HW4

March 14, 2024

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Course:	ME 036049
Homerwork:	No. 4

1 Computation

1.0.1 Part a

Here I will use the 1D Unsteady Diffusion PINNs model for different diffusion coefficients and compare the final results. I will import a file called *PINN_Classes* where I stored the definitions of the different models.

[ ]:
```
import torch
import torch.nn as nn
from torch.autograd import grad
import torch.functional as F
import numpy as np
import matplotlib.pyplot as plt
from PINN_Classes import Diffusion_PINNs_1D
```

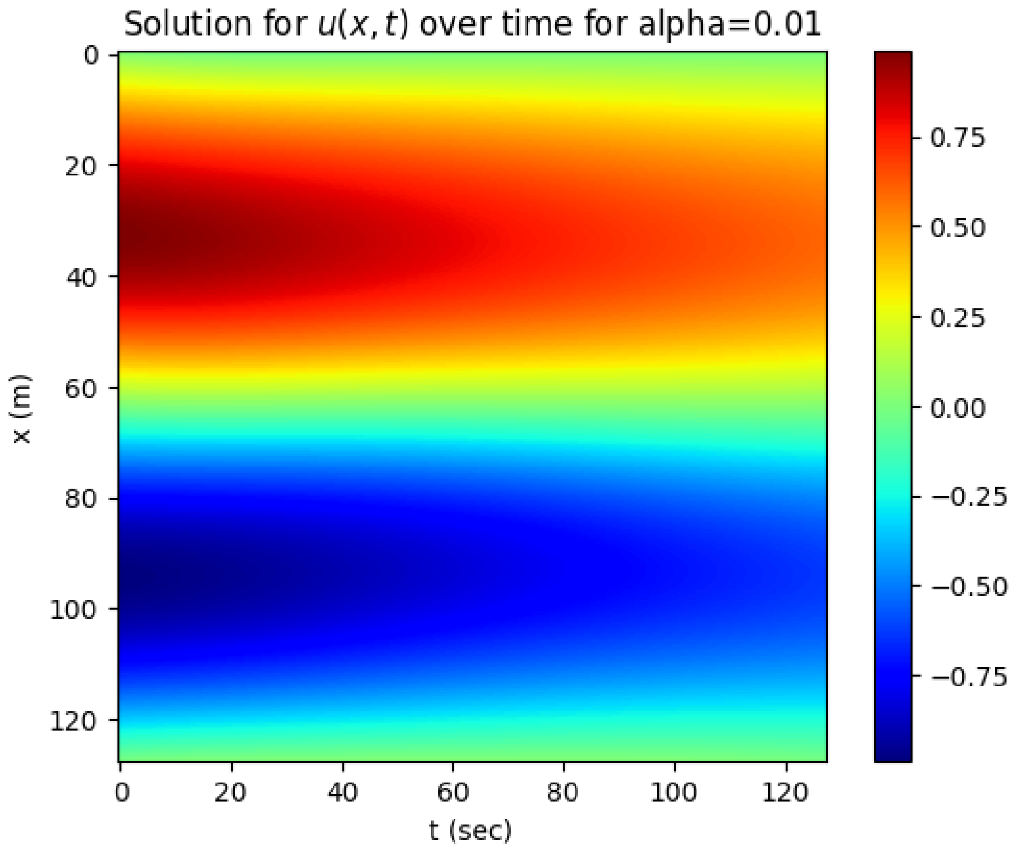
Setting up the use cases

[ ]:
```
# num of points in the domain
Nx, Nt = 128, 128

# define domain dimensions and resolution
Lx_initial, Lx_final = 0, 1
t_initial, t_final = 0, 1
dx = (Lx_final - Lx_initial) / (Nx - 1)
dt = (t_final - t_initial) / (Nt-1)

# initiallize input parameters as tensors
x = torch.zeros(Nx, Nt)
t = torch.zeros(Nx, Nt)
for i in range(Nx):
    for j in range(Nt):
        x[i,j] = Lx_initial + dx * i
        t[i,j] = t_initial + dt * j
```

