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Course: M.Tech (Aerospace Engineering)

Subject: AE 291 (Matrix Computations)

SAP No.: 6000007645

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Importing the necessary libraries

[1]:
```
import numpy as np
```

[2]:
```
from matplotlib import cm
```

[3]:
```
import matplotlib.pyplot as plt
```

[4]:
```
import sys
```

Problem:

Solving 2D Poisson's problem using Steepest Descent and Conjugate Gradient iterative methods

Consider the 2D Poisson's equation in the domain Ω = [0,1] $\times$ [0, 1], the unit square:

$$-\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} = f \qquad in \qquad \Omega, \tag{1}$$

with the boundary condition

$$u = g \qquad on \qquad \partial\Omega \tag{2}$$

where f and g are given functions, and $\partial\Omega$ represents the boundary of Ω. Eq. 1 can be discretized using the centered Finite difference method (as explained in the class).

Consider the case where f = 0, and g is given as,

$$g(x, y) = \begin{cases} 0 & if\ x = 0 \\ y & if\ x = 1 \\ (x-1)sin(x) & if\ y = 0 \\ x(2-x) & if\ y = 1 \end{cases}$$

Write two separate codes; one for Steepest Descent (SD) and other for Conjugate Gradient (CG) for solving the discretized Poisson's equation. For both the methods, take the initial guess as $u^{(0)} = 0$, and consider three mesh intervals: h = 1/10, h = 1/20 and h = 1/40. The iterations should be continued until the relative change in the solution u from one iteration to another is less than 10^{-8}. More precisely, stop the iterations when

$$\frac{||u^{(k+1)} - u^{(k)}||_2}{||u^{(k+1)}||_2} < 10^{-8} \tag{3}$$

Along with the codes, submit a short report with the following items:

1. For each method (SD and CG), for each "h", plot the relative change in the solution (LHS of Eq. 3) versus the iteration index (k). In the plot, the relative change in the solution should be in base-10 logarithmic scale (For example, see the command "semilogy" in matlab)

Answer (1): Steepest Descent (SD)

Set of values of the h

[5]:
```
H = [1/10,1/20,1/40]
```

Defining the domain: Ω = [0,1] $\times$ [0, 1]

[6]:
```
x_0 = 0
```

[7]:
```
x_l = 1
```

[8]:
```
y_0 = 0
```

[9]:
```
y_l = 1
```

Function to implement the boundary conditions

$$g(x,y) = \begin{cases} 0 & if\ x = 0 \\ y & if\ x = 1 \\ (x-1)sin(x) & if\ y = 0 \\ x(2-x) & if\ y = 1 \end{cases}$$

[10]:
```
def g(x,y):
    """
    g(x,y) sets the boundary conditions at based on the coordinates of the node,␣
↪x and y.
    If the given node does not lie on the boundary then 0 will be returned.
```

```
    x: x coordinate
    y: y coordinate
    """
    if x == 0:
        return 0
    if x == 1:
        return y
    if y == 0:
        return (x-1)*np.sin(x)
    if y == 1:
        return x*(2-x)
    else:
        return 0
```

[11]:
```
def f(x,y):
    """
    f(x,y) evaluated the function f of the question based on the coordinates of␣
↪the node, x and y.
    x: x coordinate
    y: y coordinate
    """
    return 0
```

Stopping criteria:

$$\frac{||u^{(k+1)} - u^{(k)}||_2}{||u^{(k+1)}||_2} < 10^{-8} \tag{3}$$

[12]:
```
def Error_Function(u_new,u):
    """
    Error_Function(u_new,u) evaluates the error.
    u_new: u(k+1)
    u: u(k)
    """

    # Calculating the numerator
    temp = (((u_new.flatten()-u.flatten())**2).sum())**0.5

    # Calculating the denominator
    temp_1 = (((u_new.flatten())**2).sum())**0.5

    # Calculating the error
    temp = temp/temp_1

    return temp
```

