Assignment III

Github (https://github.com/bestfranklinAI/Cython-HPC-)

In [2]:
```
import numpy as np
import matplotlib.pyplot as plt
import time
import h5py
import cProfile
```

In [1]:
```
from functools import wraps
import time

times = {}

def times_init():
    times.clear()
    times["pylist"] = []
    times["pyarray"] = []
    times["nparray"] = []
    times['GPU'] = []
    times["nvidia"] = []

# decorator to time
def timefn(fn):
    @wraps(fn)
    def measure_time(*args, **kwargs):
        t1 = time.time()
        result = fn(*args, **kwargs)
        t2 = time.time()
        print(f"@timefn: {fn.__name__} took {t2 - t1} seconds")
        times[fn.__name__].append(t2 - t1)
        return result
    return measure_time
```

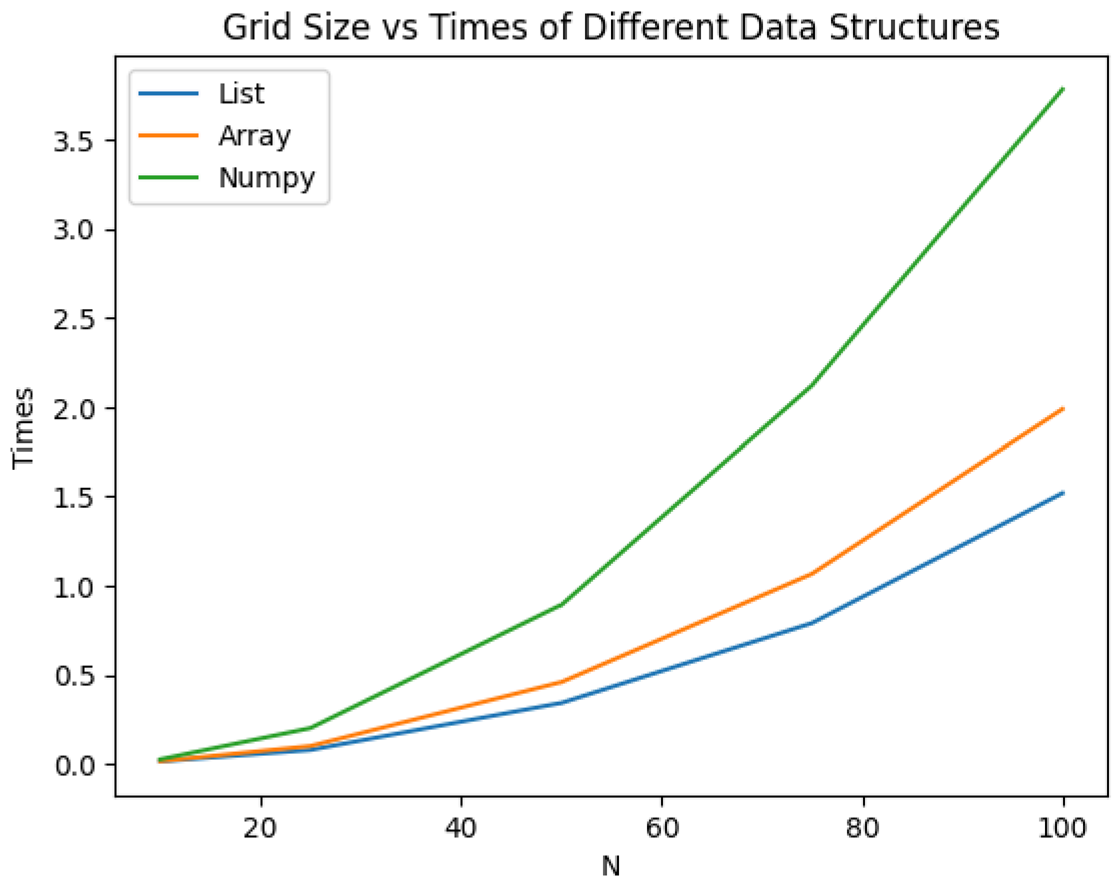
Exercise 1 - Gauss-Seidel for Poisson Solver