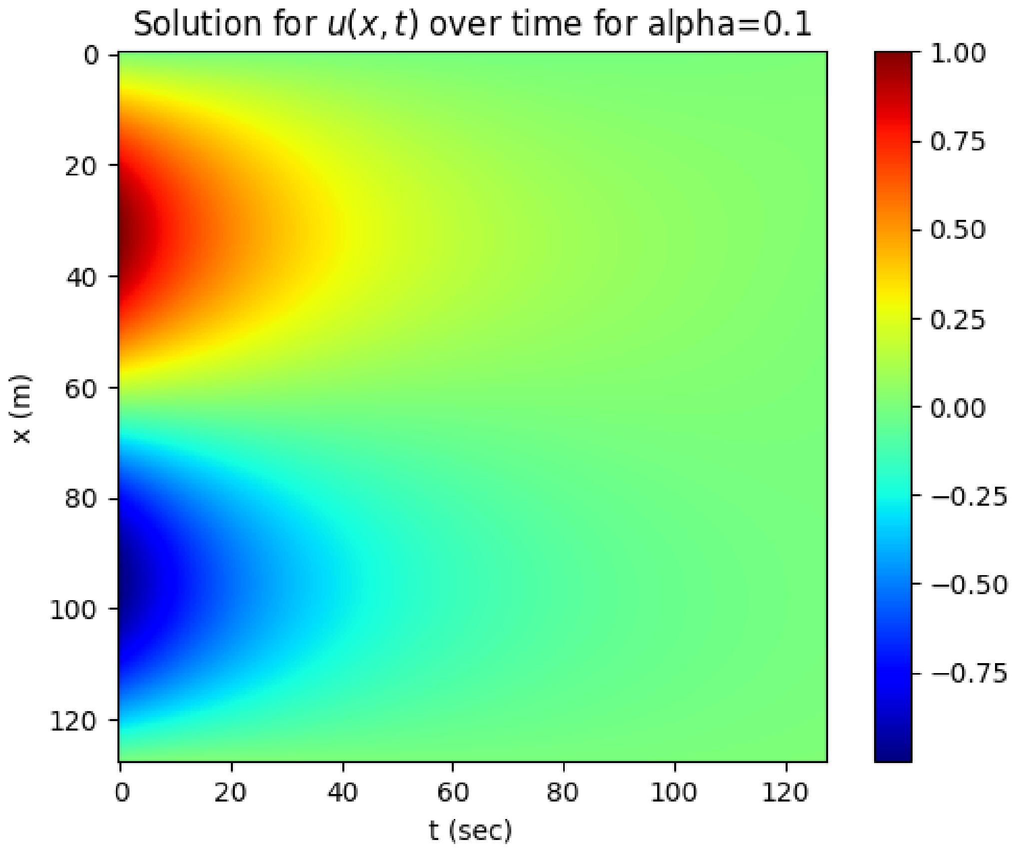
Using different models

[ ]:
```
diffusion_coefficient_cases = [0.01, 0.1, 1]
for alpha in diffusion_coefficient_cases:
    model = Diffusion_PINNs_1D(use_ffm=False, diff_coeff=alpha)
    optimizer = torch.optim.Adam(model.parameters(), lr=0.001)

    for epoch in range(1000):
    # compute various losses
        eq_loss, BC_loss, IC_loss = model.compute_loss(x.view(-1,1), t.
 ↪view(-1,1), Nx, Nt)

        # compute total loss
        total_loss = eq_loss + 20*BC_loss + 20*IC_loss

        # backward pass
        total_loss.backward()
        optimizer.step()
        optimizer.zero_grad()

        # skip by 100 epochs before printing
        if not epoch%100:
            print(f"epoch: {epoch}, loss: {total_loss}")

    u = model.forward(x.view(-1,1), t.view(-1,1)) # convert x tensor into a␣
 ↪column vector
    u_np = u.detach().numpy() # convert into a np array
    u_reshaped = u_np.reshape(Nx,Nt)

    plt.imshow(u_reshaped[:,:], cmap='jet')
    plt.title(f"Solution for $u(x,t)$ over time for alpha={alpha}")
    plt.colorbar()
    plt.xlabel("t (sec)")
    plt.ylabel("x (m)")
    plt.show()
```

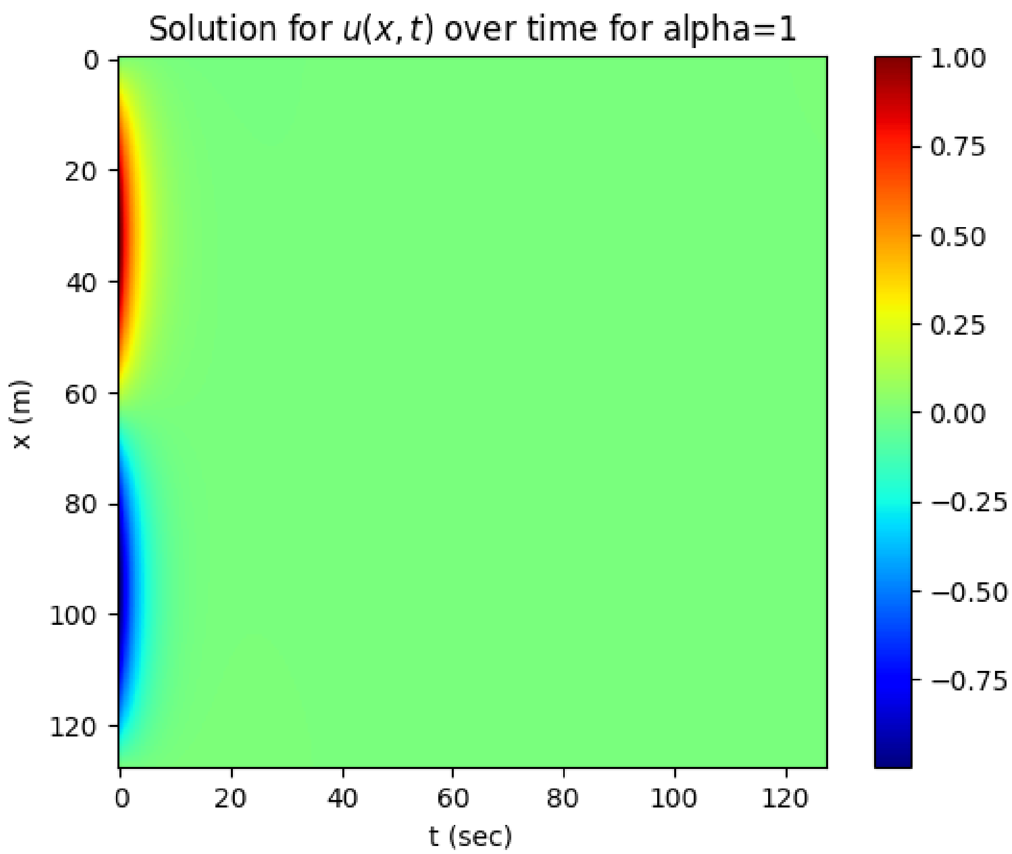
```
epoch: 0, loss: 10.401286125183105
epoch: 100, loss: 7.121054172515869
epoch: 200, loss: 0.813080906867981
epoch: 300, loss: 0.3333478569984436
epoch: 400, loss: 0.18561522662639618
epoch: 500, loss: 0.15994709730148315
epoch: 600, loss: 0.065738245844841
epoch: 700, loss: 0.04871957749128342
epoch: 800, loss: 0.031818438321352005
epoch: 900, loss: 0.025787554681301117
```




```
epoch: 0, loss: 9.952513694763184
epoch: 100, loss: 6.559505462646484
epoch: 200, loss: 0.9957858324050903
epoch: 300, loss: 0.09850098192691803
epoch: 400, loss: 0.053147584199905396
epoch: 500, loss: 0.028757719323039055
epoch: 600, loss: 0.020579200237989426
epoch: 700, loss: 0.015858598053455353
epoch: 800, loss: 0.01419171504676342
epoch: 900, loss: 0.04586707055568695
```




```
epoch: 0, loss: 11.563432693481445
epoch: 100, loss: 7.794733047485352
epoch: 200, loss: 2.0839743614196777
epoch: 300, loss: 0.2649880051612854
epoch: 400, loss: 0.1120111271739006
epoch: 500, loss: 0.045536402612924576
epoch: 600, loss: 0.034432489424943924
epoch: 700, loss: 0.017876993864774704
epoch: 800, loss: 0.013787725009024143
epoch: 900, loss: 0.13721388578414917
```



