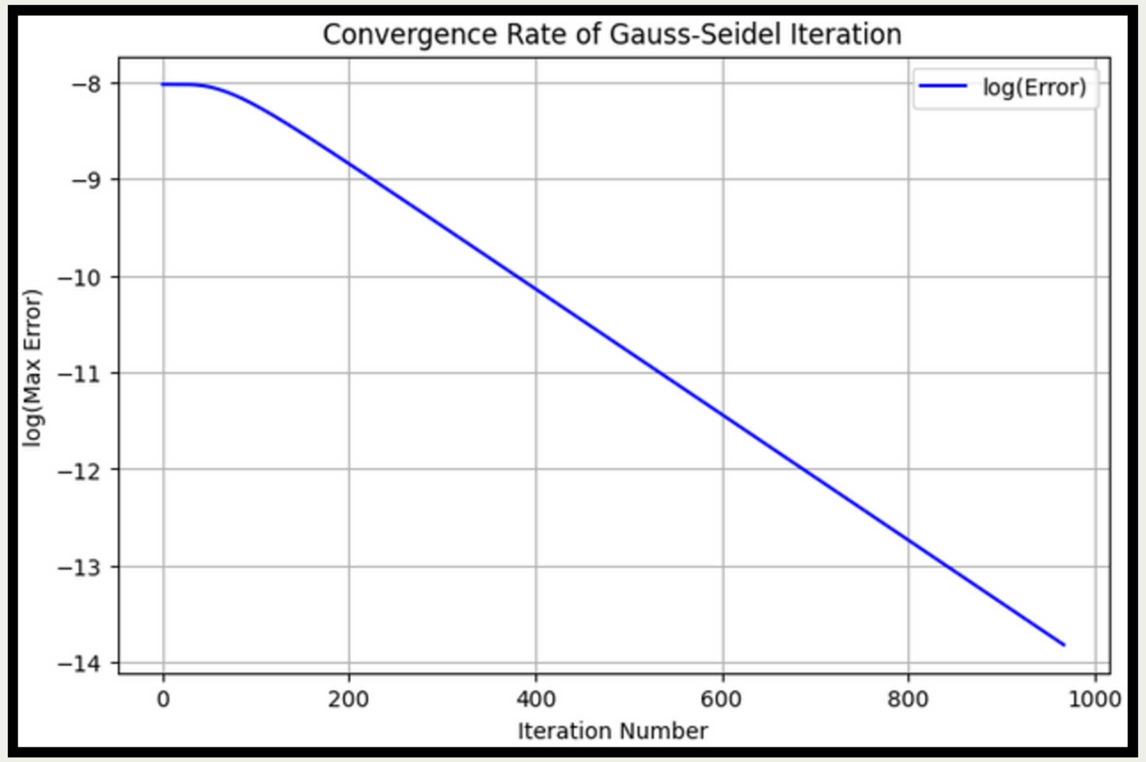
Grid = 20: 0.0038775

Grid = 30: 0.01017266

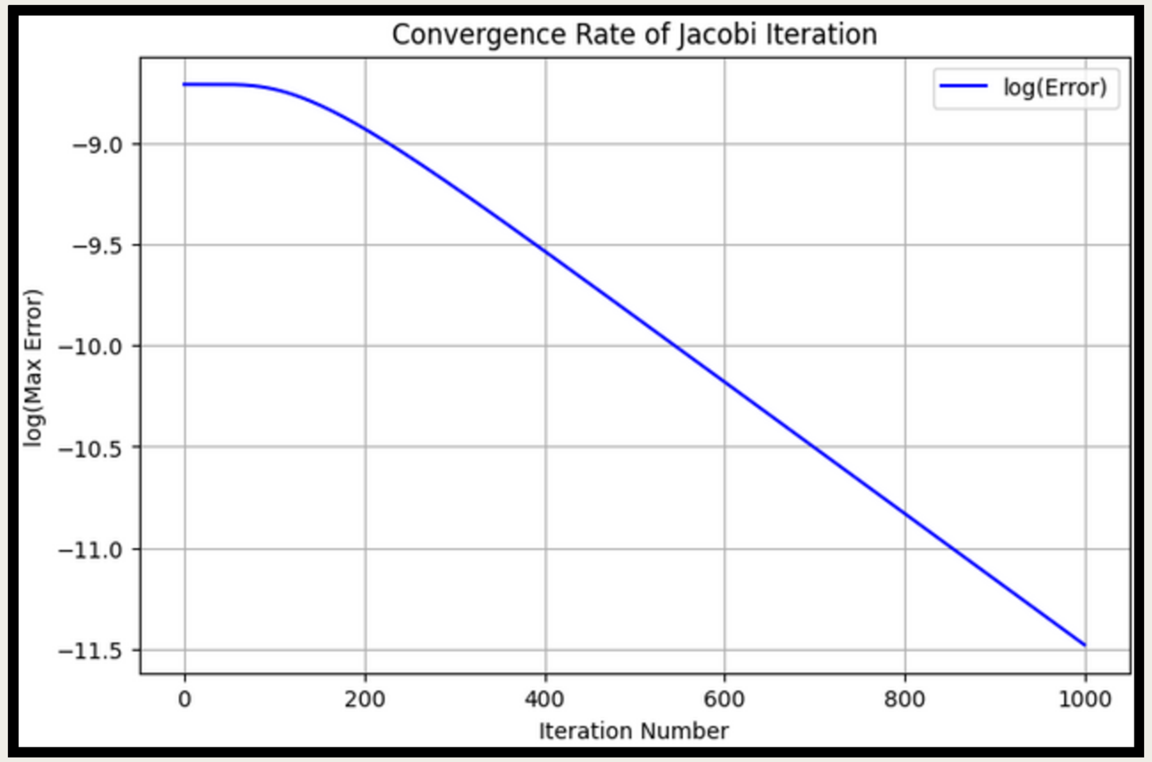
Grid = 40: 0.0325347

Grid = 80: 0.0340378

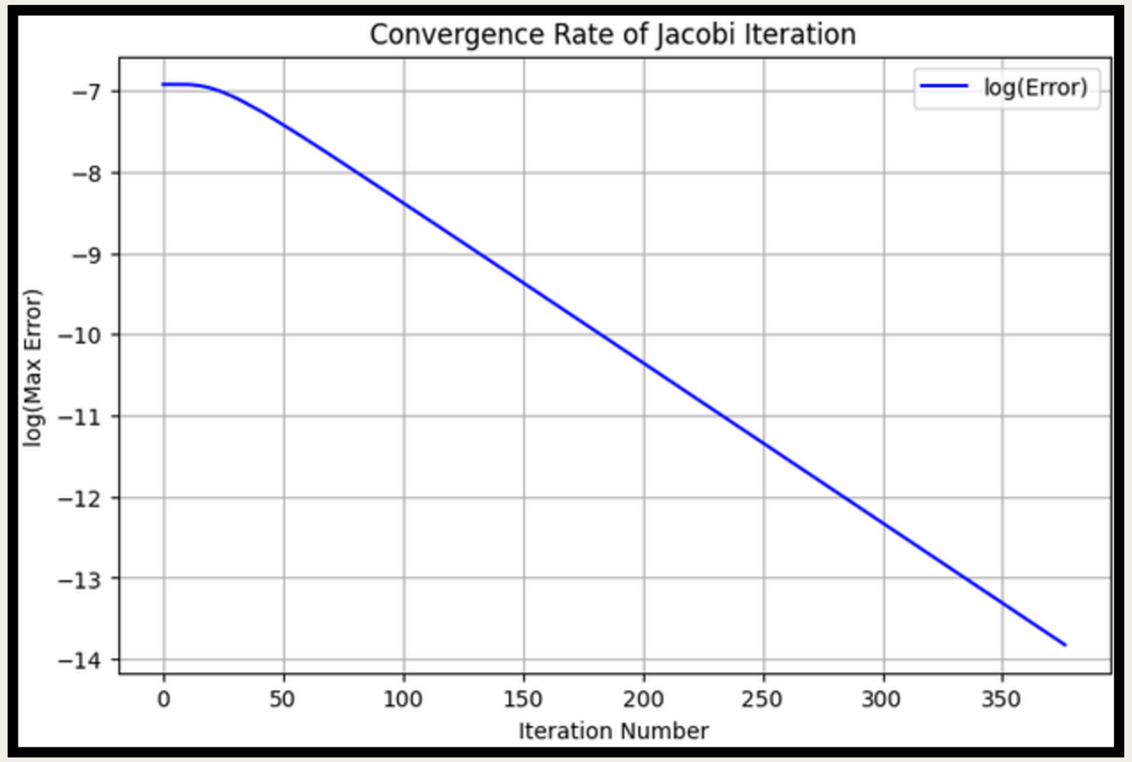

Normalized Average Error vs Grid Size
Normalized Error (Error / Grid Size)
Grid Size
0.0016
0.0014
0.0012
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
10
20
30
40
50
60
70
80
Gauss Seidel
Jacobi
SOR



