Physics-inspired and Control-Oriented Modeling of Lithium Batteries for Accurate State-of-Charge Prediction and Fast-Charging

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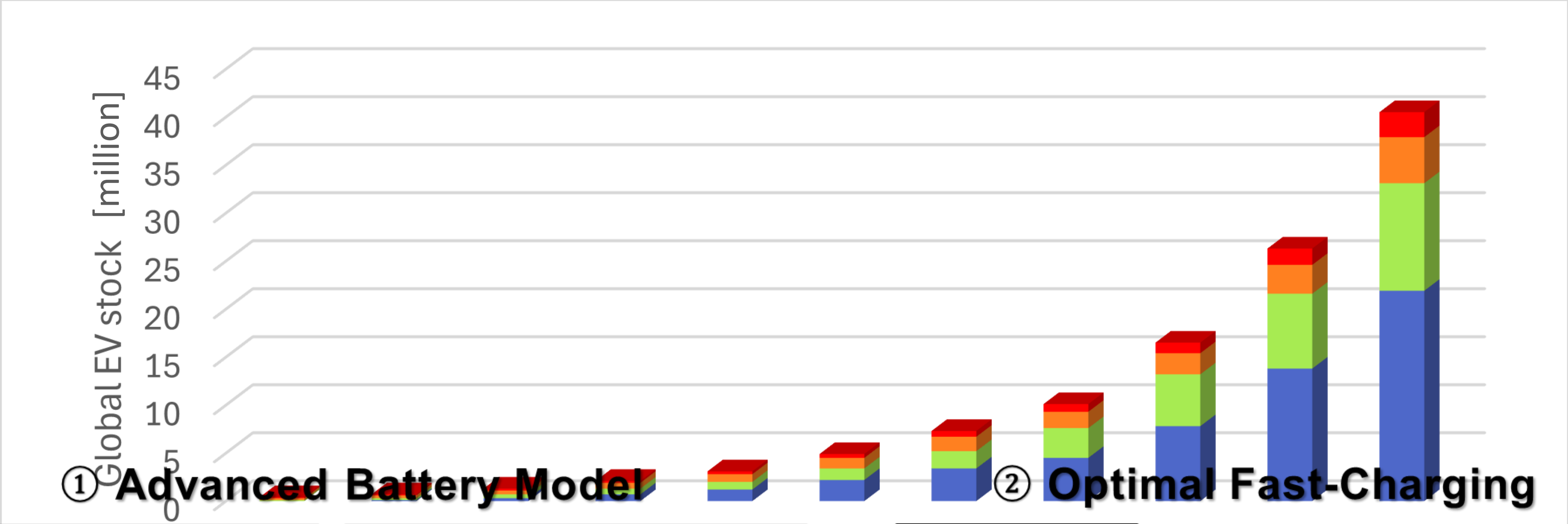
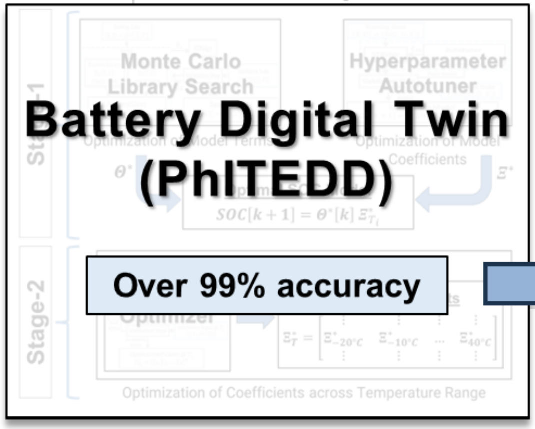
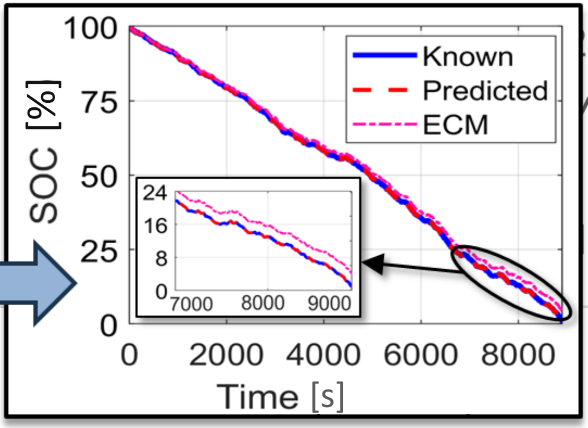
Addressing Barriers to Electric Vehicle Adoption

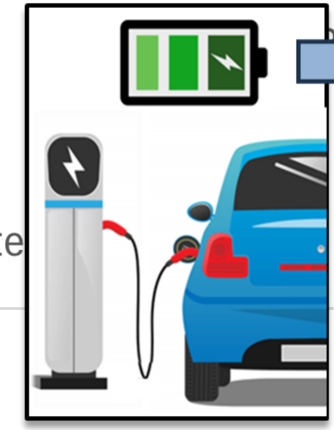


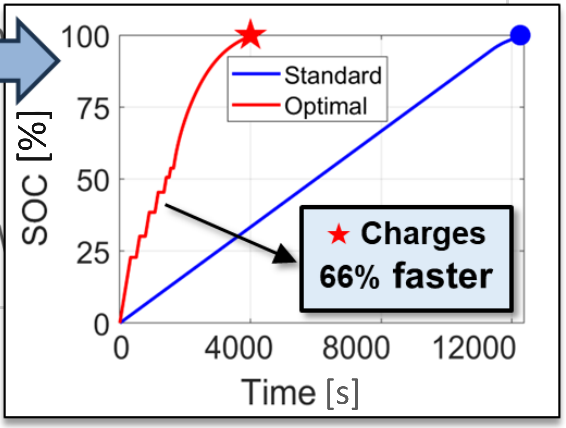
① **Advanced Battery Model**





② **Optimal Fast-Charging**





Outline

- Introduction
  - Significance of State-of-Charge dynamics (range anxiety)
  - Implications of Fast-charging (slow charging times)
  - State-of-the-art methods
  - Our proposed solution
- Methodology
  - Generic approach
  - Introducing domain knowledge to the models
  - Improve the modeling technique: Hyperparameter tuning and Monte Carlo search
  - Adaptive Learning and Optimization Approach
- Implementation and Results
  - Modeling using experimental data
  - Optimal Charging Strategy
- Summary and Future Work

INTRODUCTION

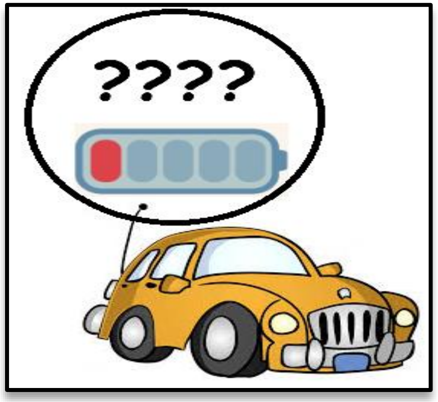
Motivation: Range Anxiety

Motivation

- Barriers to EV adoption: range anxiety
  - Fear of lacking enough energy to reach a destination
  - Due to uncertainty in range predictions
- Increased demand for advanced BMS
  - BMS (battery management system)
- Need knowledge of the battery state for increased performance/safety
  - SOC (state of charge): akin to the fuel gauge on conventional vehicles
- Direct measurements of SOC are not possible
- SOC must be obtained from available battery measurements
  - Electrical current I, voltage V, temperature T

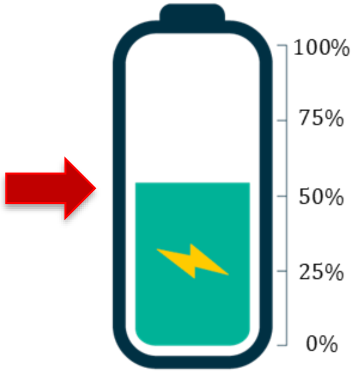
Objective

- Develop accurate, efficient and control-oriented SOC models
- Capitalize on access to battery Input/Output data
  - Achieve <u>high performance</u>, <u>improved operational safety</u>, <u>extended longevity</u>