1.0.2 Part b - Allen Cahn

[ ]:
```
from PINN_Classes import Allen_Cahn_1D_PINNs
```

Setting up the use cases

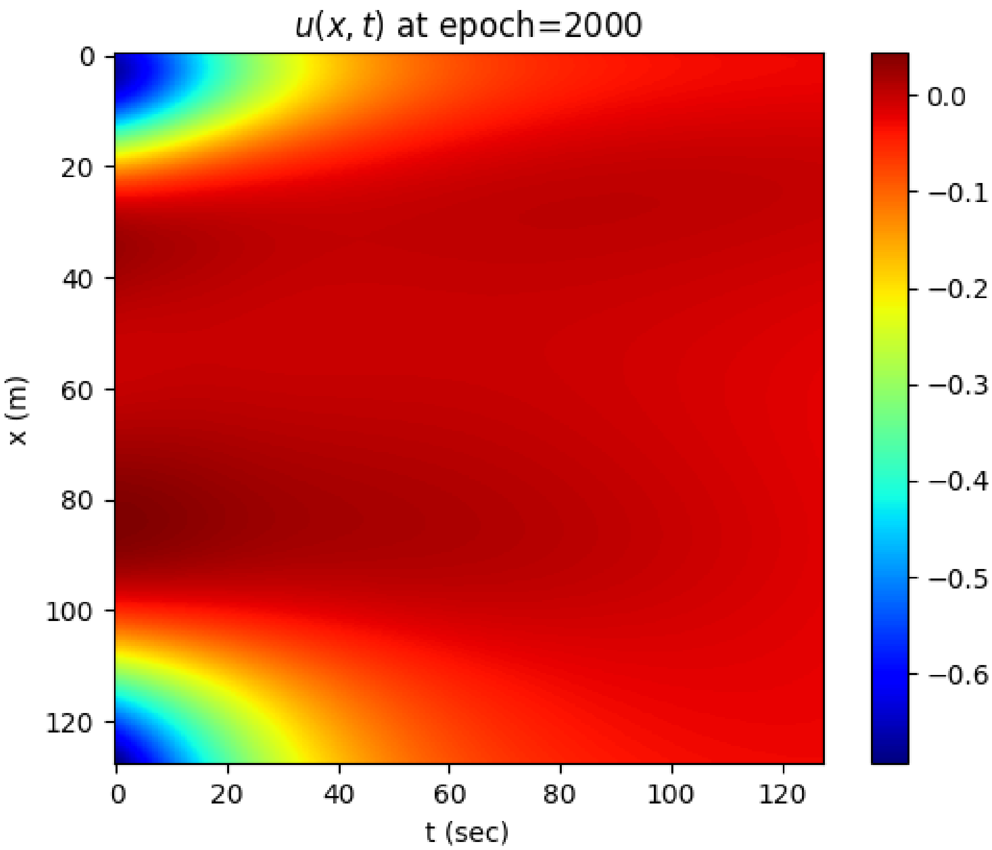
[ ]:
```
# num of points in the domain
Nx, Nt = 128, 128

# define domain dimensions and resolution
Lx_initial, Lx_final = -1, 1
t_initial, t_final = 0, 1
dx = (Lx_final - Lx_initial) / (Nx - 1)
dt = (t_final - t_initial) / (Nt-1)

# initiallize input parameters as tensors
x = torch.zeros(Nx, Nt)
t = torch.zeros(Nx, Nt)
for i in range(Nx):
    for j in range(Nt):
```

```
        x[i,j] = Lx_initial + dx * i
        t[i,j] = t_initial + dt * j
```

