Computational Physics Lab

Homework 4

108000204

Yuan-Yen Peng

Dept. of Physics, NTHU

Hsinchu, Taiwan

December 29, 2022

1 Writing Assignments

1.1 Finite difference method for solving 2D Poisson equation

The 3×3 grids with grid space h and the source term $\rho(x, y)$ can be described as:

$$u_{xx} + u_{yy} = \rho(x, y)$$

where the subscripts mean second partial derivatives of the u with x and y, respectively. Besides, we annotate (x, y) with (i, j) where i and j are from $0 \sim (3 + 1)$ (including boundaries, which are $(i, j) = (i, 0),\ (i, 4),\ (0, j),$ and $(4, j)$), and implement the Euler method for derivative; then we can get:

$$\begin{aligned}
&\frac{\partial}{\partial x}\Big(\frac{u_{i,j} - u_{i-1,j}}{h}\Big) + \frac{\partial}{\partial y}\Big(\frac{u_{i,j} - u_{i,j-1}}{h}\Big) = \rho(x, y) \\
\Rightarrow &\frac{1}{h}\Big(\frac{u_{i+1,j} - u_{i,j}}{h} - \frac{u_{i,j} - u_{i-1,j}}{h}\Big) + \frac{1}{h}\Big(\frac{u_{i,j+1} - u_{i,j}}{h} - \frac{u_{i,j} - u_{i,j-1}}{h}\Big) = \rho(x, y) \\
\Rightarrow &\big(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}\big) + \big(u_{i,j+1} - 2u_{i,j} + u_{i,j-1}\big) = \rho(x, y)h^2 \\
\Rightarrow &\ 4_{i,j} - u_{i-1,j} - u_{i+1,j} - u_{i,j-1} - u_{i,j+1} = \rho(x, y)h^2 \qquad \text{(I)}
\end{aligned}$$

In the wake of knowing the general form of the solution, we apply the boundary conditions; here boundaries are all zeros (i.e., $u_{0,j},\ u_{i,0},\ u_{4,j},$ and $u_{i,4} = 0$). Exploiting all i and j, we can get LHS of eq.(I) in the matrix form $\mathbf{A}$ and RHS in the vector form $\mathbf{b}$ with source term g_{ij} which represents the splitting of the source function $\rho(x, y)$:

$$\mathbf{A} = \begin{bmatrix}
\begin{bmatrix} 4 & -1 & 0 \\ -1 & 4 & -1 \\ 0 & -1 & 4 \end{bmatrix} & \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} & \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \\
\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} & \begin{bmatrix} 4 & -1 & 0 \\ -1 & 4 & -1 \\ 0 & -1 & 4 \end{bmatrix} & \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \\
\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} & \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} & \begin{bmatrix} 4 & -1 & 0 \\ -1 & 4 & -1 \\ 0 & -1 & 4 \end{bmatrix}
\end{bmatrix}$$

and

$$
\mathbf{b} = -h^2 \left[\begin{array}{c} g_{11} \\ g_{12} \\ g_{13} \\ \hdashline g_{21} \\ g_{22} \\ g_{23} \\ \hdashline g_{31} \\ g_{32} \\ g_{33} \end{array}\right]
$$

2 Programming Assignments

2.1 $\rho_{22} = 1$ and else are zeros

Homework's figure in the last problem is 4×4, but the question asks the 3×3 matrix. Thus, I generate the two results in Figure1, the left one uses the definition of the left bottom corner, and the other (right) implements the center of the grid as a benchmark.

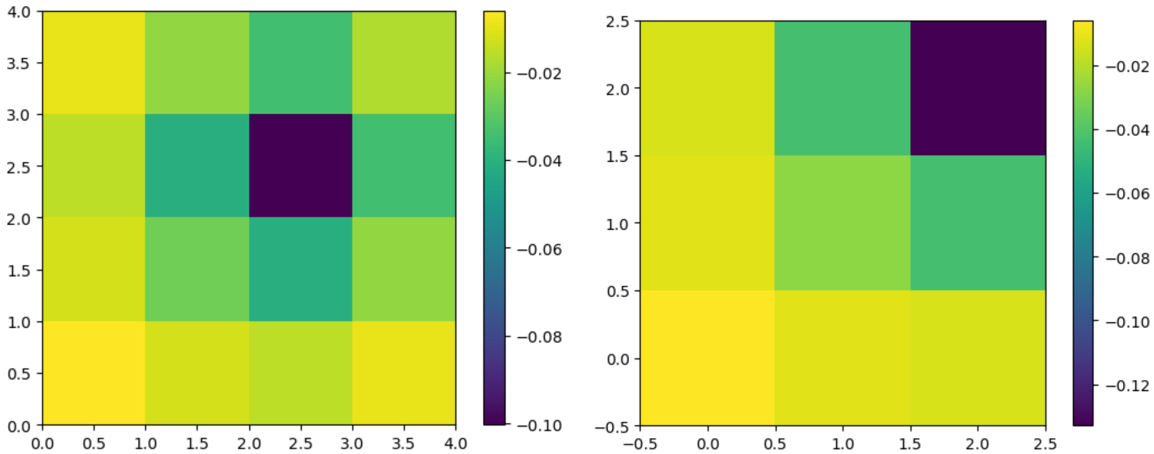

Figure 1: These figures are the solution of the potential u. The left is the 4×4 grid; the right is the 3×3 grid. Both of them are with the source $\rho_{22} = 1$ and the others are zeros.

2.2 2D Poisson's equation with a given source with periodic boindary

In this subsection (also the below's subsections), we exploit the finite difference method with the sparse matrix to solve the equation:

$$
\rho(x, y) = e^{-\frac{5}{4}r_1^2} + \frac{3}{2} \times e^{-r_2^2}
$$

with the domain $\mathscr{D}\{[-5 < x < 5] \times [-5 < y < 5]\}$ in the 128×128 grid.

