THE AEROSPACE CORPORATION

Data-Driven and Physics-Informed Li-ion Battery Performance Modeling

Space Power Workshop

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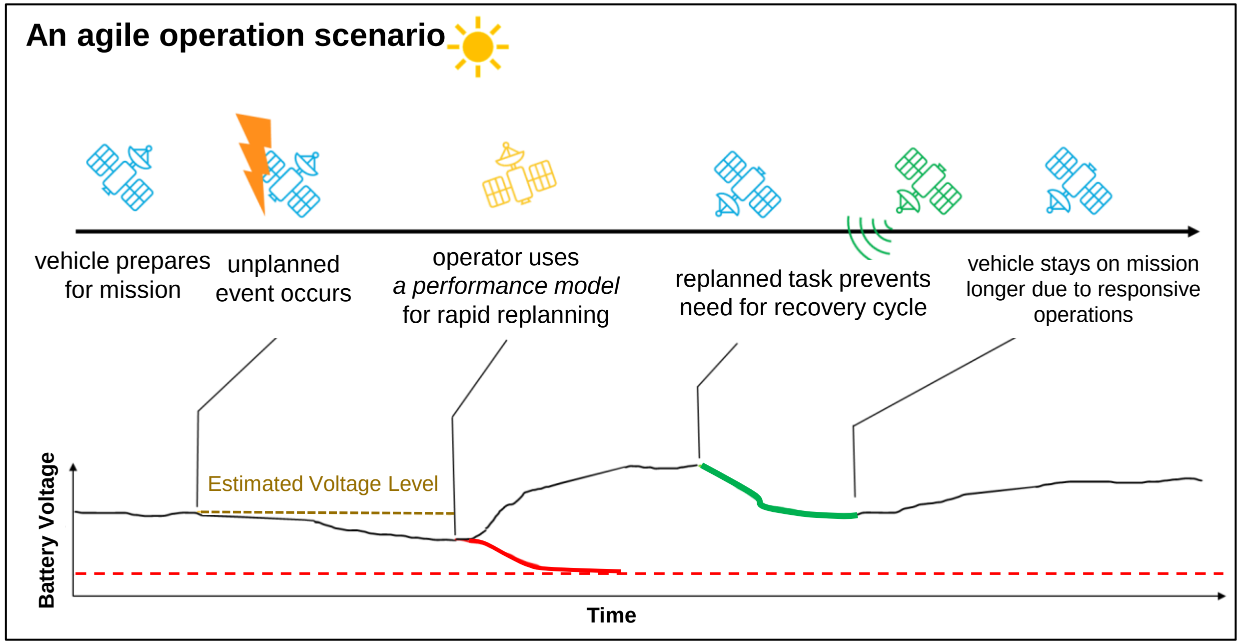
April 2025

Motivation

The Need for Intelligent Energy Management in Space

- Space missions are becoming increasingly complex, driving the need for agile space operations
  - Requires real-time adaptation and optimization of spacecraft missions based on changing circumstances
  - Operators must be prepared to respond intelligently to unexpected events and make decisions
- Agile space operations could significantly impact EPS, particularly batteries, by introducing dynamic demands
- Examples include:
  - Maneuvering spacecraft to avoid space debris
  - Rapid reconfiguration of communication systems to handle varying data transmission needs



Agile space operations require real-time energy management solutions to handle unpredictable power demands

Battery Model Development Approach

Data-Driven and Physics-Informed Li-ion Battery Performance Modeling

- To support agile scenarios, the goal of our battery model is to **predict** a forecast of future **cell voltage** given information about the present cell voltage and a context window of past and future **current**

Context

C_t

$C_t = [\ldots, -1, -1, -1, -3, -3, ..]$

system current

V_t → **Battery Model** → F_t

Predictions

Priors

$V_t = 3.13$

present cell voltage

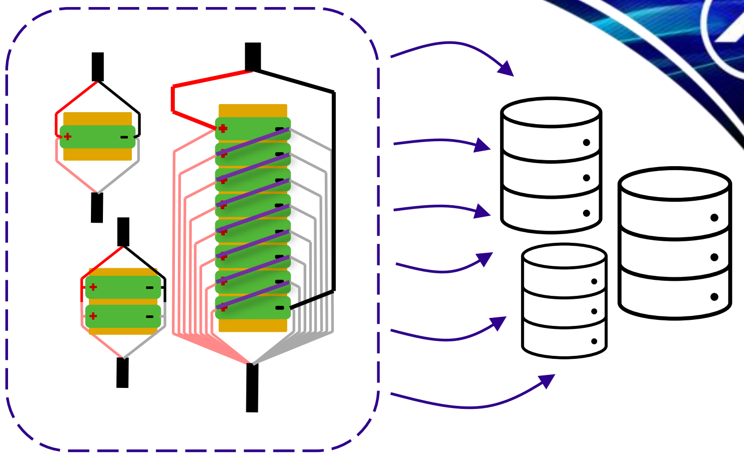
$F_t = [2.96, 2.71, ..]$

cell voltage forecast

$$F_t = f(C_t, V_t)$$

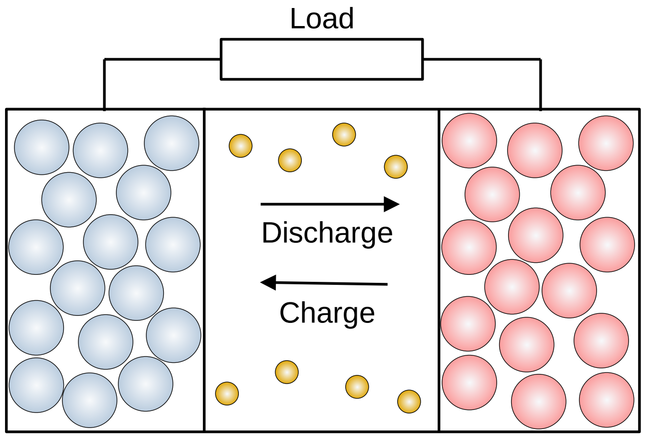
- **Formulation**
  - *Model Inputs*
    - Context of $C_t =$ ***past and future system current, past voltage***
    - Prior of $p_t =$ ***present cell voltage***
  - *Model Outputs*
    - Predict forecast of $F_t =$ ***future cell voltage***

