Hybrid Physics-Based and Data-Driven Modeling
with Calibrated Uncertainty
for Li-Ion Battery Degradation Diagnosis and Prognosis

Jing Lin, Yu Zhang, Edwin Khoo {lin_jing, zhang_yu, edwin_khoo}@i2r.a-star.edu.sg

Institute for Infocomm Research, A*STAR, Singapore

December 14, 2021
NeurIPS 2021 workshop on Tackling Climate Change with Machine Learning

Necessity of Modeling and Predicting LIB Degradation

CREATING GROWTH, ENHANCING LIVES

Lithium-Ion Battery (LIB)

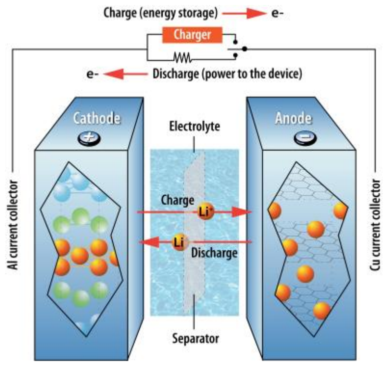
- LIB is pivotal to electrifying transportation and storing intermittent renewable energy
- Degradation and failure limit LIB's durability and safety

Utility of Modeling Degradation

- Faster and cheaper design-test iterations
- More effective online management strategy: monitoring, early warning, predictive maintenance

Challenges in SOH Evolution Modeling and RUL Prediction

- Various complicated physio-chemical mechanisms not well understood
- Strong and nonlinear dependence on usage patterns



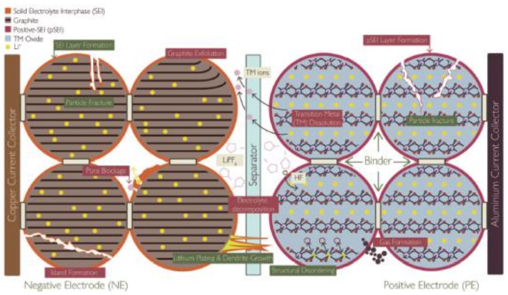


Image credit: Argonne National Lab (top); Edge et al. PCCP-2021 (bottom)

Evaluating Existing Work along Three Dimensions

CREATING GROWTH, ENHANCING LIVES

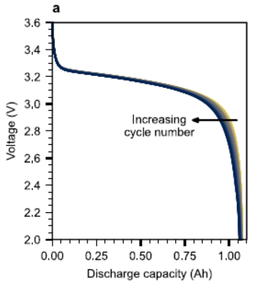
1. Must usage histories be assumed or provided?
   - Assume certain usage amount, like 100 cycles? (e.g. Severson et al. 2019)
   - Assume particular cycling patterns, like 4C discharge? (e.g. Strange and dos Reis 2021)
   - This dependence can significantly limit generalizability
2. Is degradation dynamics explicitly modeled?
   - Predicting $C(Q_{\text{tot}} = ?) = 0.8C_0$ through $\mathrm{d}C/\mathrm{d}Q_{\text{tot}}$ or not?
   - Modeling dynamics yields higher adaptability and generalizability
3. How much prior physical knowledge is explicitly incorporated?
   - Purely data-driven
   - Equivalent-circuit-model-based (ECM)
   - Physics-based

Q_{tot} is the total charge throughput (charging/discharging). C and C_0 are actual and nominal capacity, respectively.

Three Main Existing Approaches to Degradation Modeling

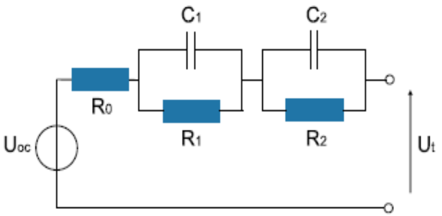
Purely Data-Driven

- Trained on charge/discharge curves and crafted features
- Agnostic of, but specific to certain cell chemistry/format and cycling pattern



ECM-based

- Enable fast real-time simulation for monitoring
- Lack of diagnostic insights and unable to predict degradation



Purely physics-based

- Gives physical insights by modeling different degradation modes
- Fitting protocol unclear and accuracy not yet systematically tested

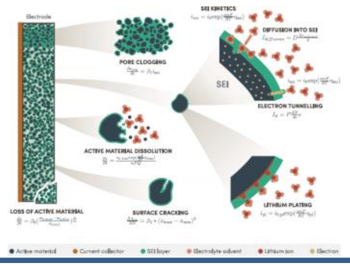


Image credit: Attia et al. JECS-2021 (top); Li et al. JES-2020 (middle); Reniers et al. JECS-2019 (bottom)

Our Proposed Physics-Data Hybrid Framework

Goal

Studying the accuracy limit of modeling for online battery degradation diagnosis and prognosis with **well-calibrated uncertainty**, putting computational costs aside temporarily.