Task 1.1

In [3]:
```
import array
import random
import numpy as np
import matplotlib.pyplot as plt

@timefn
def pylist(f, iterations):
    newf = [row.copy() for row in f]
    for _ in range(iterations):
        for i in range(1, len(newf) - 1):
            for j in range(1, len(newf) - 1):
                newf[i][j] = 0.25 * (newf[i][j + 1] + newf[i][j - 1] +
                                     newf[i + 1][j] + newf[i - 1][j])
```

```
    return newf

@timefn
def pyarray(f, iterations):
    newf = f.copy()
    for _ in range(iterations):
        for i in range(1, len(newf) - 1):
            for j in range(1, len(newf) - 1):
                newf[i][j] = 0.25 * (newf[i][j + 1] + newf[i][j - 1] +
                                     newf[i + 1][j] + newf[i - 1][j])
    return newf

@timefn
def nparray(f, iterations):
    newf = f.copy()
    for _ in range(iterations):
        # newf[1:-1, 1:-1] = 0.25 * (newf[1:-1, 2:] + newf[1:-1, :-2] +
        #                            newf[2:, 1:-1] + newf[:-2, 1:-1])
        for i in range(1,newf.shape[0]-1):
            for j in range(1,newf.shape[1]-1):
                newf[i,j] = 0.25 * (newf[i,j+1] + newf[i,j-1] +
                                     newf[i+1,j] + newf[i-1,j])
    return newf

Ns = [10, 25, 50, 75, 100]

if __name__ == "__main__":
    times_init()
    for n, N in enumerate(Ns):
        print(f"N = {N}")
        a = [[random.uniform(1, 100) for _ in range(N)] for _ in range(N)
        # Python list
        pylist(a, 1000)
        # Python array
        pyarray([array.array('f', row) for row in a], 1000)
        # Numpy array
        nparray(np.array(a), 1000)
        print(f"@timefn: pylist took {times['pylist'][n]} seconds")
        print(f"@timefn: pyarray took {times['pyarray'][n]} seconds")
        print(f"@timefn: nparray took {times['nparray'][n]} seconds")
    plt.plot(Ns, times["pylist"], label="List")
    plt.plot(Ns, times["pyarray"], label="Array")
    plt.plot(Ns, times["nparray"], label="Numpy")
    plt.title("Grid Size vs Times of Different Data Structures")
    plt.legend(loc="upper left")
    plt.xlabel("N")
    plt.ylabel("Times")
    plt.show()
```

```
N = 10
@timefn: pylist took 0.016114234924316406 seconds
@timefn: pyarray took 0.01741194725036621 seconds
@timefn: nparray took 0.027540922164916992 seconds
N = 25
@timefn: pylist took 0.08029794692993164 seconds
@timefn: pyarray took 0.10222697257995605 seconds
@timefn: nparray took 0.20291566848754883 seconds
N = 50
@timefn: pylist took 0.3435990810394287 seconds
@timefn: pyarray took 0.4604320526123047 seconds
@timefn: nparray took 0.8927969932556152 seconds
N = 75
@timefn: pylist took 0.7912530899047852 seconds
@timefn: pyarray took 1.0671000480651855 seconds
@timefn: nparray took 2.1202292442321777 seconds
N = 100
@timefn: pylist took 1.5192461013793945 seconds
@timefn: pyarray took 1.988356113433838 seconds
@timefn: nparray took 3.7797138690948486 seconds
```



Task 1.2

gaussseidel.py

In [6]:
```
from line_profiler import profile

@profile
def gauss_seidel(f):
    newf = f.copy()
    for i in range(1,newf.shape[0]-1):
        for j in range(1,newf.shape[1]-1):
```

```
                newf[i,j] = 0.25 * (newf[i,j+1] + newf[i,j-1] +
                                        newf[i+1,j] + newf[i-1,j])
    return newf

if __name__ == "__main__":
    N = 100
    x = np.array([[random.uniform(1, 100) for _ in range(N)] for _ in ran
    for i in range(1000):
        x = gauss_seidel(x)
```

In [7]:
```
! python -m kernprof -l gaussseidel.py
! python -m line_profiler gaussseidel.py.lprof
```

```
Wrote profile results to gaussseidel.py.lprof
Inspect results with:
python -m line_profiler -rmt "gaussseidel.py.lprof"
Timer unit: 1e-06 s

Total time: 9.26955 s
File: gaussseidel.py
Function: gauss_seidel at line 5

Line #      Hits         Time  Per Hit   % Time  Line Contents
==============================================================
     5                                           @profile
     6                                           def gauss_seidel(f):
     7      1000       3747.0      3.7      0.0      newf = f.copy()
     8     99000      10503.0      0.1      0.1      for i in range(1, new
f.shape[0] - 1):
     9   9702000     965605.0      0.1     10.4          for j in range(1,
newf.shape[1] - 1):
    10  28812000    5625909.0      0.2     60.7              newf[i, j] =
0.25 * (newf[i, j + 1] + newf[i, j - 1] +
    11  19208000    2663623.0      0.1     28.7
newf[i + 1, j] + newf[i - 1, j])
    12
    13      1000        165.0      0.2      0.0      return newf
```

