APC 524 Final Project:

Implementing a Navier-Stokes Solver and Physics Informed Neural Network for Simulating Two-Dimensional Fluid Flow Around a Cylinder

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1 Introduction

The Navier–Stokes (NS) equations describe fluid dynamics and have been applied to weather prediction, glacier dynamics, oceanography, thermal conduction, aircraft design, and architecture [5]. Despite their widespread use, analytic solutions exist only for a few constrained cases. As a result, the finite difference method (FDM) and finite element method (FEM) have become popular numerical approaches for obtaining approximate solutions [14]. These methods are computationally expensive, often requiring hundreds or thousands of core-hours to produce meaningful accurate results, and the largest simulations often require specialized hardware for effective scalability [8].

Recent advances in physics informed neural networks (PINNs) allow for high resolution and physically consistent approximations of the NS equations [7] [4] [6]. PINNs are supervised neural networks that take advantage of their capabilities as universal function approximators to incorporate model equations, such as partial differential equations, directly into the loss function during training [11]. This new loss term, known as the equation loss, is derived from the underlying physical system of equations accompanying the traditional mean square loss.

2 The Equations

The NS equations, governing the fluid flow, are expressed as:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = -\frac{1}{\rho}\frac{\partial p}{\partial x} + \nu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right), \tag{1}$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} = -\frac{1}{\rho}\frac{\partial p}{\partial y} + \nu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right), \tag{2}$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \tag{3}$$

where u and v are the fluid velocities in the x and y directions, respectively, p is the pressure, ρ is the fluid density, and ν is the kinematic viscosity.

3 Overview

This project contains the following features:

1. An implementation of a modular Navier-Stokes solver using the Finite Difference Method.
   (a) A python class to define arbitrary environments and environmental conditions.
   (b) Modular boundary conditions allowing for many environment types to be investigated.
   (c) Modular and composable objects that allow for complex environments to be modeled and simulated.
2. A Physics Informed Neural Network that approximates a Navier-Stokes solver.
   (a) A python class to initialize, train, and test the Navier-Stokes PINN model.
   (b) Input-output manager to simplify preparation of training and testing datasets.
   (c) Plotting manager to facilitate in simple visualization of model inference.
3. Unit tests implemented with "pytest" and automated testing using GitHub Actions.

4 Joseph Lockwood's Contributions

4.1 A derivation and implementation of an NS solver to simulate the two-dimensional cylinder wake flow.

I implemented the initial finite-element Navier-Stokes (NS) solver [3] to simulate two-dimensional cylinder wake flow – the focus of which was on incompressible, viscous fluid flow [9]. The inclusion of viscosity in the model and the application of no-slip boundary conditions [13] is required to capture the nuanced behavior of real fluid flows often found in engineering applications. The presence of a square obstacle in the flow field allows us to investigate complex phenomena like separation, and vortex-shedding and wake formation [15, 1].

4.1.1 Implementation

The solver was implemented in Python, utilizing NumPy for efficient array computations. It initializes the velocity and pressure fields, and defines a cylinder obstruction in the flow. The update functions for velocity and pressure discretize the NS equations using finite difference methods. The solver handles complex phenomena like vortex shedding, illustrated in the simulations around the cylinder. Regular plotting intervals offer visual insights into the evolving fluid dynamics.

4.1.2 Equations for Velocity and Pressure Update

The velocity and pressure updates incorporate advection, pressure gradients, and diffusion:

$$u_{next} = u - u \cdot dt \cdot \frac{\partial u}{\partial x} - v \cdot dt \cdot \frac{\partial u}{\partial y} - \frac{dt}{\rho}\frac{\partial p}{\partial x} + \nu \cdot dt \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right), \tag{4}$$

$$v_{next} = v - u \cdot dt \cdot \frac{\partial v}{\partial x} - v \cdot dt \cdot \frac{\partial v}{\partial y} - \frac{dt}{\rho}\frac{\partial p}{\partial y} + \nu \cdot dt \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right). \tag{5}$$