[13]:
```
Tolerance = 1e-8
```

A dictionary to store errors

[14]:
```
Error = {}
```

A dictionary to store u

[15]:
```
U = {}
```

A dictionary to store meshgrids

[16]:
```
X_Y_dict = {}
```

Function to calculate the product of two matrices

[17]:
```
def MatMul(A,B):
    """
    MatMul(A,B) multiply two matrices A and B of compatible sizes
    NOTE: This function is a generic matrix multiplication function.
    """

    # We are copying A and B because we will be reshaping them
    a = A.copy()
    b = B.copy()

    # Checking the dimension of a
    if len(a.shape) > 2:
        print(f"A is NOT a matrix.")
        sys.exit()

    # Checking the dimension of b
    if len(b.shape) > 2:
        print(f"B is NOT a matrix.")
        sys.exit()

    # a will be I x J
    # b will be J x K

    I = a.shape[0]

    # To take care of the vectors
    if len(a.shape) < 2:
        J = 1
    else:
        J = a.shape[1]

    # To take care of the vectors
```

```
    if len(b.shape) < 2:
        K = 1
    else:
        K = b.shape[1]

    # Checking if the dimensions of A and B are compatible for multiplication or␣
↪NOT.
    if J != b.shape[0]:
        print(f"Dimensions of A and B are NOT compatible.")
        sys.exit()

    # Prod matrix will store the results
    Prod = np.zeros((I,K))

    # a will be I x J
    a = a.reshape(I,J)

    # b will be J x K
    b = b.reshape(J,K)

    # Multiplying the matrix A and matrix B
    for i in range(I):
        for j in range(J):
            for k in range(K):
                Prod[i][k] = Prod[i][k] + (a[i][j]*b[j][k])

    # Returning the matrix product
    return Prod
```

Discretization:

$$-\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} = f \qquad in \qquad \Omega$$

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -f \qquad in \qquad \Omega$$

$$\Delta x = \Delta y = h$$

$$\frac{u_{(i+1,j)} - 2u_{(i,j)} + u_{(i-1,j)}}{h^2} + \frac{u_{(i,j+1)} - 2u_{(i,j)} + u_{(i,j-1)}}{h^2} = f_{(i,j)}$$

or,

$$\frac{u_{(i+1,j)} - 2u_{(i,j)} + u_{(i-1,j)} + u_{(i,j+1)} - 2u_{(i,j)} + u_{(i,j-1)}}{h^2} = f_{(i,j)}$$

or,

$$\frac{u_{(i+1,j)} + u_{(i,j+1)} - 4u_{(i,j)} + u_{(i-1,j)} + u_{(i,j-1)}}{h^2} = f_{(i,j)}$$

or,

$$u_{(i+1,j)} + u_{(i,j+1)} - 4u_{(i,j)} + u_{(i-1,j)} + u_{(i,j-1)} = h^2 f_{(i,j)}$$

or,

$$u_{(i+1,j)} + u_{(i,j+1)} - 4u_{(i,j)} + u_{(i,j-1)} + u_{(i-1,j)} = h^2 f_{(i,j)}$$