Task 1.3

In [9]:
```
!cython -a gaussseidel.pyx
```

```
/opt/miniconda3/envs/hpc/lib/python3.10/site-packages/Cython/Compiler/Mai
n.py:381: FutureWarning: Cython directive 'language_level' not set, using
'3str' for now (Py3). This has changed from earlier releases! File: /User
s/franklin/Codes/COMP/High Performance Computing (KTH)/HW3/gaussseidel.pyx
  tree = Parsing.p_module(s, pxd, full_module_name)
```

```
Generated by Cython 3.0.12

Yellow lines hint at Python interaction.
Click on a line that starts with a "+" to see the C code that Cython generated for it.

Raw output: gaussseidel.c

+01: import numpy as np
+02: import random
   __pyx_t_2 = __Pyx_ImportDottedModule(__pyx_n_s_random, NULL); if (unlikely(!__pyx_t_2)) __PYX_ERR(0, 2, __pyx_L1_error)
   __Pyx_GOTREF(__pyx_t_2);
   if (PyDict_SetItem(__pyx_d, __pyx_n_s_random, __pyx_t_2) < 0) __PYX_ERR(0, 2, __pyx_L1_error)
   __Pyx_DECREF(__pyx_t_2); __pyx_t_2 = 0;
 03:
 04:
 05:
+06: def gauss_seidel(f):
+07:     newf = f.copy()
+08:     for i in range(1, newf.shape[0] - 1):
+09:         for j in range(1, newf.shape[1] - 1):
+10:             newf[i, j] = 0.25 * (newf[i, j + 1] + newf[i, j - 1] +
+11:                                  newf[i + 1, j] + newf[i - 1, j])
 12:
+13:     return newf
```

Task 1.4

In [10]:

```
!cython -a gauss.pyx
```

```
/opt/miniconda3/envs/hpc/lib/python3.10/site-packages/Cython/Compiler/Mai
n.py:381: FutureWarning: Cython directive 'language_level' not set, using
'3str' for now (Py3). This has changed from earlier releases! File: /User
s/franklin/Codes/COMP/High Performance Computing (KTH)/HW3/gauss.pyx
  tree = Parsing.p_module(s, pxd, full_module_name)
```

```
Generated by Cython 3.0.12

Yellow lines hint at Python interaction.
Click on a line that starts with a "+" to see the C code that Cython generated for it.

Raw output: gauss.c

+01: # cython: boundscheck=False, wraparound=False, cdivision=True
+02: import numpy as np
 03: cimport numpy as np
 04:
+05: def cython_gauss_seidel(np.ndarray[double, ndim=2] f, int iterations=1000):
 06:     """Cython-optimized Gauss-Seidel solver (Task 1.4)."""
+07:     cdef int i, j, it, n = f.shape[0]
+08:     cdef int m = f.shape[1]
+09:     cdef np.ndarray[double, ndim=2] newf = f.copy()
 10:
+11:     for it in range(iterations):
+12:         for i in range(1, n-1):
+13:             for j in range(1, m-1):
+14:                 newf[i, j] = 0.25 * (newf[i, j+1] + newf[i, j-1] +
+15:                                      newf[i+1, j] + newf[i-1, j])
+16:     return newf
```

Task 1.5

In [ ]:

```
import torch
import cupy as cp
```

In [ ]:
```
@timefn
def GPU(f, iterations=1000, device=None):
    if device is None:
        device = torch.device("cuda" if torch.cuda.is_available() else "c
    f = f.to(device)
    for it in range(iterations):
        f = 0.25 * (torch.roll(f, shifts=1, dims=0) +
                    torch.roll(f, shifts=-1, dims=0) +
                    torch.roll(f, shifts=1, dims=1) +
                    torch.roll(f, shifts=-1, dims=1))
    return f
```

In [ ]:
```
def GPU_iterations(n):
  grid_size = n
  f_torch = torch.zeros((grid_size, grid_size), dtype=torch.float32)
  f_torch[grid_size//2, grid_size//2] = 1.0
  result_torch = GPU(f_torch, iterations=100)
  print('Max value:', result_torch.max().item())
```