The pressure update, derived from the Poisson equation to ensure incompressibility, is given by:

$$\begin{aligned} p_{next} = \frac{1}{2 \cdot (dx^2 + dy^2)} \Big(& (p_{i+1,j} + p_{i-1,j}) \cdot dy^2 \\ & + (p_{i,j+1} + p_{i,j-1}) \cdot dx^2 \\ & - \rho \cdot ((u_{i+1,j} - u_{i-1,j})/(2 \cdot dx) + (v_{i,j+1} - v_{i,j-1})/(2 \cdot dy))^2 \cdot dx^2 \cdot dy^2 \Big). \end{aligned} \tag{6}$$

The simulation begins by initializing the velocity fields (representing fluid velocity in the x and y directions) and the pressure field. These initial conditions set the starting state of the fluid flow. The solver then discretizes the Navier-Stokes equations, which govern fluid motion, using finite difference methods in both time and space. To evolve the fluid dynamics over time, the solver employs update equations for velocity and pressure.

4.2 Unit testing

A comprehensive suite of unit tests has been implemented to ensure the robustness and reliability of the code. These tests encompass various aspects of the project, including the functionality of classes and methods, and the integrity of the environment setup. The testing approach was mainly implemented to test the reliability of each step in the solution process. The tests were designed to leverage the modular structure of the solver, enabling the examination of various functional components and critical variables within each of the utilized solver files. Consequently, a multitude of unit tests were developed to confirm the correct functioning of these distinct code segments.

Another key test is to ensure the Classes are properly initialized with default values. This test is vital for confirming that the simulation environment is set up correctly before any specific conditions or changes are applied. Additionally, we have also added tests targeted towards validating the internal mechanics of the Environment class, particularly ensuring that the methods responsible for updating matrices are functioning as expected. This is essential for the accuracy and reliability of the simulation's core computational algorithms.

These tests emphasize the importance of both verification and validation in software development. Verification ensures that the code meets set requirements and functions correctly, while validation confirms that these requirements make sense and serve the intended purpose. The tests implemented here serve as a testament to these principles, ensuring that the code not only works correctly but also fulfills its intended role effectively.

In line with the overarching principles of testing, the tests are designed to be adversarial, aiming to rigorously challenge and scrutinize the code rather than simply confirming its functionality. This approach ensures that any potential defects are identified and addressed, thereby enhancing the reliability and robustness of the code. The tests also serve as documentation, explicitly stating the expectations and requirements of the code, and they play a crucial role in growing confidence in its reliability among users.

4.3 Speed and efficiency

I integrated Python's cProfile [10] module as a step in identifying performance bottlenecks and speed of runs. This also allows for a concise comparison of the speed of the finite element NS solver against the PINN approximation. cProfile provides a detailed report on call frequency and duration of the code, which were pivotal in analyzing the efficiency. This integration was a key part of the process, allowing me to gather comprehensive performance data.

Subsequently, I executed the simulation with cProfile enabled, capturing essential performance metrics. This was critical in understanding how different segments of my code impacted the overall runtime, providing a clear overview of the simulation's performance landscape. For the analysis of the profiling data, I utilized SnakeViz [12], a sophisticated graphical viewer designed for Python profiling data. This analysis was integral in visualizing and decoding performance bottlenecks, highlighting areas where optimization was necessary (Fig. 1). The benefits of this process were multifaceted. Firstly, profiling pinpointed specific functions or methods that consumed substantial time, guiding me towards target areas for optimization. Moreover, it facilitated efficient allocation of computational resources by illuminating the most resource-intensive parts of the code, thereby aiding in more informed decisions regarding optimization.

With these insights, I embarked on optimizing and refining the code. By adjusting algorithms and refactoring, I was able to significantly improve the application's performance. This process not only enhanced the efficiency of the code but also its quality and scalability, elevating the overall standard of the software. Additionally, these optimizations led to time and cost efficiencies,