Let,

$$I = I(i,j) = (n_x \times i) + j$$

So,

$$u_{(i,j)} = u_I$$

So,

$$I(i,j-1) = (n \times i) + j - 1$$

or,

$$I(i,j-1) = I - 1$$

So,

$$u_{(i,j-1)} = u_{I-1}$$

Also,

$$I(i,j+1) = (n_x \times i) + j + 1$$

or,

$$I(i,j+1) = I + 1$$

So,

$$u_{(i,j+1)} = u_{I+1}$$

Also,

$$I(i-1,j) = (n_x \times (i-1)) + j$$

or,

$$I(i-1,j) = I - n_x$$

So,

$$u_{(i-1,j)} = u_{I-n_x}$$

Also,

$$I(i+1,j) = (n_x \times (i+1)) + j$$

or,

$$I(i+1,j) = I + n_x$$

So,

$$u_{(i+1,j)} = u_{I+n_x}$$

So,

$$u_{I+n_x} + u_{I+1} - 4u_I + u_{I-1} + u_{I-n_x} = h^2 f_I$$

Function to calculate the product of A and any vector

[18]:
```
def MatMul_A_Vector(b,n,n_x):
    """
    MatMul_A_Vector(b,n,n_x) multiply matrix A for this particular case and a␣
↪generic vector b of compatible sizes.
    NOTE: We are exploiting the sparse nature of the matrix A.
    NOTE: This function is specific to this problem only and NOT a generic␣
↪matrix multiplication function.
    """

    # A will be I x J
    # b will be J x K

    I = n

    # Checking the dimension of b
    if len(b.shape) != 2:
        if b.shape[1] != 1:
            print(f"b is NOT a vector.")
            sys.exit()

    # Checking if the dimensions of A and b are compatible for multiplication or␣
↪NOT.
    if b.shape[0] != n:
        print(f"Dimensions of A and b are not compatible.")
        sys.exit()

    J = n

    K = 1

    # Prod matrix will store the results
    Prod = np.zeros((I,K))

    # b will be J x K
    b = b.reshape(J,K)

    # Doing the matrix multiplication by only multiplying the non-zero elements

    for i in range(0,n_x):
```

```
        Prod[i][0] = b[i][0]

    for i in range(n_x,I-n_x):
        if (i%n_x == 0) or ((i+1)%n_x == 0):
            Prod[i][0] = b[i][0]
        else:
            Prod[i][0] = Prod[i][0] + (-4*b[i][0])
            Prod[i][0] = Prod[i][0] + (b[i+1][0])
            Prod[i][0] = Prod[i][0] + (b[i-1][0])
            Prod[i][0] = Prod[i][0] + (b[i+n_x][0])
            Prod[i][0] = Prod[i][0] + (b[i-n_x][0])

    for i in range(I-n_x,I):
        Prod[i][0] = b[i][0]

    # Returning the matrix product
    return Prod
```

Steepest Descent (SD) Algorithm for Au = b

$r^{(0)} \leftarrow (b - Au^{(0)})$

$P^{(0)} \leftarrow r^{(0)}$

do until convergence:

$q^{(k)} \leftarrow AP^{(k)}$

$\alpha^{(k)} \leftarrow \frac{(P^{(k)})^T r^{(k)}}{(P^{(k)})^T q^{(k)}}$

$u^{(k+1)} \leftarrow (u^{(k)} + \alpha^{(k)} P^{(k)})$

$r^{(k+1)} \leftarrow (r^{(k)} + \alpha^{(k)} q^{(k)})$

$P^{(k+1)} \leftarrow r^{(k+1)}$

$k \leftarrow (k+1)$

[19]:
```
def SD_Solver(r,u,U,Error,Tolerance,f,x,y,h,n,n_x,n_y):
    """
    SD_Solver(A,b,u,U,Error,Tolerance,f,x,y,h,n_x,n_y): Solves the given poisson␣
 ↪equation using the Steepest Descent (SD) method
    r: r is the residual but b is stored in r, where Au = b and r = b-(Au)
    u: Initial value of u in the computational domain
    U: Dictionary to store u for different values of h
    Error: Dictionary to store error at each iterations for different values of h
    Tolerance: Stopping Criteria
    f: RHS of the equation
    x: X Meshgrid
    y: Y Meshgrid
    h: Grid Spacing
```

```
    n: Total number of grid points
    n_x: Number of the grid points in the x-directions
    n_y: Number of the grid points in the y-directions
    """

    # Intializing the tolerance achieved
    temp = Tolerance + 1

    # Error over iterations for some particular h
    error = []

    # Steepest Descent (SD) algorithm

    # Calculating the residual
    # r = b-(Au)
    r = r-MatMul_A_Vector(u,n,n_x)

    # While loop until the stopping criteria is met
    while temp >= Tolerance:
        u_old = u.copy()
        P = r.copy()
        # q = AP
        q = MatMul_A_Vector(P,n,n_x)
        alpha = MatMul(P.T,r)/MatMul(P.T,q)
        u = u + (alpha*P)
        r = r - (alpha*q)

        # Calculating the relative error
        temp = Error_Function(u,u_old)

        # Storing the errors corresponding to each iteration
        error.append(temp)

    # Storing u in the dictionary for some particular h
    U[h] = u_old.reshape((n_x,n_y))

    # Storing error in the dictionary for some particular h
    Error[h] = error
```