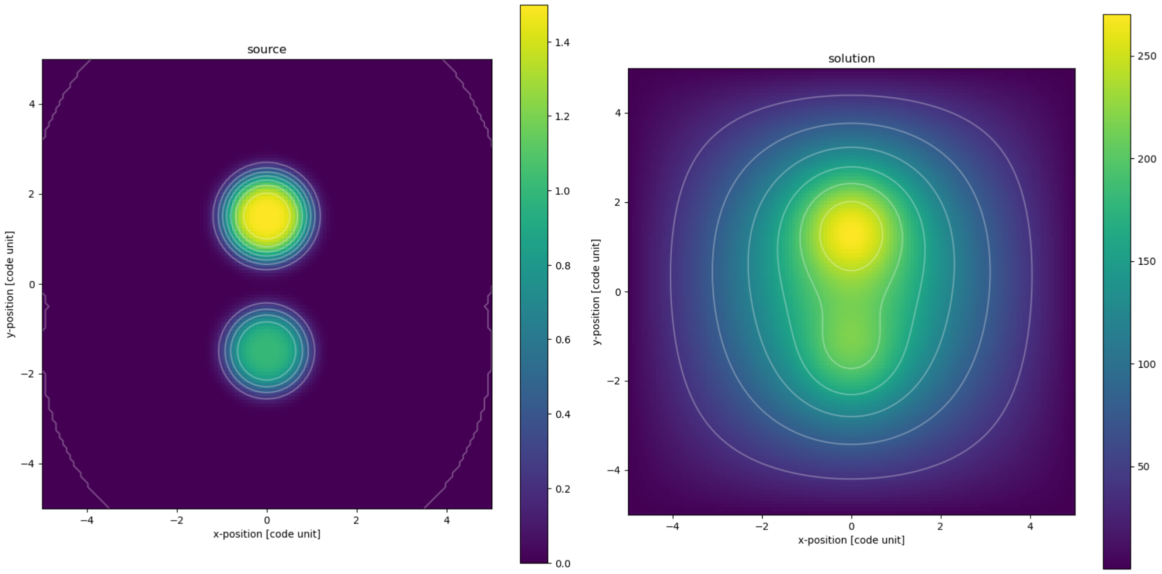

Figure 2: The left is the source function with the scheme with periodic boundary; the right is the solution of the corresponding potential for this Poisson's equation also with the periodic boundary exploiting the sparse matrix method. Moreover, this "periodic boundary" will be updated in each run during finite difference algorithm execution.

2.3 Error convergence comparison between different algorithms

We utilize three different methods learned in the lecture to investigate the error convergence of this Poisson's equation. The first method we used is the Jacobi method and the second is the Gauss-Seidel method, and the last method is the successive over-relaxation method with $w = 1.2,\ 1,5,$ and 2.0. However, in SOR (successive over-relaxation method), it might be "diverge", so we plot two schemes to research the convergence rate, one is all converge and the other is one of them diverge, please see in Figure3.

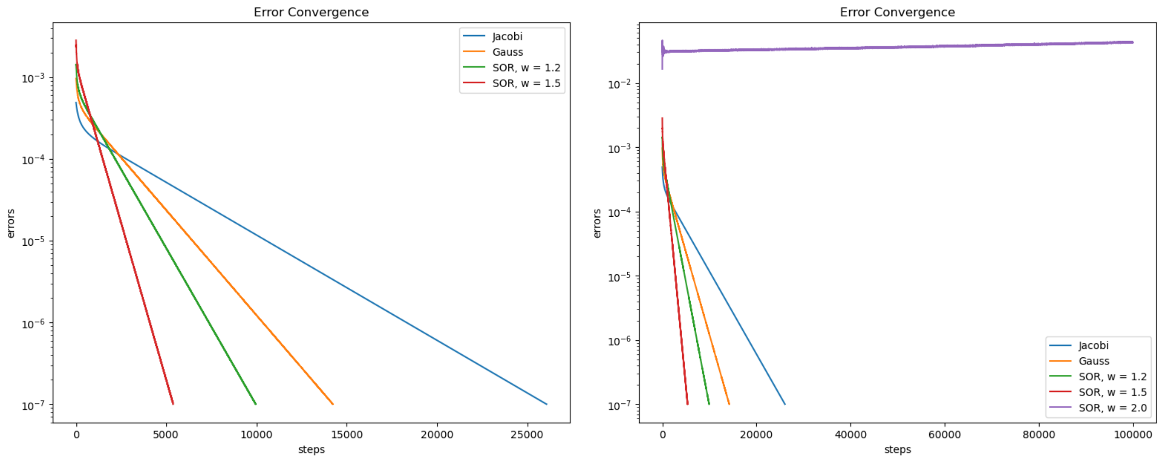

Figure 3: These two figures have the log-scale y-axis; normal scale x-axis so as to show errors as functions of iterations. The left is all of the methods are converged; the right scheme is the one diverge situation ($w = 2.0$, purple line).

It is manifestly that the Jacobi method is the slowest one and then is the Gauss-Seidel method, and the fastest is the SOR method. In this scenario, although SOR is the fastest when $w = 1.5$, it will diverge with $w = 2.0$ (Figure3-right)! The fastest (SOR with $w = 1.5$) is approximately 4.5 times faster than the slowest (Jacobi) as the error tolerance is $\sim 10^{-6}$.

2.4 Resolution vs time with different methodologyies

In this subsection, we will discuss different grid sizes; that is, different resolutions (32×32, 64×64, and 128×128). Additionally, we exploit the methods of the sparse matrix, Jacobi, Gauss-Seidel, and SOR with $w = 1.2,\ 1.5$ as well. Setting tolerance $\epsilon = 10^{-7}$, the resolutions vs time show in Figure4.

