Summer Internship for Damien Beecroft

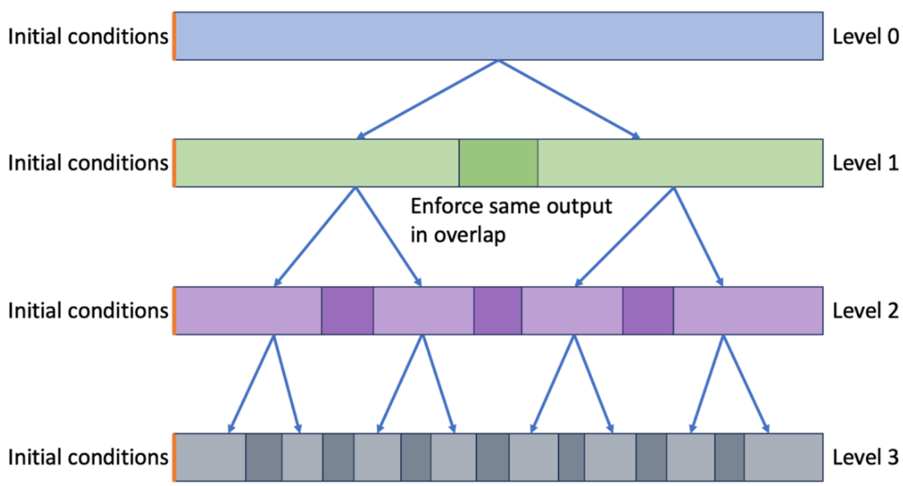
Advisors: Amanda Howard, Panos Stinis

June 28, 2023

Physics-informed neural networks, or PINNs, have shown great promise in learning the solution to partial differential equations. However, there are still cases where PINNs fail to train. This summer, we will develop new techniques for cases where PINNs fail to train.

This document serves only as a suggested outline, and creativity is encouraged. The remaining weeks will be filled in as we see how the results develop. Many extensions are possible, including training deep operator networks (DeepONets) for a range of input parameters, or switching to model other dynamical systems.

The suggested reading for each week consists of background information that you may find helpful as you work. I suggest you write a short, 1-2 sentence, summary of each paper and add it a working document after reading each paper. This will be the introduction to your final report, and later the introduction for a publication based on your work. Articles are available through PNNL when you're logged into the VPN.



We will consider a multifidelity domain decomposition approach, where a PINN is trained in the full domain first. Then, the full domain training is used as a low fidelity prediction for a prediction in a subdivided domain. Two PINNs are trained in level 1, and the domains overlap so initial conditions are not needed to train the subdomain that occurs for later time. This process is repeated until the desired accuracy is reached across the domain.

We will be working with Alexander Heinlein, who is an expert in domain decomposition. We will start by testing this setup on the case of an undamped pendulum, to see if we can overcome the issue of converging to fixed points for long time. If successful, we will move to more complex examples. Creativity is encouraged in designing training algorithms.

To Do

Reading:

- Parallel Physics-Informed Neural Networks via Domain Decomposition: `https://arxiv.org/pdf/2104.10013.pdf`
- Fourier Analysis Sheds Light on Deep Neural Networks: `https://arxiv.org/abs/1901.06523`

Coding:

- Figure out how to run code on Marianas
- Pendulum
  - Run the domain decomposition code in `Pendulum_DD`
  - Point selection and evaluation
    - Make sure that the code does not evaluate every network at all points. Only evaluate networks on points within the support of their weight function. There are two potential methods for how to do this.
      - Change the data generator function to only generate output points in a given domain
      - Once you are given a point, check whether or not the point is in the support of the weight function.
    - Work on parallelization of neural networks defined on different sub-domains.
    - Testing
      - Running with and without the residual driven point selection
      - Look at the sensitivity of the weights of the loss function
    - Do testing on how high we can get the maximum time of the pendulum. Currently it is at 10. Can we get it to 20? 50?
- Wave Equation
- Allen-Cahn
- Lorenz

Week 1

Videos:

- Stanford CS229M Lecture 13 (Neural Tangent Kernel): `https://www.youtube.com/watch?v=btphvvnad0A&list=RDCMUCBa5G_ESCn8Yd4vw5U-gIcg&index=1`

Reading:

- PINNs: `https://www.sciencedirect.com/science/article/pii/S0021999118307125`
- Multifidelity PINN: `https://arxiv.org/pdf/1903.00104.pdf`
- Multifidelity DeepONets: `https://arxiv.org/pdf/2204.09157.pdf`
- Multifidelity Continual Learning: `https://arxiv.org/pdf/2304.03894.pdf`
- Fixed points and PINNs: `https://arxiv.org/pdf/2203.13648.pdf`
- Multilevel Domain Decomposition for PINNs: `https://arxiv.org/pdf/2306.05486.pdf`
- Point selection for PINNs: `https://www.sciencedirect.com/science/article/pii/S0045782522006260`
- Respecting Causality is All you Need: `https://arxiv.org/pdf/2203.07404.pdf`

Coding:

I was sent the pendulum code by Amanda. I took some time this week to go through it and get a feel for what is going on. I have not run the code since I do not have my PNNL laptop. I plan to have the code up and running early next week.

Week 2

Reading:

- A Method for Representing Periodic Functions and Enforcing Exactly Periodic Boundary Conditions with Deep Neural Networks: `https://arxiv.org/pdf/2007.07442.pdf`
- How and Why PINNs Fail to Train: `https://arxiv.org/pdf/2007.14527.pdf`
  - Neural Tangent Kernel Convergence and Generalization: `https://arxiv.org/abs/1806.07572`
  - Deep Neural Networks as Gaussian Processes: `https://arxiv.org/abs/1711.00165`

Coding:

- Get access to Marianas
- Set up GitHub repository
- Set up GitHub repository on Marianas and pull code from `pnnl_research`
- Run Amanda's code locally
- Plot solutions from Amanda's code

Week 3

Notes:

- I went through the original code Amanda sent me slowly to understand exactly how it works.
- I went through the altered code in `Pendulum_DD` to understand exactly how it works.
- I realized that the problem of only applying neural networks to points within their domains can be solved with a rather simple sorting algorithm.

Coding

- Implementing domain sorting code.

Week 4

Week 5

Week 6

Week 7

Week 8

Week 9

Week 10