Data-driven Model



Big data *No physics*	Some data Some physics	Small data All physics

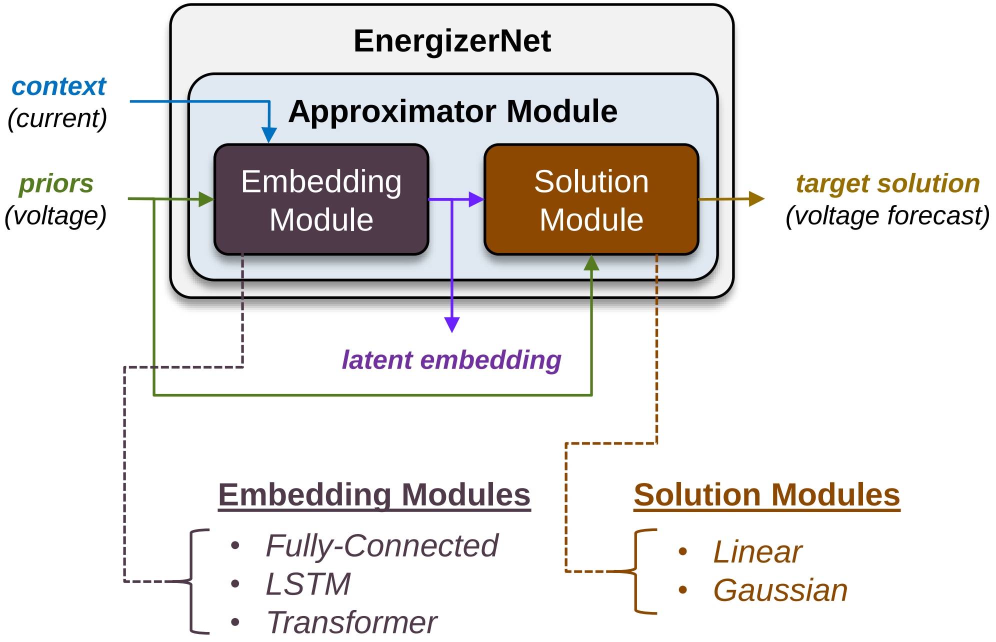
Physics-informed Model

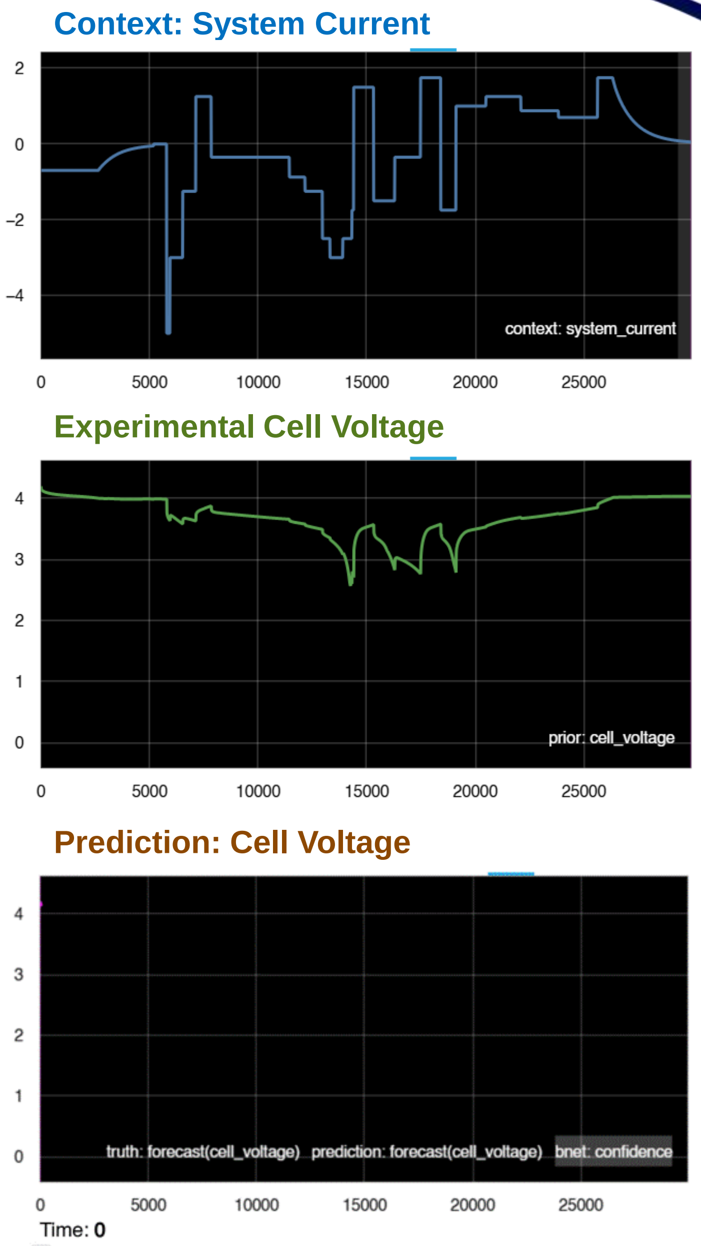


Anode Electrolyte Cathode

Data-Driven Model (EnergizerNet) Architecture

Embedding-Solution Modular Architecture





- **Data-driven model**
  - *input*: *prior cell voltage value* and *system current context window*
  - *output*: forecast of *future cell voltage values*
- **Recursive Forecasting of Telemetry**
  - Future prior voltages are estimated as a *consensus of past voltage forecasts*

A modular architecture that outputs both target solutions and latent embeddings of inputs

Data-Driven Model: Training Data Design Approach

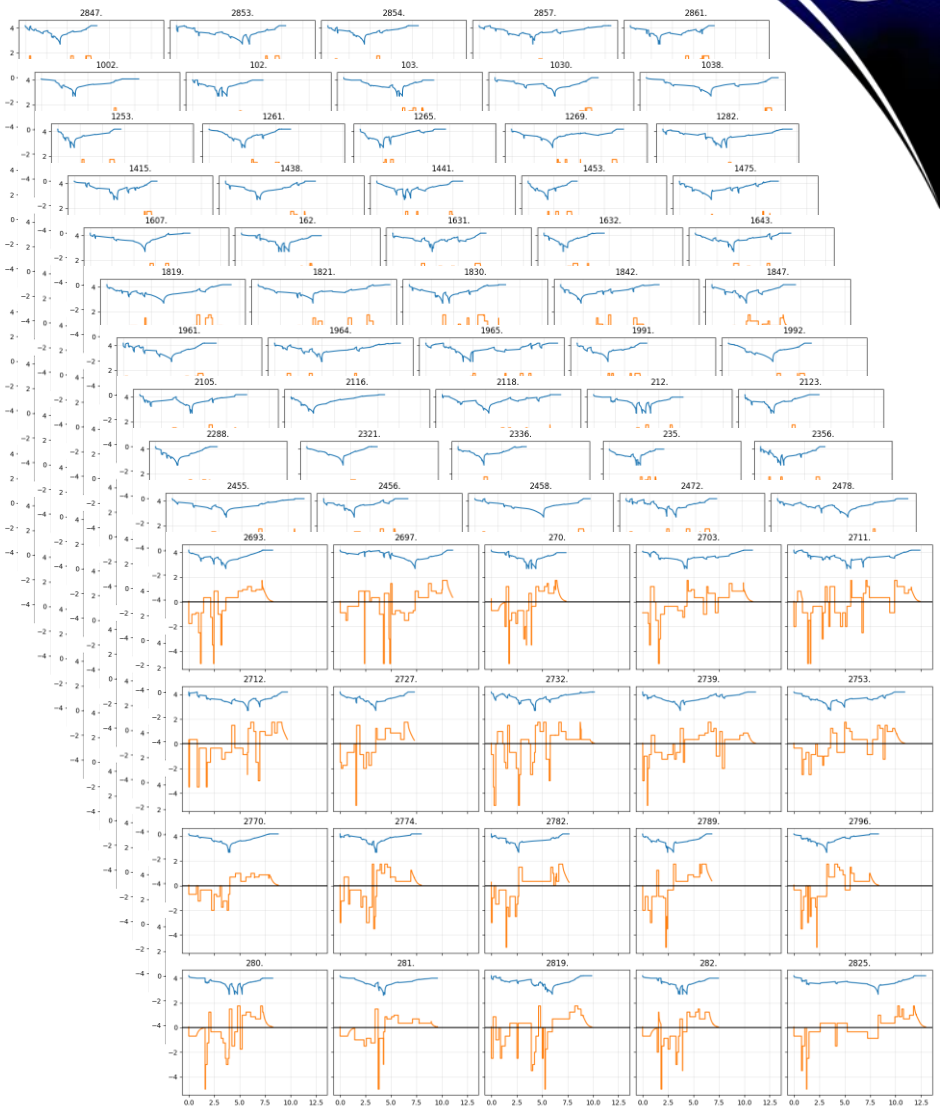
A model is only as good as its training data

- **Training data considerations:**
  - Most performance variability occurs at transitions (change in charge/discharge current)

- **Design approach:**

1. Hold as many conditions constant as possible to simplify the initial solution
   - SOH *(assume BOL, limit test time on any individual cell)*
   - Environment *(generate all data at 20°C)*
2. Create many combinations of the remaining variables to capture the bandwidth of performance
   - Current *(vary charge/discharge current)*
   - SOC *(continue varying current over full capacity of cell)*

- This design resulted in a matrix of [SOC, Current] pairs that were distributed over hundreds of "drive cycle"-style profiles.

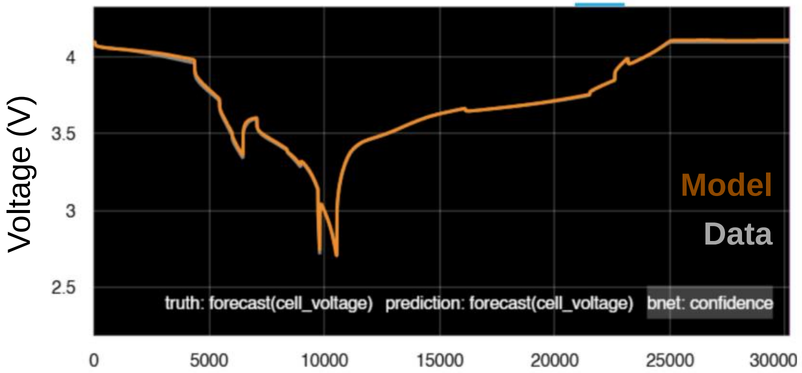


Generated a comprehensive dataset (850 drive cycles) using NMC-based Li-ion cells

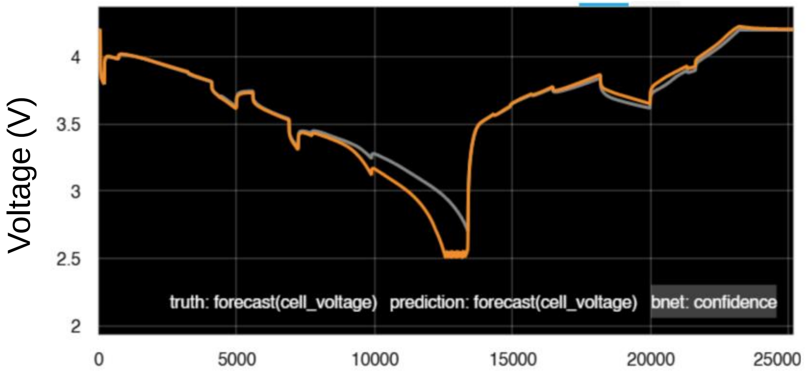
Data-driven Model Results

Assessing Model Accuracy and Confidence

- Data-driven model predicts voltage responses given system current
- Quantifying confidence assessments
  - Enables operators to make informed decisions by highlighting areas where predictions are robust
  - Guides further data collection efforts to improve model accuracy in underrepresented regions



Good fit

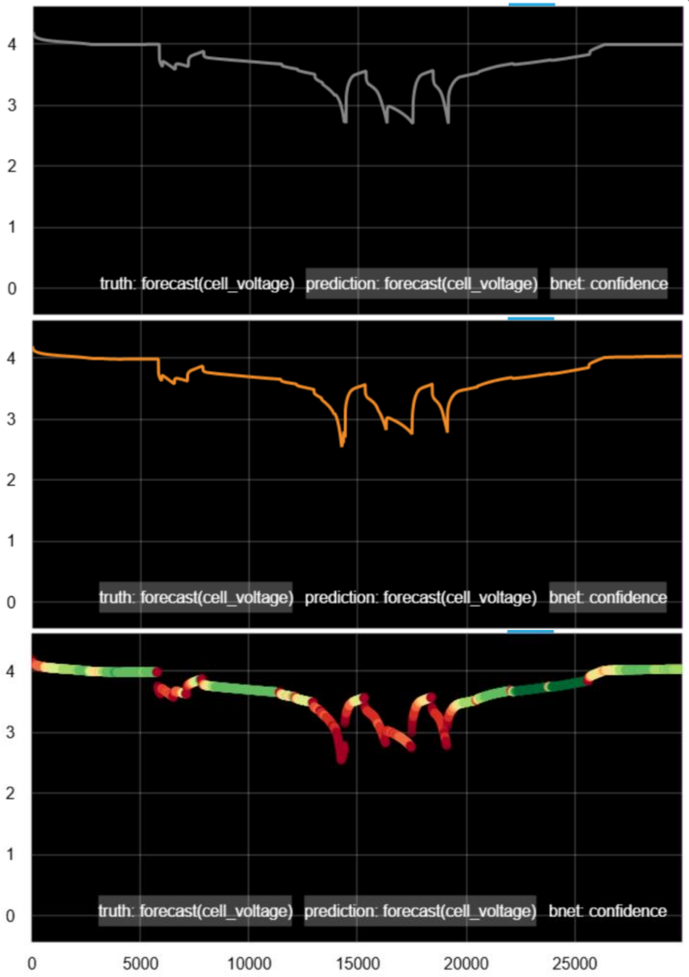


Poor fit

Ground Truth Cell Voltage Signal

Forecast Cell Voltage Signal

Confidence Assessments



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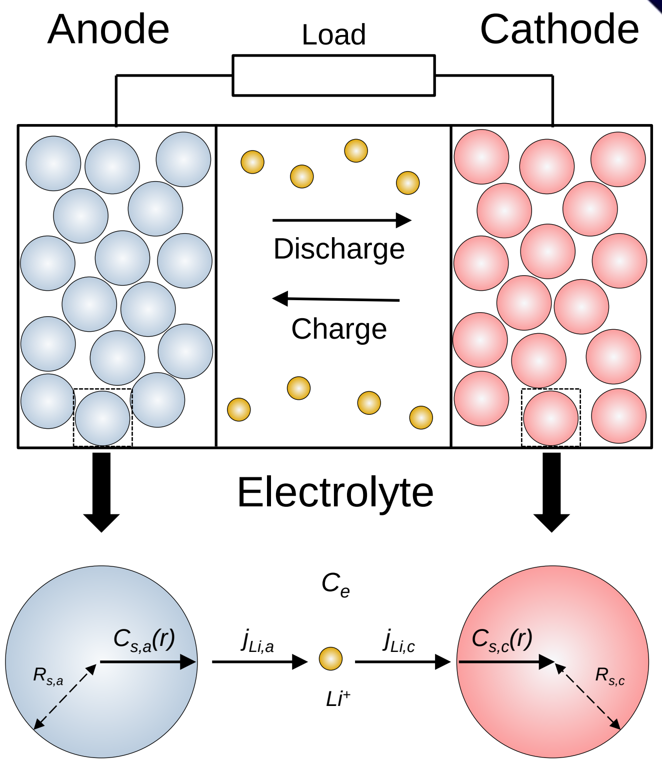
Physics-informed Model Background

Integrating Physical Principles into Battery Modeling

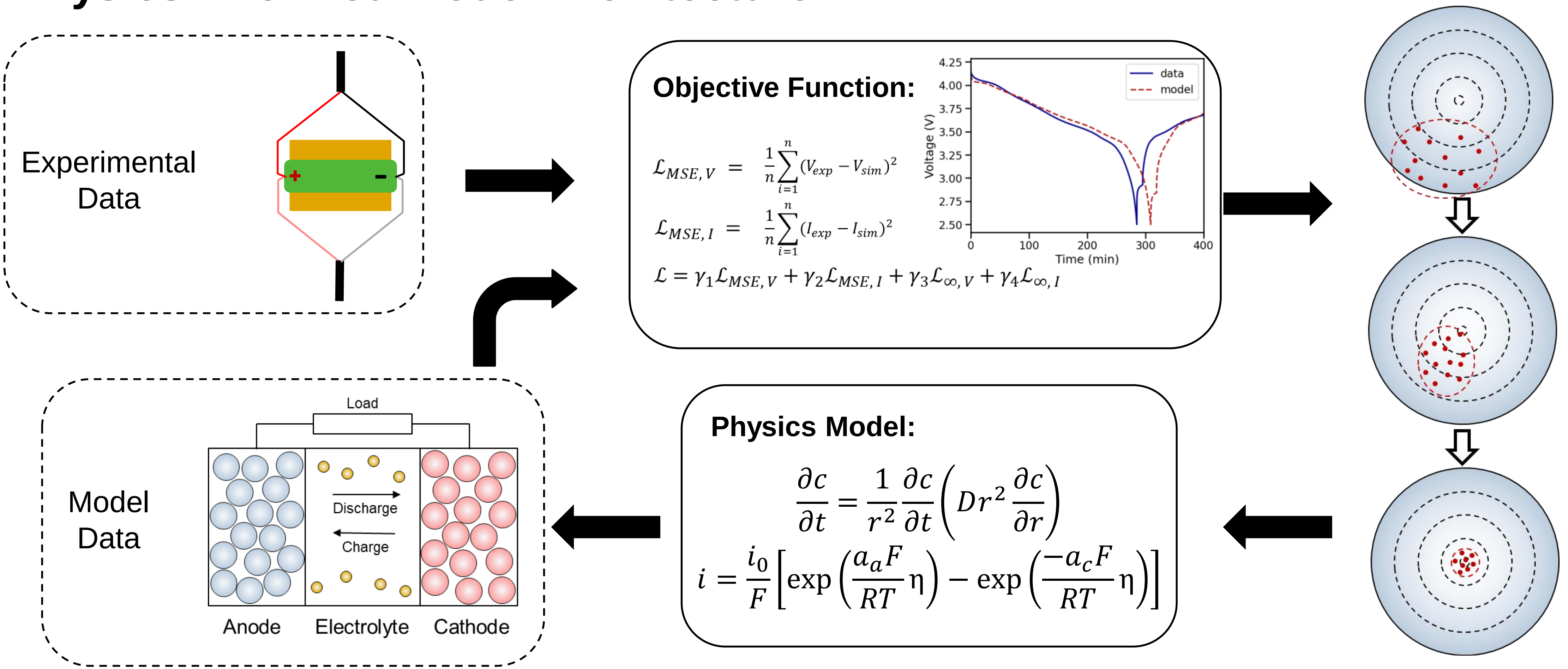
- Our physics-informed model relies on a P2D (pseudo-two dimensional) approach
  - The P2D Li-ion cell model assumes radial symmetry and one-dimensional charge transport within the electrode materials
  - The parameters include electrochemical constants (diffusion coefficients, reaction rates), geometrical parameters (electrode thickness, active area), and thermodynamic properties

- Determining these parameters is challenging due to the complexity of electrochemical phenomena
  - It often requires requires both destructive and non-destructive, complex electrochemical experiments
  - This model involves a total of 23 physics-based parameters



The pseudo-2D battery model incorporates complex electrochemical parameters

Physics-informed Model Architecture

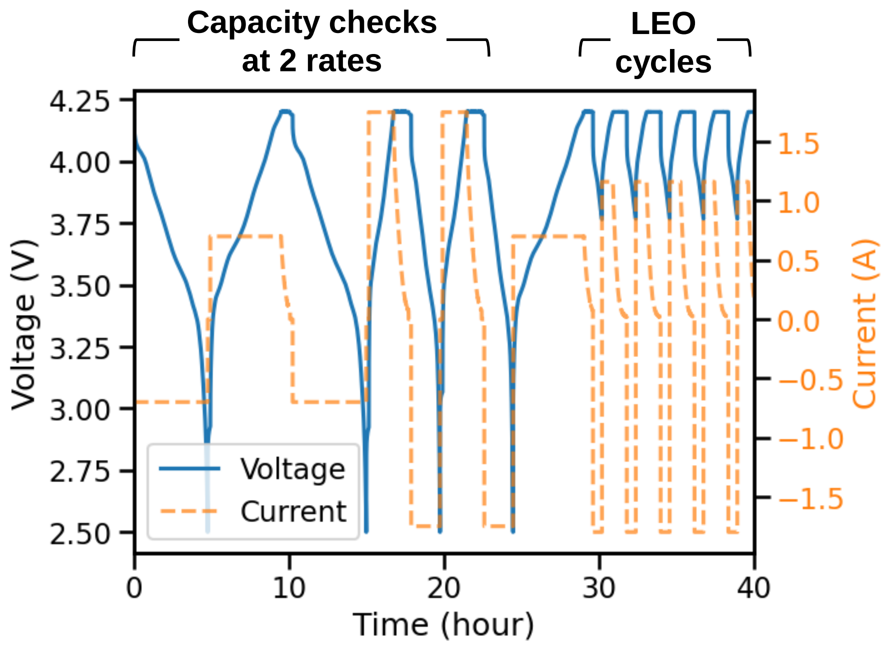


- Optimization algorithm iteratively adjusts model parameters by exploring the parameter space based on fitness evaluations
  - It utilizes gradient-free, covariance matrices to guide the search direction and accelerate convergence towards optimal parameters
- Goal is to minimize the difference between model predictions and experimental data (loss function)
  - Ensures that the model adheres to physical laws while fitting the data

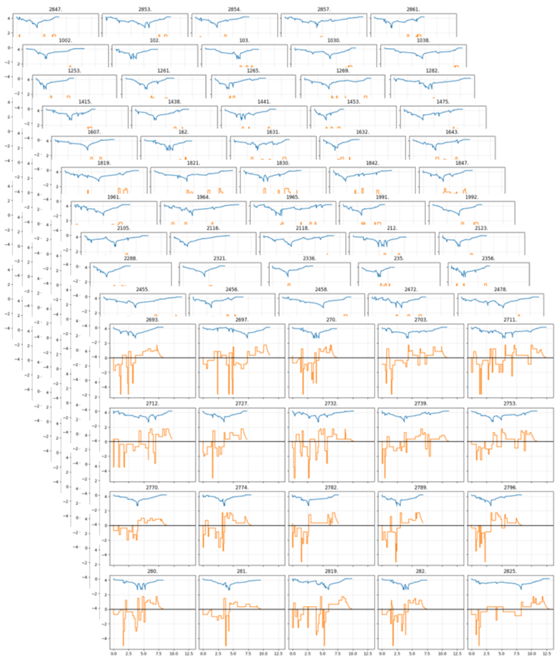
Physics-informed Model: Training Data Design Approach

Efficient Data Utilization for Physics-Informed Models

- **Training data considerations:**
  - The physics-informed approach incorporates fundamental electrochemical principles (needs OCV)
  - Requires significantly less training data compared to data-driven approach (roughly 2 days vs 2 months)
- The training dataset consists of charge/discharge cycles at 2 different rates
  - Include a few Low Earth Orbit (LEO) cycles for realistic operational scenarios



Physics-informed Training dataset

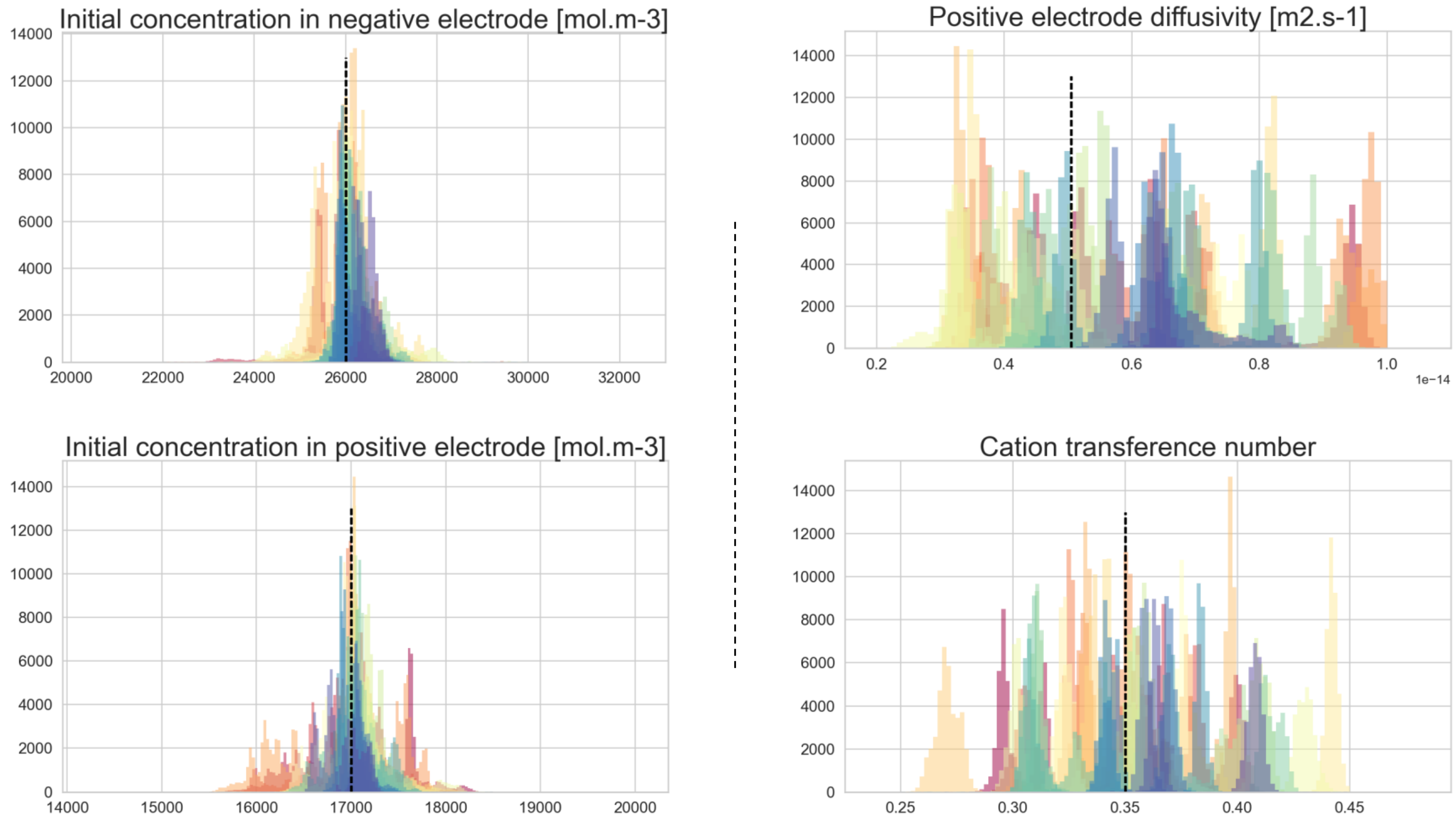


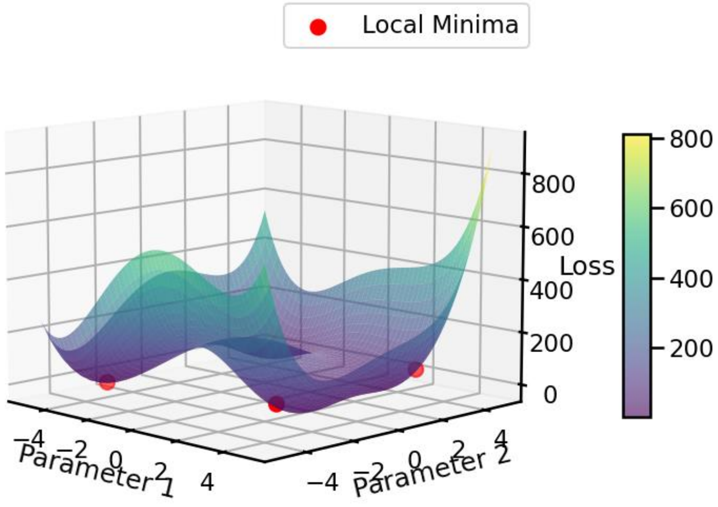
Data-driven model Training dataset

The physics-informed approach requires minimal data, focusing on key charge/discharge cycles to capture essential battery behaviors

Physics-informed Model

CMA-ES Optimization: Achieving Accurate Parameter Estimation





- Challenge of local minima due to a large number of model parameters
- Multiple parameter sets can yield similar loss values

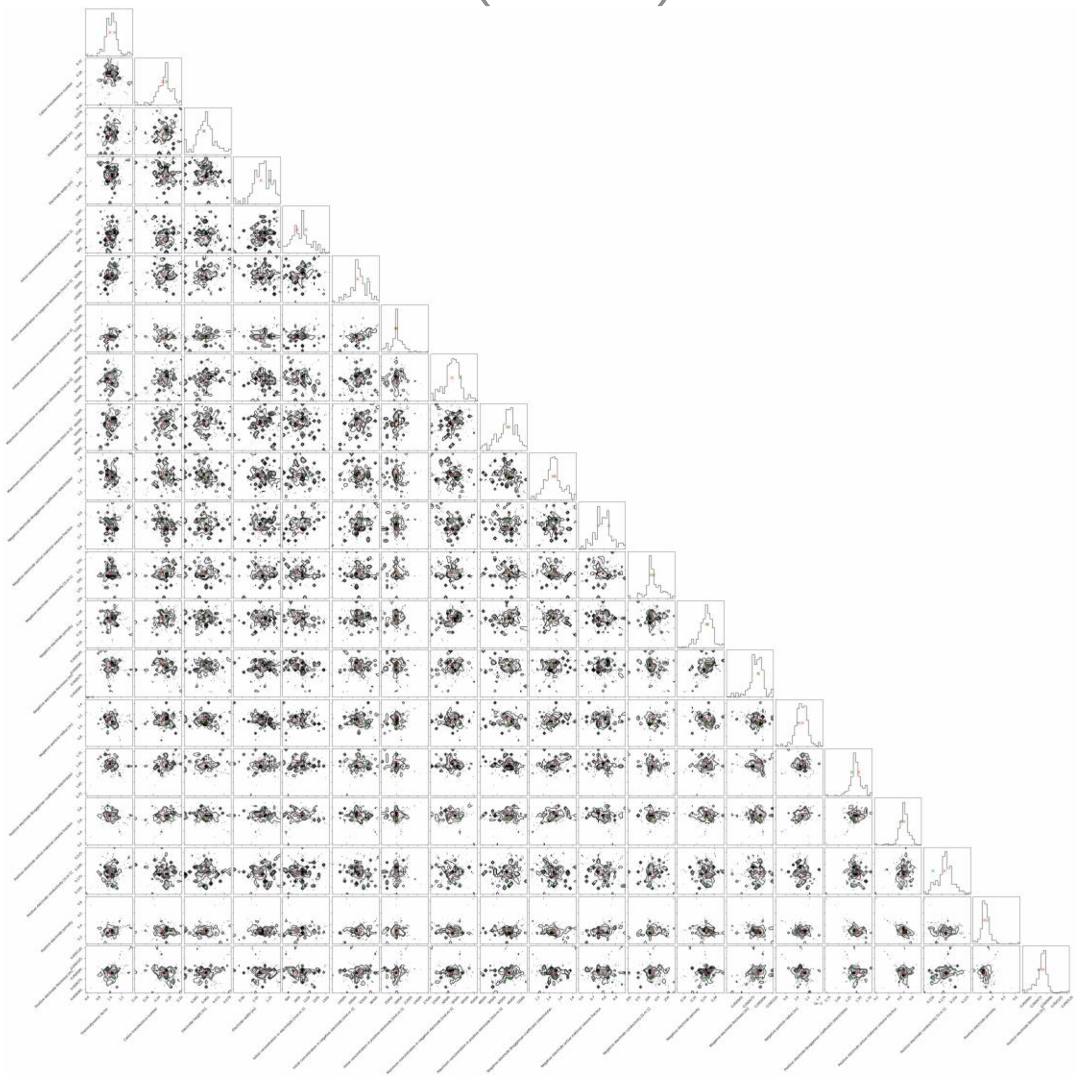
Challenges of finding global optima due to high-dimensional parameter space