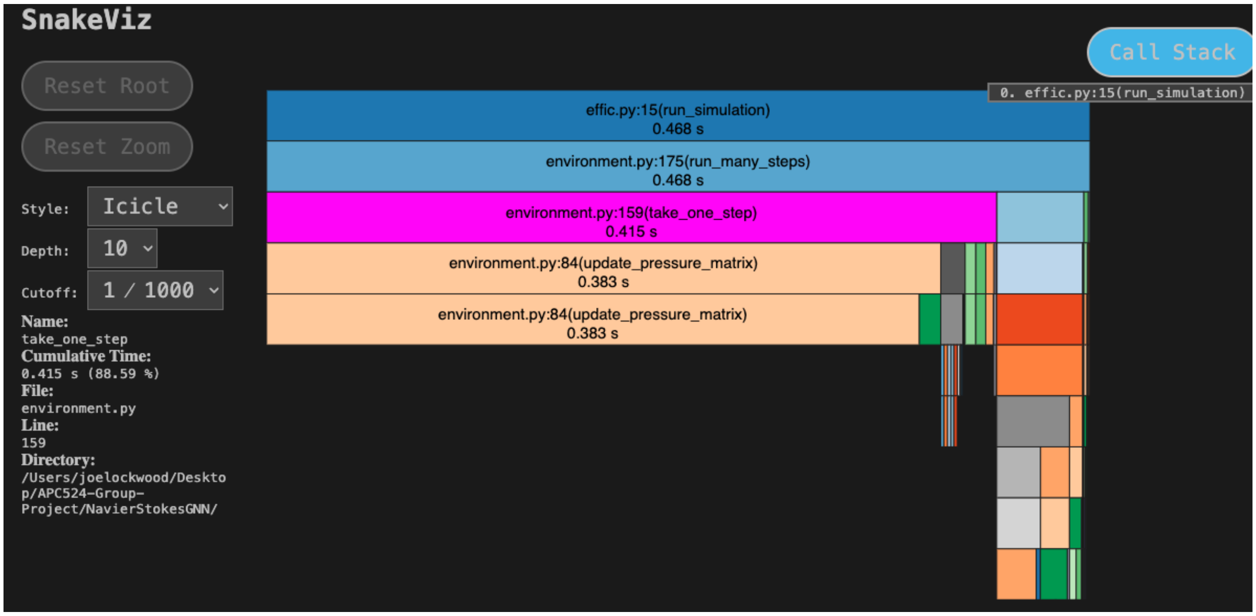

Figure 1: Sophisticated graphical viewer designed for Python profiling data using SnakeViz.

particularly beneficial in environments where computational resources are charged. The data-driven approach provided by profiling enabled me to make informed decisions, concentrating my efforts on modifications that offered substantial performance improvements.

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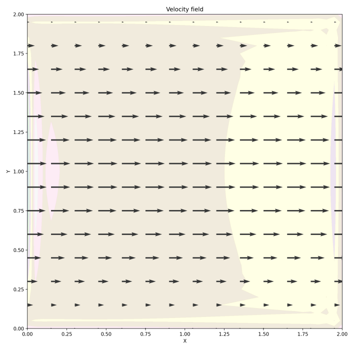
5 Aaron Spaulding's Contributions

5.1 An implementation of a Finite Difference Navier-Stokes solver to simulate the two-dimensional cylinder wake flow.

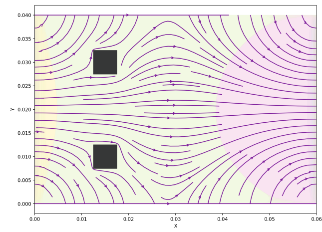
I implemented a solver for the Navier-Stokes equations using a Finite Difference(FD) method. This approach allows us to simulate fluid flows in two dimensions quickly and has been applied to many fluid related problems such as weather prediction, aerodynamics, and oceanography. I implemented this solver in python using the NumPy library for efficient array computations. The solver initializes the velocity and pressure fields and tracks changes and interactions between "parcels" of fluid interacting with each other. Each parcel is stationary and has a velocity and pressure associated with it that is updated at each time step to track the flux into and out of the parcel. This solver type enables efficient quick simulations at the cost of using fixed time steps and a fixed grid size. I implemented this solver following the equations derived by Joseph as well as work published from Barba et al.[2].

5.1.1 Environment Setup

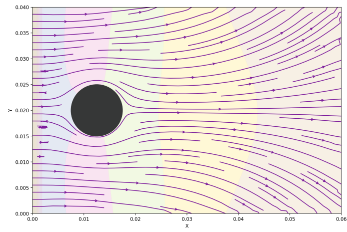
I designed the solver environment to be flexible and modular so users could easily define different size and resolution environments. The environment has a customizable grid, with adjustable resolution, time step, and fluid properties. This was implemented as a python "Environment" Class inside a module. The "Environment" class also includes automatic plotting routines that enable quick visualization of the fluid flow.