Range Anxiety

Fuel Gauge



SOC: charge level

Motivation: Slow Charging Times

Motivation

- EV adoption is hindered by slow charging times
- Level 2 chargers (240V) are most common
  - US-DOT: 10-hours to charge EV (0% - 80%)
- **Charging EV takes much longer than refueling ICEV**
  - ICEV (internal combustion engine vehicle)

- Demand for improved battery technologies
  - **minimize charge time, maintain safe operation**

Objective

- Charging strategy to increase performance & mitigate aging
- Test efficacy of our solution
  - Manufacturer recommended charging procedure
  - Alternative fast-charging procedure

Slow Charging Times

Level 2 chargers: common in home, workplace, and public settings
transportation.gov

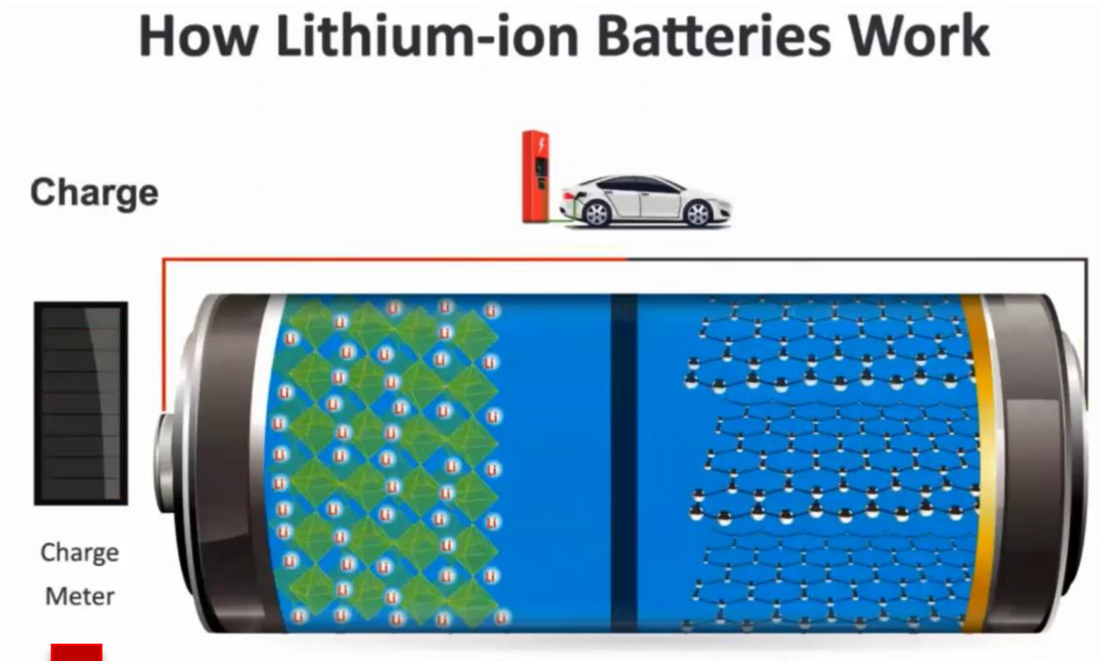
Lithium-ion Battery

System of Interest: Li-ion Battery (LiB)

- Complex nonlinear dynamical system
  - Varying operating modes (temperature), Degradation (capacity fade)

Objective

- Charge battery as fast as possible
- Need advanced controls to optimize performance & safety
- Need accurate knowledge of battery state (e.g., SOC)



https://www.energy.gov/node/2697942

Challenges

- LiB cycle-life is influenced by charging protocol
- Trade-off between charging-speed and lifespan
- Fast-charging risks: high currents, high temperatures
- High temperatures result in thermal degradation
  - deterioration of battery performance and lifespan
  - electrolyte decomposition, lithium plating, side reactions

- Accurate modeling often requires physics-based methods [1]
  - Has high computational complexity: not suited for real-time
  - High modeling cost: needs knowledge of battery composition

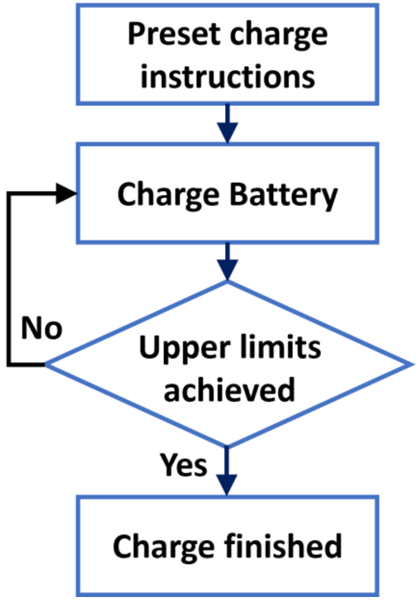
[1] Doyle, M., et al. Modeling of galvanostatic charge and discharge of the lithium/polymer/insertion cell.

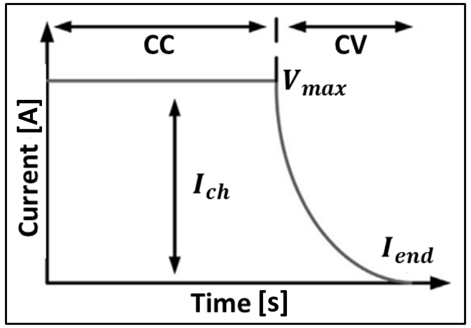
Literature Review: Passive Fast Charging

- Fast charging has been explored through:
  - Passive charging strategies
  - Active charging strategies

Passive charging techniques [2]

- Model-free methods with predefined charging profiles
- Defined by current (I), voltage (V), and/or power (P) constraints
- Methods include:
  - Constant-current constant-voltage (CC-CV)
- Ignore the response of the battery
  - **Can result in unsafe operation: high temperatures (T)**
- Solutions can violate safety constraints





CC-CV

[2] Gao, Y., et al. Classification and review of the charging strategies for commercial lithium-ion batteries.

State-of-the-art: Fast Charging

Passive Charging Strategies

Constant Current Constant Voltage (CCCV)

- Anseán, D., et al. (2016). Fast charging technique for high power LiFePO4 batteries: A mechanistic analysis of aging.
- Shi, R., et al. (2017). Constant current fast charging of electric vehicles via a DC grid using a dual-inverter drive.

Multi-stage CC (MSCC)

- Tahir, M., et al. (2023). Overview of multi-stage charging strategies for Li-ion batteries
- Lee, C. H., et al. (2021). Taguchi-based optimization of the four-stage constant current charge pattern.

Positive Pulse Charging (PPC)

- Purushothaman, B. K., et al. (2005). Reducing mass-transport limitations by application of special pulsed current modes.
- Aryanfar, A., et al. (2014). Dynamics of lithium dendrite growth and inhibition: pulse charging.
- Jeong, Y. T., et al. (2023). Insight into pulse-charging for lithium plating-free fast-charging lithium-ion batteries.

Active Charging Strategies

Linear Quadratic Control

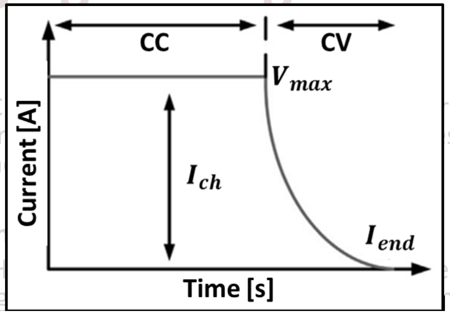
- Fang, H., Wang, Y., & C… -involved battery charging management for electr… s. IEEE Transactions on Control Systems Techn…

Pontryagin's minimum prin…

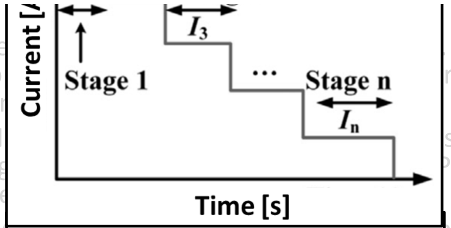
- Park, S., Lee, D., Ahn, H… cember). Optimal control of battery fast charging… nciple. In 2020 59th IEEE Conference on Decisio… IEEE.