In [ ]:
```
Ns = [10, 25, 50, 75, 100]


times_init()
for n in Ns:
    print(f"N = {N}")
    GPU_iterations(N)
```

```
N = 10
@timefn: GPU took 0.007311344146728516 seconds
Max value: 52.40863037109375
N = 25
@timefn: GPU took 0.0073566436767578125 seconds
Max value: 52.669822692871094
N = 50
@timefn: GPU took 0.007281780242919922 seconds
Max value: 54.40192413330078
N = 75
@timefn: GPU took 0.007548093795776367 seconds
Max value: 55.23120880126953
N = 100
@timefn: GPU took 0.007348775863647461 seconds
Max value: 55.676395416259766
```

Task 1.6

In [ ]:
```
import cupy as cp
```

In [ ]:
```
@timefn
def nvidia(f, iterations=1000):
    for it in range(iterations):
        f = 0.25 * (cp.roll(f, shift=1, axis=0) +
                    cp.roll(f, shift=-1, axis=0) +
                    cp.roll(f, shift=1, axis=1) +
```

```
                        cp.roll(f, shift=-1, axis=1))
    return f
```

In [ ]:
```
def nvidia_iterations(n):


  grid_size = n
  f_cupy = cp.zeros((grid_size, grid_size), dtype=cp.float64)
  f_cupy[grid_size//2, grid_size//2] = 1.0
  result_cupy = nvidia(f_cupy, iterations=100)
  cp.cuda.Stream.null.synchronize()
  print('Max value:', cp.max(result_cupy).get())
```

In [ ]:
```
Ns = [10, 25, 50, 75, 100]


times_init()
for n in Ns:
    print(f"N = {N}")
    nvidia_iterations(N)
```

```
N = 10
@timefn: nvidia took 0.03714108467102051 seconds
Max value: 55.39032454040849
N = 25
@timefn: nvidia took 0.034827232360839844 seconds
Max value: 54.55565667689732
N = 50
@timefn: nvidia took 0.036354780197143555 seconds
Max value: 55.951031270515635
N = 75
@timefn: nvidia took 0.0346524715423584 seconds
Max value: 54.61823762353901
N = 100
@timefn: nvidia took 0.0458371639251709 seconds
Max value: 54.921316716800376
```

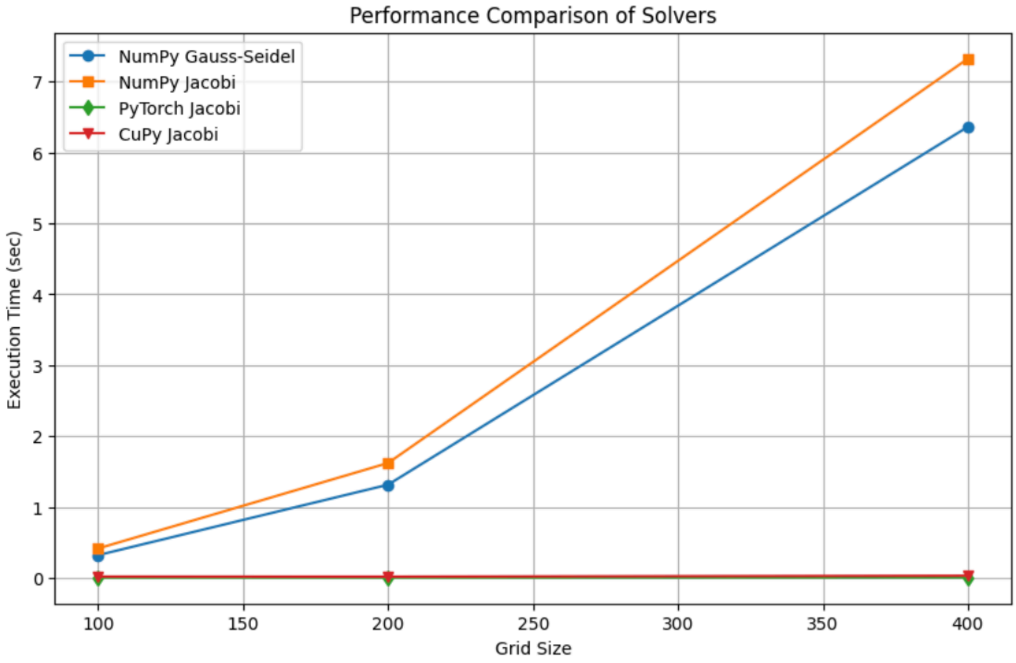
Task 1.7

In [15]:
```
import gauss

def benchmark(func, *args, **kwargs):
    start = time.perf_counter()
    result = func(*args, **kwargs)
    end = time.perf_counter()
    return result, end - start

grid_sizes = [100, 200, 400]
gs_times = []
jacobi_times = []
cython_times = []
pytorch_times = []
cupy_times = []
```

```
iterations = 50  # Use a smaller number for demonstration purposes
```