Convergence Rate of Gauss-Seidel Iteration
log(Error)
log(Max Error)
Iteration Number



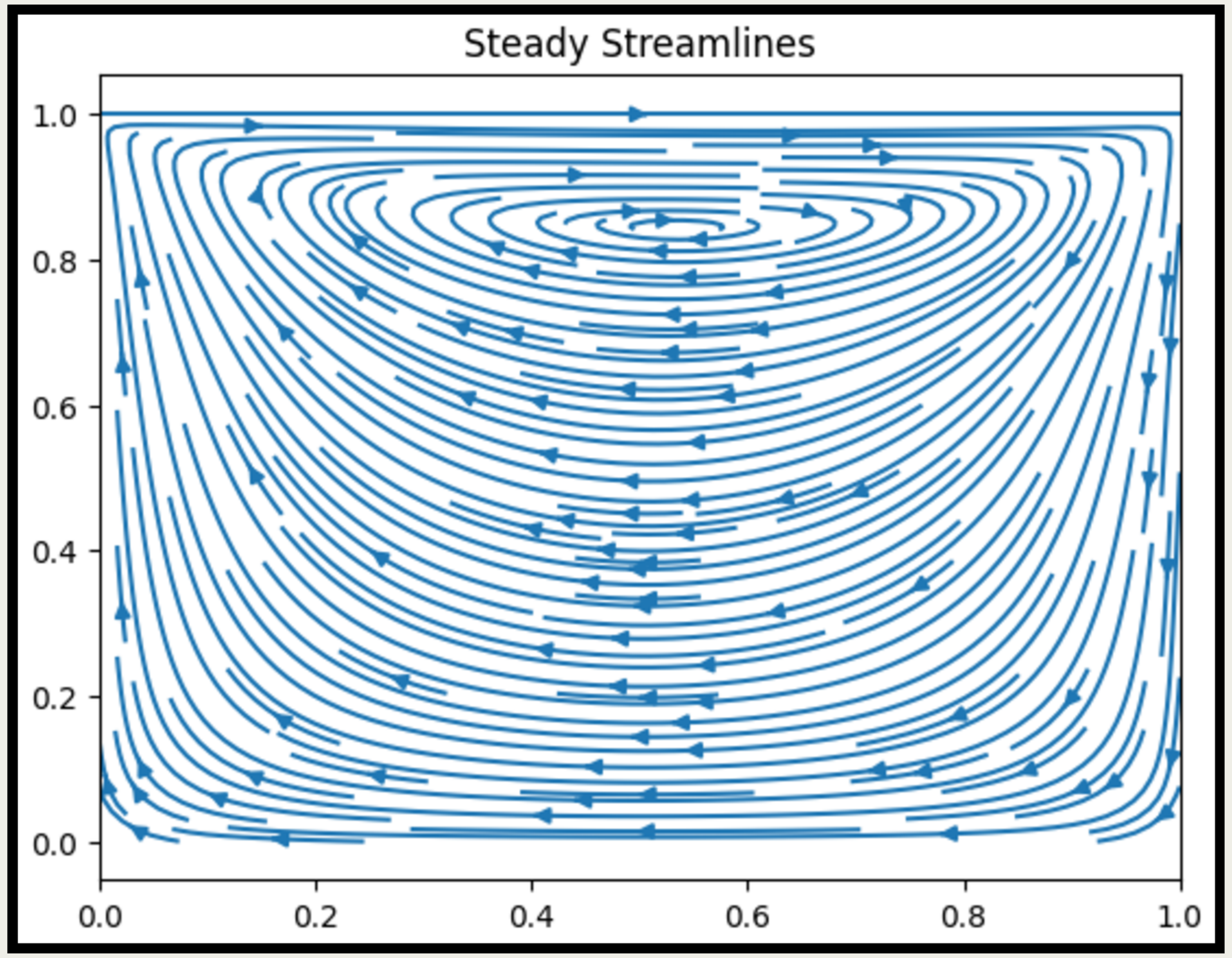
Convergence Rate of Jacobi Iteration
log(Error)
log(Max Error)
Iteration Number

