Navier-Stokes Equation

The Navier-Stokes equations describes the physics of fluid dynamics and is used in many different fields from oceanography to aircraft wing design to pollution analysis and many more. This equation describes how temperature and density are related to the velocity and pressure fields of fluid in motion.

The equations are defined as:

$$egin{aligned} u_t + \lambda_1(uu_x + vu_y) + p_x - \lambda_2(u_{xx} + u_{yy}) &= 0 \ v_t + \lambda_1(uv_x + vv_y) + p_y - \lambda_2(v_{xx} + v_{yy}) &= 0 \ \ t \in [0,20]; x \in [1,8]; y \in [-2,2] \end{aligned}$$

We will created a Physics Informed Neural Network (PINN) to solve these differential equations and for the given boundary conditions. Unlike the Burger's or Allen-Cahn PINNs, this model will utilize previously sampled data to help train the network.

1. Import Python Packages

This implementation will uses some common data science packages:

- Pytorch: package of machine learning tools, including user-friendly neural network functions
- Pandas / Numpy: collection of data reading and manipulation tools
- Matplotlib: package of data visualization tools

Additionally, this notebook supports CPU and GPU computing so the default device will be checked and used for processing

```
import time
import os
import scipy.io
import numpy as np
import torch
import torch.nn as nn
from torch.autograd import Variable
import matplotlib.pyplot as plt
from matplotlib import colors
%matplotlib inline
os.environ['KMP_DUPLICATE_LIB_OK']='True'

# Looks to see if GPU is available, if not sets default to CPU. Allows the models to be
device = torch.device("cuda:0" if torch.cuda.is_available() else "cpu")
```

2. Map Model and Data Directories

If the files are in the same folder as this notebook, these values can remain as just the file name

```
In [2]: filepath_to_load_model = 'NS_model.pt' #<--- change to None (no parenthesis) if you wan
filepath_to_save_model = 'NS_model.pt' #<--- change to new file name if you do not want
data_filepath = 'cylinder_nektar_wake.mat'</pre>
```

3. Read in Sample Data

Dataset provided for exact values of u(t,x,y), v(t,x,y), and p(t,x,y) sampled over various values of t, x, and y. A .mat file provides the values that must be extracted and reformatted for processing by the model. This data will be used to test the model output and compute the loss function.

```
In [3]:
         # Function reads in sample data from .mat file
         # puts data in proper orientation for processing/training
         def read data(file):
             # read .mat file contents
             data = scipy.io.loadmat(file)
             # read data columns
             U star = data['U star']
             p_star = data['p_star']
             t star = data['t']
             X_star = data['X_star']
             \# get number of x and t values in list
             N = X star.shape[0]
             T = t_star.shape[0]
             # extract data from column cells
             XX = np.tile(X_star[:, 0:1], (1, T))
             YY = np.tile(X star[:, 1:2], (1, T))
             TT = np.tile(t star, (1, N)).T
             UU = U_star[:, 0, :]
             VV = U_star[:, 1, :]
             pp = p_star
             # flatten data into appropriate dimension: (size, 1)
             x = XX.flatten()[:, None] # NT x 1
             y = YY.flatten()[:, None] # NT x 1
             t = TT.flatten()[:, None] # NT x 1
             u = UU.flatten()[:, None] # NT x 1
             v = VV.flatten()[:, None] # NT x 1
             p = pp.flatten()[:, None] # NT x 1
             # delete unnecessary variables to save RAM. May be necessary for GPU on limited RAM
             del data, U_star, p_star, t_star, X_star, N, T, XX, YY, TT, UU, VV, pp
             # return the input and output variables in proper format
             return x,y,t,u,v,p
         # read in values from .mat file
         x, y, t, u, v, p = read data(data filepath)
```

4. Define the Algorithm Architecture

Requirements: 3 inputs (t,x,y), 2 outputs (Ψ ,p), and 2 constant values (λ_1,λ_2)

The model can be created using any combination of valid hidden layers; however, the more complex the network, the more data and computational power is required to train the model. On the opposite side, if the network is too simplistic, it may not be able to learn the characteristics of the data.