In [ ]:
```
for size in grid_sizes:
    print(f"\nGrid Size: {size}")
    f = np.zeros((size, size), dtype=np.float64)
    f[size//2, size//2] = 1.0

    # NumPy Gauss-Seidel
    _, t_gs = benchmark(pylist, f, iterations)
    gs_times.append(t_gs)
    print(f"NumPy Gauss-Seidel: {t_gs:.4f} sec")

    # NumPy Jacobi
    _, t_jacobi = benchmark(nparray, f, iterations)
    jacobi_times.append(t_jacobi)
    print(f"NumPy Jacobi: {t_jacobi:.4f} sec")

    # Cython Gauss-Seidel
    _, t_cython = benchmark(gauss.cython_gauss_seidel, f, iterations)
    cython_times.append(t_cython)
    print(f"Cython Gauss-Seidel: {t_cython:.4f} sec")

    # PyTorch Jacobi
    f_torch = torch.from_numpy(f).float()
    _, t_torch = benchmark(GPU, f_torch, iterations)
    pytorch_times.append(t_torch)
    print(f"PyTorch Jacobi: {t_torch:.4f} sec")

    # CuPy Jacobi
    f_cupy = cp.array(f)
    cp.cuda.Stream.null.synchronize()
    start = time.perf_counter()
    _ = nvidia(f_cupy, iterations)
    cp.cuda.Stream.null.synchronize()
    t_cupy = time.perf_counter() - start
    cupy_times.append(t_cupy)
    print(f"CuPy Jacobi: {t_cupy:.4f} sec")

# Plotting the performance comparison
plt.figure(figsize=(10, 6))
plt.plot(grid_sizes, gs_times, 'o-', label='NumPy Gauss-Seidel')
plt.plot(grid_sizes, jacobi_times, 's-', label='NumPy Jacobi')
# plt.plot(grid_sizes, cython_times, '^-', label='Cython Gauss-Seidel')
plt.plot(grid_sizes, pytorch_times, 'd-', label='PyTorch Jacobi')
plt.plot(grid_sizes, cupy_times, 'v-', label='CuPy Jacobi')
plt.xlabel('Grid Size')
plt.ylabel('Execution Time (sec)')
plt.title('Performance Comparison of Solvers')
plt.legend()
plt.grid(True)
plt.show()
```

```
Grid Size: 200
@timefn: pylist took 1.3143630027770996 seconds
NumPy Gauss-Seidel: 1.3145 sec
@timefn: nparray took 1.6195251941680908 seconds
NumPy Jacobi: 1.6200 sec
@timefn: GPU took 0.0039255619049072266 seconds
PyTorch Jacobi: 0.0040 sec
@timefn: nvidia took 0.01689743995666504 seconds
CuPy Jacobi: 0.0174 sec

Grid Size: 400
@timefn: pylist took 6.364067554473877 seconds
NumPy Gauss-Seidel: 6.3642 sec
@timefn: nparray took 7.324380874633789 seconds
NumPy Jacobi: 7.3245 sec
@timefn: GPU took 0.006232738494873047 seconds
PyTorch Jacobi: 0.0063 sec
@timefn: nvidia took 0.029954910278320312 seconds
CuPy Jacobi: 0.0306 sec
```



The one with GPU has seen significant improvement in speed, while the numpy one without GPU remains as the slowest.

In [17]:
```
import gauss

N = 100
arr = np.array([[random.uniform(1, 100) for _ in range(N)] for _ in range
gauss.cython_gauss_seidel(arr, 1000)
```

Out[17]:
```
array([[15.34998779,  7.07198273, 81.27156397, ..., 81.17868071,
        12.78488569, 23.94690078],
       [10.70246122, 25.64927854, 48.9316945 , ..., 53.5949884 ,
        28.08956988, 14.02130493],
       [35.21869902, 35.89098334, 42.99400896, ..., 47.35310207,
        31.95710213,  3.31183442],
       ...,
       [26.34357973, 49.54888343, 53.67329496, ..., 51.67885644,
        48.68880392, 43.92562834],
       [83.51624529, 58.22263926, 54.80784311, ..., 56.30646543,
        51.41483171, 46.19858131],
       [ 4.24149496, 45.01758808, 52.68768298, ..., 65.5521781 ,
        54.46547618, 17.12217905]])
```

Task 1.8

In [18]:
```
final_grid, _ = benchmark(gauss.cython_gauss_seidel, f, iterations)


with h5py.File('final_grid.h5', 'w') as hf:
    hf.create_dataset('grid', data=final_grid)

print('Final grid saved to final_grid.h5')
```

```
Final grid saved to final_grid.h5
```

Bonus Exercise - Fast Fractal Fun with Cython & GPUs

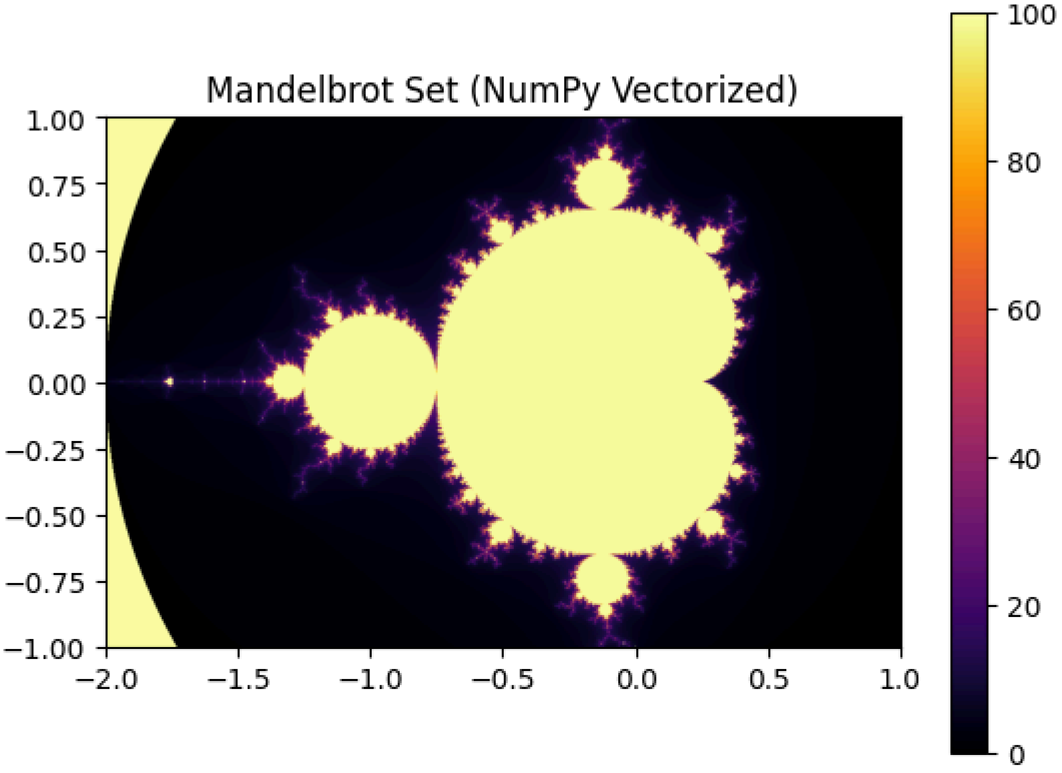
Pure Python

In [ ]:
```
import numpy as np
import time

def mandelbrot_python(width, height, x_min, x_max, y_min, y_max, max_iter
    x_vals = np.linspace(x_min, x_max, width)
    y_vals = np.linspace(y_min, y_max, height)
    image = np.zeros((height, width), dtype=int)

    for i in range(height):
        for j in range(width):
            c = complex(x_vals[j], y_vals[i])
            z = 0 + 0j
            for n in range(max_iter):
                if abs(z) > 2:
                    image[i, j] = n
                    break
                z = z * z + c
            else:
                image[i, j] = max_iter
    return image
```

numpy

In [ ]:
```
import numpy as np
import matplotlib.pyplot as plt

def mandelbrot_numpy(width, height, x_min, x_max, y_min, y_max, max_iter=
    x_vals = np.linspace(x_min, x_max, width)
    y_vals = np.linspace(y_min, y_max, height)
    X, Y = np.meshgrid(x_vals, y_vals)
    C = X + 1j * Y

    Z = np.zeros_like(C, dtype=np.complex128)
    M = np.full(C.shape, max_iter, dtype=np.int32)
    mask = np.ones(C.shape, dtype=bool)

    for i in range(max_iter):
        Z[mask] = Z[mask] ** 2 + C[mask]
```