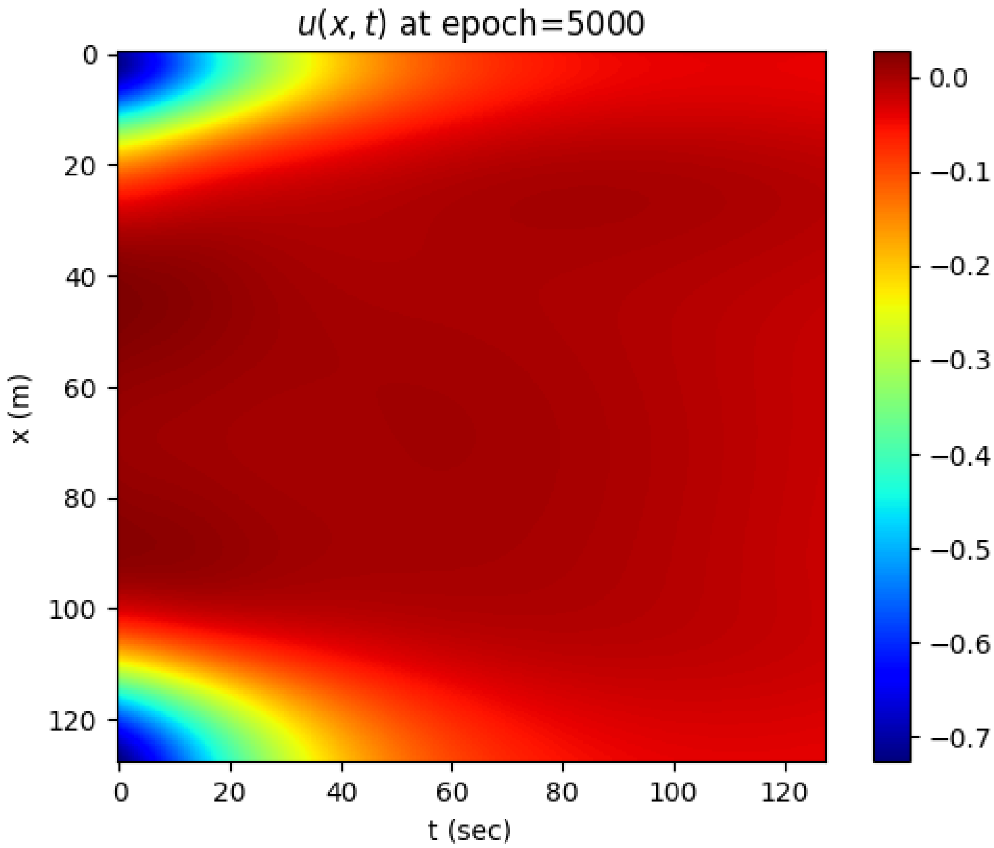
[ ]:
```
model = Allen_Cahn_1D_PINNs()
optimizer = torch.optim.Adam(model.parameters(), lr=0.001)
num_of_epochs = 20000
losses_history = np.zeros((num_of_epochs, 4))

for epoch in range(num_of_epochs):
# compute various losses
    eq_loss, BC_loss, IC_loss = model.compute_loss(x.view(-1,1), t.view(-1,1),␣
 ↪Nx, Nt)

    # compute total loss
    total_loss = eq_loss + 20*BC_loss + 20*IC_loss

    # save date for losses history
    losses_history[epoch, 0] = total_loss
    losses_history[epoch, 1] = eq_loss
    losses_history[epoch, 2] = BC_loss
    losses_history[epoch, 3] = IC_loss

    # backward pass
    total_loss.backward()
    optimizer.step()
    optimizer.zero_grad()

    # skip by 500 epochs before every print
    if not epoch%500:
        print(f"epoch: {epoch}, loss: {total_loss}")

    # plot solutions by the end of [5000, 15000, 20000] epochs
    if epoch+1 in [2000, 5000, 15000, 20000]:
        u = model.forward(x.view(-1,1), t.view(-1,1)) # convert x tensor into a␣
 ↪column vector
        u_np = u.detach().numpy() # convert into a np array
        u_reshaped = u_np.reshape(Nx,Nt)
        plt.imshow(u_reshaped[:,:], cmap='jet')
        plt.colorbar()
        plt.title(f"$u(x,t)$ at epoch={epoch+1}")
        plt.xlabel("t (sec)")
        plt.ylabel("x (m)")
        plt.show()


plt.plot(losses_history)
plt.title("Losses History")
```

```
plt.legend(["Total Loss", "PDE Loss", "BC Loss", "IC Loss"])
```

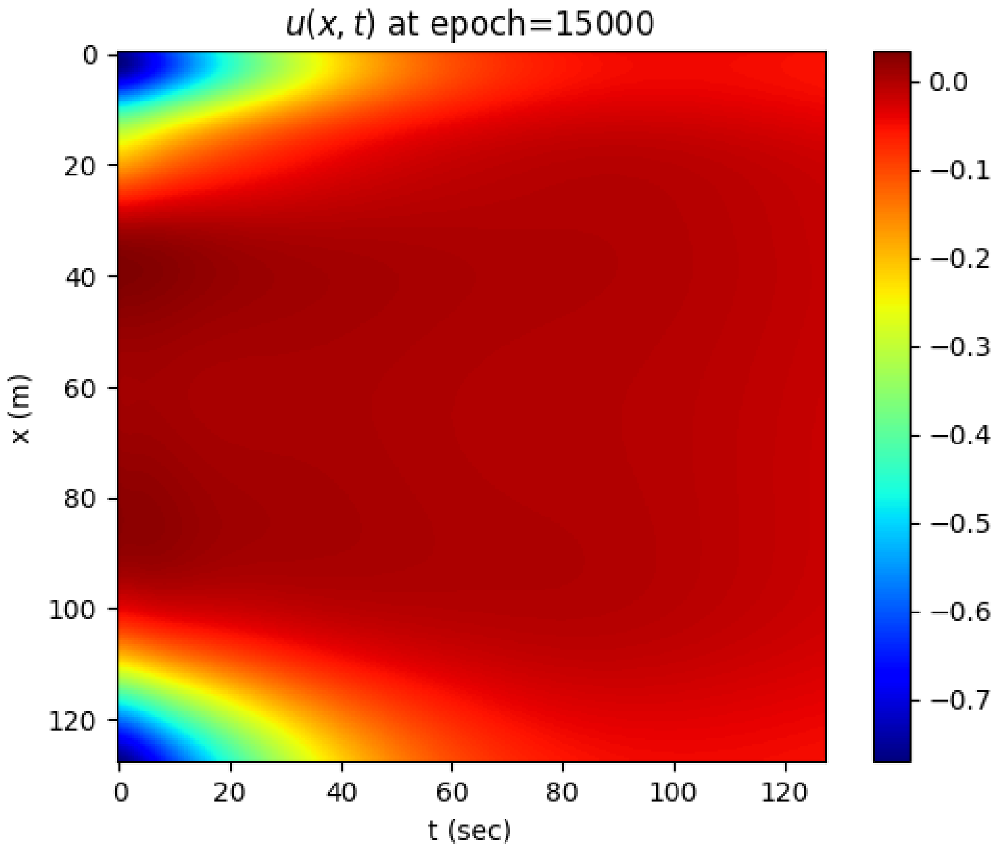
```
epoch: 0, loss: 3.6087818145751953
epoch: 500, loss: 1.0110085010528564
epoch: 1000, loss: 1.0136874914169312
epoch: 1500, loss: 0.9320902228355408
```