Model Predictive Control

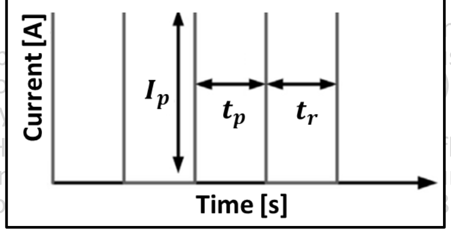
- Berliner, M. D., Cogswe… (2022). A mixed continuous-discrete ap… ries while maximizing lifetime. IFAC-PapersOn…
- Klein, R., Chaturvedi, N… sen, R., & Kojic, A. (2011, June). Optimal charging… Proceedings of the 2011 american Control Confe…
- Kujundžić, G., Ileš, Š., M… al charging of valve-regulated lead-acid bat… trol. Applied Energy, 187, 189-202.
- Kolluri, S., Aduru, S. V.,… nian, V. R. (2020). Real-time nonlinear model p… sing physics-based models for advanced lithium-io… . Journal of The Electrochemical Society…
- Liu, J., Li, G., & Fathy, H… flatness approach for the health-conscious nonlin… m-ion batteries. IEEE Transactions on Contro… 89.



CCCV



MSCC



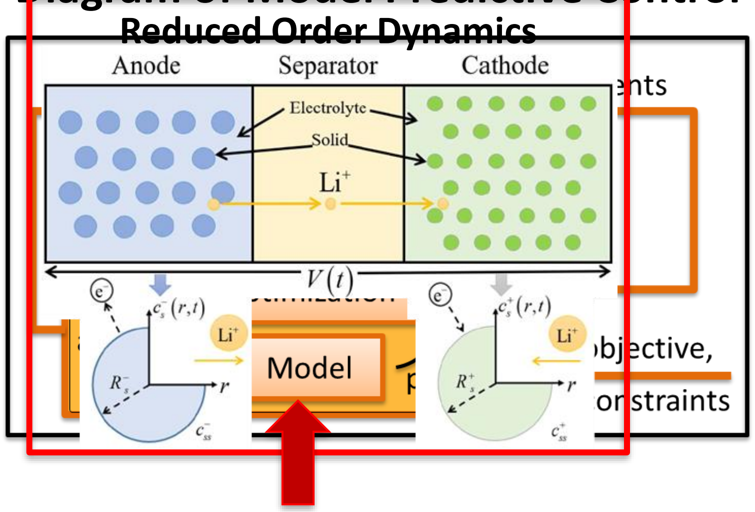
PPC

Literature Review: Active Fast Charging

Model-based methods: include 2 steps

- Step-1: Use model to calculate battery states (e.g., SOC)
  - Reduced-order electrochemical model
  - Empirical models and state observers
- Step-2: Use control/optimization scheme to improve performance
  - Closed-loop optimization problem
  - minimize time to reach a SOC | **maximize SOC within charging duration**
- Common approach: model predictive control (MPC) [3,4]
  - Can handle complex dynamics
  - Can include safety constraints to mitigate aging
  - High computational cost
  - Simplified models: can be inaccurate; don't capture battery's full range
  - Can lead to conservative or infeasible solutions

Diagram of Model Predictive Control



[3] Kujundžić, G., et al. Optimal charging of valve-regulated lead-acid batteries based on model predictive control.
[4] Kolluri, S., et al. Nonlinear MPC strategies using physics-based models for lithium-ion battery management system

State-of-the-art: Fast Charging

Passive Charging Strategies

Constant Current Con

- Anseán, D., & Gor ... ng technique for high power LiFePO4 ba ... aging.
- Shi, R., & Lehn, P. ... fast charging of electric vehicles via a DC g

Multi-stage CCCV

- Ta ... ging st
- Lee, C. H., & Ji ... zation of the four-stage constant

Pulse C

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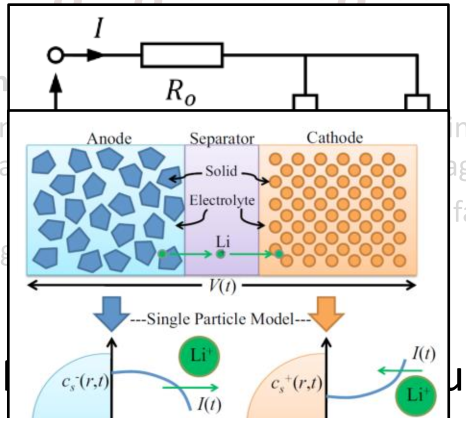
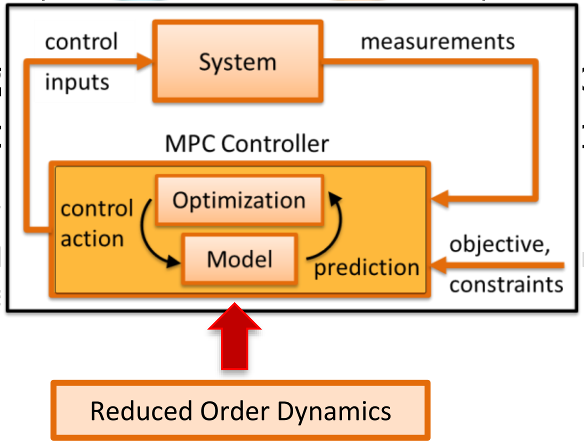
- Jeong, Y. T., & ... rging for lithium plating-free fas

Charging ... uit Model



Charg ... del
(reduc ... del)

Model Predictive Control



Active Charging Strategies

Linear Quadratic Control

- Fang, H., & Chen, J., et al. (2016). Health-aware battery charging management for electric vehicles: Linear quadratic strategies.

Pontryagin's minimum principle

- Park, S., & Moura, S., et al. (2020). Optimal control of battery fast charging based-on Pontryagin’s minimum principle.

Model Predictive Control (MPC)

- Berliner, M. D., & Braatz, R. D., et al. (2022). A mixed continuous-discrete approach to fast charging of li-ion batteries.
- Klein, R., & Chaturvedi, N. A., et al. (2011). Optimal charging strategies in lithium-ion battery.
- Kujundžić, G., & Vašak, M., et al. (2017). Optimal charging of valve-regulated lead-acid batteries based on model predictive control.
- Kolluri, S., & Braatz, R. D., et al. (2020). Nonlinear MPC strategies using physics-based models for Li-ion battery management system.
- Liu, J., & Fathy, H. K., et al. (2016). An extended differential flatness approach for the health-conscious nonlinear MPC of Li-ion batteries.