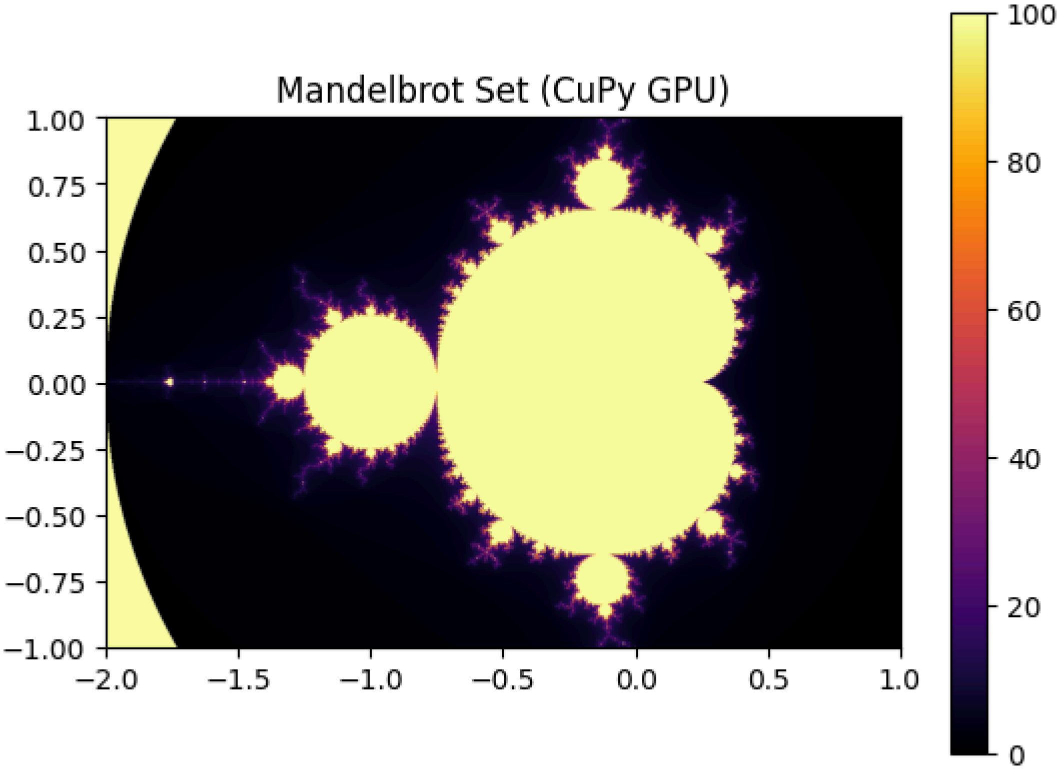
```
        mask = (np.abs(Z) <= 2)
        M[mask] = i

    return M

width, height = 1000, 800
x_min, x_max, y_min, y_max = -2, 1, -1, 1
image = mandelbrot_numpy(width, height, x_min, x_max, y_min, y_max)

plt.imshow(image, cmap='inferno', extent=[x_min, x_max, y_min, y_max])
plt.colorbar()
plt.title("Mandelbrot Set (NumPy Vectorized)")
plt.show()
```



Cupy

In [ ]:
```
import cupy as cp
import matplotlib.pyplot as plt

def mandelbrot_gpu(width, height, x_min, x_max, y_min, y_max, max_iter=10
    x_vals = cp.linspace(x_min, x_max, width)
    y_vals = cp.linspace(y_min, y_max, height)
    X, Y = cp.meshgrid(x_vals, y_vals)
    C = X + 1j * Y

    Z = cp.zeros_like(C, dtype=cp.complex128)
    M = cp.full(C.shape, max_iter, dtype=cp.int32)
    mask = cp.ones(C.shape, dtype=bool)

    for i in range(max_iter):
        Z[mask] = Z[mask] ** 2 + C[mask]
        mask = (cp.abs(Z) <= 2)
        M[mask] = i

    return cp.asnumpy(M)
```

```
width, height = 1000, 800
image = mandelbrot_gpu(width, height, -2, 1, -1, 1)

plt.imshow(image, cmap='inferno', extent=[-2, 1, -1, 1])
plt.colorbar()
plt.title("Mandelbrot Set (CuPy GPU)")
plt.show()
```