(a) Simulation of fluid flowing in a pipe. The top and bottom boundary conditions are set as no-slip conditions, while the left and right are set as periodic boundary conditions.



(b) Simulation of a fluid flowing around two boxes. Boundary conditions for all sides are set as fixed velocity conditions. The boundary conditions for the boxes are set as no-slip conditions are updated dynamically as each box is added to the environment.



(c) A simulation of fluid flow around a cylinder. Here the right, top, and bottom sides have no slip conditions while the left side has a fixed velocity boundary condition. The boundary conditions around the cylinder are automatically updated at simulation time.

Figure 2: The modular boundary conditions, customizable environment, and composable objects allows for easy simulation of complex environments with very different conditions and requirements.

5.1.2 Boundary Conditions

To extend this modularity I abstracted different types of boundary conditions common in fluid simulations. I implemented four different boundary conditions for each edge of the environment. Each of these boundary conditions is fully modular and can be mixed and matched for each simulation environment.

1. **No-Slip Boundary Condition**: This boundary condition is used to simulate a solid boundary where fluid flows are zero in both the parallel and perpendicular directions to the boundary. This is seen on the inside of pipes, along buildings and objects, and against the ground.

2. **Fixed Velocity Boundary Condition**: This boundary condition is used to simulate a boundary where fluid flows are fixed in the parallel direction to the boundary. This could be used to simulate a fan, an inlent valve, or the top of a boundary layer where the fluid is moving at a constant velocity.

3. **Periodic Boundary Condition**: This boundary condition is used to simulate a boundary where fluid flows are periodic in the parallel direction to the boundary. This can be used to simulate repeating simulations such as a section of pipe where the input and output ends are similar.

4. **Free Slip Boundary Condition**: This boundary condition is used to simulate a boundary where fluid flows are zero in the perpendicular direction to the boundary. This can be used to simulate a boundary where the fluid is free to move in the parallel direction but cannot move in the perpendicular direction.

5.1.3 Objects in the Environment

Objects inside environments also interact with fluid flows and affect the velocity and pressure fields. To enable modular simulations, I also implemented an "Object" Class that can be used to place arbitrary objects in the environment. I implemented a "Rectangle" Class that inherits from the abstract "Object" Class that automatically manages boundary conditions of the added object and updates the velocity and pressure fields during simulation. I also implemented a "Cylinder" Class that also inherits from the abstract "Object" Class.

These can be combined to make complex simulations with multiple objects interacting with each other and the fluid flow.

5.1.4 Example Simulation Setup

```python
from navier_stokes_fdm import Environment
from navier_stokes_fdm import Rectangle
import navier_stokes_fdm.boundary_condition as bc


U = 1  # m/s
dimension = 0.005

boundary_conditions = [
    bc.TopSideFixedVelocityBoundaryCondition(u_value=U, v_value=0),
    bc.BottomSideFixedVelocityBoundaryCondition(u_value=U, v_value=0),
    bc.LeftSideFixedVelocityBoundaryCondition(u_value=U, v_value=0),
    bc.RightSideFixedVelocityBoundaryCondition(u_value=U, v_value=0),
]


x1, y1 = 0.0125, (0.04 / 2) - (dimension / 2)
objects = [Rectangle(x1, y1, x1 + dimension, y1 + dimension)]


a = Environment(
    F=(1.0, 0.0),
    len_x=0.06,
    len_y=0.04,
    dt=0.00000015,
    dx=0.0001,
    boundary_conditions=boundary_conditions,
    objects=objects,
    rho=0.6125  # kg/ m
    nu=3e-5  #  m  /s
)

a.run_many_steps(480)
a.plot_streamline_plot(title="", filepath="../Figures/box_example_streamline.png")
```

5.2 Unit testing

To further ensure code functionality I implemented unit tests using "pytest" for the boundary conditions. Each test creates an environment, applies a boundary condition, and checks to see if the boundary condition has been applied correctly.

5.2.1 Automated Unit Testing with GitHub Actions

To make sure that changes to the code do not break functionality, I implemented automated testing using GitHub Actions. I wrote a GitHub Action that runs the "pytest" unit tests on every pull request and commit to the repository.

