Physics-Informed Neural Network Modeling of Li-ion Batteries

Preprint

Malik Hassanaly,[1] Peter Weddle,[1] Kandler Smith,[1]
Subhayan De,[2] Alireza Doostan,[2] and Ryan N. King[1]

1 National Renewable Energy Laboratory
2 University of Colorado Boulder

Presented at the 242nd Electrochemical Society Meeting
Atlanta, Georgia
October 9-13, 2022

NREL is a national laboratory of the U.S. Department of Energy
Office of Energy Efficiency & Renewable Energy
Operated by the Alliance for Sustainable Energy, LLC

This report is available at no cost from the National Renewable Energy Laboratory (NREL) at www.nrel.gov/publications.

Contract No. DE-AC36-08GO28308

Conference Paper
NREL/CP-2C00-82015
August 2022

Physics-Informed Neural Network Modeling of Li-ion Batteries

Preprint

Malik Hassanaly,[1] Peter Weddle,[1] Kandler Smith,[1]
Subhayan De,[2] Alireza Doostan,[2] and Ryan N. King[1]

1 National Renewable Energy Laboratory
2 University of Colorado Boulder

Suggested Citation
Hassanaly, Malik, Peter Weddle, Kandler Smith, Subhayan De, Alireza Doostan, and Ryan N. King. 2022. *Physics-Informed Neural Network Modeling of Li-ion Batteries: Preprint*. Golden, CO: National Renewable Energy Laboratory. NREL/CP-2C00-82015. https://www.nrel.gov/docs/fy22osti/82015.pdf.

NREL is a national laboratory of the U.S. Department of Energy
Office of Energy Efficiency & Renewable Energy
Operated by the Alliance for Sustainable Energy, LLC

This report is available at no cost from the National Renewable Energy Laboratory (NREL) at www.nrel.gov/publications.

Contract No. DE-AC36-08GO28308

Conference Paper
NREL/CP-2C00-82015
August 2022

National Renewable Energy Laboratory
15013 Denver West Parkway
Golden, CO 80401
303-275-3000 • www.nrel.gov

NOTICE

This work was authored in part by the National Renewable Energy Laboratory, operated by Alliance for Sustainable Energy, LLC, for the U.S. Department of Energy (DOE) under Contract No. DE-AC36-08GO28308. Funding provided by the U.S. Department of Energy Office of Science, Advanced Scientific Computing Research. The views expressed herein do not necessarily represent the views of the DOE or the U.S. Government. The U.S. Government retains and the publisher, by accepting the article for publication, acknowledges that the U.S. Government retains a nonexclusive, paid-up, irrevocable, worldwide license to publish or reproduce the published form of this work, or allow others to do so, for U.S. Government purposes.

This report is available at no cost from the National Renewable Energy Laboratory (NREL) at www.nrel.gov/publications.

U.S. Department of Energy (DOE) reports produced after 1991 and a growing number of pre-1991 documents are available free via www.OSTI.gov.

Cover Photos by Dennis Schroeder: (clockwise, left to right) NREL 51934, NREL 45897, NREL 42160, NREL 45891, NREL 48097, NREL 46526.

NREL prints on paper that contains recycled content.

Physics-informed neural network modeling of Li-ion batteries

Malik Hassanaly[1], Peter Weddle[1], Kandler Smith[1], Subhayan De[2], Alireza Doostan[2], and Ryan N. King[1]

[1] National Renewable Energy Laboratory, Golden CO
[2] University of Colorado Boulder, Boulder CO

Keywords: *Physics-informed neural network, Lithium-ion battery, Battery degradation, Pseudo two-dimensional model*

Li-ion batteries (LIB) are a promising solution to enable the storage of intermittent energy sources due to their high energy density. However, LIBs are known to significantly degrade after about 1000 charge-discharge cycles. LIBs degrade following different degradation modes and at a rate that depends on the operating conditions (e.g., external temperature, load). To plan the installation of batteries, appropriate understanding and prediction capabilities of their lifecycle is needed. In particular, the LIB degradation model needs to be transferable to variable operating conditions throughout the LIB lifetime. To this end, degradation models of individual LIB battery properties are sought to allow for sufficient granularity in the degradation model.

