Master's Thesis 2026

Title

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Title

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Title

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Abstract

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

Acknowledgements

List of Acronyms

BC boundary condition.

DFN Doyle-Fuller-Newman model.

EV electric vehicle.

FE finite element.

FFE Fourier feature embedding.

IC initial condition.

Li lithium.

LiB lithium-ion battery.

NCA Nickel Cobalt Aluminum.

NMC Nickel Manganese Cobalt.

NN neural network.

PDE partial differential equation.

PINN physics-informed neural network.

RWF random weight factorization.

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

Literture from RISE

- **Matty 2025 MSc thesis Chalmers** - Modelling of Electrode Swelling in Lithium ion Batteries.pdf. Thesis work from 2025 at VCC on multiscale modelling of cyclic swelling of batteries. This thesis introduces the topic of electro-chemo-mechanical modelling of batteries, and the current thesis will explore if/how AI/ML-methods can be used for upscaling the response, going from the corresponding micro/meso- to macroscale.

- **Asheri 2023** - Data-driven multiscale simulation of solid-state batteries via machine learning.pdf. Paper from a group in Darmstadt, Germany (work done with VW), where they train a surrogate model (based on NN) on a large set of simulation data, which is afterwards employed to predict the cell performance (for solid-state batteries, which in general or from a modelling perspective, is very similar to conventional batteries).

- **Meyer and Ekre 2023** – Thermodynamically consistent neural network plasticity modelling and discovery of evolution laws. Very nice paper from Knut and Fredrik (another previous, Chalmers-Fredrik) on using thermodynamically consistent NN for plasticity modelling and discovery of evolution laws.

- **Panahi et al 2025** - Fast and generalisable parameter-embedded neural operators for lithium-ion battery simulation.pdf. Recent paper from RWTH Aachen+Imperial on machine learning surrogates for battery modelling.

- **Guo 2025** - Uncovering the impact of battery design parameters on health and lifetime using short charging segments.pdf. Recent paper from Uppsala+Aalborg on ML framework for corresponding problem.

- **Schmid 2024** - Sequential Multi-Scale Modeling Using an Artificial Neural Network-Based Surrogate Material Model for Predicting the Mechanical Behavior of a Li-Ion Pouch Cell Under Abuse Conditions.pdf. Long, but relatively self-explanatory, title. Basically, this paper uses a similar approach, but for the pure mechanical response of batteries under mechanical impact loading (or what is referred to as abuse conditions).

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, has the lowest density out of all solids and it also 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^+ $Li \rightarrow Li^+ + e^-$
- What equations are governing? (Thermodynamics, Mechanics, electric, chemical). The Doyle-Fuller-Newman model (DFN) seems to be the gold-standard when it comes to modeling (DFN).
- 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) [2].
- How to make NNs PINNs? Regularization term in the loss function that penalizes NN solutions that aren't physically viable.

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

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

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

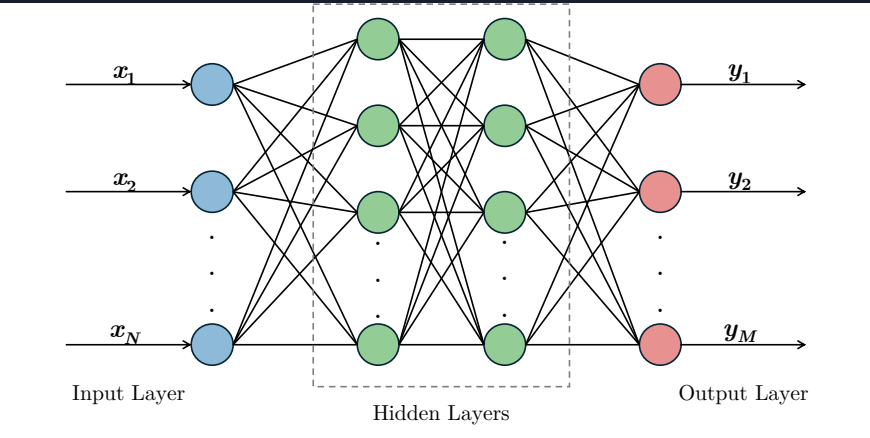

FIG 2.1: Schematic view of a neural network where each circle represents a single neuron. An input signal $\boldsymbol{X} = \{\boldsymbol{x}_i\}_{i=0}^{N}$ enters the model in the input layer, proceeds through the hidden layers, and exits from the output layer. This process produces an output $\boldsymbol{Y}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

2.3.1 Pipeline for the Training Procedure

Following the suggested pipeline from Wang *et al.*, the initial step is to ensure inputs and outputs are within the same range through non-dimensionalization of the PDE system [3]. Unevenly distributed values might: negatively influence the training process leading to unstable convergence, prevent the model from finding important correlations, it could also prevent vanishing gradient phenomenon through a more balanced initialization scheme. In practice, non-dimensionalization is done by reducing the system to a dimensionless version by first choosing some fundamental units or characteristics, and then scaling the remaining parameters such that all terms are dimensionless and of first order. An example of non-dimensionalization for Navier-Stoke

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \vec{\nabla})\boldsymbol{u} = -\frac{1}{\rho}\vec{\nabla}p + \nu\nabla^2\boldsymbol{u} \longmapsto \frac{\partial \boldsymbol{u}^*}{\partial t^*} + (\boldsymbol{u}^* \cdot \vec{\nabla}^*)\boldsymbol{u}^* = -\vec{\nabla}^* p^* + \frac{1}{\mathrm{Re}}\nabla^{*2}\boldsymbol{u}^*,$$

where $\boldsymbol{u}^* = \boldsymbol{u}/U$, $\vec{\nabla}^* = L\vec{\nabla}$, $t^* = tU/L$, and $p^* = p/(\rho U^2)$

The subsequent step is to design the NN architecture that could represent the PDE. Wang *et al.* recommends using either Fourier feature embedding (FFE) or random weight factorization (RWF) to accelerate the convergence [3]. Lastly, the training procedure should contain loss balancing, casual training and/or curriculum training.

3
Method

Here's the method

4
Results and Discussion

Here are the results

5
Conclusion

Here's the conclusion

Bibliography

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Appendix A: Extra Stuff

In Fig. A.1, ...

Fig A.1: hej