Key Ingredients

- Base physical models: pseudo-2-dimensional (P2D) + various degradation mechanisms
- Characterizing degradation status by a set of model parameters
- **Uncertainty quantification** and statistical model residual modeling
- Data assimilation for online state and parameter estimation
- Measurements from published battery datasets (e.g. Severson et al. 2019)

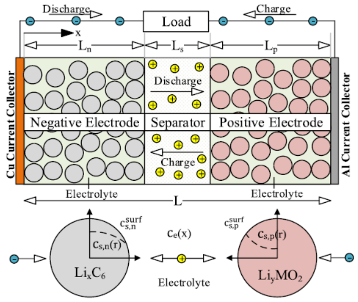
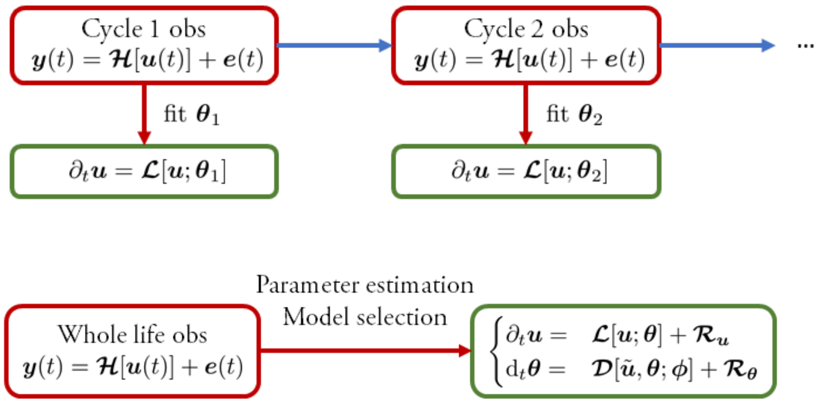


Image credit: Jokar et al. JPS-2016

Step 1&2: Parametric Study for Physical Models and Degradation

- Step 1: Fit P2D parameters to cells degraded to different extent
- Step 2: Select degradation models and fit parameters to whole-life data



Goals

1. Protocol for parameter fitting and model selection with **well-calibrated uncertainty**
2. More refined parametric characterization of SOH indicating degradation extent

Step 3: Statistical Modeling of Residuals in Physical Models

Whole life obs
$$\boldsymbol{y}(t) = \boldsymbol{\mathcal{H}}[\boldsymbol{u}(t)] + \boldsymbol{e}(t)$$

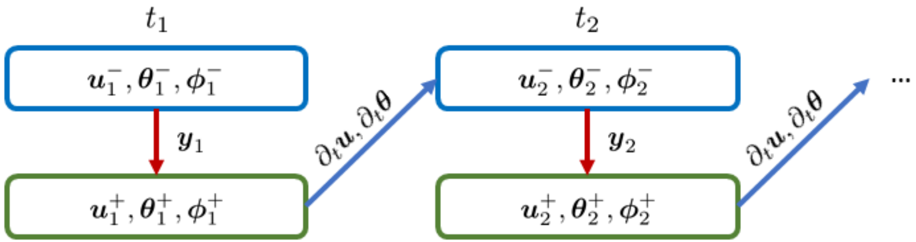
$\xrightarrow[\text{Model selection}]{\text{Parameter estimation}}$

$$\begin{cases} \partial_t \boldsymbol{u} = & \boldsymbol{\mathcal{L}}[\boldsymbol{u}; \boldsymbol{\theta}] + \boldsymbol{\mathcal{R}}_{\boldsymbol{u}} \\ \mathrm{d}_t \boldsymbol{\theta} = & \boldsymbol{\mathcal{D}}[\tilde{\boldsymbol{u}}, \boldsymbol{\theta}; \boldsymbol{\phi}] + \boldsymbol{\mathcal{R}}_{\boldsymbol{\theta}} \end{cases}$$

Candidate Approaches

- Characterize model residuals by certain stochastic processes (e.g. Gaussian processes)
- Characterize uncertain functional dependence of parameters on conditions
- Any uncertain functions could be identified by domain knowledge and/or statistical learning

Step 4: Integrating into BMS-like Online Diagnosis and Prognosis



- Use sequentially measured data to correct state and parameters in a principled way
- Both accuracy and **uncertainty calibration** count
- Ample flexibility to decide which parameters can be fixed and which must be inferred online
- May not be computationally feasible in real-time applications yet, but still yield valuable insights

CREATING GROWTH, ENHANCING LIVES

CREATING GROWTH, ENHANCING LIVES

Institute for Infocomm Research

I²R

THANK YOU

www.a-star.edu.sg/i2r