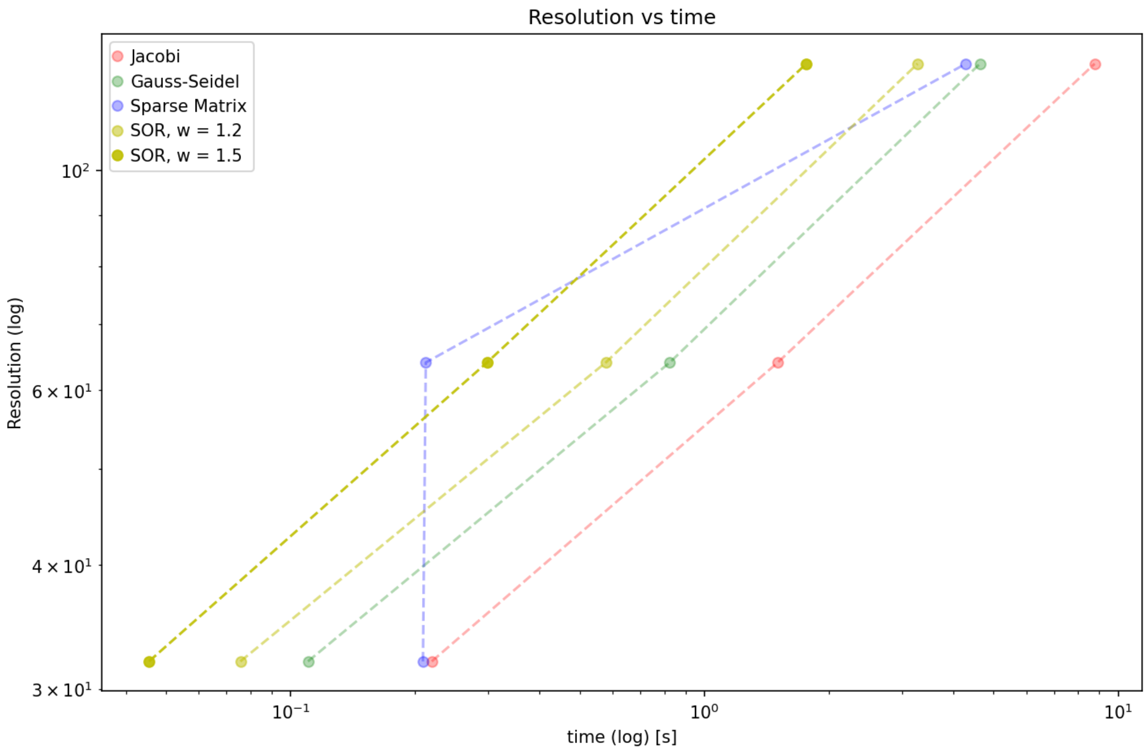

Figure 4: This figure shows different algorithms to solve Poisson's equation in (subsection 2.2). The tendency of these methods, excluding sparse matrix, require more time to iterate to the tolerance ($\epsilon = 10^{-7}$). The outcomes are the same consequent analysis in the aforementioned subsections; i.e., Jacobi is the slowest, Gauss-Seidel is the middle and the SOR is the fastest (besides, $w = 1.5$ is more efficient than $w = 1.3$). On the other hand, the behavior of the sparse matrix method does not act the same as others. It takes the least time among others when the resolution is 64×64. Likewise, in low resolution (32×32), the sparse matrix method is only faster than Jacobi, but in the largest resolution (128×128), it drills faster than Jacobi and also the Gauss-Seidel. Here, we can briefly sum up, if the size (resolution) is in "some proper range", such as 64×64, we can adopt `scipy`'s sparse solver! It is more well organized than others.

3 Codes

All the codes are transferred from jupyterlab or python codes; hence, if you want to re-run them, please see the source code in the attached files or my GitHub repository:

<https://github.com/gary20000915/Comphyslab-HW4.git>

3.1 `solvers.py`

```
import numpy as np
from numba import njit, prange

from .mesh import Mesh2D
```

```python
"""
Solver to solve for Laplace/Poisson's equation

"""

@njit(parallel=True)
def generate_g(g, buff_size, nx, ny, x, y):
    for i in prange(nx+2*buff_size):
        for j in prange(ny+2*buff_size):
            r1 = np.square(x[i] + 1.5) + np.square(y[j])
            r2 = np.square(x[i] - 1.5) + np.square(y[j])
            g[i, j] = np.exp(-5 * 0.25 * np.square(r1)) + 3 * 0.5 * np.exp(-np.square(r2))

    return g

def set_boundary(g, x, y, nx, ny, buff_size, mesh: Mesh2D):
    generate_g(g, buff_size, nx, ny, x, y)
    UL = g[-1,:]
    LR = g[:,-1]
    boundary = np.array([[UL],[LR],[UL],[LR]])
    mesh[0, :] = boundary[0]
    mesh[ny+buff_size, :] = boundary[1]
    mesh[:, 0] = boundary[2]
    mesh[:, nx+buff_size] = boundary[3]


@njit(parallel = True)
def j_kernel(u, u_temp, x, y, nx, ny, g, buff_size):
    for i in prange(1, nx + 2*buff_size - 1, 1):
        for j in prange(1, ny + 2*buff_size - 1, 1):
            r1 = np.square(x[i] + 1.5) + np.square(y[j])
            r2 = np.square(x[i] - 1.5) + np.square(y[j])
            g[i, j] = np.exp(-5 * 0.25 * np.square(r1)) + 3 * 0.5 * np.exp(-np.square(r2))
            u[i, j] = 0.25 * (u_temp[i+1, j] + u_temp[i, j+1] + u_temp[i-1, j] + u_temp[i, j-1] + g[i, j])
    return u

@njit(parallel = True)
def gs_kernel(u, x, y, nx, ny, g, buff_size):
    for i in prange(1, nx + 2*buff_size - 1, 1):
        for j in prange(1, ny + 2*buff_size - 1, 1):
            r1 = np.square(x[i] + 1.5) + np.square(y[j])
            r2 = np.square(x[i] - 1.5) + np.square(y[j])
            g[i, j] = np.exp(-5 * 0.25 * np.square(r1)) + 3 * 0.5 * np.exp(-np.square(r2))
            u[i, j] = 0.25 * (u[i+1, j] + u[i, j+1] + u[i-1, j] + u[i, j-1] + g[i, j])
    return u

@njit(parallel = True)
```

```python
def SOR_kernel(u, u_temp, x, y, nx, ny, g, buff_size, w):
    for i in prange(1, int(nx + 2*buff_size - 1), 1):
        for j in prange(1, int(ny + 2*buff_size - 1), 1):
            r1 = np.square(x[i] + 1.5) + np.square(y[j])
            r2 = np.square(x[i] - 1.5) + np.square(y[j])
            g[i, j] = np.exp(-5 * 0.25 * np.square(r1)) + 3 * 0.5 * np.exp(-np.square(r2))
            u[i, j] = 0.25 * (u[i+1, j] + u[i, j+1] + u[i-1, j] + u[i, j-1] + g[i, j])
            u[i, j] = (1-w) * u_temp[i,j] + w * u[i, j]
    return u

def solve(name, tor, mesh: Mesh2D, **kwargs):
    u         = mesh.get_mesh()
    x         = mesh.get_x()
    y         = mesh.get_y()
    nx        = mesh.get_nx()
    ny        = mesh.get_ny()
    g         = mesh.get_xx()
    buff_size = mesh.get_buff_size()

    err     = 10
    err_arr = np.array([])
    n       = 0

    while err > tor:
        u_temp = np.copy(u)
        set_boundary(g, x, y, nx, ny, buff_size, u)

        if name == "Jacobi":
            u = j_kernel(u, u_temp, x, y, nx, ny, g, buff_size)
        elif name == "Gauss":
            u = gs_kernel(u, x, y, nx, ny, g, buff_size)
        elif name == "SOR":
            u = SOR_kernel(u, u_temp, x, y, nx, ny, g, buff_size, kwargs['w'])
        else:
            print("Error: unknown kernel!")
            break

        err = np.sqrt(np.sum(np.square(u - u_temp))) / (nx * ny)
        err_arr = np.append(err_arr, err)
        n += 1
        # check
        # if n % 100 == 0:
        #     print(err, tor)
            # print(u)
            # plt.imshow(u.reshape(nx+2*buff_size, ny+2*buff_size), origin = 'lower', extent=[-1, 1, -1, 1])
            # plt.colorbar()
            # plt.contour(u, colors = 'white', extent=[-1, 1, -1, 1])
        if n == 1e5:
            break
```

```
        return u.reshape(nx+2*buff_size, ny+2*buff_size), err_arr, n



if __name__=='__main__':

    nx, ny = 4, 4
    buff_size=1
    tor = 1e-10
    # boundary = np.zeros((4, nx + 2*buff_size))
    # boundary[0] =np.ones(nx + 2*buff_size)
    mesh = Mesh2D(nx = nx, ny = ny, buff_size=buff_size)

    u = solve("Jacobi", tor, mesh)[1]
    print(u)
    print("TEST")
```

3.2 mesh.py

```
"""
This file define classes for generating 2D meshes.

"""
import numpy as np
from numba import jit, int32, float64
from numba.experimental import jitclass

class Mesh2D:
    def __init__(self, nx:int = 10, ny:int = 10, buff_size = 1, xmin = 0,
        xmax = 1, ymin = 0, ymax = 1):
        self._nx = nx
        self._ny = ny
        self._nbuff = buff_size
        self._xmin = xmin
        self._xmax = xmax
        self._ymin = ymin
        self._ymax = ymax

        self._setup()

        return

    def _setup(self):
        self._dx = (self._xmax - self._xmin) / (self._nx + 1)
        self._dy = (self._ymax - self._ymin) / (self._ny + 1)

        self._istart = self._nbuff
        self._istartGC = 0
        self._iend = self._nbuff + self._nx - 1
        self._iendGC = 2 * self._nbuff + self._nx - 1
        self._nxGC = 2 * self._nbuff + self._nx
```

```
        self._jstart = self._nbuff
        self._jstartGC = 0
        self._jend = self._nbuff + self._ny - 1
        self._jendGC = 2 * self._nbuff + self._ny - 1
        self._nyGC = 2 * self._nbuff + self._ny

        x = np.linspace(self._xmin, self._xmax, self._nxGC)
        y = np.linspace(self._ymin, self._ymax, self._nyGC)
        xx, yy = np.meshgrid(x, y, indexing='ij')
        self._mesh = xx * 0
        self._xx = xx
        self._yy = yy
        self._x = x
        self._y = y

        return

    def get_nx(self):
        return int(self._nx)
    def set_nx(self, nx):
        self._nx = nx
        self._setup()
        return

    def get_ny(self):
        return int(self._ny)
    def set_ny(self, ny):
        self._ny = ny
        self._setup()
        return

    def get_buff_size(self):
        return int(self._nbuff)
    def set_buff_size(self, buff_size):
        self._nbuff = buff_size
        self._setup()
        return

    def get_xmin(self):
        return self._xmin
    def set_xmin(self, xmin):
        self._xmin = xmin
        self._setup()
        return

    def get_xmax(self):
        return self._xmax
    def set_xmax(self, xmax):
        self._xmax = xmax
        self._setup()
        return