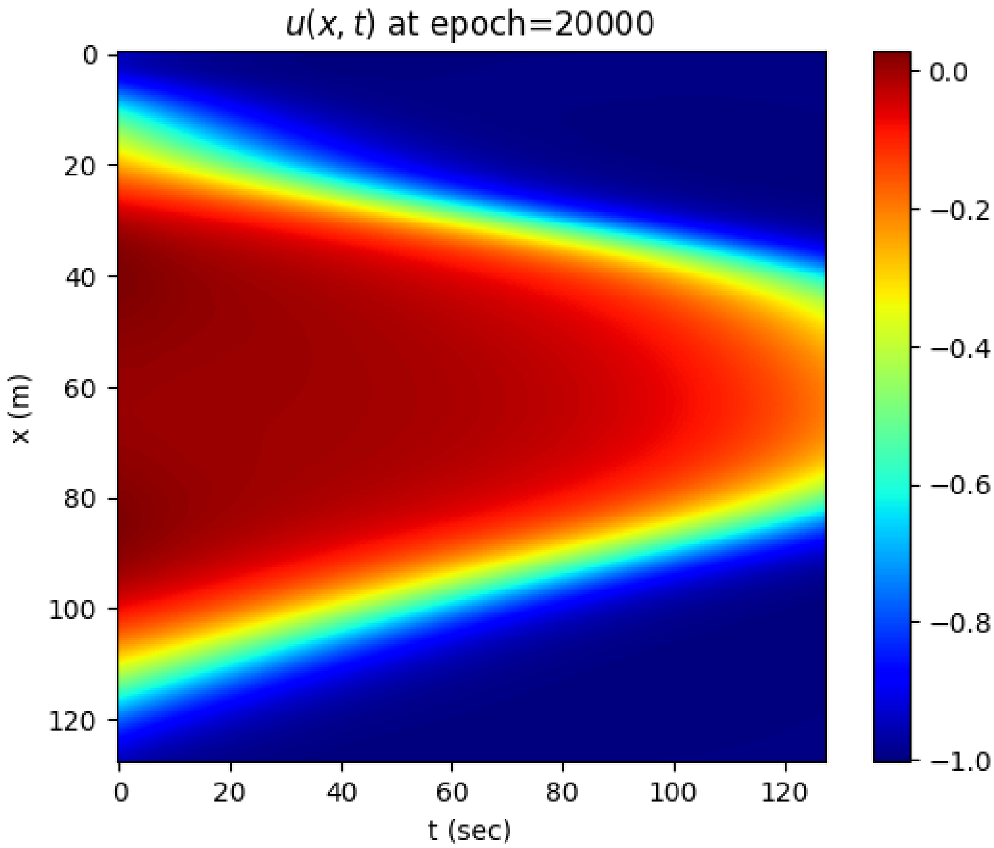

```
epoch: 2000, loss: 0.9170194268226624
epoch: 2500, loss: 0.909360945224762
epoch: 3000, loss: 0.9045158624649048
epoch: 3500, loss: 0.900154173374176
epoch: 4000, loss: 0.8981761336326599
epoch: 4500, loss: 0.8964554667472839
```



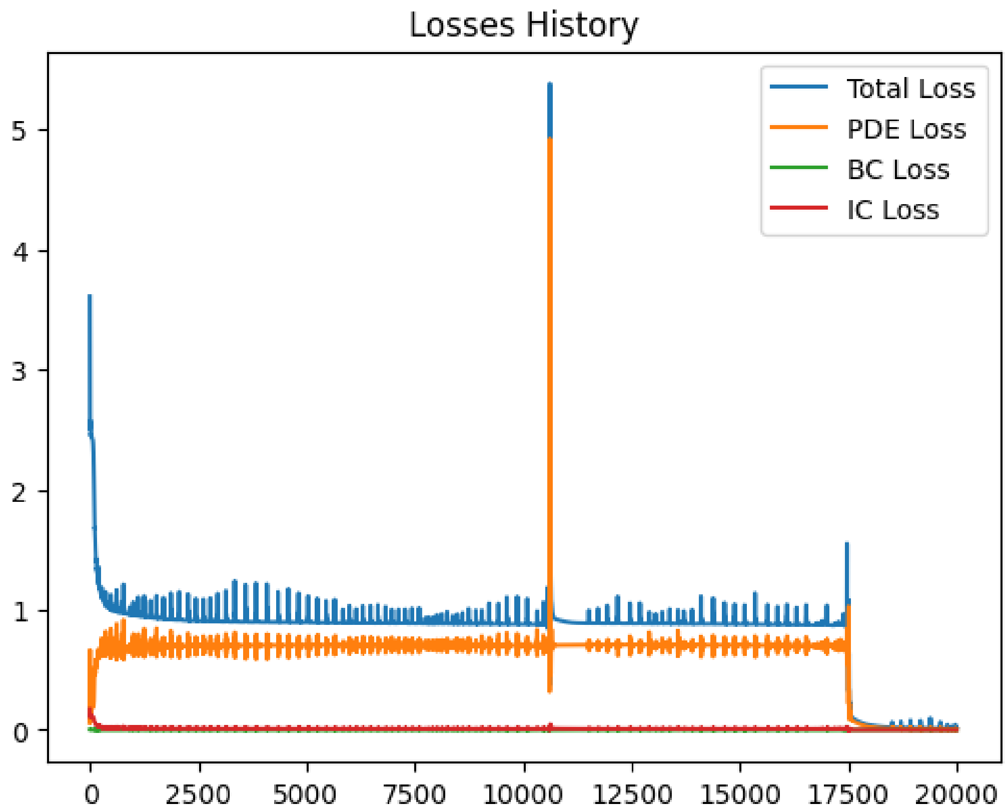

```
epoch: 5000, loss: 0.8942526578903198
epoch: 5500, loss: 0.893661379814148
epoch: 6000, loss: 0.8957456350326538
epoch: 6500, loss: 0.8938789367675781
epoch: 7000, loss: 0.8908458948135376
epoch: 7500, loss: 0.8863319754600525
epoch: 8000, loss: 0.9134286642074585
epoch: 8500, loss: 0.8846665024757385
epoch: 9000, loss: 0.882631778717041
epoch: 9500, loss: 0.8815603852272034
epoch: 10000, loss: 0.8795162439346313
epoch: 10500, loss: 0.8761231899261475
epoch: 11000, loss: 0.8998742699623108
epoch: 11500, loss: 0.8882033824920654
epoch: 12000, loss: 0.8873723149299622
epoch: 12500, loss: 0.8871829509735107
epoch: 13000, loss: 0.885071337223053
epoch: 13500, loss: 0.8840809464454651
epoch: 14000, loss: 0.8830869197845459
epoch: 14500, loss: 0.8822808861732483
```




```
epoch: 15000, loss: 0.8809372782707214
epoch: 15500, loss: 0.8792852759361267
epoch: 16000, loss: 0.8766546845436096
epoch: 16500, loss: 0.8734652996063232
epoch: 17000, loss: 0.8757535219192505
epoch: 17500, loss: 0.5533410906791687
epoch: 18000, loss: 0.0392947793006897
epoch: 18500, loss: 0.020056897774338722
epoch: 19000, loss: 0.01487440150231123
epoch: 19500, loss: 0.012701889500021935
```