This model was created using:

- Input layer (3 variables)
- 8 Hidden layers (20 neurons)
- Output layer (2 variables)

```
In [4]:
         # Defines the network class
         class Net(nn.Module):
             def init (self):
                 super(Net, self).__init__()
                 # Placeholder for lambda constant values that will be learned by model
                 self.lambda 1 = nn.Parameter(torch.randn(1, requires grad= True))
                 self.lambda 2 = nn.Parameter(torch.randn(1, requires grad= True))
                 # Construct the neural network architecture
                 # Using 3-variable input layer, 8X20 hidden layers, 2-variable output layer
                 self.hidden_layer1 = nn.Linear(3,20)
                 self.hidden layer2 = nn.Linear(20,20)
                 self.hidden layer3 = nn.Linear(20,20)
                 self.hidden_layer4 = nn.Linear(20,20)
                 self.hidden layer5 = nn.Linear(20,20)
                 self.hidden_layer6 = nn.Linear(20,20)
                 self.hidden layer7 = nn.Linear(20,20)
                 self.hidden layer8 = nn.Linear(20,20)
                 self.output layer = nn.Linear(20,2)
             def forward(self, t,x,y):
                 # Connects each of the layers together. Accepts 3 input parameters: t, x, y
                 inputs = torch.cat([t,x,y],axis=1)
                 layer1 out = torch.sigmoid(self.hidden layer1(inputs))
                 layer2 out = torch.sigmoid(self.hidden layer2(layer1 out))
                 layer3 out = torch.sigmoid(self.hidden layer3(layer2 out))
                 layer4_out = torch.sigmoid(self.hidden_layer4(layer3_out))
                 layer5 out = torch.sigmoid(self.hidden layer5(layer4 out))
                 layer6 out = torch.sigmoid(self.hidden layer6(layer5 out))
                 layer7 out = torch.sigmoid(self.hidden_layer7(layer6_out))
                 layer8 out = torch.sigmoid(self.hidden layer8(layer7 out))
                 output = self.output layer(layer8 out)
                 return output
         #initialize a new network
         net = Net()
         #map the network to the default device type (GPU/CPU)
         net = net.to(device)
```

5. Define PDE functions

We just defined a Neural Network (NN) to take inputs $\mathbf{t}, \mathbf{x}, \mathbf{y}$ and return $\hat{\Psi}, \hat{P}$. This can be represented as the following equation:

$$NN(t,x,y)=|\hat{\Psi},\hat{p}|$$

where;

$$egin{aligned} \hat{u}(t,x,y) &= \hat{\Psi}_y \ \hat{v}(t,x,y) &= -\hat{\Psi}_x \end{aligned}$$

Therefore, the NN outputs must satisfy the Navier-Stokes PDEs as shown below:

$$egin{aligned} \hat{u}_t + \lambda_1 (\hat{u}\hat{u}_x + \hat{v}\hat{u}_y) + \hat{p}_x - \lambda_2 (\hat{u}_{xx} + \hat{u}_{yy}) &= 0 \ \hat{v}_t + \lambda_1 (\hat{u}\hat{v}_x + \hat{v}\hat{v}_y) + \hat{p}_y - \lambda_2 (\hat{v}_{xx} + \hat{v}_{yy}) &= 0 \end{aligned}$$