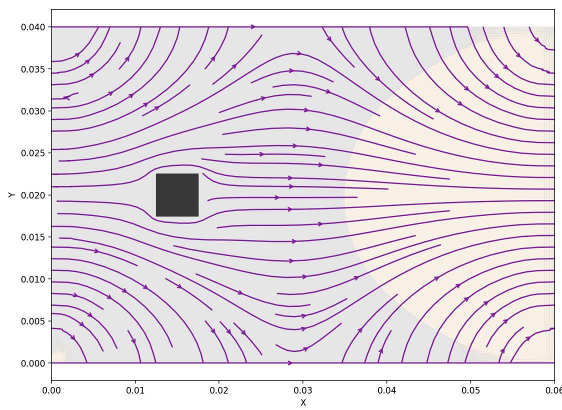
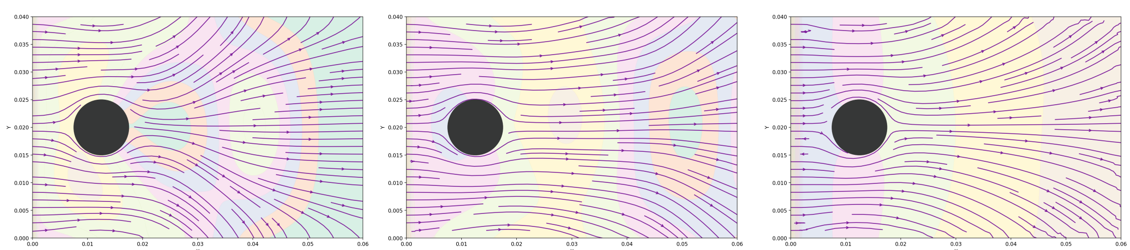


Figure 3: Example streamline plot of a fluid flow around a box. Each boundary is assigned a fixed velocity. Shading represents the pressure field with lighter colors indicating regions of lower pressure. Streamlines are shown in purple.

5.3 Simulation of a fluid flow around a cylinder

To simulate the fluid flow around a cylinder I initialized a simulation environment of $6cm$ by $4cm$ with a $5mm$ cylinder. I set ρ to be $0.6125\frac{kg}{m^3}$ and ν to be $3 * 10^{-5}\frac{m^2}{s}$. These values are physically plausible for air. The left side boundary condition was set to a fixed velocity of $1\frac{m}{s}$, and the top, right, and bottom boundaries were set as free slip conditions. The dt was set to $0.15\mu s$, and each step was a total of 30 time steps, or $4.5\mu s$. Every $4.5\mu s$ I generated and saved the streamline plot for analysis. Three selected frames are shown in Figure 4.

The simulation was stable until 10 time steps. After this point the simulation diverged. A longer simulation could be completed using a higher resolution grid, or by using smaller time steps.



(a) $9\mu s$ (b) $13.5\mu s$ (c) $45\mu s$

Figure 4: Three time steps of the FD simulation of fluid flow around a a cylinder. The pressure field is shown by the shading while streamlines are shown in purple.

6 Fairuz Ishraque's Contributions

6.1 Navier-Stokes Physics Informed Neural Network solver to simulate two-dimensional cylinder wake flow

I implemented a physics informed neural network that can train on limited simulation data and approximate the physical evolution of fluid flow described by the NS equations. My PINN model is based on the same principles as the one described in Raissi et al.[11], where the NS equations are encoded into the equations loss term. If we consider the non-dimensional NS equations below:

$$u_t + (uu_x = vu_y) = -p_x + \frac{1}{Re}(u_{xx} + u_{yy}) \tag{7}$$

$$v_t + (uv_x = vv_y) = -p_y + \frac{1}{Re}(v_{xx} + v_{yy}) \tag{8}$$

where Re is the Reynolds number, we can formulate two equation loss functions for the PINN.

$$f := u_t + (uu_x = vu_y) + p_x - \frac{1}{Re}(u_{xx} + u_{yy}) \tag{9}$$

$$g := v_t + (uv_x = vv_y) + p_y - \frac{1}{Re}(v_{xx} + v_{yy}) \tag{10}$$

Combining these equation loss functions with the data loss results in the following mean-squared error term:

$$MSE := \frac{1}{N}\Sigma_{i=1}^{N}(|u(t^i, x^i, y^i) - u^i|^2 + |v(t^i, x^i, y^i) - v^i|^2) + \frac{1}{N}\Sigma_{i=1}^{N}(|f(t^i, x^i, y^i)|^2 + |g(t^i, x^i, y^i)|^2) \tag{11}$$

The first term in equation (11) minimizes data loss from the model approximation, while the second term minimizes equation loss, since f and g are supposed to be zero according to the NS equations.

