ME 697 - Project Check Point 1

**Due Date:** 2/2/2025

# Project Objective

The project aims to replicate the process of writing a paper/report in scientific machine learning. In summary, you will have to conduct a literature review, select a paper to replicate, implement the code of the paper following best practices, and write a six-page report.

# Project Timeline

The project timeline is as follows:

* **Project Checkpoint 1 (this assignment). Due 2/2/2025.** You must identify a specific paper from the list below to read in detail, identify your weaknesses on the topic covered, and start building your background knowledge to understand its material. More details below.
* **Project Checkpoint 2. Due 3/2/2025.** By this time, you should have read your chosen paper in detail and understood the mathematics of the paper. More details on the assignment will follow.
* **Project Checkpoint 3. Due 4/6/2025.** By this time, you should have implemented the first version of the code and solved a synthetic verification example. More details on the assignment will follow.
* **Project Report. Due 5/10.** By this time, you should have replicated the examples of the paper. It doesn’t matter if you have successfully replicated everything. You don’t have to be 100% successful in replicating the paper to get the full grade. More details on the assignment will follow.

# Paper Selection

You must pick **one of the following papers** to replicate:

* **Surrogate modeling**
  + Sun et al., 2020, Surrogate modeling for fluid flows based on physics-constrained deep learning without simulation data, Computer Methods in Applied Mechanics and Engineering, <https://doi.org/10.1016/j.cma.2019.112732>
  + Batzner et al., 2022, E(3)-equivariant graph neural networks for data-efficient and accurate interatomic potentials, Nature Communications, <https://www.nature.com/articles/s41467-022-29939-5>
  + Kontolati et al., 2023, On the influence of over-parameterization in manifold-based surrogates and deep neural operators, Journal of Computational Physics, <https://doi.org/10.1016/j.jcp.2023.112008>
* **Inverse problems**
  + Alberts et al., 2023, Physics-informed information field theory for modeling physical systems with uncertainty quantification, Journal of Computational Physics, <https://doi.org/10.1016/j.jcp.2023.112100>
  + Karnakov et al., 2024, Solving inverse problems in physics by optimizing a discrete loss: Fast and accurate learning without neural networks, Proceedings of the National Academy of Science, <https://doi.org/10.1093/pnasnexus/pgae005>
* **Dynamical systems**
  + Brunton et al., 2016, Discovering governing equations from data by sparse identification of nonlinear dynamical systems, Proceedings of the National Academy of Science, <https://www.pnas.org/doi/abs/10.1073/pnas.1517384113>
  + Cenedese et al., 2022, Data-driven modeling and prediction of non-linearizable dynamics via spectral submanifolds, Nature Communications, <https://www.nature.com/articles/s41467-022-28518-y>
  + Kontolati et al., 2024, Learning nonlinear operators in latent spaces for real-time predictions of complex dynamics in physical systems, Nature Communications, <https://www.nature.com/articles/s41467-024-49411-w>

# Project Check Point 1

*Write this page and submit it on gradescope.*

**Name: Shaunak Mukherjee**

**Date: 02/02/2025**

**Did you use generative AI? Which one did you use? How did you use it?**

*You can use generative AI to help you edit your text. But you will be responsible for correcting your write-up.*

**Yes, I used ChatGPT. I used it to make the texts more cohesive. It definitely writes better English than me.**

# Understand what the suggested papers are about

* Read the abstracts and skim through all suggested papers.
* Google the authors’ names and/or paper titles and try to find if they have codes that replicate their papers or a lecture video explaining the paper. Both of these will help you understand the paper faster. Feel free to discuss your findings with others on the discussion forums.

*Nothing to report.*

# Read more carefully the papers you find more interesting

Pick two papers that you find interesting and dedicate about one or two hours to each one of them to dig a little deeper. You can read them a bit more carefully. You can watch the YouTube videos you found, etc. Your goal is to learn more so that you can make an informed choice moving forward.

*I watched the following videos*

*I evaluated two papers E(3)-equivariant graph neural networks by Batzner et al 2022 and*

*I picked this paper- E(3)-equivariant graph neural networks for data-efﬁcient and accurate interatomic potentials by Batzner et al. Nat. Comm. 2022, 13, 2453 based on useful videos on youtube.*

[*https://www.youtube.com/watch?v=oePOO8bN7Co*](https://www.youtube.com/watch?v=oePOO8bN7Co)

[*https://www.youtube.com/watch?v=ZR1NTBPBDOo*](https://www.youtube.com/watch?v=ZR1NTBPBDOo)

[*https://www.youtube.com/watch?v=JwYPVP-vm6A*](https://www.youtube.com/watch?v=JwYPVP-vm6A)

# What is the paper you picked?

*E(3)-equivariant graph neural networks for data-efﬁcient and accurate interatomic potentialsby Batzner et al. Nat. Comm. 2022, 13, 2453*

# What is the big problem/need addressed by the paper?

# What is the specific objective of the paper?

*Your answer here.*

# What are the gaps in your background knowledge you would have to cover to understand the paper fully?

*Identify your knowledge gaps. Do you understand the mathematical terminology? Is there a reference to a specific mathematical topic you are unfamiliar with? It is okay if you are unfamiliar with the topic which will be covered in class. However, it is also okay if an unfamiliar topic is not covered in class. Push yourself a little bit. You will not be penalized for selecting a difficult topic. Your answer here. Delete this italic text.*

*I am familiar with atomic potentials, advanced quantum mechanics and group theory. I am also familiar with CNN.*