Literature Review: Existing Modeling Approaches

- ❑ Coulomb Counting [5]
  - Current integration normalized by capacity
  - Simple implementation, low complexity
  - Prone to drift due to measurement errors

$$SOC[k] = SOC[k-1] + \int_0^{kh} \frac{I(t)}{C_{bat}} dt$$

Where:

- $SOC[k]$ SOC at time kh [%]
- $SOC[k-1]$ Initial SOC [%]
- I Electrical current [A]
- $t = kh$ Time [h]
- h Sampling time
- C_{bat} Battery capacity [Ah]

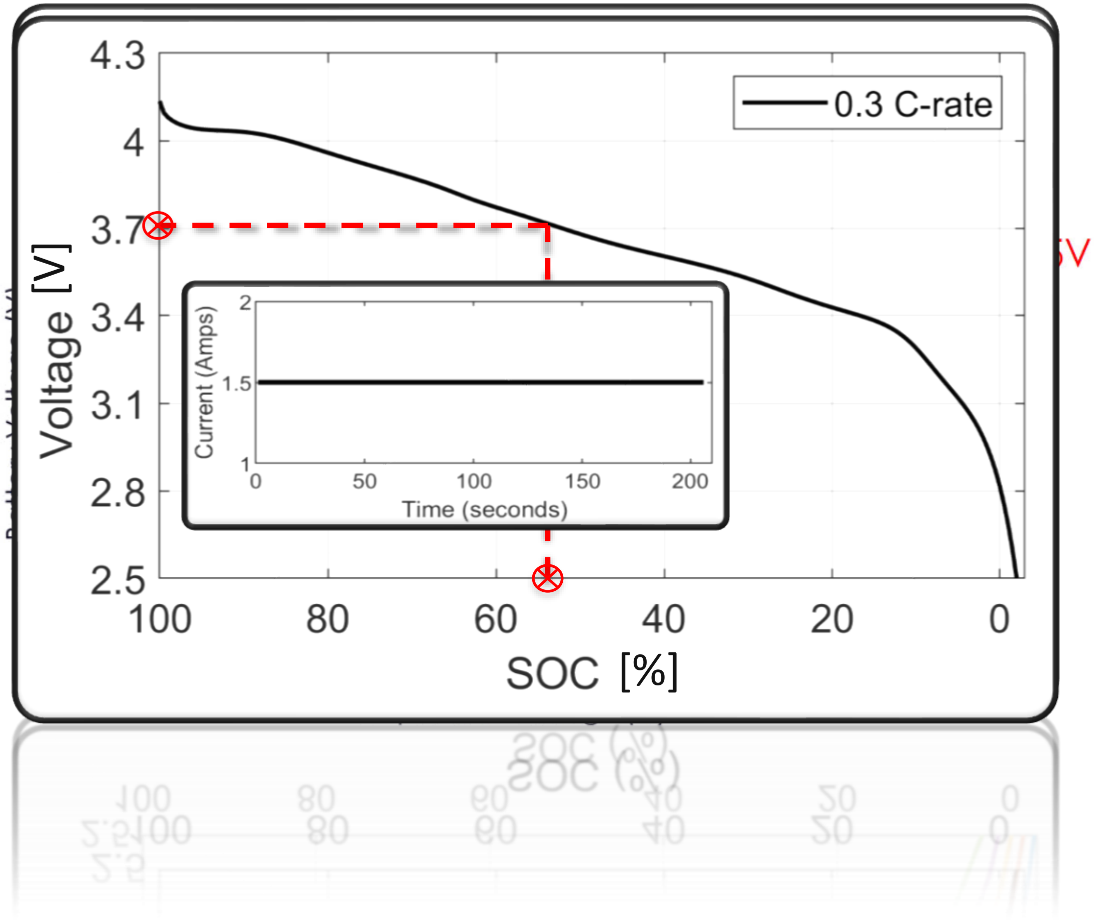
[5] Ng, K. S., et al. Enhanced coulomb counting method for estimating state-of-charge and state-of-health of lithium-ion batteries.

Literature Review: Existing Modeling Approaches

✓ Coulomb Counting

❑ Open Circuit Voltage (OCV) method [6]

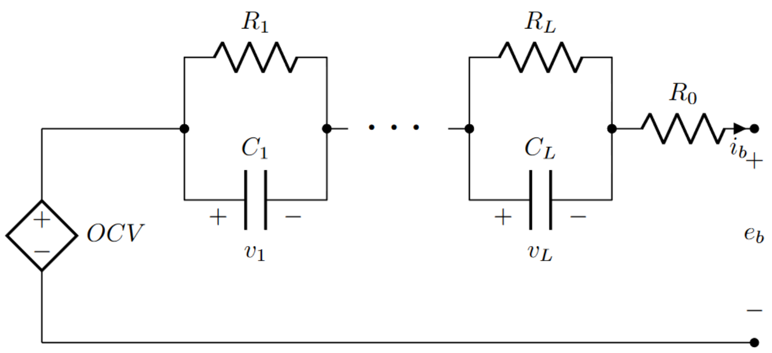
- Empirical mapping between voltage and SOC
- Simple implementation, low complexity
- Limited operational range, needs multiple mappings
- LiBs have relatively flat charge/discharge curves
  - Small voltage change over wide SOC range



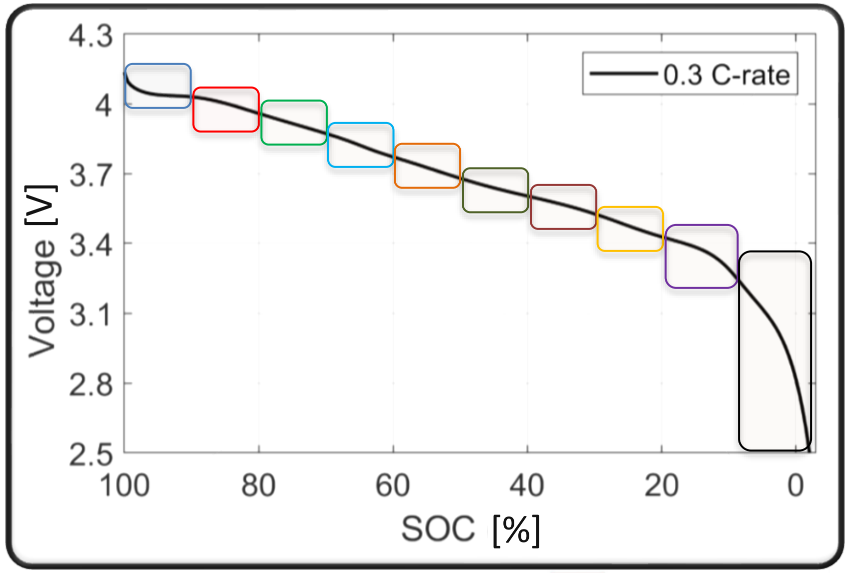
[6] Zheng, F., et al. Influence of different open circuit voltage tests on state of charge online estimation for lithium-ion batteries.
[-] *Lithium-ion state of charge (SOC) measurement - coulomb counter method - OCV*. PowerTech Systems - PowerTech Systems. (n.d.). https://www.powertechsystems.eu/home/tech-corner/lithium-ion-state-of-charge-soc-measurement/

Literature Review: Existing Modeling Approaches

- ✓ Coulomb Counting
- ✓ Open Circuit Voltage (OCV) method
- ❑ Equivalent circuit modeling (ECM) [7]
  - Uses electrical components to describe the battery behavior
    - Resistors and capacitors
  - Developed from measurable battery data
  - Narrow operating range, requires multiple models
  - Poor low SOC and low temperature performance



Equivalent Circuit Model Diagram [7]



[7] Natella, D., et al. A co-estimation framework for SOC and parameters of LiB with robustness to usage conditions.