```

```
        def get_ymin(self):
            return self._ymin
        def set_ymin(self, ymin):
            self._ymin = ymin
            self._setup()
            return

        def get_ymax(self):
            return self._ymax
        def set_ymax(self, ymax):
            self._ymax = ymax
            self._setup()
            return

        def get_istart(self):
            return self._istart
        def set_istart(self, istart):
            self._istart = istart
            self._setup()
            return

        def get_istartGC(self):
            return self._istartGC
        def set_istartGC(self, istartGC):
            self._istartGC = istartGC
            self._setup()
            return

        def get_iend(self):
            return self._iend
        def set_iend(self, iend):
            self._iend = iend
            self._setup()
            return

        def get_iendGC(self):
            return self._iendGC
        def set_iendGC(self, iendGC):
            self._iendGC = iendGC
            self._setup()
            return

        def get_jstart(self):
            return self._jstart
        def set_jstart(self, jstart):
            self._jstart = jstart
            self._setup()
            return

        def get_jstartGC(self):
            return self._jstartGC
        def set_jstartGC(self, jstartGC):
            self._jstartGC = jstartGC
```

```python
            self._setup()
            return

        def get_jend(self):
            return self._jend
        def set_jend(self, jend):
            self._jend = jend
            self._setup()
            return

        def get_jendGC(self):
            return self._jendGC
        def set_jendGC(self, jendGC):
            self._jendGC = jendGC
            self._setup()
            return

        def get_mesh(self):
            return self._mesh
        def set_mesh(self, mesh):
            self._mesh = mesh
            if (mesh.size != self._mesh.size):
                print("error! size conflict!")
            return

        def get_xx(self):
            return self._xx
        def set_xx(self, xx):
            self._xx = xx
            self._setup()
            return

        def get_yy(self):
            return self._yy
        def set_yy(self, yy):
            self._yy = yy
            self._setup()
            return

        def get_x(self):
            return self._x
        def set_x(self, x):
            self._x = x
            self._setup()
            return

        def get_y(self):
            return self._y
        def set_y(self, y):
            self._y = y
            self._setup()
            return
```

```python
        def get_nx(self):
            return self._nx
        def set_nx(self, nx):
            self._nx = nx
            self._setup()
            return

        def get_ny(self):
            return self._ny
        def set_ny(self, ny):
            self._ny = ny
            self._setup()
            return


if __name__=='__main__':
    mesh = Mesh2D(nx = 3, ny = 3, buff_size=1)
    # mesh.set_nx(32)
    # mesh.set_ny(32)

    u = mesh.get_mesh()
    nx = mesh.get_nx()
    ny = mesh.get_ny()
    buff = mesh.get_buff_size()

    print(u)
    print(f"Testing ... nx={nx}, ny={ny}, buff ={buff}")
    print('Done')
```

3.3 1_finite_difference.ipynb

```python
# %% [markdown]
# ### 1. Finite Difference method for solving discrete Laplace Equation

# %%
%reset -f

import numpy as np
import matplotlib.pyplot as plt
from scipy import linalg
from scipy.sparse import csc_matrix
from scipy.sparse import dia_array
from scipy.sparse import dia_matrix
import scipy.sparse.linalg as splinalg
from numba import njit, prange

# %%
N = 4
min, max = -1, 1
dx = (max - min) / N

# %%
```

```python
def generate_D(n):
    ex = np.ones(n)
    data = np.array([-1 * ex, 4 * ex, -1 * ex])
    offsets = np.array([-1, 0, 1])

    return dia_matrix((data, offsets), shape=(n, n)).toarray()

# %%
@njit(parallel = True)
def kernel(N, A, D, I):
    for i in prange(N):
        for j in prange(N):
            if i == j:
                for ii in prange(N):
                    for jj in prange(N):
                        A[ii+N*i, jj+N*j] = D[ii, jj]

            if np.abs(i - j) == 1:
                for ii in prange(N):
                    for jj in prange(N):
                        A[ii+N*i, jj+N*j] = I[ii, jj]

    return A

# %%
def generate_A(N):
    A = np.zeros((N ** 2, N ** 2))
    D = generate_D(N)
    I = -np.identity(N)
    A = kernel(N, A, D, I)
    return A

# %%
def generate_b(N, dx):
    b = np.zeros(N ** 2).reshape(N, N)
    b[2, 2] = -1 * np.square(dx)
    plt.imshow(b, origin = 'lower')
    plt.colorbar()
    return b.reshape(N ** 2)

# %%
# solve
def solve(N, dx):
    a = generate_A(N)
    a = csc_matrix(a) # transform to the fitting matrix
    b = generate_b(N, dx)
    x = splinalg.spsolve(a, b).reshape(N, N)
    return x

# %%
u = solve(N, dx)
print(u)
```

```
# %%
plt.imshow(u, origin = 'lower', extent = [0,4,0,4])
plt.colorbar()
```

3.4 2_finite_difference.ipynb

```
# %% [markdown]
# ### Finite Difference method for solving discrete Laplace Equation

# %%
%reset -f

import numpy as np
import matplotlib.pyplot as plt
from matplotlib.pyplot import figure
from scipy import linalg
from scipy.sparse import csc_matrix
from scipy.sparse import dia_array
from scipy.sparse import dia_matrix
import scipy.sparse.linalg as splinalg
from numba import njit, prange

# %%
N = 128
min, max = -5, 5
dx = (max - min) / N

x = np.linspace(-5, 5, N)
y = np.linspace(-5, 5, N)
g = np.zeros([N, N])

# %%
def generate_D(n):
    ex = np.ones(n)
    data = np.array([-1 * ex, 4 * ex, -1 * ex])
    offsets = np.array([-1, 0, 1])

    return dia_matrix((data, offsets), shape=(n, n)).toarray()

# %%
@njit
def kernel(N, A, D, I):
    for i in prange(N):
        for j in prange(N):
            if i == j:
                for ii in prange(N):
                    for jj in prange(N):
                        A[ii+N*i, jj+N*j] = D[ii, jj]

            if np.abs(i - j) == 1:
                for ii in prange(N):
                    for jj in prange(N):
```

```python
                    A[ii+N*i, jj+N*j] = I[ii, jj]

    return A

# %%
def generate_A(N):
    A = np.zeros((N ** 2, N ** 2))
    D = generate_D(N)
    I = -np.identity(N)
    A = kernel(N, A, D, I)
    return A

# %%
@njit
def generate_g(g, N, x, y):
    for i in prange(N):
        for j in prange(N):
            r1 = np.square(x[i] + 1.5) + np.square(y[j])
            r2 = np.square(x[i] - 1.5) + np.square(y[j])
            g[i, j] = np.exp(-5 * 0.25 * np.square(r1)) + 3 * 0.5 *
                np.exp(-np.square(r2))

    return g

# %%
ans = generate_g(g, N, x, y)

figure(figsize=(10, 10), dpi=100)
plt.imshow(ans, origin = 'lower', extent=[-5, 5, -5, 5])
plt.colorbar()
plt.contour(ans, colors = 'w', alpha = .3, extent=[-5, 5, -5, 5])
plt.title('source')
plt.xlabel('x-position [code unit]')
plt.ylabel('y-position [code unit]')
plt.show()
plt.close()

# %%
def generate_b(N, g, dx):
    # boundaries
    # b = np.zeros(N ** 2)
    b = g.reshape(N, N)
    b[-1,:] = b[1,: ]
    b[:,-1] = b[:,-1]
    b = b.reshape(N ** 2)
    # source
    b += - g * np.square(dx)
    return b

# %%
# solve
def solve(N, g, dx, x, y):
    g = generate_g(g, N, x, y).reshape(N ** 2)
```

```
    a = generate_A(N)
    a = csc_matrix(a) # transform to the fitting matrix
    b = generate_b(N, g, dx)
    x = splinalg.spsolve(a, b).reshape(N, N)
    return x

# %%
u = solve(N, g, dx, x, y)
# %timeit solve(N, g, dx, x, y)

# %% [markdown]
# parallel: 6.31 s ± 29.3 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
# nopython: 6.08 s ± 136 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)

# %%
figure(figsize=(10, 10), dpi=100)
plt.imshow(u, origin = 'lower', extent=[-5, 5, -5, 5])
plt.colorbar()
plt.contour(u, colors = 'w', alpha = .3, extent=[-5, 5, -5, 5])
plt.title('solution')
plt.xlabel('x-position [code unit]')
plt.ylabel('y-position [code unit]')
plt.show()
plt.close()
```

3.5 3_iteractive_methods.ipynb

```
# %% [markdown]
# # Laplace Equation & Possion Equations
#
# In this Lab, we will learn how to numerically solve Laplace and Possion equations, which are common equations in electromagnestism and gravitational problems.

# %% [markdown]
# There should be two files under `./poisson_solver`.\
# 1. `mesh.py` handles the mesh grids we will used in this Lab.\
# 2. `solvers.py` handles all corresponding iterative solvers for Laplace/Poisson Equation.

# %%
%reset -f

import numpy as np
import numba as na
import matplotlib.pyplot as plt
from matplotlib.pyplot import figure
import time as time
from poisson_solver.mesh import Mesh2D
from poisson_solver.solvers import *
```

```python

# %% [markdown]
# ## Exercise 4: Jacobi method
#
# 1. Test your Mesh2D class to see if you could generate the grids we
    need for this calculation
# 2. Implement the Jacobi meothd in `./poisson_solver/solver.py`.
# 3. Write a function called `updata_boundary()` to update the boundary
    conditions.\