I implemented the PINN using the NumPy and Tensorflow2 libraries in python. Implementation with the Tensorflow2 library makes the model significantly more readable and modular. Additionally, I structured the model code following object-oriented design principles to make the model more user friendly.

6.1.1 PINN Training and Testing Data

For this initial PINN model implementation, I decided to use the high quality cylinder wake-flow simulation data from Raissi et al. [11], which was acquired by evolving the domain described in Figure 5. I have assumed a uniform free stream velocity profile imposed at the left boundary, a zero pressure outflow condition imposed at the right boundary located 25 diameters downstream of the cylinder, and periodicity for the top and bottom boundaries of the $[15, 25] \times [8, 8]$ domain. The free stream velocity is $u_\infty = 1$, the cylinder diameter is $D = 1$, and the Reynold's number is set to $Re = 100$. The training and testing data subdomain has been identified in with the black rectangle in the figure below. Additionally, the training data arrays are also visualized in Figure 5, where the scattered points in the arrays representing the streamwise (u) and transverse (v) velocity components indicate the $N = 5000$ training data (less than 1% of available data). Testing data are selected as select slices from the u and v arrays (the colorful slices in Figure 5 bottom)

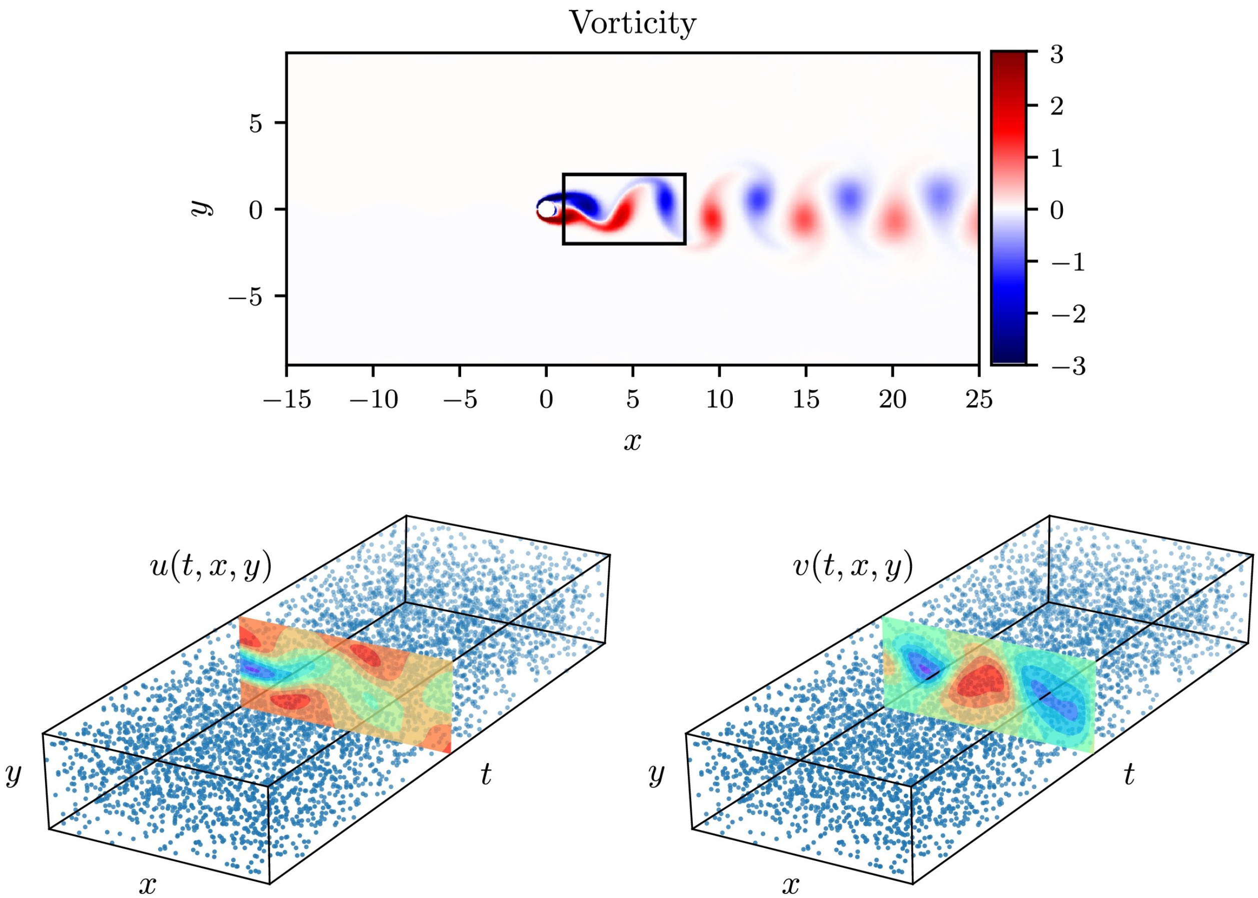


Figure 5: (Top) Incompressible flow and dynamic vortex shedding past a circular cylinder at Re = 100. Notice the black rectangle outlining the extent of the training/testing data for our PINN. (Bottom) Location of the training data points and the testing data slices in the $u(t, x, y)$ and $v(t, x, y)$ arrays. [11]

6.1.2 PINN Model Setup

I wrote the PINN model in terms of Python classes. First, I wrote the "NeuralNetwork" class that uses abstract methods to enforce essential neural network methods (`initialize_NN`, `neural_net`, `loss`, `train`, and `predict`) on classes that inherit from it. Next I had the class "PhysicsInformedNN" inherit from "NeuralNetwork", where, in addition to implementing the required methods, I also implemented additional utility methods to help with model initialization and physics-informed equation loss.

6.1.3 PINN Input-Output Handler