To satisfy these equations, the model output must be decomposed to get the variables \hat{u} , \hat{v} , and \hat{p} along with the first and second order derivatives that are required in the above equations. The resulting functions can then be inputted into the PDEs for calculation. For loss function testing, this function will return the two PDE results along with the functions of \hat{u} , \hat{v} , and \hat{p} for comparison to the sampled data

```
In [5]:
         # Function to deconstruct output variables and define PDEs to solve
         def f(t, x, y, net):
             # get current working lambda values
             lambda1 = net.lambda 1
             lambda2 = net.lambda 2
             # predict results given input values for t,x,y
             psi_p = net(t, x, y)
             # model outputs 2 variables. Assign first output to Psi(t,x,y), second to P(t,x,y)
             psi = psi_p[:, 0].reshape(-1,1)
             p = psi_p[:, 1].reshape(-1,1)
             # decompose velcoty function
             # calculate u(t,x,y) = dPsi/dy and v(t,x,y) = -dPsi/dx
             u = torch.autograd.grad(psi.sum(), y, create graph=True)[0]
             v = -torch.autograd.grad(psi.sum(), x, create_graph=True)[0]
             # calculate first order derivatives for PDE
             u t = torch.autograd.grad(u.sum(), t, create graph=True)[0]
             u_x = torch.autograd.grad(u.sum(), x, create_graph=True)[0]
             u_y = torch.autograd.grad(u.sum(), y, create_graph=True)[0]
             v_t = torch.autograd.grad(v.sum(), t, create_graph=True)[0]
             v_x = torch.autograd.grad(v.sum(), x, create_graph=True)[0]
             v_y = torch.autograd.grad(v.sum(), y, create_graph=True)[0]
             p_x = torch.autograd.grad(p.sum(), x, create_graph=True)[0]
             p_y = torch.autograd.grad(p.sum(), y, create_graph=True)[0]
             # calculate second order derivatives for PDE
             u xx = torch.autograd.grad(u x.sum(), x, create graph=True)[0]
             u_yy = torch.autograd.grad(u_y.sum(), y, create_graph=True)[0]
             v_xx = torch.autograd.grad(v_x.sum(), x, create_graph=True)[0]
```

```
v_yy = torch.autograd.grad(v_y.sum(), y, create_graph=True)[0]

# calculate PDEs
f_u = u_t + lambda1*(u*u_x + v*u_y) + p_x - lambda2*(u_xx + u_yy)
f_v = v_t + lambda1*(u*v_x + v*v_y) + p_y - lambda2*(v_xx + v_yy)

# delete unnecessary variables to save RAM. May be necessary for GPU on limited RAM del lambda1, lambda2, psi_p, psi, u_t, u_x, u_y, v_t, v_x, v_y, u_xx, u_yy, v_xx, v

# return functions of velocity, pressure and PDE results
return u, v, p, f_u, f_v

# define default loss function as the mean squared error
mse_cost_function = torch.nn.MSELoss()

# define the optimizer function
optimizer = torch.optim.Adam(net.parameters())
```

6. Train the Model

This model will be trained over n number of iterations with a batch size of x randomly chosen data points. Both of these values can be adjusted for better training performance.

To train the model, the optimizer will attempt to reduce the model loss down to zero. Therfore, the loss function must be defined to incorporate the information gained by attempting to solve the PDEs and the error between the output values and the sampled exact values.

To calculate the loss, Mean Squared Error (MSE) will be used on the model outputs.:

$$MSE = \frac{1}{N} \sum (Value_{actual} - Value_{predicted})^2$$

Recalling from steps 3 and 5, we have two PDEs that have been defined along with the model outputs and the associated exact values. When calculating the loss, the function should be created in a way where the best loss value will be 0. In order to achieve this for our model, the predicted values can be compared with the exact values to get the error between the two. Additionally, since the PDEs are supposed to equal zero, this error can be used to calculate the loss as well. Each of these components results in a loss function of:

$$egin{aligned} MSE_{outputs} &= rac{1}{N} \sum \left(\left| u - \hat{u}
ight|^2 + \left| v - \hat{v}
ight|^2 + \left| p - \hat{p}
ight|^2
ight) \ MSE_{PDEs} &= rac{1}{N} \sum \left(\left| PDE_u
ight| + \left| PDE_v
ight|
ight) \ Loss &= MSE_{outputs} + MSE_{PDEs} \end{aligned}$$