Our Solution: Battery Modeling

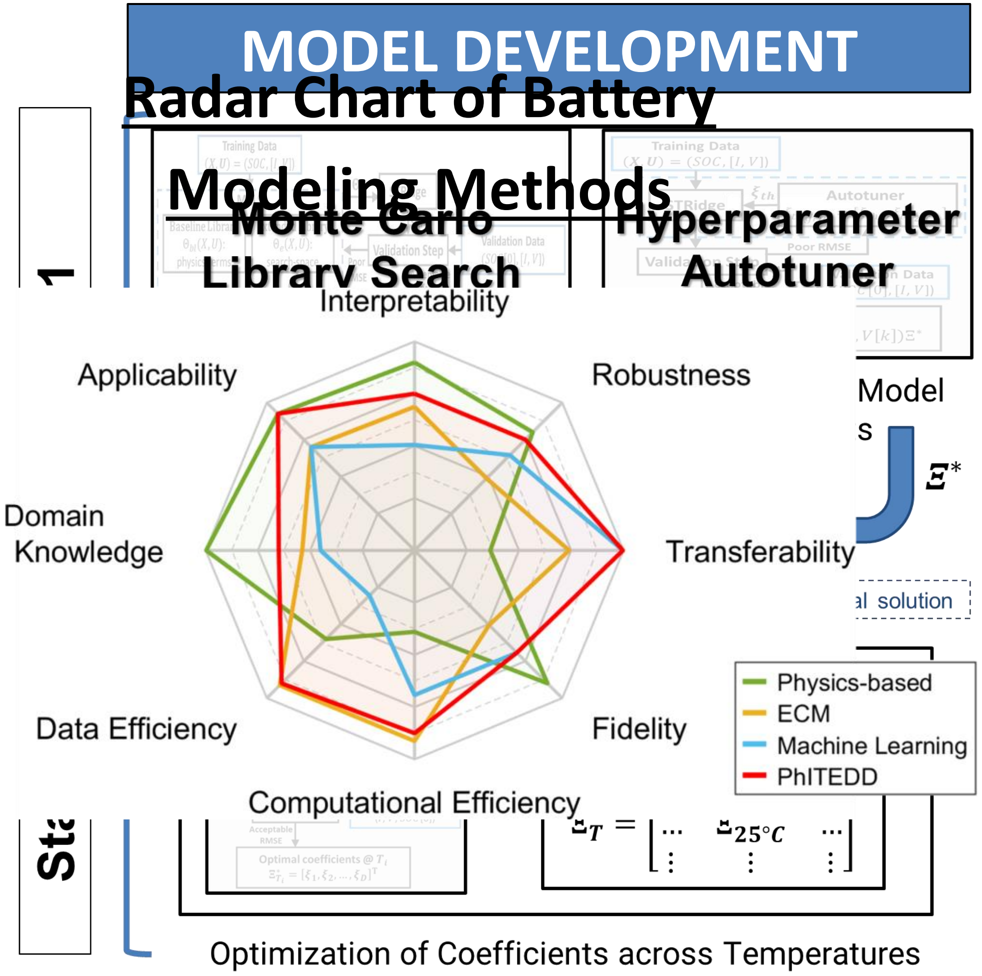
Existing Modeling methods

- ✓ Coulomb Counting
- ✓ Open Circuit Voltage (OCV) method
- ✓ Equivalent circuit modeling (ECM)

Our Solution: Battery Digital Twin

❑ Explicit data-driven modeling (**PhITEDD**)

- Identifies sparse models from input/output data
- Simple architecture: library of terms & set of coefficients
  - Library terms: transformations of measurement data
  - Coefficients: denote importance of each term
- Tunable modeling approach - specialized for LiB
  - Introduce domain knowledge: physics informed
  - Models re-calibrated on new data (temperature)
- Optimal model: accurate, efficient, valid across operating range
  - SOC levels (0% to 100%), Temperature ($-20°\mathrm{C}$ to $40°\mathrm{C}$)
- **Physics-informed & Temperature-dependent Explicit Data-driven**



METHODOLOGY

Sparse Identification of Nonlinear Dynamics (SINDyC)

- Often physical systems have **few terms** that define the dynamics
- Dynamics represented with function ($f(\cdot)$) of states (x) and inputs (u)

$$x[k+1] = f(x[k], u[k])$$

- $f(\cdot)$ can be represented with a **library ($\Theta(\cdot)$)** that consist of linear and nonlinear terms (candidate transformations) of x and u

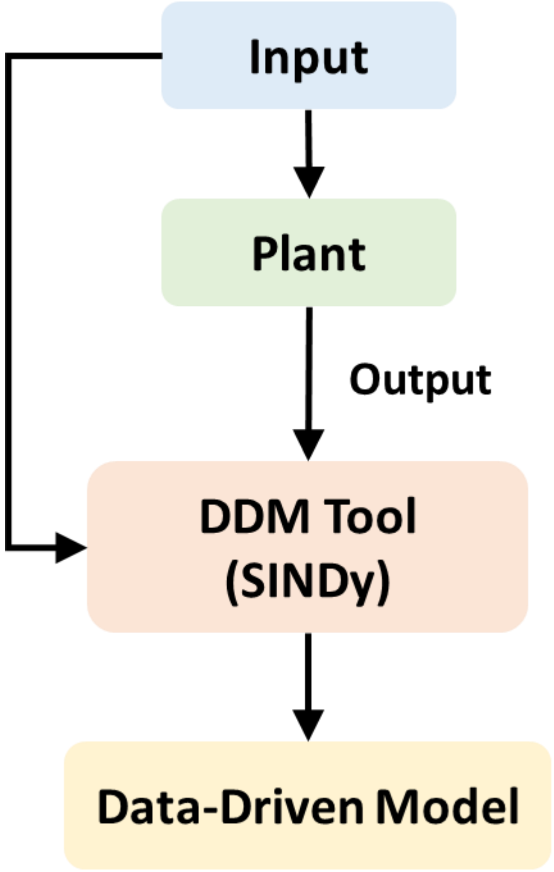
$$\Theta(\mathrm{X}, \mathrm{U}) = \begin{bmatrix} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ X & X^2 & \cdots & \sin(X) & \cdots & U & U^2 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$

where X and U time series data matrices

- The sparse nonlinear model is given by the combination of the library

  $\Theta(\mathrm{X}, \mathrm{U})$ and a set of coefficients/weights Ξ:

$$\boldsymbol{X'} = \boldsymbol{\Theta}(\boldsymbol{X}, \boldsymbol{U})\boldsymbol{\Xi}$$



[8] Brunton, S., et al. Sparse identification of nonlinear dynamics with control (SINDYc).

Identifying sparse vector of coefficients Ξ

Model

$$\boxed{\boldsymbol{X}' = \boldsymbol{\Theta}(\boldsymbol{X}, \boldsymbol{U})\boldsymbol{\Xi}}$$

- Set of coefficients, one for every library term

$$\Xi = [\xi_1 \quad \xi_2 \quad \cdots \quad \xi_D]^T$$

- Sparsity Promoting Regularization (Ridge, ℓ_2 norm)
  - Minimizes error between known data (X') and predicted data ($\Theta\Xi$)
  - Penalizes the count of non-zero coefficients with λ
- Sequentially thresholded ridge regression (STRidge)
  - Eliminates coefficients with small magnitudes, less than ξ_{th}
  - If $|\xi_i| < \xi_{th} \Rightarrow \xi_i = 0$

$$\Xi^* = \text{argmin}_{\Xi}(\|X' - \Theta\Xi\|_2 + \lambda\|\Xi\|_2 + \xi_{th}\|\Xi\|_0)$$

- Sparse (simpler) models are more generalizable

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[9] Kulkarni, C. S., et al. Sparse regression and adaptive feature generation for the discovery of dynamical systems

Challenges with Nonlinear Sparse Modeling

Challenges:

- Generic libraries (e.g., polynomial terms) only work for simple/known problems
- Selecting the optimal library terms from a vast pool of candidates is challenging
  - Method can learn incorrect representation of the data
- Varying hyperparameters can produce significantly different models
  - Method can fit the wrong nonlinear model, even with good library terms
- Dependence on a single dataset for model development
  - Challenging to create model that works well under changing operating conditions (e.g. temperature)

Our Solutions:

- Physics-informed set of library terms
  - Including domain knowledge to the learning process
- Monte Carlo Library Search of additional nonlinear terms
  - Improved accuracy and generalizability with tailored library
- Automated hyperparameter tuning with training and validation error and sparsity
  - Optimal balance between accuracy and complexity
- Re-calibration of model coefficients for distinct operating condition
  - Ensures efficacy across full operating spectrum, while maintaining minimal complexity