[20]:
```
X_Y_dict
```

[20]: {}

[21]:
```
# Iterating over different values of h (Mesh Interval)
for h in H:

    # Mesh intervals
```

```
dx = h
dy = h

# Number of grid points in x-directions
n_x = int((x_l-x_0)/h + 1)

# Number of grid points in y-directions
n_y = int((y_l-y_0)/h + 1)

# Total number of grid points
n = n_x*n_y

# A matrix to store grid numbering associated with a particular h
I = np.zeros((n_x,n_y),dtype = np.int32)

# A matrix to store the solution associated with a particular h
u = np.zeros((n_x,n_y))

# Creating a meshgrid
x = np.arange(x_0,x_l+dx,dx)
y = np.arange(y_0,y_l+dy,dy)
X,Y = np.meshgrid(x,y,indexing = "ij")

# Storing meshgrids
X_Y_dict[h] = (X,Y)

# Applying the boundary conditions and storing the grid numbers
for i in range(u.shape[0]):
    for j in range(u.shape[1]):

        # Applying the boundary conditions
        u[i,j] = g(x[i],y[j])

        # Storing the grid numbers
        I[i,j] = int((n_x*i)+j)

# Storing u as a vector
u_linear = u.flatten()

# Treating vector as a matrix
u_linear = u_linear.reshape(u_linear.shape[0],1)

# RHS vector stored as matrix
b = np.zeros((n,1))

# Applying the boundary conditions
for i in range(u.shape[0]):
```

```
        for j in range(u.shape[1]):
            if i == 0:
                b[I[i,j],0] = u_linear[I[i,j]] + ((h**2)*f(x[i],y[j]))
            if i == (u.shape[0]-1):
                b[I[i,j],0] = u_linear[I[i,j]] + ((h**2)*f(x[i],y[j]))
            if j == 0:
                b[I[i,j],0] = u_linear[I[i,j]] + ((h**2)*f(x[i],y[j]))
            if j == (u.shape[1]-1):
                b[I[i,j],0] = u_linear[I[i,j]] + ((h**2)*f(x[i],y[j]))
            b[I[i,j],0] =  b[I[i,j],0] + ((h**2)*f(x[i],y[j]))

    # Intializing the u at the current iteraion with zeros
    u = np.zeros(((int((x_l-x_0)/dx))+1,(int((y_l-y_0)/dy))+1))

    # Applying the boundary conditions to u
    for i in range(u.shape[0]):
        for j in range(u.shape[1]):
            u[i,j] = g(x[i],y[j])

    # Solving the system of equation using SD Method
    # NOTE: b will be modified after the excution of this function
    SD_Solver(b,u_linear,U,Error,Tolerance,f,x,y,h,n,n_x,n_y)

    # Number of iterations required
    iteraions = len(Error[h])

    # Printing the value of h
    print(f"For h = {h}:")

    # Printing the number of iterations required
    print(f"Number of iterations required: {iteraions}\n\n")
```