To handle all the data input, output, and preparation when training and testing the PINN, I implemented the I/O handler class "NavierStokesPINN_IO". The methods included in this I/O handler class help with data loading and data reduction (`parse_data_file`), randomly selecting training data (`select_training_data`), selecting data for testing (`select_test_data`), and saving model prediction results (`save_predict_data`, and `save_multi_predict_data`). Since several methods in this class depend on the implementation of another class method, I have implemented exception checks to make sure methods in I/O handler are used in a proper order.

6.1.4 PINN Plotting Handler

I also implemented a simple plotter class called "NavierStokesPINN_Plotter"that can take the I/O Handler class as an input and use parsed data as well as saved model prediction data to create and save two-dimensional plots comparing model prediction and exact ground truth values for each predicted variable (u, v, and p).

6.1.5 Example PINN Model Run

```python
import numpy as np
import tensorflow as tf
import matplotlib.pyplot as plt
from navier_stokes_pinn.PINN import PhysicsInformedNN
from navier_stokes_pinn.input_output import NavierStokesPINN_IO
from navier_stokes_pinn.plotting import NavierStokesPINN_Plotter


IO_manager = NavierStokesPINN_IO("navier_stokes_pinn/data", "navier_stokes_pinn/output
    ")
IO_manager.parse_data_file('cylinder_nektar_wake.mat')

# Selecting training data
IO_manager.select_training_data(N_train=5000)

# Extract training data from IO_manager
training_data = IO_manager.training_data

# Casting the training data into tensorflow
x_train = tf.cast(training_data['x_train'], dtype=tf.float32)
y_train = tf.cast(training_data['y_train'], dtype=tf.float32)
t_train = tf.cast(training_data['t_train'], dtype=tf.float32)
u_train = tf.cast(training_data['u_train'], dtype=tf.float32)
v_train = tf.cast(training_data['v_train'], dtype=tf.float32)

# Setting model architechture
layers = [3, 20, 20, 20, 20, 20, 20, 20, 20, 2]

# Setting Reynold's Number
Re = 100

# Initializing the PINN model
# Model training support TensorFlow 2 and GPU acceleration
model = PhysicsInformedNN(x_train, y_train, t_train, u_train, v_train, Re, layers)
# Train PINN model
model.train(2000, learning_rate=1e-3)
# Select test data at a time snapshot to test run inference and test the trained model
time_snapshot = 100
IO_manager.select_test_data(time_snapshot)
test_data = IO_manager.test_data
# Run inference and save predicted data
IO_manager.save_predict_data(model, 'example_prediction_100.npz')

# Plot the predicted data and save the plot with plotting class
Plot_manager = NavierStokesPINN_Plotter("navier_stokes_pinn/data", "navier_stokes_pinn
    /plots", IO_manager)
# Saves the u, v. and p values at the timestep 100
Plot_manager.plot_compare_predictions('example_prediction_100.npz', time_snapshot)
```