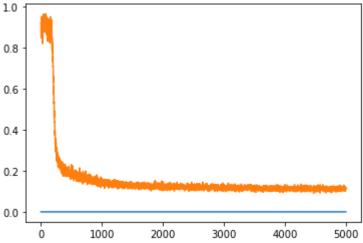
For each iteration of training, this loss function will be calculated and the result will be used by the optimizer to adjust the neural network. Graphing the loss function over time should result in an exponentially decreasing function that converges towards zero.

```
In [6]: # set number of iterations desired for training
   iterations = 5000
   losses = []
```

```
start = time.time()
# Load the current working version of the model
# Allows training to resume from last saved model
# Comment out line if no model has been created yet
if filepath to load model is not None:
    net.load state dict(torch.load(filepath to load model,map location=device))
# for the number of iterations defined
for epoch in range(iterations):
    # clear the optimizer for new input
    optimizer.zero grad()
    # identify the batch size (number of training points per iteration)
    N train = 200
    # randomly sample data to match batch size
    idx = np.random.choice(len(x), N train, replace=False)
    x train = x[idx,:]
    y_train = y[idx,:]
    t_train = t[idx,:]
    u train = u[idx,:]
    v_train = v[idx,:]
    p train = p[idx,:]
    # define zeros as same length as batch size
    # will be used to calculate MSE
    zeros = np.zeros((N train,1))
    # convert training date to tensor format
    pt_x = Variable(torch.from_numpy(x_train).float(), requires_grad=True).to(device)
    pt_t = Variable(torch.from_numpy(t_train).float(), requires_grad=True).to(device)
    pt y = Variable(torch.from numpy(y train).float(), requires grad=True).to(device)
    pt_u = Variable(torch.from_numpy(u_train).float(), requires_grad=True).to(device)
    pt v = Variable(torch.from numpy(v train).float(), requires grad=True).to(device)
    pt_p = Variable(torch.from_numpy(p_train).float(), requires_grad=True).to(device)
    pt_zeros = Variable(torch.from_numpy(zeros).float(), requires_grad=True).to(device)
    # delete unnecessary variables to save RAM. May be necessary for GPU on limited RAM
    del x_train, y_train, t_train, u_train, v_train, p_train, zeros
    # get output from model given the input parameters
    u_hat, v_hat, p_hat, f_u, f_v = f(pt_t, pt_x, pt_y, net)
    # calculate error between predicted outputs (u hat, v hat, p hat) and exact solutions
    mse_u = mse_cost_function(u_hat, pt_u)
    mse v = mse cost function(v hat, pt v)
    mse_p = mse_cost_function(p_hat, pt_p)
    # calculates error in PDE function
    # functions should equal 0 so mse calculated between 0 and PDE results (f u, f v)
    mse_f_u = mse_cost_function(f_u, pt_zeros)
    mse_f_v = mse_cost_function(f_v, pt_zeros)
    # sum all calculated error to get loss
    loss = mse u + mse v + mse p + mse f u + mse f v
    # delete unnecessary variables to save RAM. May be necessary for GPU on limited RAM
    del u_hat, v_hat, p_hat, f_u, f_v, mse_u, mse_v, mse_p, mse_f_u, mse_f_v
```

```
# use back propagation to pass the resulting loss backwards through the model
    # optimizer attempts to reduce the loss to zero
    loss.backward()
    optimizer.step()
    with torch.autograd.no grad():
        # adds the current loss to a list for future analysis/graphing
        losses.append(float(loss.data))
        # prints out status update every n iteration
        if (epoch+1)%1000 == 0:
            print(epoch+1, "Training Loss:", round(float(loss.data),5))
            # saves current working copy of model in case of crash
            torch.save(net.state_dict(), filepath_to_save_model)
# save final trained model
torch.save(net.state_dict(), filepath_to_save_model)
# print completion message
print('Completed',epoch+1,'iterations in',round((time.time()-start)/60,0), 'minutes')
# show graph of loss over training iterations
xs = list(range(len(losses)))
ys = np.zeros((len(losses),1))
plt.plot(xs,ys)
plt.plot(xs,losses)
plt.show()
```

```
1000 Training Loss: 0.15573
2000 Training Loss: 0.11585
3000 Training Loss: 0.11418
4000 Training Loss: 0.12025
5000 Training Loss: 0.11093
Completed 5000 iterations in 6.0 minutes
```



8. Analyzing the Results

Overall performance of the model can be evaluated using the known sample data and the models outputs. Loss between the outputted functions can be calculated and used to track accuracy. Model performance can also be visualized by graphing the predicted functions against the exact values.

Unfortunately, since this function operates in larger than 3 dimension, data must be visualized by keep some input values constant.