[ ]: <matplotlib.legend.Legend at 0x23fb3517c40>

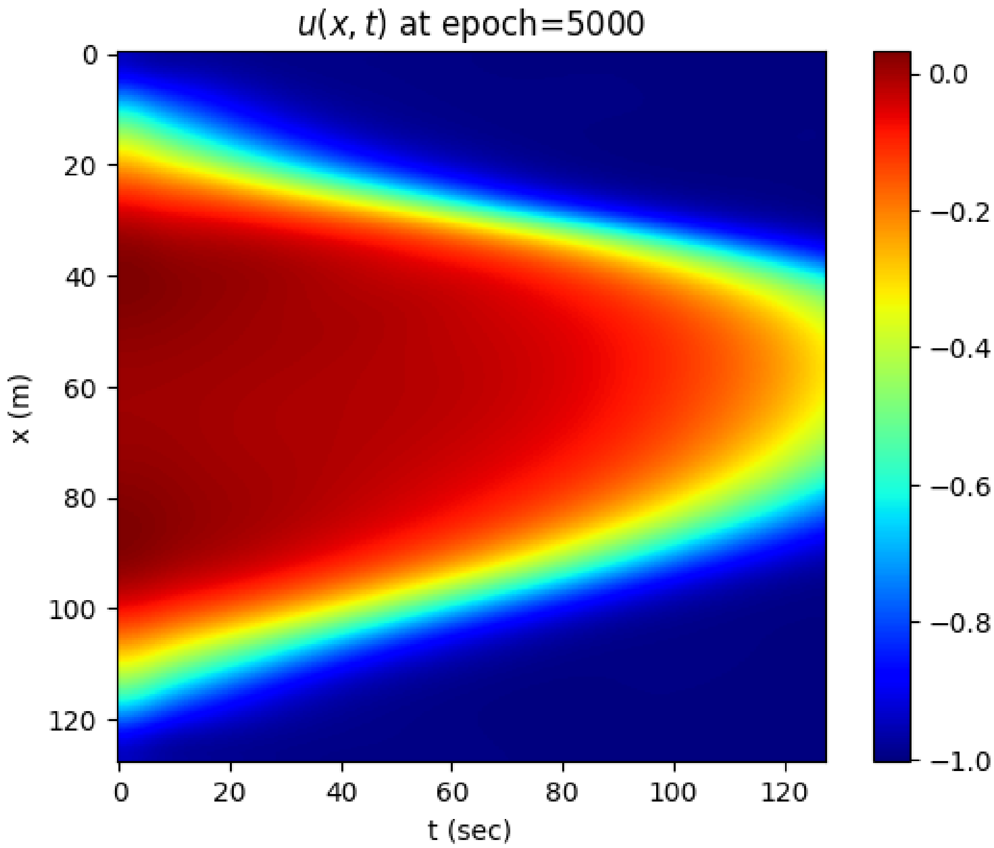


1.0.3 Part d - Studying the effect of FFMs

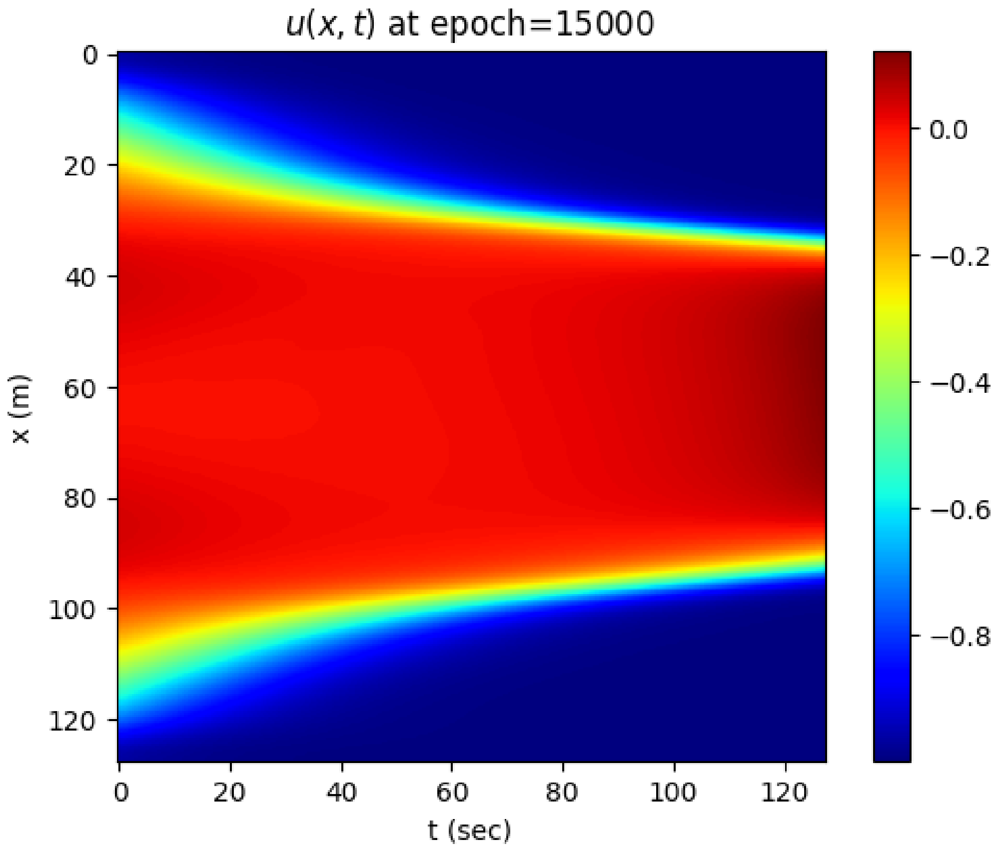
```
[ ]: model = Allen_Cahn_1D_PINNs(use_ffm=True)
optimizer = torch.optim.Adam(model.parameters(), lr=0.001)
num_of_epochs = 20000
losses_history = np.zeros((num_of_epochs, 4))

for epoch in range(num_of_epochs):
# compute various losses
    eq_loss, BC_loss, IC_loss = model.compute_loss(x.view(-1,1), t.view(-1,1),
 ↪Nx, Nt)

    # compute total loss
    total_loss = eq_loss + 20*BC_loss + 20*IC_loss

    # save date for losses history
    losses_history[epoch, 0] = total_loss
    losses_history[epoch, 1] = eq_loss
    losses_history[epoch, 2] = BC_loss
    losses_history[epoch, 3] = IC_loss
```

```
    # backward pass
    total_loss.backward()
    optimizer.step()
    optimizer.zero_grad()

    # skip by 500 epochs before every print
    if not epoch%500:
        print(f"epoch: {epoch}, loss: {total_loss}")