#    Where to put this `update_boundary()` function is up to you.\
#    You could put it either inside the `Mesh2D` class, in `solvers.py`,
    or here.

# %% [markdown]
# ## Exercise 5: Gauss-Seidel Meothd.
#
# 1. Implement the Gauss-Seidel meothd in your solver.
# 2. Repeat exercise 4. for the Gauss-Seidel meothd.
# 3. Compare the error convergence between Jacobi and Gauss-Seidel

# %%
def setup():
    tor       = 1e-7
    xmin, xmax = -5, 5
    ymin, ymax = -5, 5
    nx, ny   = 128, 128
    buff_size = 1

    mesh = Mesh2D(nx = nx, ny = ny, buff_size = buff_size)
    mesh.set_xmin(xmin)
    mesh.set_xmax(xmax)
    mesh.set_ymin(ymin)
    mesh.set_ymax(ymax)

    return tor, mesh

# %%
'''
Jacobi
'''
ini = setup()
t1 = time.time()
# name == Gauss or Jacobi or SOR
j_arr = solve("Jacobi", ini[0], ini[1])
j_u   = j_arr[0]
j_err = j_arr[1]
j_n   = j_arr[2]
j_N = np.linspace(0, int(j_n), int(j_n))
t2 = time.time()

'''
Gauss-Seidel
'''
```

```
    ini = setup()
    t3 = time.time()
    # name == Gauss or Jacobi or SOR
    g_arr = solve("Gauss", ini[0], ini[1])
    g_u   = g_arr[0]
    g_err = g_arr[1]
    g_n   = g_arr[2]
    g_N = np.linspace(0, int(g_n), int(g_n))
    t4 = time.time()

    '''
    SOR
    '''
    ini = setup()
    t5 = time.time()
    # name == Gauss or Jacobi or SOR
    w1, w2, w3 = 1.2, 1.5, 2.0

    s1_arr = solve("SOR", ini[0], ini[1], w = w1)
    s1_u   = s1_arr[0]
    s1_err = s1_arr[1]
    s1_n   = s1_arr[2]
    s1_N = np.linspace(0, int(s1_n), int(s1_n))
    # prune the margins
    s1_u = np.delete(s1_u, (0, -1), 0)
    s1_u = np.delete(s1_u, (0, -1), 1)

    ini = setup()
    s2_arr = solve("SOR", ini[0], ini[1], w = w2)
    s2_u   = s2_arr[0]
    s2_err = s2_arr[1]
    s2_n   = s2_arr[2]
    s2_N = np.linspace(0, int(s2_n), int(s2_n))
    # prune the margins
    s2_u = np.delete(s2_u, (0, -1), 0)
    s2_u = np.delete(s2_u, (0, -1), 1)

    ini = setup()
    s3_arr = solve("SOR", ini[0], ini[1], w = w3)
    s3_u   = s3_arr[0]
    s3_err = s3_arr[1]
    s3_n   = s3_arr[2]
    s3_N = np.linspace(0, int(s3_n), int(s3_n))
    # prune the margins
    s3_u = np.delete(s3_u, (0, -1), 0)
    s3_u = np.delete(s3_u, (0, -1), 1)
    t6 = time.time()

    print("Jocobi -> Time = ", np.round((t2-t1), 2))
    print("Gauss -> Time = ", np.round((t4-t3), 2))
    print("SOR -> Time = ", np.round((t6-t5), 2))
    print("Done!")
```

```
# %% [markdown]
# ### Visualize your results

# %%
'''
Jacobi
'''
# prune the margins
j_u = np.delete(j_u, (0, -1), 0)
j_u = np.delete(j_u, (0, -1), 1)

figure(figsize=(8, 8), dpi=100)
plt.imshow(j_u, origin = 'lower', extent=[-5, 5, -5, 5])
plt.colorbar()
plt.contour(j_u, colors = 'w', alpha = .3, extent=[-5, 5, -5, 5])
plt.title("Jacobi")
plt.show()

'''
Gauss-Seidel
'''
# prune the margins
g_u = np.delete(g_u, (0, -1), 0)
g_u = np.delete(g_u, (0, -1), 1)

figure(figsize=(8, 8), dpi=100)
plt.imshow(g_u, origin = 'lower', extent=[-5, 5, -5, 5])
plt.colorbar()
plt.contour(g_u, colors = 'w', alpha = .3, extent=[-5, 5, -5, 5])
plt.title("Gauss-Seidel")
plt.show()

'''
SOR
'''
figure(figsize=(8, 8), dpi=100)
plt.imshow(s1_u, origin = 'lower', extent=[-5, 5, -5, 5])
plt.colorbar()
plt.contour(s1_u, colors = 'w', alpha = .3, extent=[-5, 5, -5, 5])
plt.title(f"SOR, with w = {w1}")
plt.show()

# %% [markdown]
# ### Error convergence.
#
# To see how it converge, we could make a of Error vs. Iteration times
   to see how it converges.

# %%
figure(figsize=(9, 7), dpi=100)
plt.yscale('log')
plt.plot(j_N, j_err, label = "Jacobi")
plt.plot(g_N, g_err, label = "Gauss")
```

```
        plt.plot(s1_N, s1_err, label = f"SOR, w = {w1}")
        plt.plot(s2_N, s2_err, label = f"SOR, w = {w2}")
        plt.plot(s3_N, s3_err, label = f"SOR, w = {w3}")
        plt.xlabel("steps")
        plt.ylabel("errors")
        plt.title("Error Convergence")
        plt.legend(loc = 'best')
```