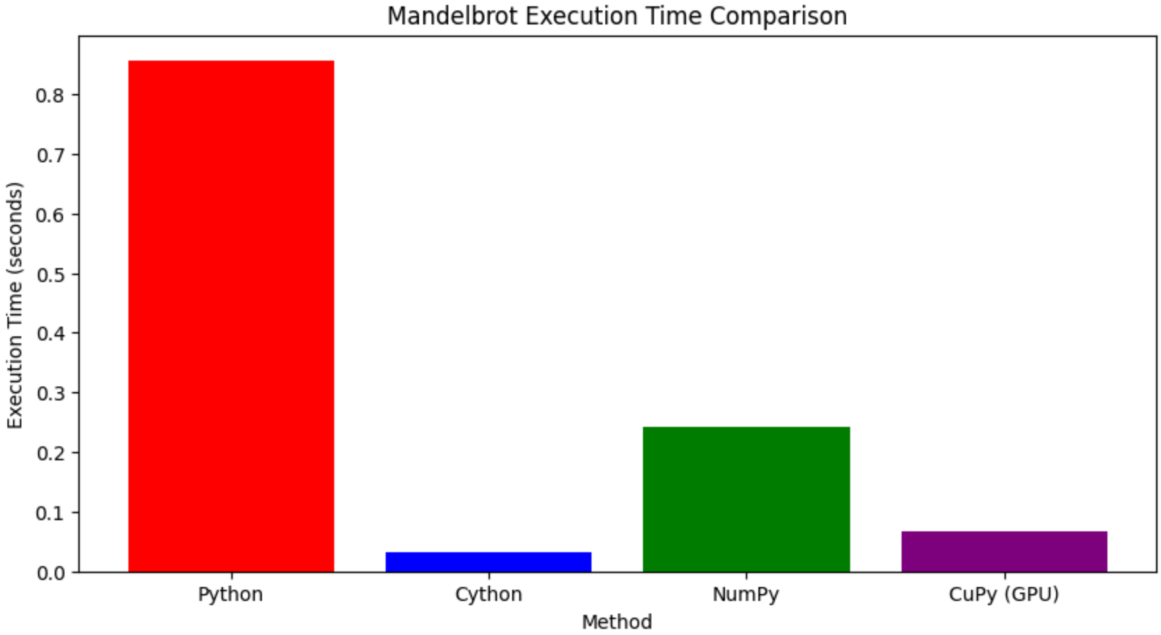
Comparison

In [ ]:
```
import sys
sys.path.append(r"build/lib.win-amd64-cpython-312")
```

In [ ]:
```
import time
import matplotlib.pyplot as plt
import mandelbrot_cython

width, height = 500, 500
x_min, x_max, y_min, y_max = -2, 1, -1, 1
max_iter = 100

def time_execution(func, *args):
    start = time.time()
    func(*args)
    return time.time() - start

times = {
    "Python": time_execution(mandelbrot_python, width, height, x_min, x_m
    "Cython": time_execution(mandelbrot_cython.mandelbrot_set_cython, wid
    "NumPy": time_execution(mandelbrot_numpy, width, height, x_min, x_max
    "CuPy (GPU)": time_execution(mandelbrot_gpu, width, height, x_min, x_
}

for method, t in times.items():
```

```
    print(f"{method} execution time: {t:.4f} seconds")


plt.figure(figsize=(10, 5))
plt.bar(times.keys(), times.values(), color=['red', 'blue', 'green', 'pur
plt.xlabel("Method")
plt.ylabel("Execution Time (seconds)")
plt.title("Mandelbrot Execution Time Comparison")
plt.show()
```

```
Python execution time: 0.8559 seconds
Cython execution time: 0.0316 seconds
NumPy execution time: 0.2410 seconds
CuPy (GPU) execution time: 0.0666 seconds
```



When comparing the performance of NumPy and CuPy, a significant factor affecting execution time is data transfer between CPU and GPU. NumPy operations are executed on the CPU, while CuPy operations run on the GPU. If data is frequently transferred between the two, it can significantly slow down execution.