    # plot solutions by the end of [5000, 15000, 20000] epochs
    if epoch+1 in [5000, 15000, 20000]:
        u = model.forward(x.view(-1,1), t.view(-1,1)) # convert x tensor into a␣
 ↪column vector
        u_np = u.detach().numpy() # convert into a np array
        u_reshaped = u_np.reshape(Nx,Nt)
        plt.imshow(u_reshaped[:,:], cmap='jet')
        plt.title(f"$u(x,t)$ at epoch={epoch+1}")
        plt.colorbar()
        plt.xlabel("t (sec)")
        plt.ylabel("x (m)")
        plt.show()


plt.plot(losses_history)
plt.title("Losses History")
plt.legend(["Total Loss", "PDE Loss", "BC Loss", "IC Loss"])
```

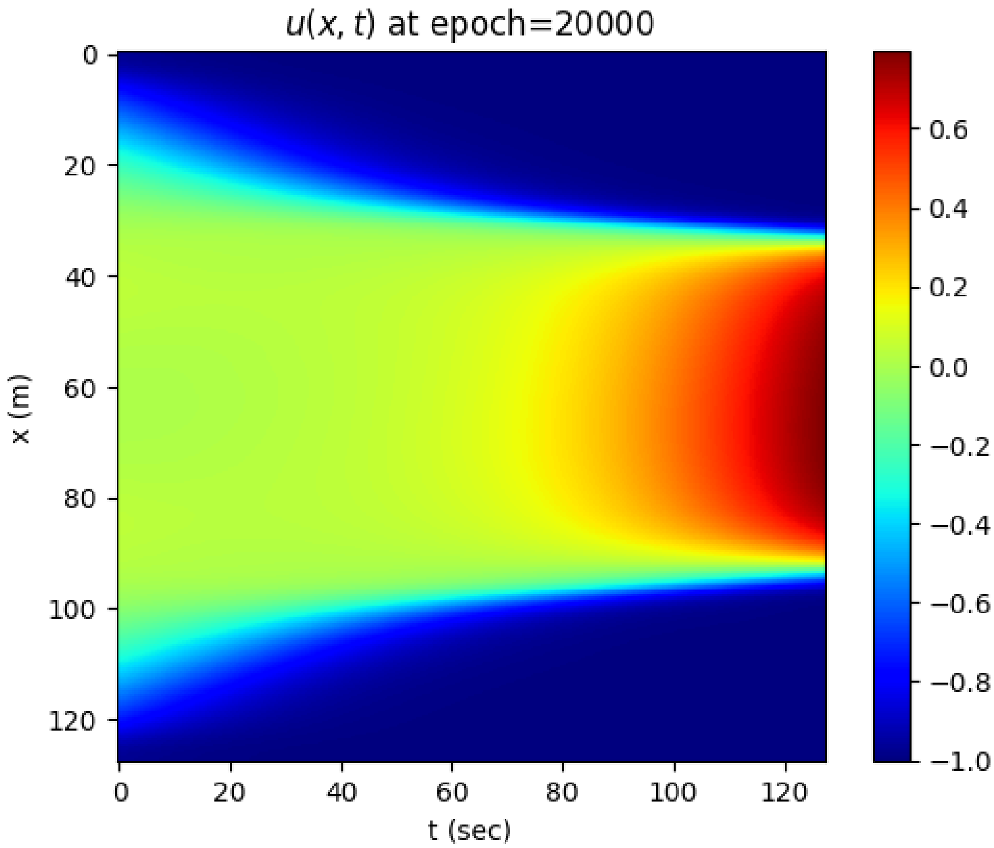
```
epoch: 0, loss: 2.7488596439361572
epoch: 500, loss: 0.8861088156700134
epoch: 1000, loss: 0.05930585414171219
epoch: 1500, loss: 0.03926784545183182
epoch: 2000, loss: 0.0315205380320549
epoch: 2500, loss: 0.02909487672150135
epoch: 3000, loss: 0.025914005935192108
epoch: 3500, loss: 0.024264851585030556
epoch: 4000, loss: 0.022779766470193863
epoch: 4500, loss: 0.021603386849164963
```