High-fidelity numerical models of LIBs such as the pseudo-two-dimensional (P2D) model have been shown to accurately represent the charge-discharge-cycle of an LIB if the physical parameters used in the model are accurately estimated. Given observations of battery charge-discharged cycles, the objective is to use the P2D model to infer the values of all the battery properties, throughout the battery life. To prevent overfitting and account for the sparse data availability, the overarching objective is to enable Bayesian calibration to solve the inverse problem. Given the number of physical parameters, and the number of cycles to simulate, adjusting parameters directly via P2D forward runs is computationally intractable.

This work describes the development of a surrogate model that would replace numerical integration of the P2D equations to significantly reduce the cost of the forward runs. To capture parameter dependencies, a physics-informed neural network (PINN) is developed as a surrogate substitute for the P2D model. The inverse modeling approach is illustrated in Fig. 1 (top). The PINN is advantageous as it needs little to no observational data, which avoids offsetting the reduced inference computational cost with an increased training data generation burden. However, PINNs are notoriously difficult to train in stiff dynamical systems such as the P2D equations. Here, we discuss the specific training procedure that is adopted to efficiently cover parameter space, handle model stiffness, enforce initial, boundary conditions, and treat variables of different magnitudes. Furthermore, a verification procedure akin to ones used in computational fluid dynamics is implemented to ensure that the right governing equations are implemented. An emphasis is placed on verifying the governing equation even in presence of numerical errors.

The training procedure and loss convergence are described to highlight training instabilities encountered. In addition, the training cost is evaluated and put in perspective of the forward integration of the P2D equations. Through ablation studies, we discuss what model components are the most critical to appropriately capture P2D solutions.

The trained PINN is validated against numerical solutions of the P2D model (sample results are shown in Fig. 1 bottom). In particular, it is assessed whether the PINN can replicate numerical solutions for parameter values not represented in the training data which is key in ensuring that the surrogate can be used for parameter calibration.

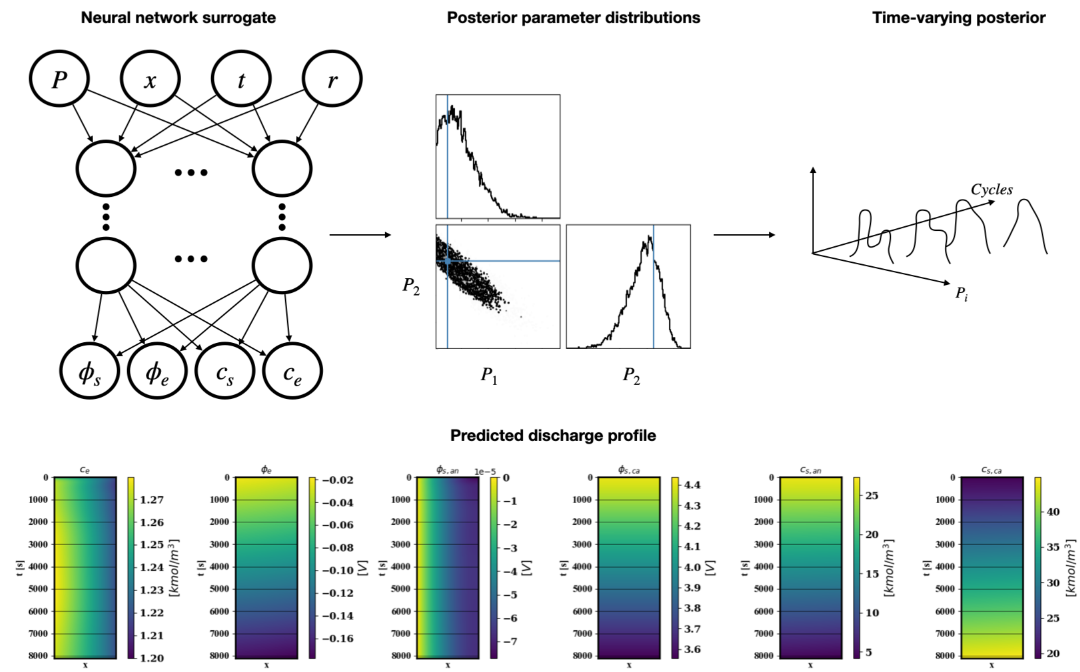

Figure 1: Top: inverse modeling approach of the battery degradation model. Bottom: sample predicted battery state discharge profile.