6.2 Unit Testing

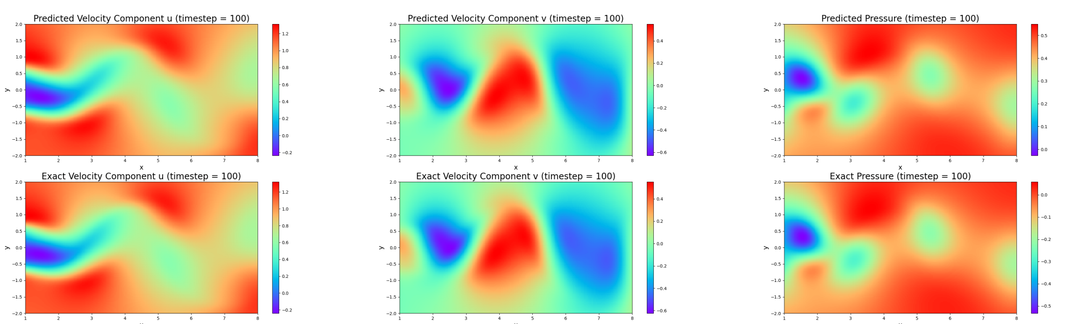
I used unit testing to verify proper initialization and functionality of the PINN model. I also wrote unit tests to verify proper implementation of each method of the IO Handler class. Almost every aspect of the PINN codebase short of training the model was covered through the testing. I chose not to implement a test to verify the `train` method for the PINN since it would be quite time consuming when running automatic testing through Github Actions.

6.3 Adding model run saver to the FD solver in "Environment" class

I added the functionality to save the entire model run for the finite difference NS solver implemented by Aaron. If the saver is set to True, the NS solver saves all relevant data for each timestep of the model evolution into a .mat file. This capability creates a path to connect the results of the NS finite difference solver and the implemented PINN model.

6.4 PINN Prediction Results

After training on the 5000 data points, I employed PINN model to reconstruct the u, v, and p for several timesteps provided in the test data. The results of the model inference for the timestep 100 are show in Figure 6



(a) u (b) v (c) w

Figure 6: The PINN predictions compared to ground truth values for the time step 100

Note that the predictions results for u and v are very accurate (with mean errors 0.06 and 0.6 respectively), which can be expected, since a small amount of data from these arrays was used for the PINN training. However, looking at the pressure prediction in Figure 6c, it is clear that, while the pressure field is represented well qualitatively, all the values are off by a constant (notice the colorbars in Figure 6c). This is evident in the calculated mean error of approximately 2.6. Further pressure predictions at other timesteps are visualized in a .gif format here (`https://github.com/acs14007/APC524-Group-Project.git`).This is quite impressive, since no pressure data was used for the PINN training. Thus the pressure approximations by the model resulted from the integrated equation loss terms. The offset in the predicted pressure field can be explained by the nature of Navier-Stokes system, since the pressure is only identifiable upto a constant [11].

7 Conclusion

In this project, we have used the Navier-Stokes equations to investigate an important test case of turbulent fluid flow. We have built a user-accessible and highly modular algorithmic Navier-Stokes solver and simulated the cylinder wake flow phenomena. We have also implemented a physics informed neural network and used it to run inversions on a cylinder wake flow dataset for an unknown pressure field. Future steps include additional rigorous testing of the project code and better integration of the finite difference and the PINN solvers.

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