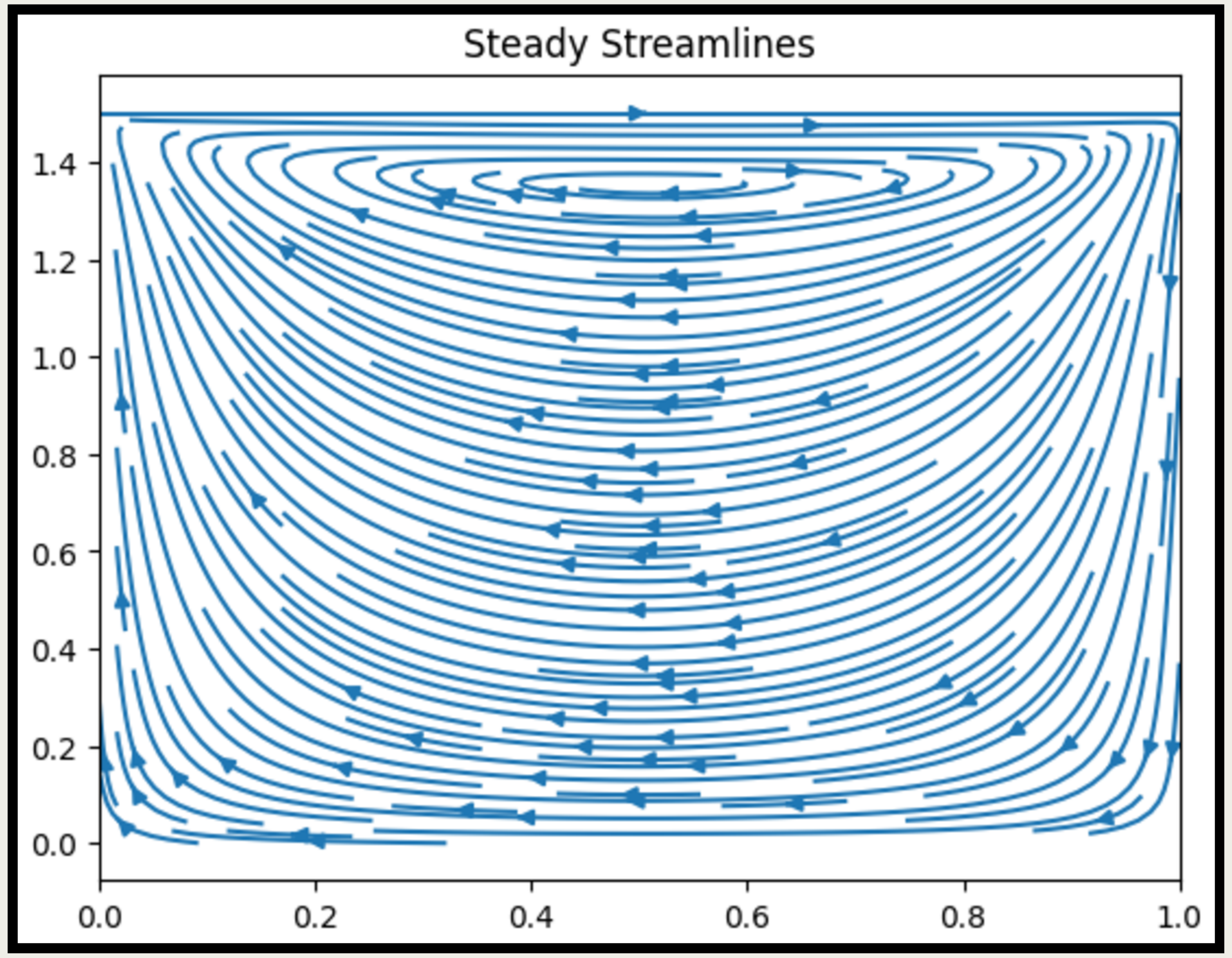


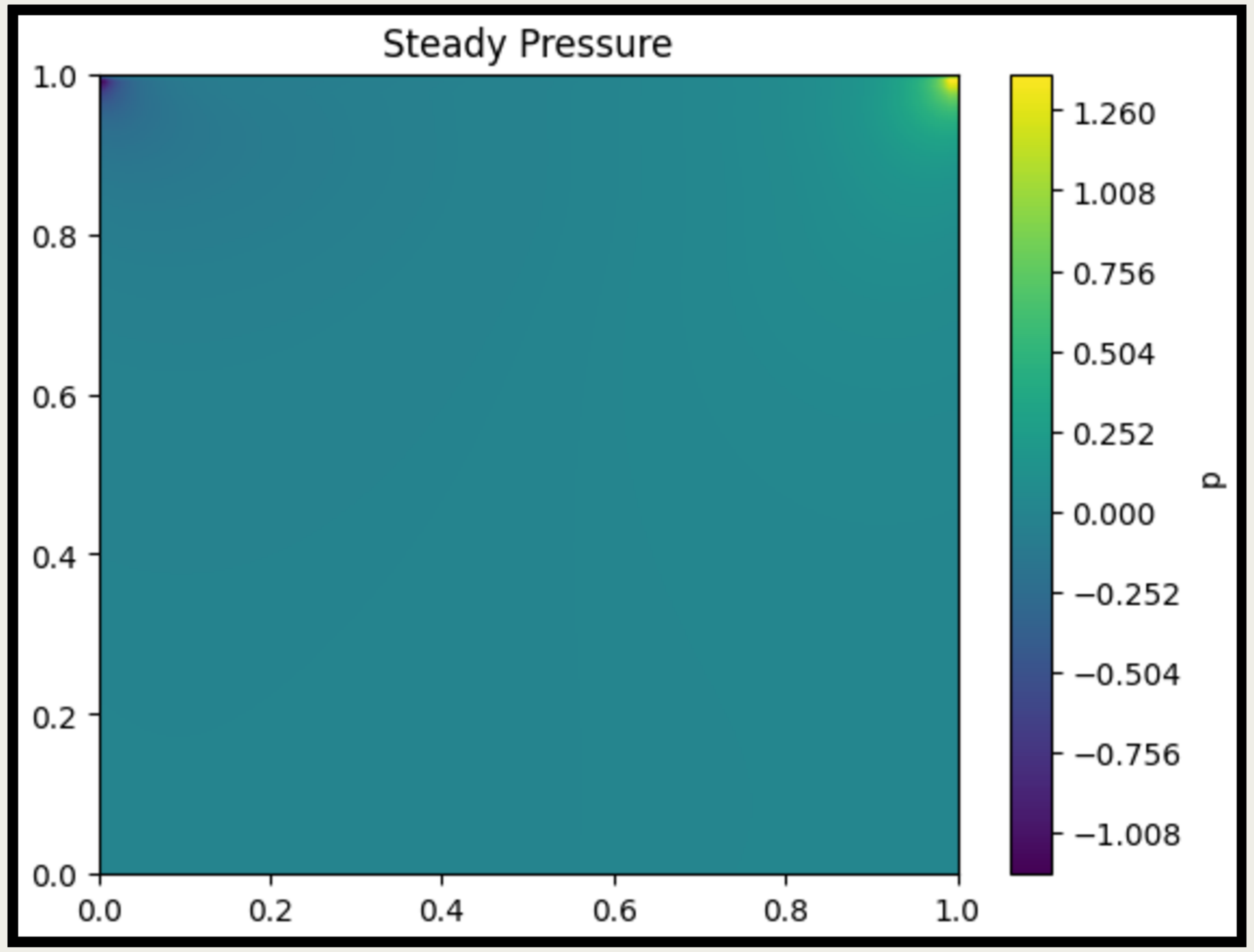
Convergence Rate of Jacobi Iteration
log(Error)
log(Max Error)
Iteration Number

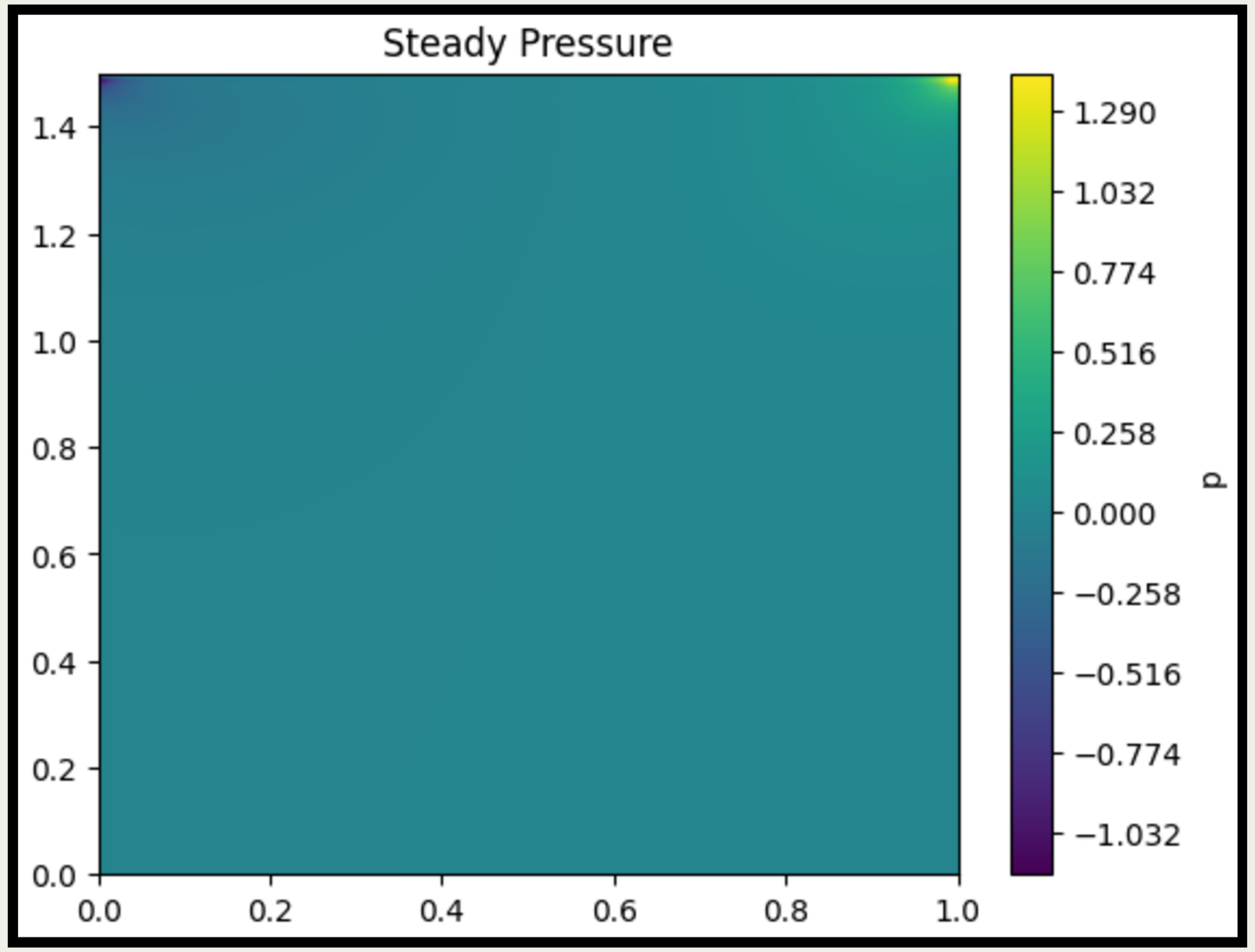
Assignment Problems

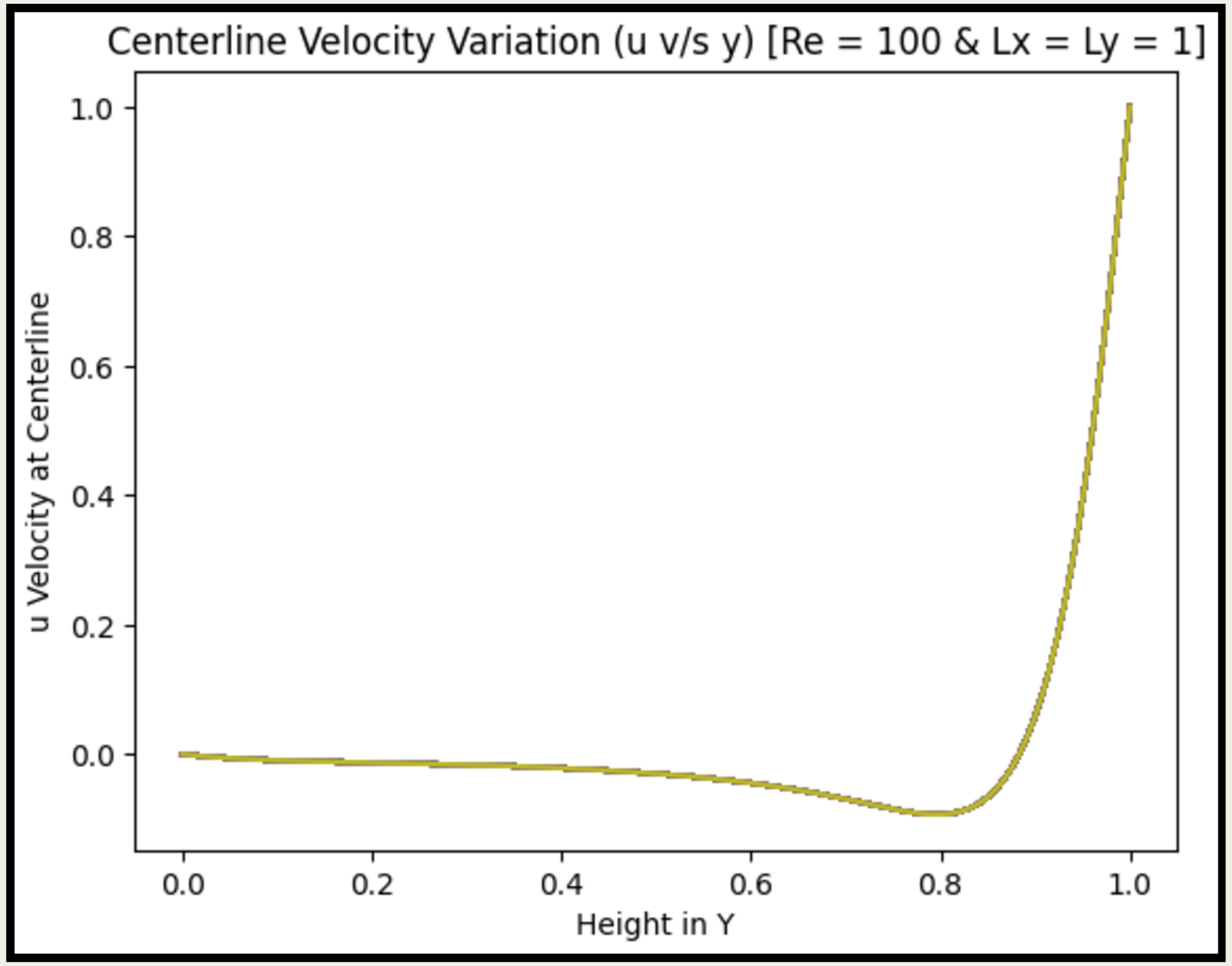
Question 3:

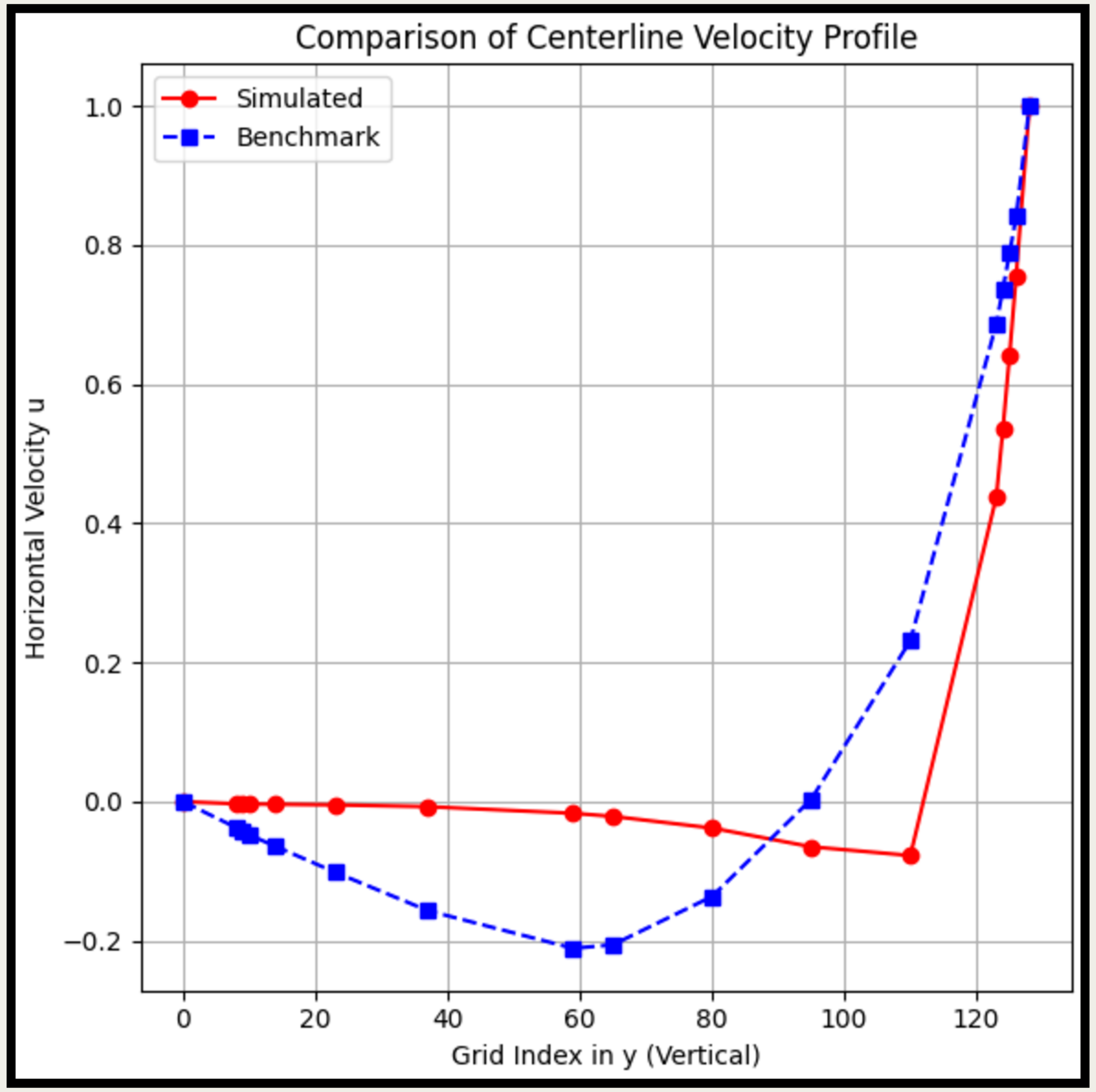

Steady Streamlines
0.0
0.2
0.4
0.6
0.8
1.0


Steady Streamlines
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4


Steady Pressure
1.260
1.008
0.756
0.504
0.252
0.000
−0.252
−0.504
−0.756
−1.008
p


Steady Pressure
1.290
1.032
0.774
0.516
0.258
0.000
−0.258
−0.516
−0.774
−1.032
p


Centerline Velocity Variation (u v/s y) [Re = 100 & Lx = Ly = 1]
u Velocity at Centerline
Height in Y
0.0
0.2
0.4
0.6
0.8
1.0


Comparison of Centerline Velocity Profile
Simulated
Benchmark
Horizontal Velocity u
Grid Index in y (Vertical)
−0.2
0.0
0.2
0.4
0.6
0.8
1.0
0
20
40
60
80
100
120

Numerical Methods for Droplet Impact

- Russo et al. (2020) – VOF in OpenFOAM

Mass Momentum Conservation by PISO Algorithm

Interface Tracking Method: modified version of VOF since it can handle interface deformations

Wettability is modeled via a dynamic contact-angle law

Kistler’s dynamic contact-angle model to update the contact angle as a function of contact-line velocity

Numerical Methods for Droplet Impact

- Gelissen et al. (2020) – Diffuse-Interface (Phase-Field) Model

Diffuse interface (DIM) model based on the Navier–Stokes–Korteweg (NSK) equations.
Wetting is imposed via a special solid–fluid interaction boundary condition: the wall energy is tuned so that the diffuse interface naturally exhibits a prescribed contact angle

Numerical Methods for Droplet Impact

- Liwei et al. (2019) – Particle-Dynamics (MDPD)

Many-body dissipative particle dynamics (MDPD) method to simulate droplet fragmentation on mesh screens

Particle based method

Newton's equations with conservative, dissipative, and random forces that enforce hydrodynamic behavior

Wetting induced through boundary conditions