3.6 4_iteractive_methods.ipynb

```
# %%
%reset -f

from scipy import linalg
from scipy.sparse import csc_matrix
from scipy.sparse import dia_array
from scipy.sparse import dia_matrix
import scipy.sparse.linalg as splinalg
from numba import njit, prange

import numpy as np
import matplotlib.pyplot as plt
import matplotlib
from matplotlib.pyplot import figure
import time as time
from poisson_solver.mesh import Mesh2D
from poisson_solver.solvers import *

# %%
def generate_D(n):
    ex = np.ones(n)
    data = np.array([-1 * ex, 4 * ex, -1 * ex])
    offsets = np.array([-1, 0, 1])

    return dia_matrix((data, offsets), shape=(n, n)).toarray()

# %%
@njit
def kernel(N, A, D, I):
    for i in prange(N):
        for j in prange(N):
            if i == j:
                for ii in prange(N):
                    for jj in prange(N):
                        A[ii+N*i, jj+N*j] = D[ii, jj]

            if np.abs(i - j) == 1:
                for ii in prange(N):
                    for jj in prange(N):
                        A[ii+N*i, jj+N*j] = I[ii, jj]

    return A
```

```
# %%
def generate_A(N):
    A = np.zeros((N ** 2, N ** 2))
    D = generate_D(N)
    I = -np.identity(N)
    A = kernel(N, A, D, I)
    return A

# %%
@njit
def generate_g(g, N, x, y):
    for i in prange(N):
        for j in prange(N):
            r1 = np.square(x[i] + 1.5) + np.square(y[j])
            r2 = np.square(x[i] - 1.5) + np.square(y[j])
            g[i, j] = np.exp(-5 * 0.25 * np.square(r1)) + 3 * 0.5 *
                np.exp(-np.square(r2))

    return g

# %%
def generate_b(N, g, dx):
    # boundaries
    # b = np.zeros(N ** 2)
    b = g.reshape(N, N)
    b[-1,:] = b[1,: ]
    b[:,-1] = b[:,-1]
    b = b.reshape(N ** 2)
    # source
    b += - g * np.square(dx)
    return b

# %%
# solve
def psolve(N, g, dx, x, y):
    g = generate_g(g, N, x, y).reshape(N ** 2)
    a = generate_A(N)
    a = csc_matrix(a) # transform to the fitting matrix
    b = generate_b(N, g, dx)
    x = splinalg.spsolve(a, b).reshape(N, N)
    return x

# %%
def setup(N):
  min, max = -5, 5
  dx = (max - min) / N

  x = np.linspace(-5, 5, N)
  y = np.linspace(-5, 5, N)
  g = np.zeros([N, N])

  return N, g, dx, x, y
```

```python
# %%
t0_32 = time.time()
N, g, dx, x, y = setup(32)
u = psolve(N, g, dx, x, y)
t00_32 = time.time()
t32 = np.round(t00_32 - t0_32, 5)

t0_64 = time.time()
N, g, dx, x, y = setup(64)
u = psolve(N, g, dx, x, y)
t00_64 = time.time()
t64 = np.round(t00_64 - t0_64, 5)

t0_128 = time.time()
N, g, dx, x, y = setup(128)
u = psolve(N, g, dx, x, y)
t00_128 = time.time()
t128 = np.round(t00_128 - t0_128, 5)

m = [[t32, t64, t128], [32, 64, 128]]

# %%
def setup32():
    tor       = 1e-7
    xmin, xmax = -5, 5
    ymin, ymax = -5, 5
    nx, ny    = 32, 32
    buff_size = 1

    mesh = Mesh2D(nx = nx, ny = ny, buff_size = buff_size)
    mesh.set_xmin(xmin)
    mesh.set_xmax(xmax)
    mesh.set_ymin(ymin)
    mesh.set_ymax(ymax)

    return tor, mesh

# %%
def setup64():
    tor       = 1e-7
    xmin, xmax = -5, 5
    ymin, ymax = -5, 5
    nx, ny    = 64, 64
    buff_size = 1

    mesh = Mesh2D(nx = nx, ny = ny, buff_size = buff_size)
    mesh.set_xmin(xmin)
    mesh.set_xmax(xmax)
    mesh.set_ymin(ymin)
    mesh.set_ymax(ymax)

    return tor, mesh
```

```
# %%
def setup128():
    tor      = 1e-7
    xmin, xmax = -5, 5
    ymin, ymax = -5, 5
    nx, ny   = 128, 128
    buff_size = 1

    mesh = Mesh2D(nx = nx, ny = ny, buff_size = buff_size)
    mesh.set_xmin(xmin)
    mesh.set_xmax(xmax)
    mesh.set_ymin(ymin)
    mesh.set_ymax(ymax)

    return tor, mesh

# %%
'''
Jacobi
'''
def j(name):
  if name == 32:
    ini = setup32()
  elif name == 64:
    ini = setup64()
  elif name == 128:
    ini = setup128()
  else:
    print("No such Grid!")
    quit()

  t1 = time.time()
  # name == Gauss or Jacobi or SOR
  j_arr = solve("Jacobi", ini[0], ini[1])
  t2 = time.time()

  # print(f"Jocobi{name} -> Time = ", np.round((t2-t1), 2))
  return name, np.round((t2-t1), 5)

# %%
'''
Gauss-Seidel
'''
def g(name):
  if name == 32:
    ini = setup32()
  elif name == 64:
    ini = setup64()
  elif name == 128:
    ini = setup128()
  else:
    print("No such Grid!")
```

```
        quit()

      t3 = time.time()
      # name == Gauss or Jacobi or SOR
      g_arr = solve("Gauss", ini[0], ini[1])
      t4 = time.time()

      # print(f"Gauss{name} -> Time = ", np.round((t4-t3), 2))
      return name, np.round((t4-t3), 5)

    # %%
    '''
    SOR
    '''
    def s(name):
      if name == 32:
        ini = setup32()
      elif name == 64:
        ini = setup64()
      elif name == 128:
        ini = setup128()
      else:
        print("(s1) No such Grid!")
        quit()

      t5 = time.time()
      # name == Gauss or Jacobi or SOR
      w1, w2 = 1.2, 1.5

      s1_arr = solve("SOR", ini[0], ini[1], w = w1)
      t6 = time.time()

      if name == 32:
        ini = setup32()
      elif name == 64:
        ini = setup64()
      elif name == 128:
        ini = setup128()
      else:
        print("(s2) No such Grid!")
        quit()
      t7 = time.time()
      s2_arr = solve("SOR", ini[0], ini[1], w = w2)
      t8 = time.time()

      # print(f"SOR{name} -> Time = ", np.round((t6-t5), 2))
      # print(f"SOR{name} -> Time = ", np.round((t8-t7), 2))
      return name, w1, w2, np.round((t6-t5), 5), np.round((t8-t7), 5)

    # %% [markdown]
    # ### Error convergence.
    #
```

```python
        # To see how it converge, we could make a of Error vs. Iteration times to see how it converges.

        # %%
        import matplotlib
        figure(figsize=(11, 7), dpi=150)
        matplotlib.rcParams['legend.handlelength'] = 0
        matplotlib.rcParams['legend.numpoints'] = 1
        plt.yscale('log')
        plt.xscale('log')

        j  = [[j(32)[1], j(64)[1], j(128)[1]], [[j(32)[0], j(64)[0], j(128)[0]]]]
        g  = [[g(32)[1], g(64)[1], g(128)[1]], [[g(32)[0], g(64)[0], g(128)[0]]]]
        s1 = [[s(32)[3], s(64)[3], s(128)[3]], [s(32)[0], s(64)[0], s(128)[0]]]
        s2 = [[s(32)[4], s(64)[4], s(128)[4]], [s(32)[0], s(64)[0], s(128)[0]]]

        plt.plot(j[0], j[1][0], '--o', alpha = .3, color = 'r', label = "Jacobi")
        plt.plot(g[0], g[1][0], '--o', alpha = .3, color = 'g', label = "Gauss-Seidel")
        plt.plot(m[0], m[1], '--o', alpha = .3, color = 'b', label = "Sparse Matrix")
        plt.plot(s1[0], s1[1], '--o', alpha = .5, color = 'y', label = f"SOR, w = {s(32)[1]}")
        plt.plot(s2[0], s2[1], '--o', alpha = .9, color = 'y', label = f"SOR, w = {s(32)[2]}")

        plt.xlabel("time (log) [s]")
        plt.ylabel("Resolution (log)")
        plt.title("Resolution vs time")
        plt.legend(loc = 'best')
```