Physics-informed Model: Global Parameter Optimization Approach

ML Approach: Exploring Parameter Space with Markov Chain Monte Carlo (MCMC)

- MCMC methods simulate random walks through the parameter space of the physics-informed model
  - Applied Bayesian statistical modeling and probabilistic machine learning, in which unknown parameters are inferred in terms of their probability distributions

- Used for global sensitivity analysis to:
  - Identify key parameters affecting model performance
  - Quantify uncertainty in model predictions

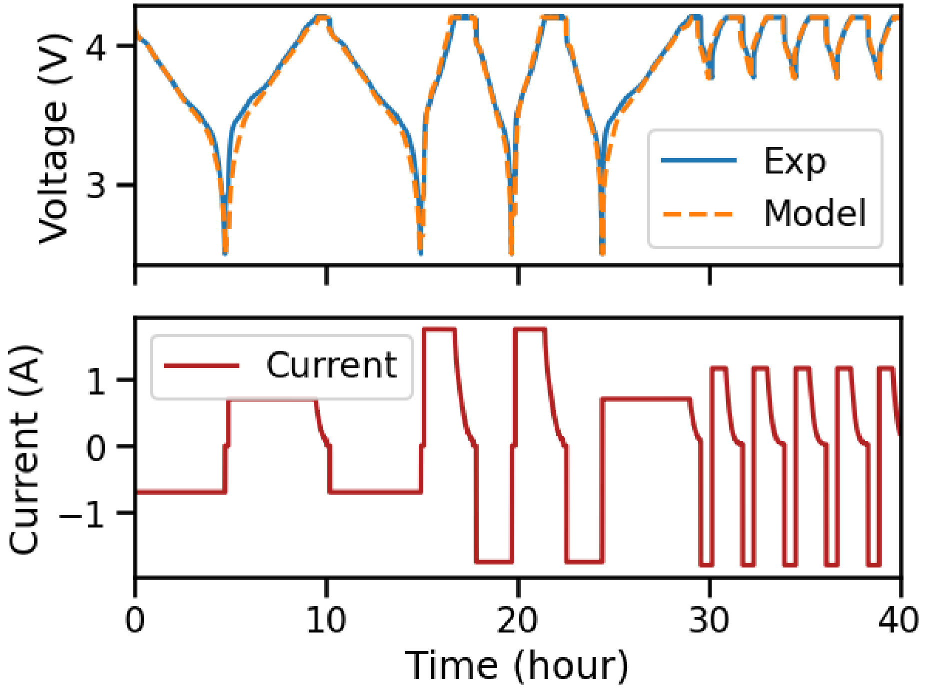


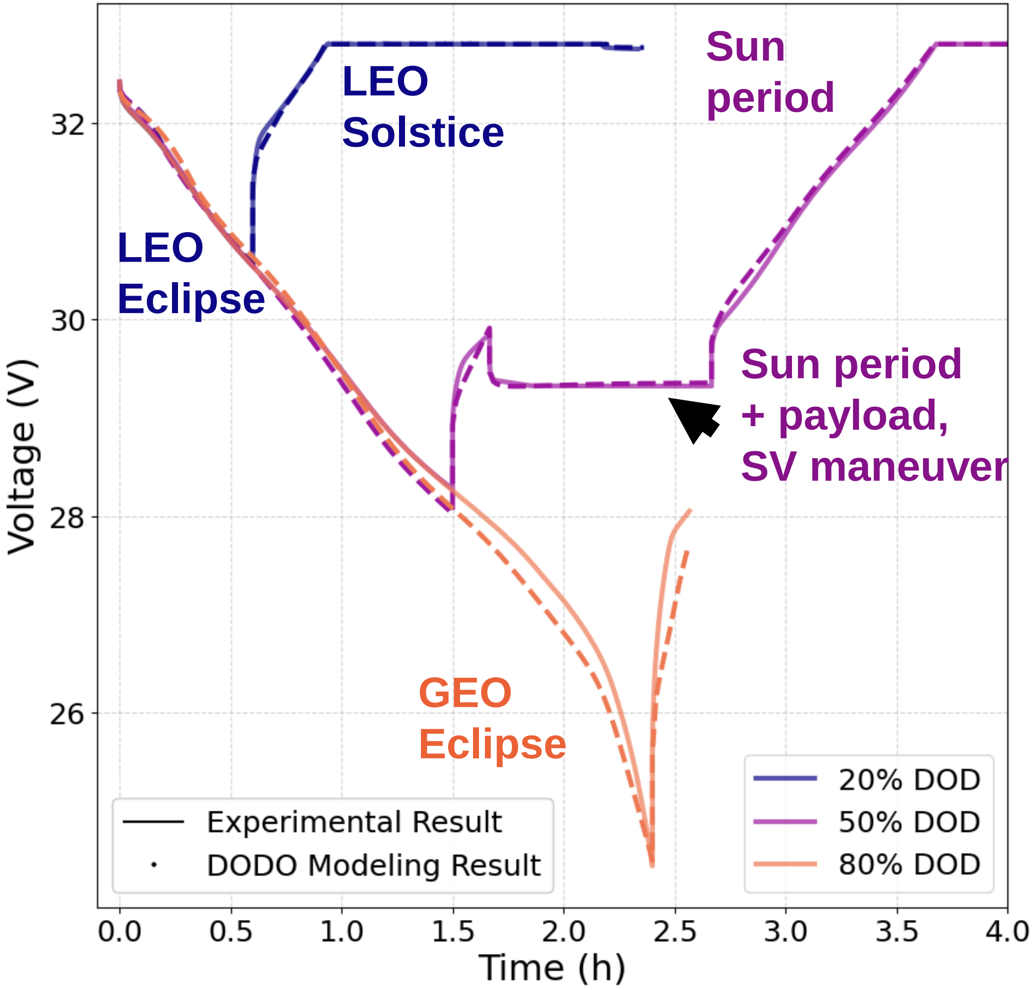
ML algorithm facilitate global sensitivity analysis, identifying key parameters and quantifying uncertainty

Physics-informed Model: Results

Validating Model Predictions

- Our model successfully predicted battery voltage with an average error of less than 42 mV.
- The physics-informed approach allows for predictions of battery performance/behavior under dynamic operating conditions