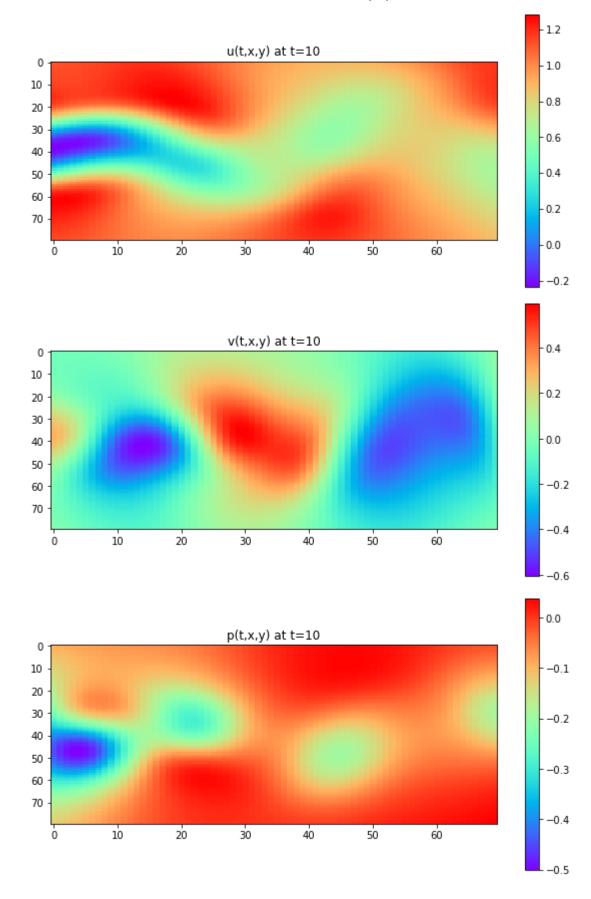
```
In [7]:
         # loads trained model for analysis
         net = Net()
         net.load state dict(torch.load(filepath to save model,map location=device))
         # Function tests the results of the model with the exact results
         def test result(x,y,t,u,v,p):
             # number of points to test
             N \text{ test} = 10000
             # ensures the random values are the same every time for comparison of model progres
             # comment line out if truly random samples are required
             np.random.seed(1234)
             # get random data points to match number of test points
             idx = np.random.choice(len(x), N test, replace=False)
             x \text{ test} = x[idx,:]
             y test = y[idx,:]
             t_test = t[idx,:]
             u test = u[idx,:]
             v_test = v[idx,:]
             p_test = p[idx,:]
             # convert variables to tensors for input into the model
             pt_x = Variable(torch.from_numpy(x_test).float(), requires_grad=True).to(device)
             pt_t = Variable(torch.from_numpy(t_test).float(), requires_grad=True).to(device)
             pt y = Variable(torch.from numpy(y test).float(), requires grad=True).to(device)
             pt_u = Variable(torch.from_numpy(u_test).float(), requires_grad=True).to(device)
             pt v = Variable(torch.from numpy(v test).float(), requires grad=True).to(device)
             pt_p = Variable(torch.from_numpy(p_test).float(), requires_grad=True).to(device)
             # Get resulting outputs from model given inputs (t,x,y)
             u_hat, v_hat, p_hat, f_u, f_v = f(pt_t, pt_x, pt_y, net)
             # calculate error of predicted values vs actual values for: u, v, p
             error = mse_cost_function(u_hat, pt_u)
             error += mse cost function(v hat, pt v)
             error += mse cost function(p hat, pt p)
             # print resulting error rate of model
             print('\nMean Squared Error:', round(float(error),5))
         # function creates 2D heat map at constant time
         def plot heat map(time, net):
             # get values between variable boundaries at constant increments
             x=np.arange(1,8,0.1)
             y=np.arange(-2,2,0.05)
             # orient values in proper format for processing
             ms x, ms y = np.meshgrid(x, y)
             xx = np.ravel(ms_x).reshape(-1,1)
             yy = np.ravel(ms y).reshape(-1,1)
             # assign all t values to inputted constant
             tt = np.ones((len(xx),1))*time
```