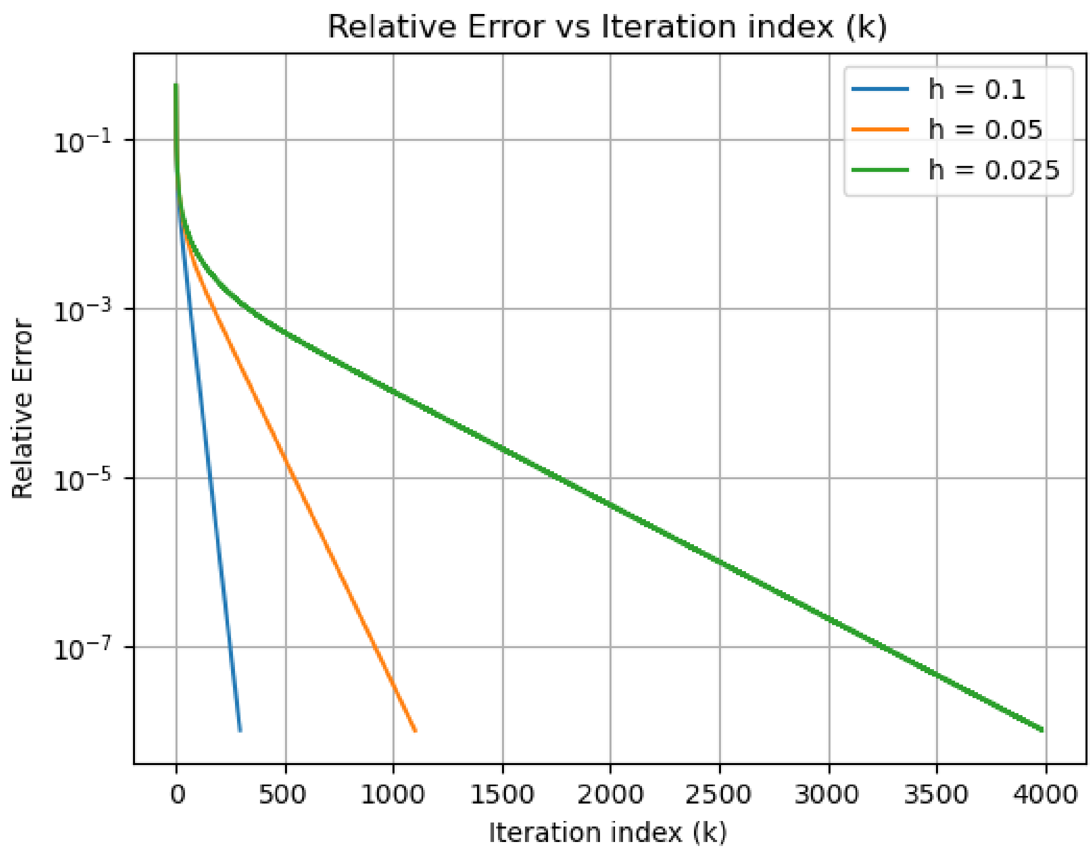
```
For h = 0.1:
Number of iterations required: 297


For h = 0.05:
Number of iterations required: 1102


For h = 0.025:
Number of iterations required: 3986
```

[22]:
```
for h,error in Error.items():
    plt.semilogy(error,label = "h = "+str(h))
```

```
plt.legend()
# NOTE: Here, the iteration index k starts from 0
plt.xlabel("Iteration index (k)")
plt.ylabel("Relative Error")
plt.title(f"Relative Error vs Iteration index (k)")
plt.grid()
plt.show()
```



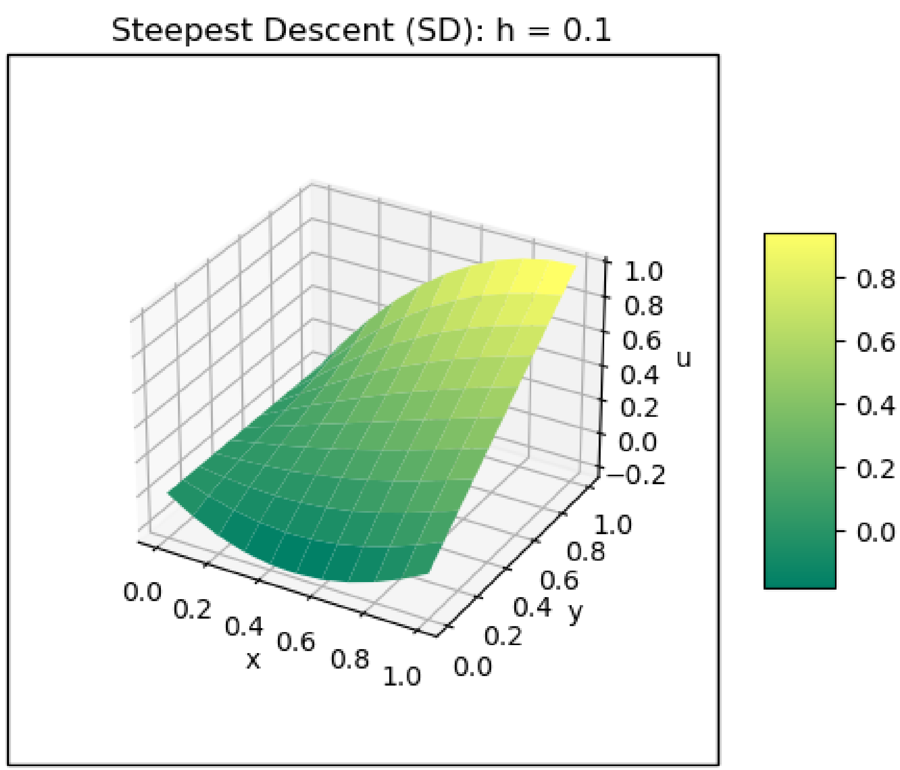
---

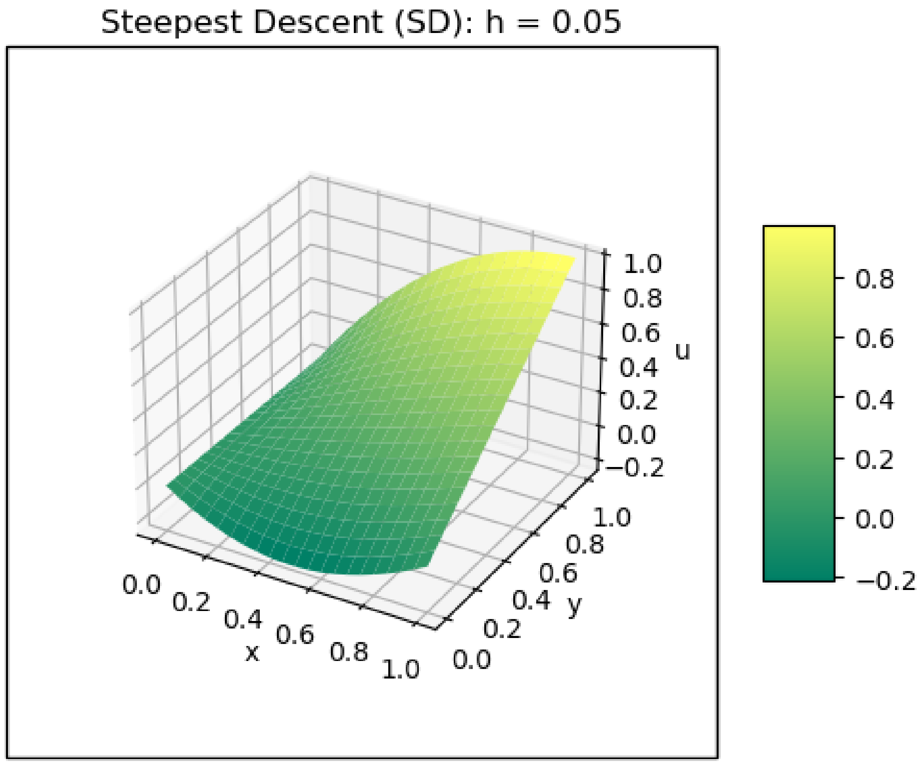
2. For each method (SD and CG), for each "h", show the 3D surface plot of the final solution u (as a function of x and y).

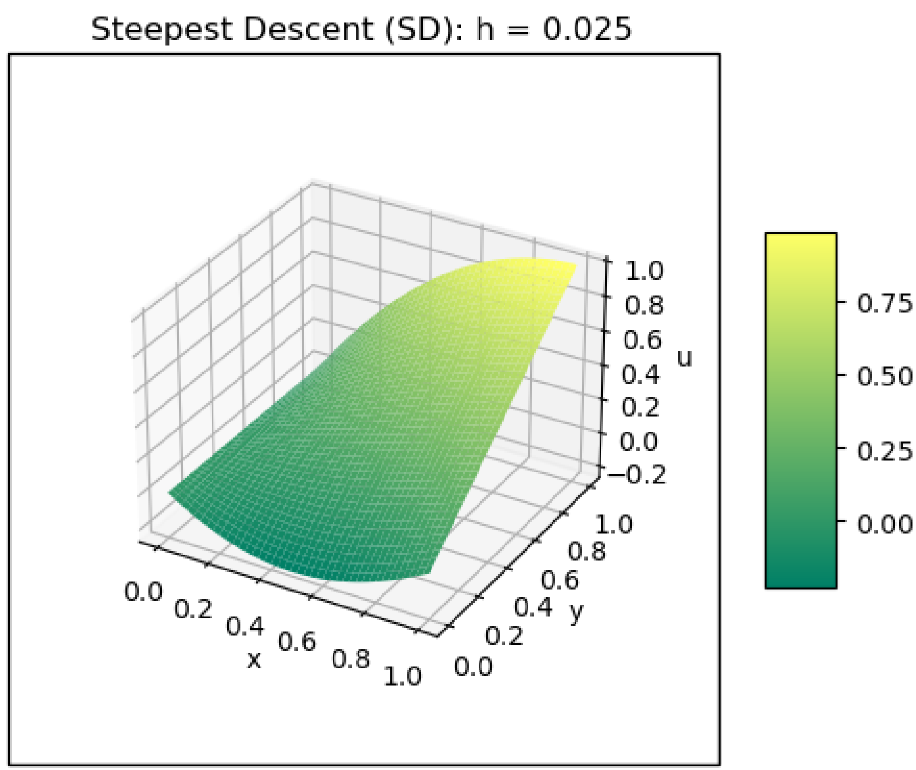
Answer (2): Steepest Descent (SD)

[23]:
```
for h,u in U.items():
    fig = plt.figure()
    ax = fig.add_subplot(projection = "3d")
```

```
    surf = ax.plot_surface(X_Y_dict[h][0], X_Y_dict[h][1], u, cmap=cm.
↪summer,linewidth=0)
    fig.colorbar(surf, shrink=0.5, aspect=5)
    ax.set_xlabel("x")
    ax.set_ylabel("y")
    ax.set_zlabel("u")
    ax.set_title(f"Steepest Descent (SD): h = {h}")
    ax.set_box_aspect(aspect=None, zoom=0.75)
    ax.patch.set_edgecolor('black')
    ax.patch.set_linewidth(1)
plt.show()
```




Steepest Descent (SD): h = 0.05
x
y
u
0.0
0.2
0.4
0.6
0.8
1.0
−0.2


Steepest Descent (SD): h = 0.025
x
y
u
0.0
0.2
0.4
0.6
0.8
1.0
−0.2
0.00
0.25
0.50
0.75

3. A table comparing the iterations required to reach the convergence criteria for Jacobi, Gauss-Seidel, Steepest Descent and Conjugate gradient for all three "h" values.

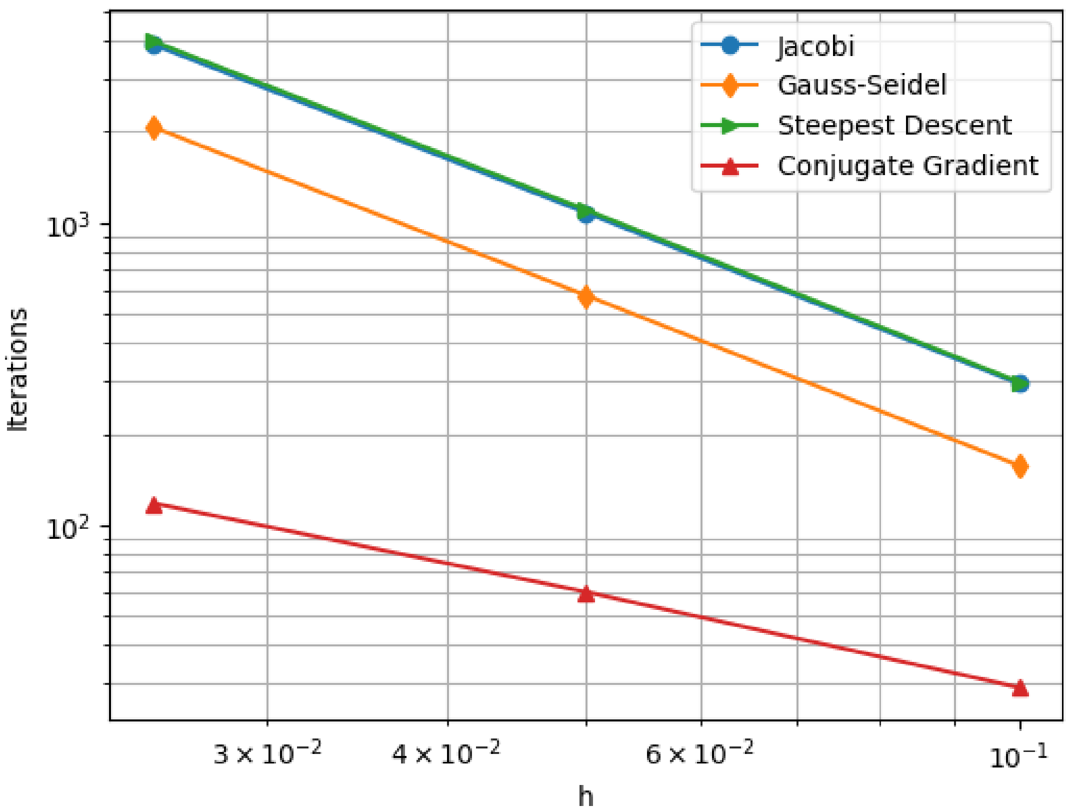
Answer (3):

Iterations required to reach the convergence criteria for Jacobi, Gauss-Seidel, Steepest Descent and Conjugate gradient

h	Jacobi	Gauss-Seidel	Steepest Descent	Conjugate gradient
$\frac{1}{10}$	293	157	297	29
$\frac{1}{20}$	1077	574	1102	60
$\frac{1}{40}$	3882	2069	3986	118

[24]:
```
J = [293,1077,3882]
GS = [157,574,2069]
SD = [297,1102,3986]
CG = [29,60,118]
```

[25]:
```
plt.loglog(H,J,"o-",label = "Jacobi")
plt.loglog(H,GS,"d-",label = "Gauss-Seidel")
plt.loglog(H,SD,">-",label = "Steepest Descent")
plt.loglog(H,CG,"^-",label = "Conjugate Gradient")
plt.legend()
plt.grid(which='minor')
plt.xlabel("h")
plt.ylabel("Iterations")
plt.show()
```



Observations:

1. Conjugate Gradient method requires considerably less iterations as compared to other methods

2. Steepest Descent method is the slowest method among all the reported methods.

3. Jacobi method is marginally faster as compared to the Steepest Descent method.

4. Gauss-Siedel method is approximately twice as fast as the Jacobi and the Steepest Descent methods.

5. As h reduces, the number of iterations required for Conjugate Gradient method increased at a slower rate as compared to the other methods

6. The rate of increase in the iterations required for Jacobi, Gauss-Seidel and Steepest Descent is almost the same. (The slopes are almost equal for these methods)