Selection of Candidate Library Terms

- The library includes:
  - Model Outputs (x): **SOC**
  - Model Inputs (u): electrical current ($\boldsymbol{I}$), voltage ($\boldsymbol{V}$)
- Model structure due to need for accurate SOC prediction from available I and V measurements

- Candidate library terms
  - Polynomial exponents (e.g., $V^2, \dots, I^2, \dots$)
  - Mixing (e.g., $V \cdot SOC, V \cdot I, \dots$)
  - Nonpolynomial exponents (e.g., $V^{1.2}, \dots, I^{2.2}, \dots$)
    - Sinusoidal transformations (e.g., $\sin(V), \dots, \cos(I), \dots$)
    - Exponential (e.g., $e^V, e^I, \dots$)
    - Integral (e.g., $\int I$)

SINDYc Model

$$SOC[k+1] = \Theta(SOC[k], I[k], V[k])\boldsymbol{\Xi}$$

$$\Theta(SOC, I, V) = \begin{bmatrix} | & | & & | & | & & | & & | \\ 1 & V^n & \cdots & V^n I^n & \sin(V) & \cdots & e^V & \cdots & \int(I) \\ | & | & & | & | & & | & & | \end{bmatrix}$$

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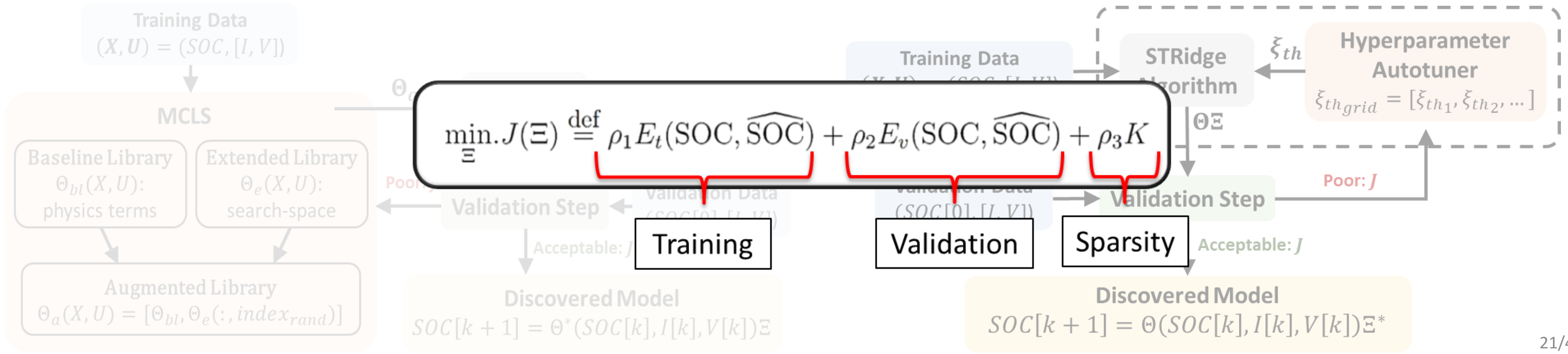
aSINDY: Library and Hyperparameter Optimization

Monte Carlo Library Search (MCLS)

- Assumption of sparse modeling holds if the function space (library) is broad
  - Coverage of the high-dimensional search-space
  - Can yield intractable problem / inefficient solution
- Random search of library terms (MCLS)
  - Efficient exploration of large search-space
  - Leads to improved performance (accuracy)

Hyperparameter Autotuning

- Sequentially thresholded ridge regression (STRidge)
  - It works by defining threshold, ξ_{th}: if $|\xi_i| < \xi_{th} \Rightarrow \xi_i = 0$
- ξ_{th} is selected from experience and/or trial-and-error
- Can fit a wrong model, even with a good library
- Automated grid-search for optimal threshold ξ_{th}^*
  - Search-space from analysis of the non-thresholded coefficients Ξ computed via pseudoinverse



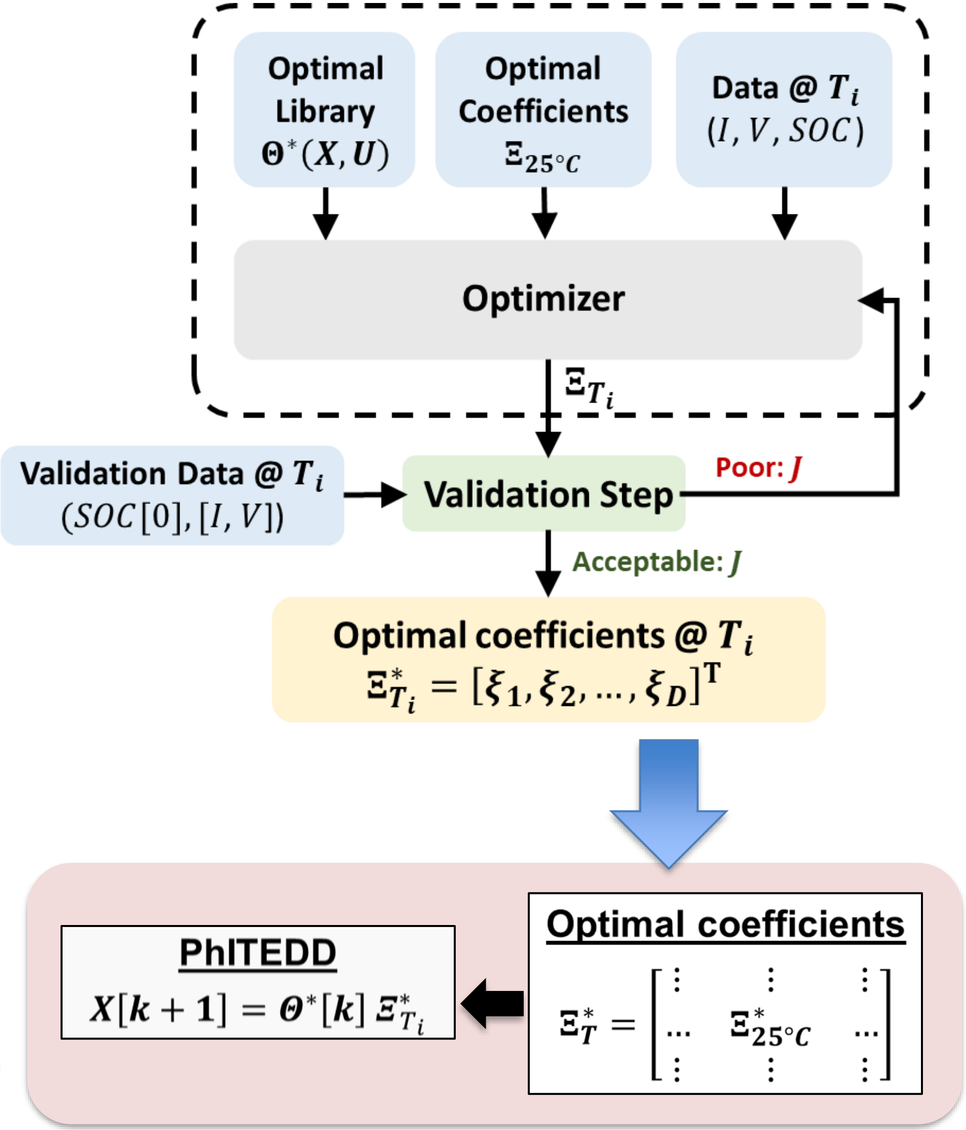
$$\min_{\Xi} . J(\Xi) \stackrel{\text{def}}{=} \underbrace{\rho_1 E_t(\mathrm{SOC}, \widehat{\mathrm{SOC}})}_{\text{Training}} + \underbrace{\rho_2 E_v(\mathrm{SOC}, \widehat{\mathrm{SOC}})}_{\text{Validation}} + \underbrace{\rho_3 K}_{\text{Sparsity}}$$

aSINDY: Re-calibration of Model Coefficients

- LiB operational range includes:
  - SOC levels: 0% to 100%
  - Temperatures (T): $-20^\circ C$ to $40^\circ C$
- Battery capacity varies depending on T
  - Reduced capacity at low temperatures
- Stage-2 optimization of model coefficients
- Allow for re-calibrating coefficient on new data
  - Different temperature conditions, T_i
- Maintains the optimal model structure (library) from MCLS
  - Maintains connection to the physics
- Optimizes accuracy in new conditions via a RMSE-based cost function