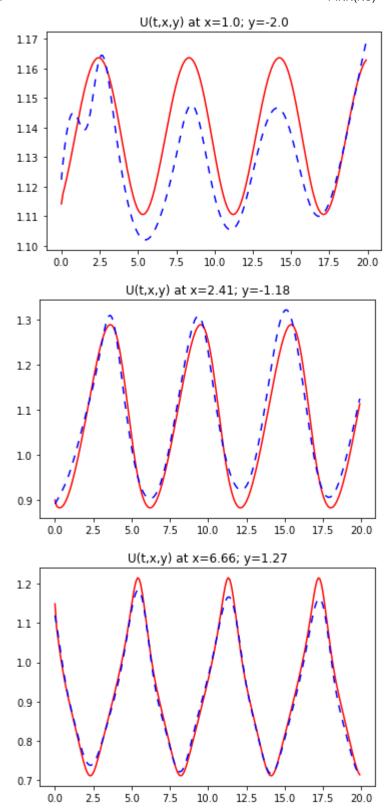
```
# convert values to tensors for model input
    pt_x = Variable(torch.from_numpy(xx).float(), requires_grad=True).to(device)
    pt_y = Variable(torch.from_numpy(yy).float(), requires_grad=True).to(device)
    pt_t = Variable(torch.from_numpy(tt).float(), requires_grad=True).to(device)
    # get model output given input values
    u_hat, v_hat, p_hat, f_u, f_v = f(pt_t, pt_x, pt_y, net)
    # arrange the output variables in 2D array for graphing
    u=np.asarray(u_hat.data)
    u=u.reshape(ms x.shape)
    v=np.asarray(v hat.data)
    v=v.reshape(ms x.shape)
    p=np.asarray(p_hat.data)
    p=p.reshape(ms_x.shape)
    # plots the 2D array for u(t,x,y)
    fig = plt.figure(figsize=(10,5))
    plt.imshow(u, cmap='rainbow', interpolation='nearest', aspect=.35)
    plt.title("u(t,x,y) at t="+str(time))
    plt.colorbar()
    plt.show()
    # plots the 2D array for v(t,x,y)
    fig = plt.figure(figsize=(10,5))
    plt.imshow(v, cmap='rainbow', interpolation='nearest', aspect=.35)
    plt.title("v(t,x,y) at t="+str(time))
    plt.colorbar()
    plt.show()
    # plots the 2D array for p(t,x,y)
    fig = plt.figure(figsize=(10,5))
    plt.imshow(p, cmap='rainbow', interpolation='nearest', aspect=.35)
    plt.title("p(t,x,y) at t="+str(time))
    plt.colorbar()
    plt.show()
# Function compares the predicted u(t,x,y) results to exact at constant t and y values
def plot_x_value(t_value, y_value, net):
    # read the exact data
    x, y, t, u, v, p = read_data(data_filepath)
    # get the x and u values at the constant t and y values
    idx = np.where((t==t value) & (y==y value))
    x = x[idx]
    xx = x.reshape(-1,1)
    u star = u[idx]
    uu = u_star.reshape(-1,1)
    # set the t and y values to their constant values
    tt = np.ones((len(xx),1))*t value
    yy = np.ones((len(xx),1))*y_value
    # convert the values to tensors for model input
    pt_x = Variable(torch.from_numpy(xx).float(), requires_grad=True).to(device)
    pt_y = Variable(torch.from_numpy(yy).float(), requires_grad=True).to(device)
    pt_t = Variable(torch.from_numpy(tt).float(), requires_grad=True).to(device)
    # get the model output for the given inputs
    u_hat, v_hat, p_hat, f_u, f_v = f(pt_t, pt_x, pt_y, net)
```

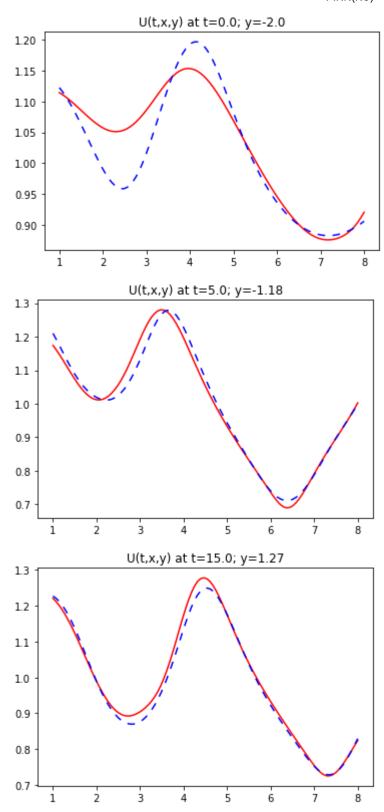
```
u=np.asarray(u hat.data)
    # plot the exact u(t,x,y) as red line
    plt.plot(x,u_star, 'red')
    # plot the predicted u(t,x,y) as dotten blue line
    plt.plot(x,u,'blue', linestyle=(0,(5,5)))
    plt.title('U(t,x,y) at t='+str(round(t value,2))+'; y='+str(round(y value,2)))
    plt.show()
# Function compares the predicted u(t,x,y) results to exact at constant t and x values
def plot y value(t value, x value, net):
    # read the exact data
    x, y, t, u, v, p = read data(data filepath)
    \# get the y and u values at the constant t and x values
    idx = np.where((t==t value) & (x==x value))
    y = y[idx]
    yy = y.reshape(-1,1)
    u_star = u[idx]
    uu = u star.reshape(-1,1)
    # set the t and x values to their constant values
    tt = np.ones((len(yy),1))*t_value
    xx = np.ones((len(yy),1))*x value
    # convert the values to tensors for model input
    pt x = Variable(torch.from numpy(xx).float(), requires grad=True).to(device)
    pt y = Variable(torch.from numpy(yy).float(), requires grad=True).to(device)
    pt_t = Variable(torch.from_numpy(tt).float(), requires_grad=True).to(device)
    # get the model output for the given inputs
    u_hat, v_hat, p_hat, f_u, f_v = f(pt_t, pt_x, pt_y, net)
    u=np.asarray(u hat.data)
    # plot the exact u(t,x,y) as red line
    plt.plot(y,u_star,'red')
    # plot the predicted u(t,x,y) as dotten blue line
    plt.plot(y,u,'blue', linestyle=(0,(5,5)))
    plt.title('U(t,x,y) at t='+str(round(t_value,2))+'; x='+str(round(x_value,2)))
    plt.show()
# Function compares the predicted u(t,x,y) results to exact at constant x and y values
def plot_t_value(x_value, y_value, net):
    # read the exact data
    x, y, t, u, v, p = read_data(data_filepath)
    # get the t and u values at the constant x and y values
    idx = np.where((x==x value) & (y==y value))
    t = t[idx]
    tt = t.reshape(-1,1)
    u star = u[idx]
    uu = u star.reshape(-1,1)
    # set the x and y values to their constant values
    xx = np.ones((len(tt),1))*x value
    yy = np.ones((len(tt),1))*y_value
```