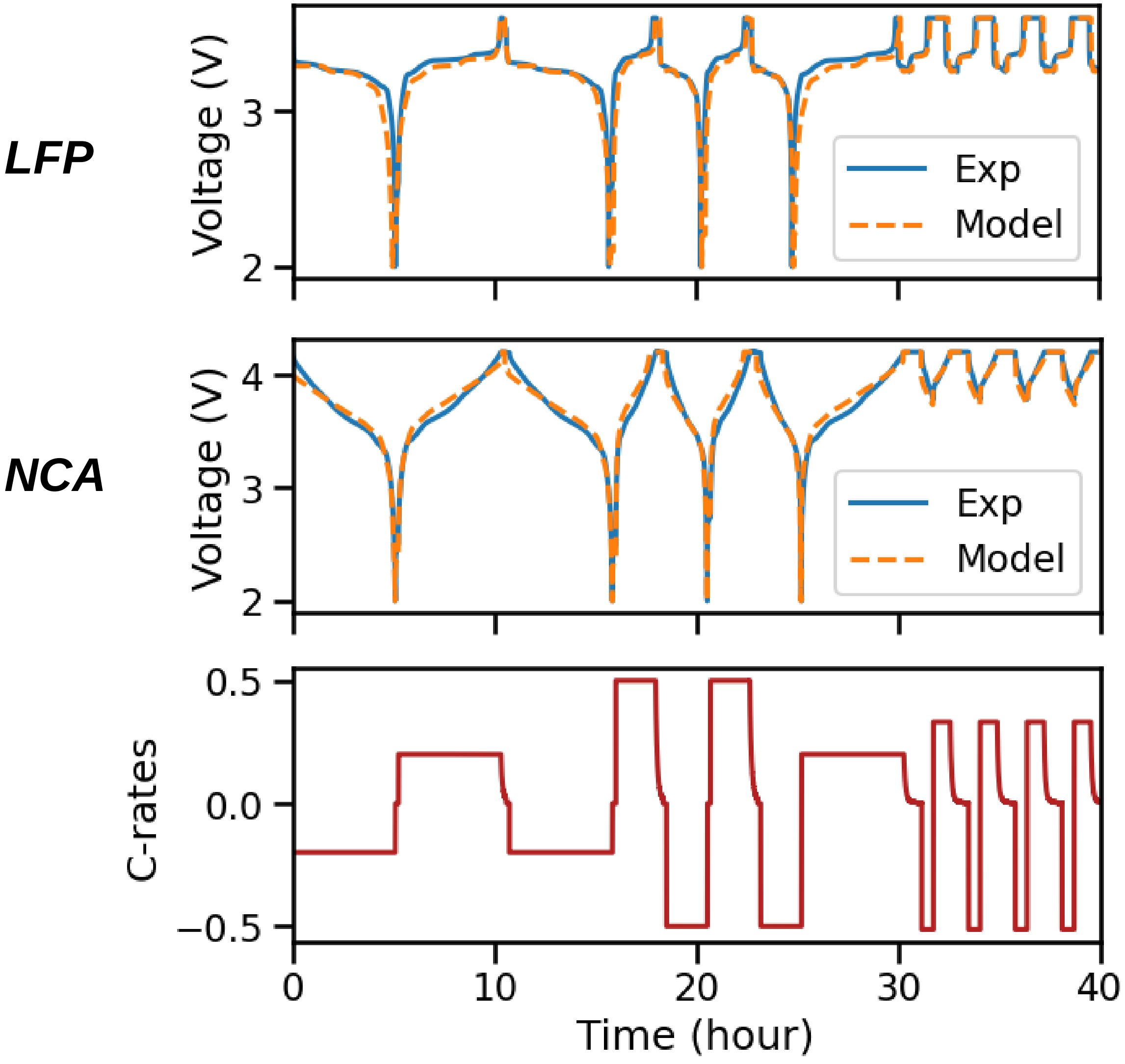
Our model demonstrates high-fidelity voltage predictions across various operational scenarios, validated against experimental data

Application of Physics-Informed Model

Versatility Across Multiple Chemistries

- Applied the physics-informed model framework to LFP and NCA chemistries
  - Results show high accuracy in predicting voltage profiles for both chemistries
  - Demonstrates model's robustness and adaptability to different battery types

- An average training data error
  - LFP: 51 mV
  - NCA: 56 mV



The physics-informed model accurately forecasts battery performance for both LFP and NCA chemistries

Summary: Comparison of Data-driven vs. Physics-informed Models

Evaluating Strengths and Limitations

Big data *No physics*	**Some data** **Some physics**	**Small data** **All physics**

- Data-driven Approach
  - Pros
    - Leverage large datasets, adaptable to various scenarios, less dependent on detailed physical understanding
  - Cons
    - Require extensive data for training, will likely struggle with extrapolation beyond training data

- Physics-informed Model
  - Pros
    - Based on fundamental physical principles, require less data, robust to extrapolation, optimized model parameters are easily transferred, updated, and deployed
  - Cons
    - Complex to develop (requires domain knowledge), parameter estimation can be challenging and computationally intensive

Data-driven models excel with large datasets but struggle with extrapolation, while physics-informed models are robust but complex to develop

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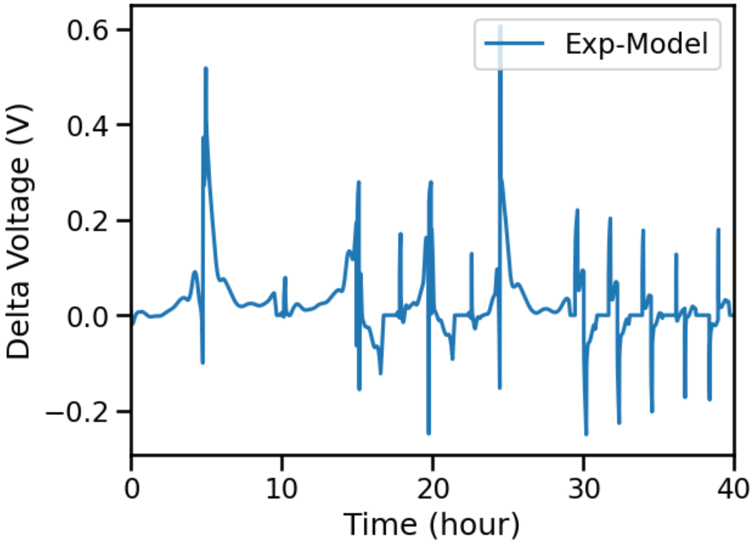
Backup

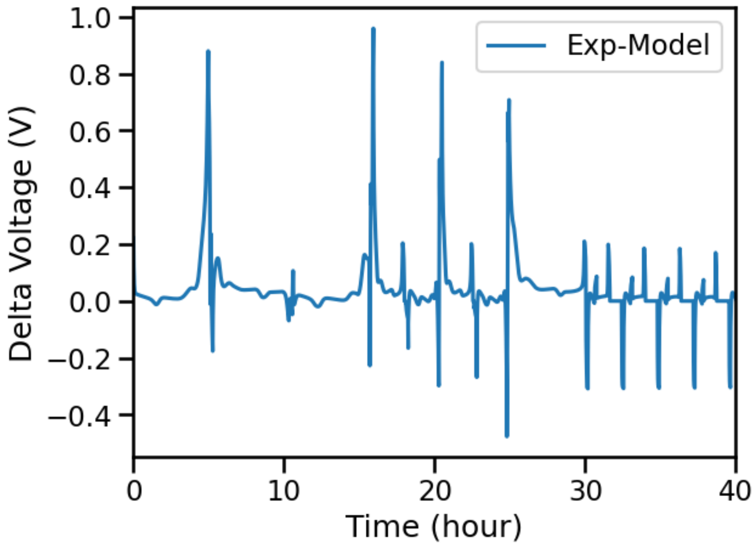
Physics-informed Model: Results

Difference between predicted and experimentally measured voltage profiles

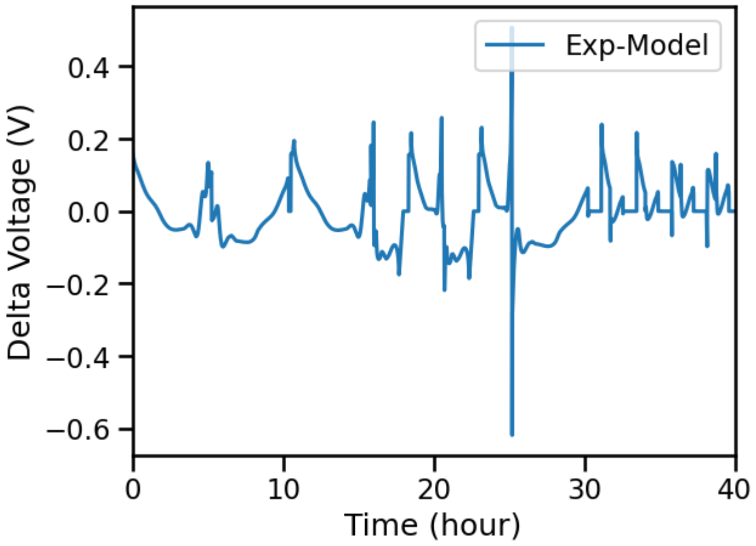
NMC



LFP



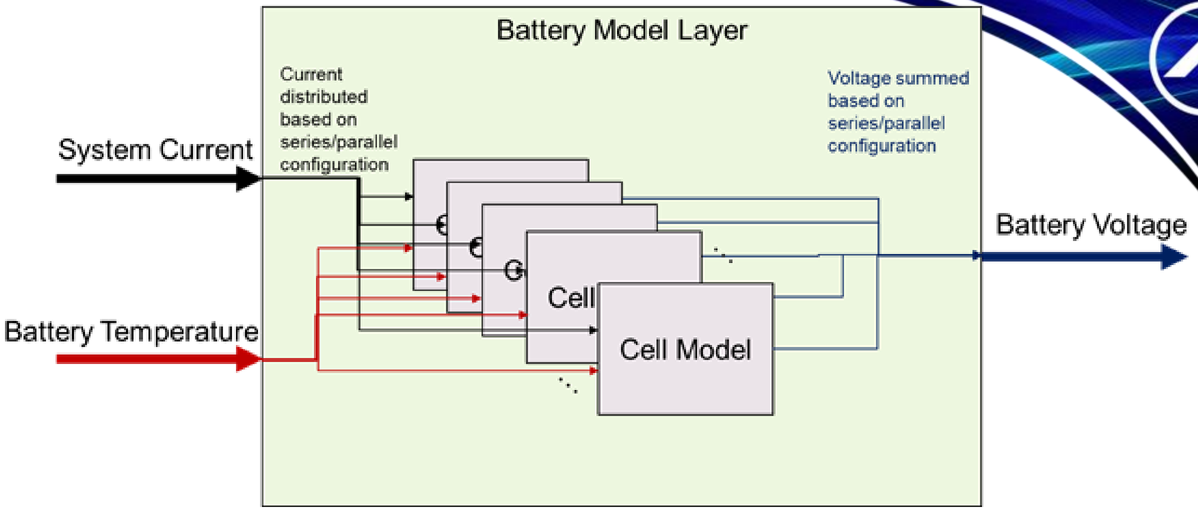
NCA



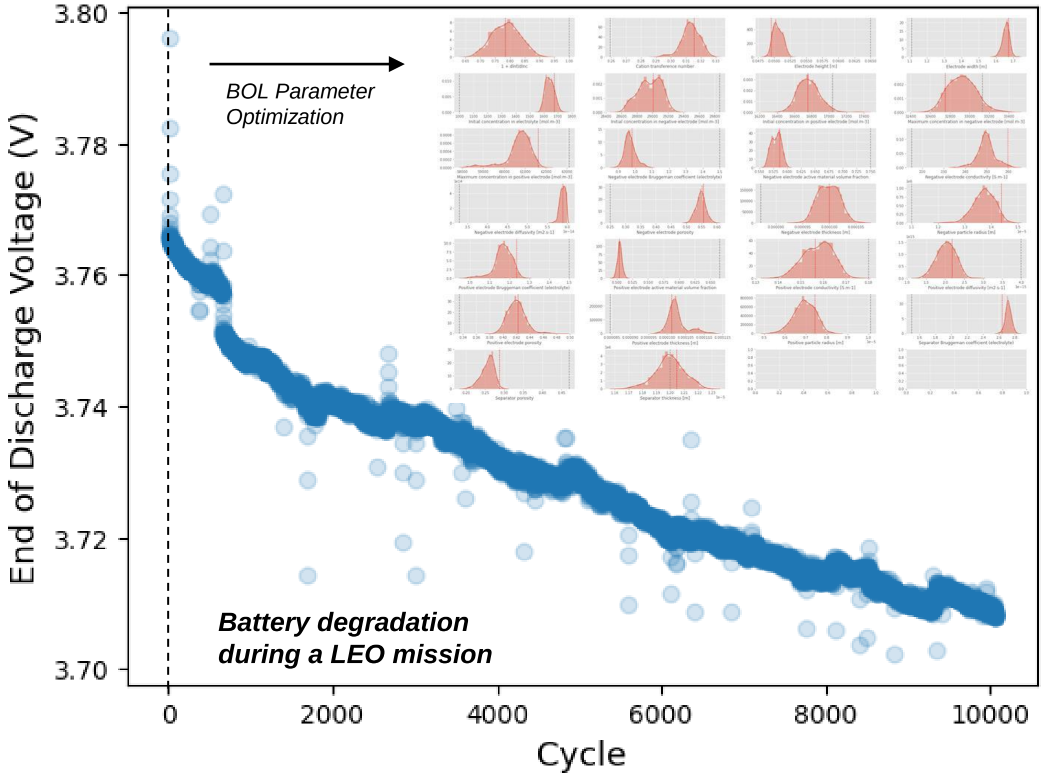
Physics-informed Model

Future Work

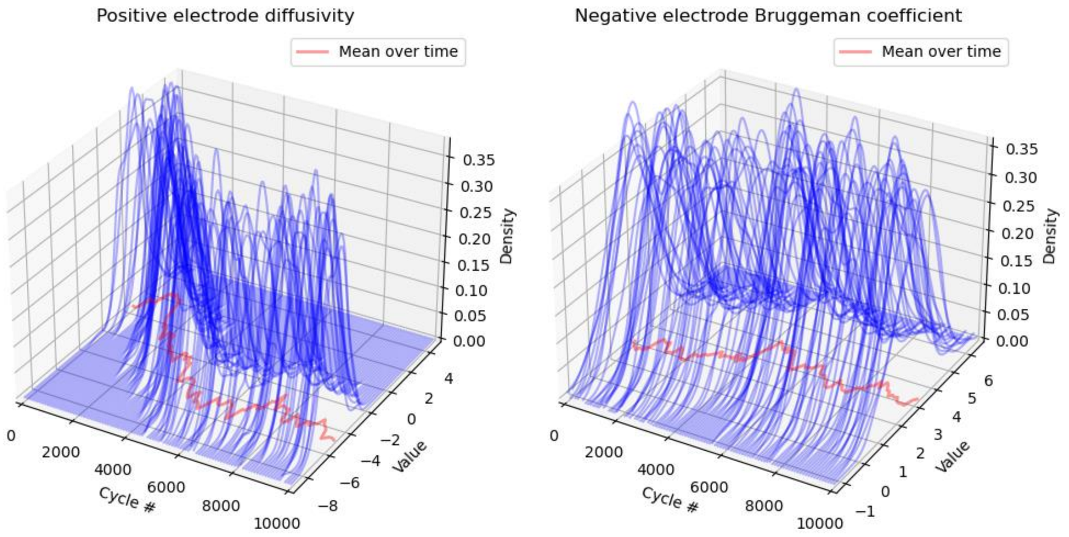
- Battery-level model integration
- Long-term performance prediction



Space Battery Model Architecture



Parameter Optimization over its Lifespan



Optimizing the optimization: loss functions

- MSE (Voltage)

$$\mathcal{L}_{MSE,V} = \frac{1}{n}\sum_{i=1}^{n}(V_{exp} - V_{sim})^2$$

- MSE (Current)

$$\mathcal{L}_{MSE,I} = \frac{1}{n}\sum_{i=1}^{n}(I_{exp} - I_{sim})^2$$

- L-Infinity norm (Voltage)

$$\mathcal{L}_{\infty,V} = |V|_{\infty} = max_i|V_{exp,i} - V_{sim,i}|$$

- L-Infinity norm (Current)

$$\mathcal{L}_{\infty,I} = |I|_{\infty} = max_i|I_{exp,i} - I_{sim,i}|$$

- Combined

$$\mathcal{L} = \gamma_1\mathcal{L}_{MSE,V} + \gamma_2\mathcal{L}_{MSE,I} + \gamma_3\mathcal{L}_{\infty,V} + \gamma_4\mathcal{L}_{\infty,I}$$