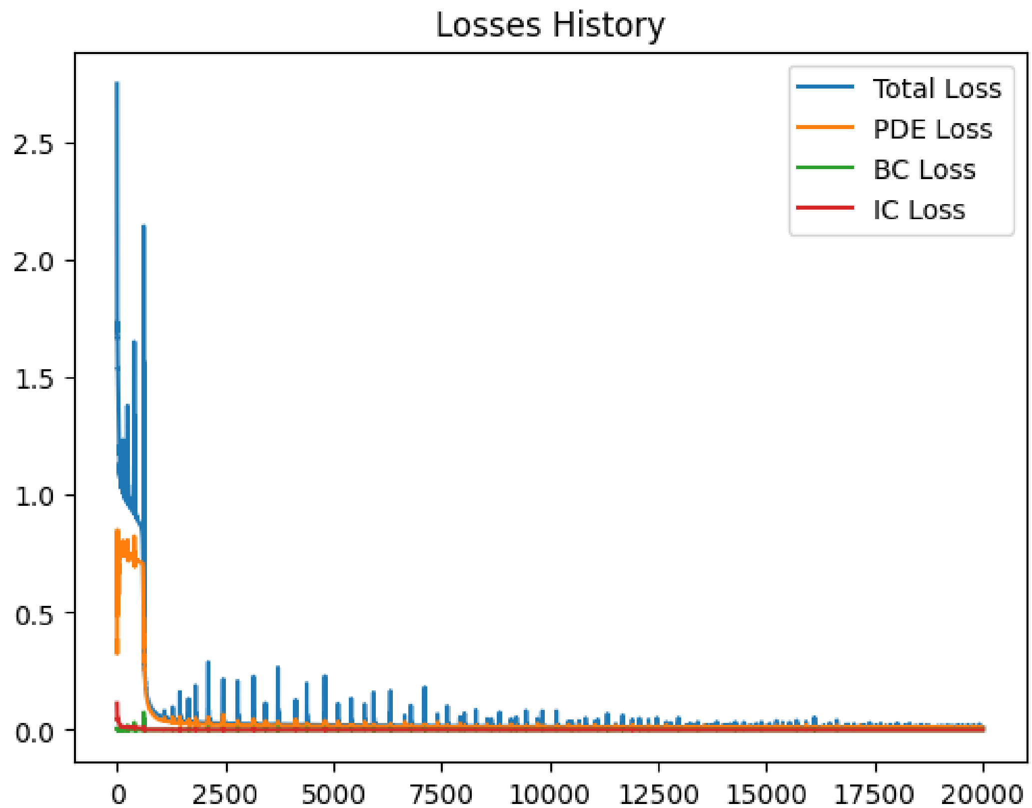

```
epoch: 5000, loss: 0.020247869193553925
epoch: 5500, loss: 0.019191797822713852
epoch: 6000, loss: 0.01826496608555317
epoch: 6500, loss: 0.0171140618622303
epoch: 7000, loss: 0.016082696616649628
epoch: 7500, loss: 0.015298517420887947
epoch: 8000, loss: 0.014574057422578335
epoch: 8500, loss: 0.014003068208694458
epoch: 9000, loss: 0.013511590659618378
epoch: 9500, loss: 0.013404212892055511
epoch: 10000, loss: 0.012786949053406715
epoch: 10500, loss: 0.01640583574771881
epoch: 11000, loss: 0.01233481615781784
epoch: 11500, loss: 0.0122213959693908\u0037
epoch: 12000, loss: 0.012052040547132492
epoch: 12500, loss: 0.012751941569149494
epoch: 13000, loss: 0.012318241409957409
epoch: 13500, loss: 0.011703806929290295
epoch: 14000, loss: 0.011653617024421692
epoch: 14500, loss: 0.012179439887404442
```




```
epoch: 15000, loss: 0.011493622325360775
epoch: 15500, loss: 0.011355290189385414
epoch: 16000, loss: 0.01130964420735836
epoch: 16500, loss: 0.011408453807234764
epoch: 17000, loss: 0.011155577376484871
epoch: 17500, loss: 0.011100772768259048
epoch: 18000, loss: 0.011020392179489136
epoch: 18500, loss: 0.011275367811322212
epoch: 19000, loss: 0.010847387835383415
epoch: 19500, loss: 0.01059894822537899
```



[ ]: <matplotlib.legend.Legend at 0x23fb3b25c90>



2 Comments

- Case without FFM - The loss function shows that after 10000 epochs there is a large spike. In addition there is a second descent after 17500 epochs. This explains why the solution at 20000 epochs is different from the solutions for 15000 and 5000 epochs.
- Case with FFM - The loss function exhibits a steady descent and the solution that took 20k without ffm is already given after 5k epochs. This suggests that the FFM allowed the PINN converge faster to begin with and is a good choice to use for this type of problem. It allows the PINNs converge to a high frequency solution better.
- In general, it takes a long time to train the PINNs so it is important to understand if the problem contains high frequency solutions or not. The PINNs still doesn't give a correct solution, so if the solution space of hyperparameters would be simulated it might help to optimally train the network.