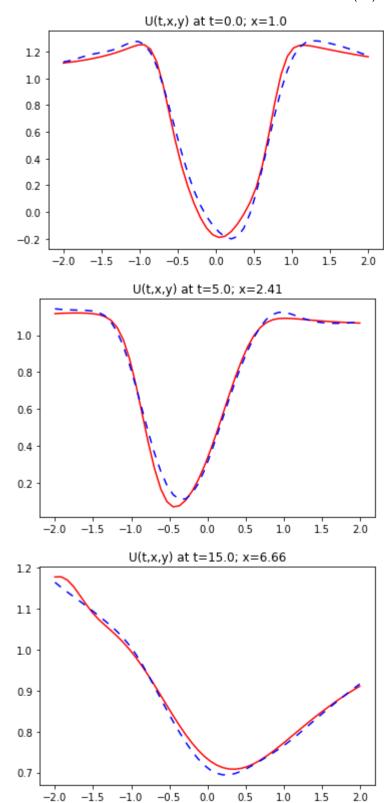
```
# convert the values to tensors for model input
    pt x = Variable(torch.from numpy(xx).float(), requires grad=True).to(device)
    pt_y = Variable(torch.from_numpy(yy).float(), requires_grad=True).to(device)
    pt_t = Variable(torch.from_numpy(tt).float(), requires_grad=True).to(device)
    # get the model output for the given inputs
    u_hat, v_hat, p_hat, f_u, f_v = f(pt_t, pt_x, pt_y, net)
    u=np.asarray(u hat.data)
    # plot the exact u(t,x,y) as red line
    plt.plot(t,u star, 'red')
    # plot the predicted u(t,x,y) as dotten blue line
    plt.plot(t,u,'blue', linestyle=(0,(5,5)))
    plt.title('U(t,x,y) at x='+str(round(x_value,2))+'; y='+str(round(y_value,2)))
    plt.show()
#test the performance of the saved model
test_result(x,y,t,u,v,p)
#plot the heat maps for u(t,x,y), v(t,x,y) and p(t,x,y)
plot heat map(10, net)
\# get the values of x, y, and t in the sample data
x vals = np.unique(x)
y_vals = np.unique(y)
t vals = np.unique(t)
# plot u(t,x,y) at constant x,y values
plot_t_value(x_vals[0],y_vals[0],net)
plot_t_value(x_vals[20],y_vals[10],net)
plot t value(x vals[80],y vals[40],net)
# plot u(t,x,y) at constant t,y values
plot_x_value(t_vals[0],y_vals[0],net)
plot_x_value(t_vals[50],y_vals[10],net)
plot_x_value(t_vals[150],y_vals[40],net)
# plot u(t,x,y) at constant t,x values
plot_y_value(t_vals[0],x_vals[0],net)
plot_y_value(t_vals[50],x_vals[20],net)
plot_y_value(t_vals[150],x_vals[80],net)
```

Mean Squared Error: 0.00174









In []: