Master's Thesis 2026

Title

Jonatan Haraldsson
Jesper Noord

Department of Industrial and Materials Science
Division of Material and Computational Mechanics
Chalmers University of Technology
Gothenburg, Sweden 2026

Title

© Jonatan Haraldsson & Jesper Noord

Supervisors:
Examiner:

Master's Thesis 2025
Department of Industrial and Materials Science
Division of Material and Computational Mechanics
Chalmers University of Technology
SE-412 96 Gothenburg

Cover:

Typeset in LaTeX
Printed by Chalmers Reproservice
Gothenburg, Sweden 2025

Title
Jonatan Haraldsson & Jesper Noord
Department of Industrial and Materials Science
Division of Material and Computational Mechanics
Chalmers University of Technology

Abstract

bla bla

Keywords: *Physics Informed Neural Network, ..., ...*

Acknowledgements

List of Acronyms

BC boundary condition. 3

EV electric vehicle. 1

FE finite element. 1

IC initial condition. 3

Li lithium. 1, 2

LiB lithium-ion battery. 1

NCA Nickel Cobalt Aluminum. 2

NMC Nickel Manganese Cobalt. 2

NN neural network. 1, 2

PDE partial differential equation. 3

PINN physics-informed neural network. 1

RMSE root-mean-squared error. 3

Contents

1
Introduction

1.1 Background

With an ever growing demand for convenient energy storage, the use of lithium-ion batteries (LiBs) in portable devices have skyrocketed over the last 30 years.

physics-informed neural network (PINN), electric vehicle (EV), lithium (Li)

Contents

- Why batteries? (Nobel prize 2019, a game changer in our modern lives, necessary for climate change)
- However, there are still problems, and the hunt for even more energy efficient batteries requires models to describe the physical properties of batteries.
- While models based on finite element (FE) can be used to simulate such systems to a high accuracy, they are often computationally costly[1]. Au contraire, data-driven models such as neural networks (NNs) are generally computationally cheap once trained, but could require large dataset to reach a satisfying accuracy. In addition, a purely data-driven approach fails to encompass prior knowledge of the underlying physics.
- To address this, PINN offers a middle-ground approach, where physical knowledge of the system can be combined with the data-driven approach of NNs. Specifically, in PINNs solutions outside of the physically viable domain are heavily penalized, hopefully forcing the NN outputs to be close to the true solution. Although first introduced during the 90s, PINNs have gained popularity with the rise of modern computational power.

1.2 Aim and Scope

2
Theory

2.1 Overview of Batteries

- A battery's parts, anode, cathode, electrolyte.
  - Anode: Primarily graphite. Light-weight, high conductivity
  - Cathode: Li-oxides commonly Nickel Manganese Cobalt (NMC) or Nickel Cobalt Aluminum (NCA).
  - Electrolyte: Up to this point mainly liquid electrolytes, however, solid-state electrolyte are in development.
  - Lithium: Why use Li in the first place? (Fun fact: Li was first discovered on Utö in the Stockholm archipelago) Li, the third lightest element on earth, has the among the lowest density out of all solids and it has a low ionization energy. With its low mass it uses less energy as it diffuses through the cell.
- The general working principle: charging and discharging. Potential negative effects that need to be considered. Heat development, or other factors affecting performance of the cell. Intercalation of Li^+
- What equations are governing? (Thermodynamics, Mechanics, electric, chemical)
- The different scales: cell vs. module vs. pack. What can be inferred from the different scales? How does microscopic properties influence macroscopic ones and vice versa.
-

2.2 Neural Networks

- General overview of neural networks. Explain neurons, weights, bias, loss function, different types of NNs. RNN??
- Motivate the use of NNs w/ the Universal Approximation Theorem, i.e., the fact that a single layer perceptron NN can achieve universallity. Put differently, any continuous function can be modelled to the desired degree of accuracy with a NN (wiki-link).

2.3 Physics Informed Neural Networks

- Generally describe the setup we're dealing with Eq. 2.1 to 2.3. Eq. 2.1 describes the partial differential equation (PDE) residual, Eq. 2.2 the initial condition (IC) and Eq. 2.3 the boundary condition (BC).
- How to make NNs PINNs? Regularization term in the loss function that penalizes NN solutions that aren't physically viable.

$$f\left(\boldsymbol{x}, t, \frac{\partial u}{\partial \boldsymbol{x}}, \frac{\partial u}{\partial t}, \boldsymbol{\lambda}\right) = 0, \quad \boldsymbol{x} \in \Omega, t \in [0, \tau], \tag{2.1}$$

$$u(\boldsymbol{x},0) = h(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega, \tag{2.2}$$

$$u(\boldsymbol{x},t) = g(\boldsymbol{x},t), \quad \boldsymbol{x} \in \partial\Omega, t \in [0, \tau]. \tag{2.3}$$

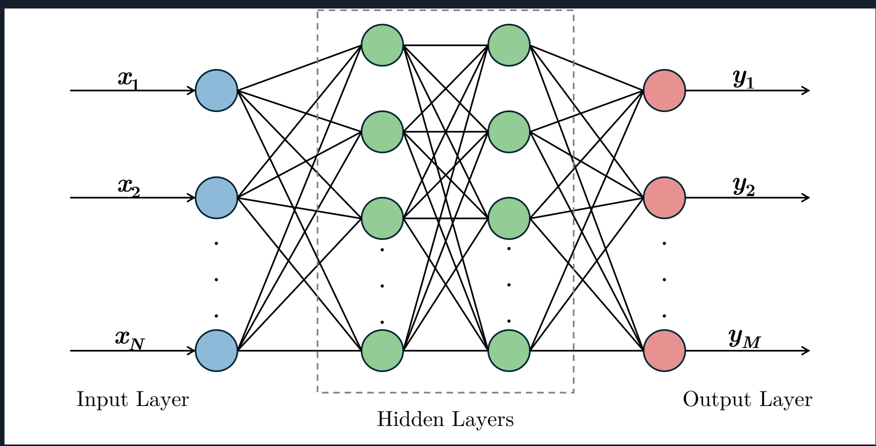

Fig 2.1: Schematic view of a neural network where each circle represents a single neuron. An input signal $\boldsymbol{X} = \{\boldsymbol{x}_i\}_{i=0}^{N}$ enters the model in the input layer, proceeds through the hidden layers, and exits from the output layer. This process produces an output $\boldsymbol{Y} = \{\boldsymbol{y}_i\}_{i=0}^{M}$, which can be interpreted as a prediction based on the input data.

Loss function, such as root-mean-squared error (RMSE).

3
Method

Here's the method

4
Results and Discussion

Here are the results

5 Conclusion

Here's the conclusion

Bibliography

[1] A. Asheri, M. Fathidoost, V. Glavas, S. Rezaei, and B.-X. Xu, “Data-driven multiscale simulation of solid-state batteries via machine learning,” *Computational Materials Science*, vol. 226, p. 112 186, 2023, ISSN: 0927-0256. DOI: https://doi.org/10.1016/j.commatsci.2023.112186. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S0927025623001805.

A

Appendix A: Extra Stuff

In Fig. A.1, ...

Fig A.1: hej