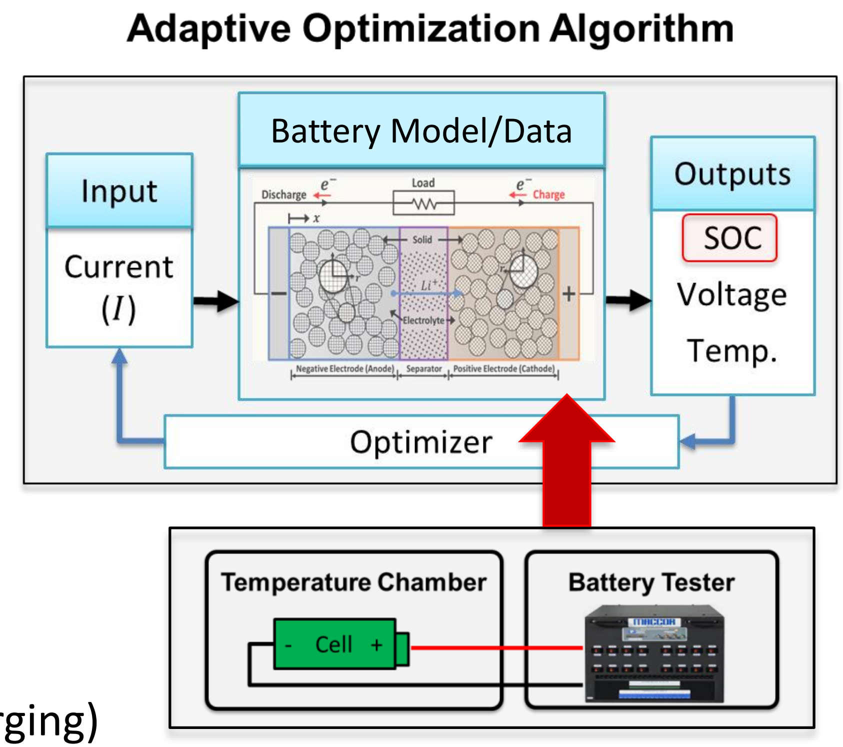
$$\min_{\Xi_{T_i}}. J(\Xi_{T_i}) \stackrel{\text{def}}{=} E_{T_i}(\text{SOC}, \widehat{\text{SOC}})$$

- Yields optimal model valid across operating conditions



Overview of Learning and Optimization Process #1

- Method based on a direct data-driven control framework
  - Searches for optimal inputs without visiting all combinations
  - Optimizes response while satisfying Input and Outputs constraints
- Optimize charging profile (I) for minimum charge-time
- Ensure safe operation and mitigate battery aging
  - Satisfy constraints: max T, max V
- Flexible data generation
  - Full-order dynamics (physics-based model) or PhITEDD
  - Applicable to actual battery
- Allows for hybrid (mixed continuous-discrete) charging framework
  - Continuous: direct simulation of operating modes (e.g., CC, CV, pulse charging)
  - Discrete: dynamic transition between operating modes
- Maximizes current; transition between operating modes to meet constraints
- Ensures solution by initializing with a sub-optimal baseline



Overview of Learning and Optimization Process #2

Learning and Optimization Process

- Step-1: Jacobian Learning
  - Learn Jacobian ($\mathbb{J}$) from input/output battery data
  - Maps the input u (I) to each of the q outputs y (SOC, V, T)

    $\Delta y_j = \mathbb{J}_j^T\,[k]\Delta u[k]\ ,\ j = [1, q],\quad \mathbb{J}_j^T\ \textit{is the } j^{th}\ \textit{row of } \mathbb{J}$
  - Jacobian is updated via RLS at every iteration

- Step-2: Optimization

  a) Conduct simulation/experiment for a given I (input u)

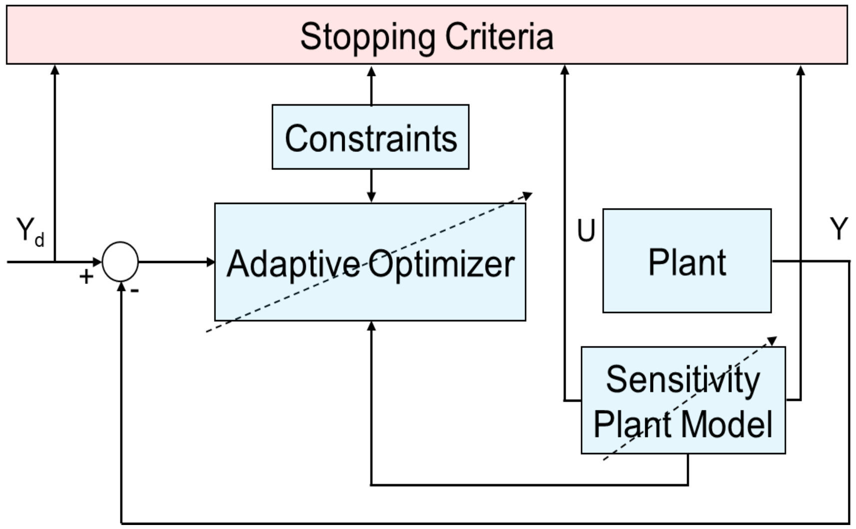
  b) Use insight from outputs and $\mathbb{J}$ to map out next I

$$u[k+1] = u[k] + [\mathbb{J}^T[k]G\left(\rho I + \mathbb{J}[k]\mathbb{J}^T[k]\right)^{-1}](y_d - y[k]))$$

$\rho > 0$: constant, I: identity, G: controller gain, y_d: target

- Initializes with a baseline solution
  - Baseline solution: constant current constant voltage (CCCV)
- Iteratively improves I until convergence to the optimum (I^*)

Diagram of Learning and Optimization Method



- Y: outputs
- U: inputs
- Y_d: target output

Optimal Charging Problem Formulation

- Maximize charge level (SOC) within a duration (t_f)
- Constraints enforced to mitigate aging effects
  - T constraints: avoid overheating / thermal degradation
  - V constraints: prevent over-charging/discharging

SOC [%]	Maximize value at t_f
Temperature [°C]	maximum: 57
Voltage [V]	maximum: 4.2
	minimum: 2.5

- Optimization problem
  - $\boldsymbol{I^*}$: optimal charging profile
  - $\boldsymbol{SOC_d}$ / $\boldsymbol{SOC(t)}$: desired SOC (100%) / SOC level from latest iteration
  - $\boldsymbol{ub}$ / $\boldsymbol{lb}$: upper/lower bounds

$$I^* = \arg\min_{I} \int_0^{t_f} (SOC(t) - SOC_d)^2 dt$$

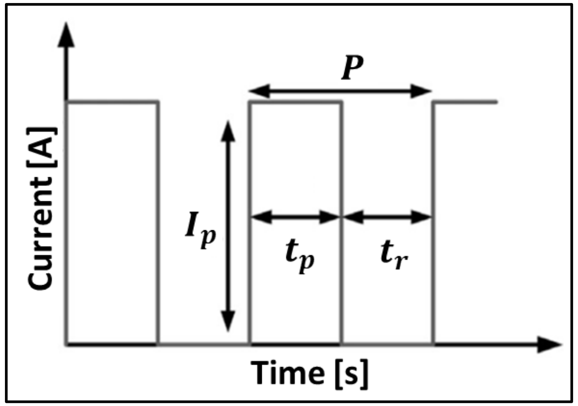
subject to the constraints: $T(t) \leq T_{ub}$

$$V_{lb} \leq V(t) \leq V_{ub}$$

<u>Solution:</u> hybrid charging strategy

1) Positive pulse charging (PPC) to apply high current
   - PPC is defined by waveform parameters
   - Proper selection can prevent side reactions
2) CV to avoid continuing temperature rise

- Initialize with information (I) from CCCV strategy
- Optimize: waveform parameters, switch to CV



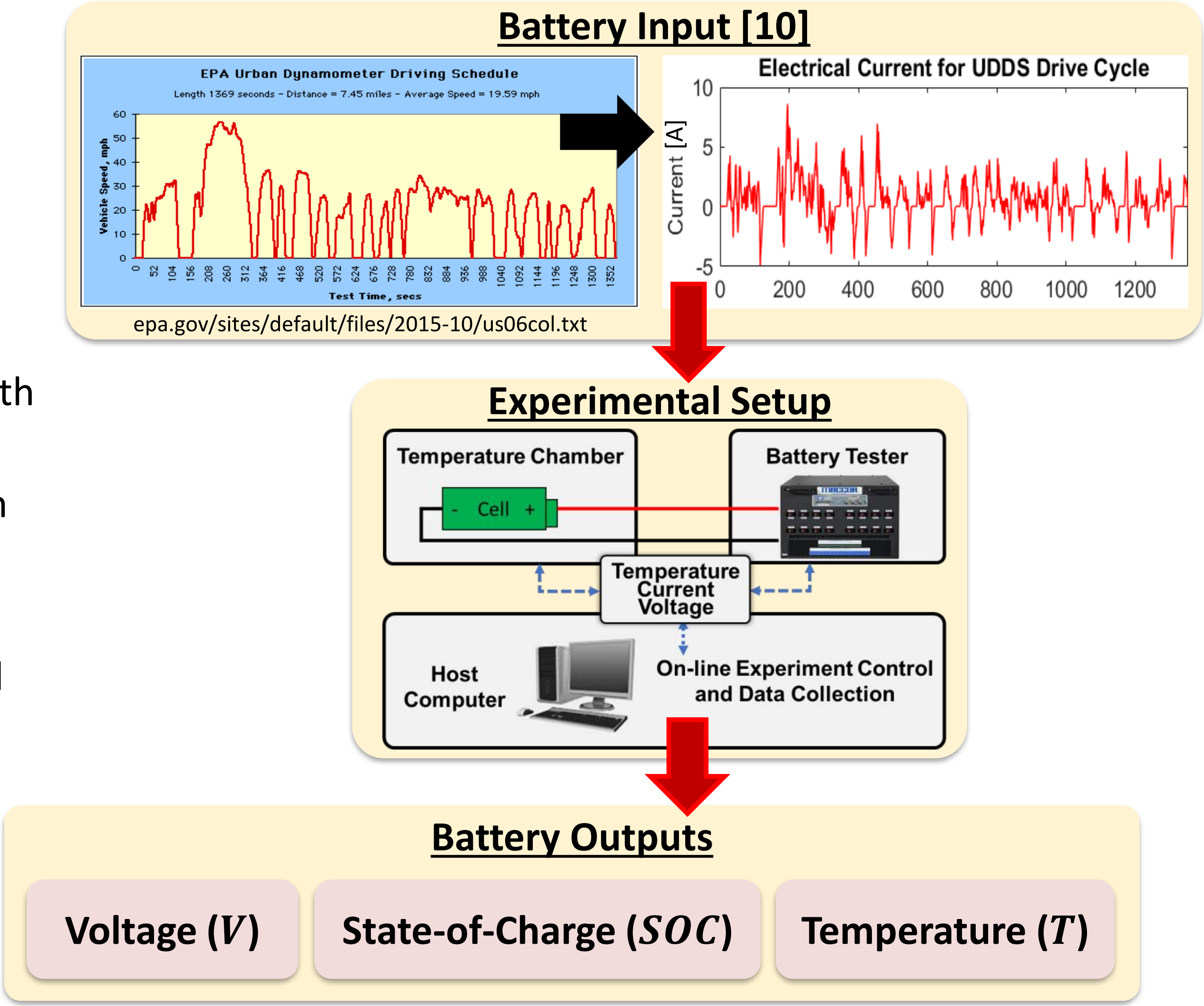
peak current (I_p), pulse on-time (t_p) relaxation time (t_r), pulse period (P)

Battery Digital Twin and Fast Charging

Experimental Data Collection

- The battery experiments conducted on LGM50 cell
  - Cylindrical cell
  - Capacity: 5Ah
  - Positive electrode: NMC 811

- The experimental procedures includes
  i. Cycling (charging/discharging) the cell three times with constant current constant voltage (CCCV)
  ii. Fully charging the battery with CCCV at the maximum allowable rate of 0.3 C-rates
  iii. Resting the cell for two hours
  iv. Employing our in-house stochastic current input until the voltage drops to the lower voltage limit of 2.5V
  v. Storing the battery input/output data.
- Similar steps were followed for the experiments corresponding to EPA cycles.



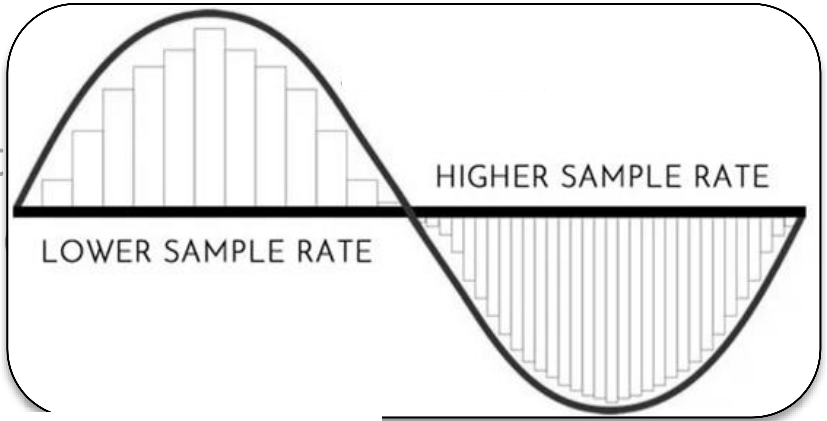
[10] Moura, S. J., et al. Genetic identification of the Doyle–Fuller–Newman model from experimental cycling of a LiFePO4 cell.

Optimizing Initial Model Parameters / Settings

- Model accuracy and complexity depend on good initial settings for the learning algorithm
- Tested different settings to obtain sparse models with good predictive performance

Study of Library Terms (Θ_{bl})

- We explored combinations of library terms and their effect
- Goal: identify the most relevant terms to characterize the S



Study of Data Sampling Rate

- Stu ... ates
  - Sampling rate: time in

$$\Theta(SOC,I,V) = \begin{bmatrix} | & | & & | & | & & | & & | \\ 1 & V^n & \cdots & V^nI^n & \sin(V) & \cdots & e^V & \cdots & \int(I) \\ | & | & & | & | & & | & & | \end{bmatrix} \; ?$$

- Goal: identify the best sampling-rate for data-driven modeling of Lithium-ion batteries

Study of Library Terms

- Test different combinations of libraries terms:
  - Polynomial exponents (**PE**)
  - Mixing (**M**)
  - Sinusoids (**S**)
  - Nonpolynomial exponents (**NE**)
  - Exponential (**Exp**)
  - Integral of current (**Int**)

PE: $$\Theta = \begin{bmatrix} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & V & V^2 & \cdots & I^2 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$

PE,S: $$\Theta = \begin{bmatrix} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & V & V^2 & \cdots & \sin(V) & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$

$$\vdots$$

Library Terms	RMSE	Number of Parameters	Notes
PE, M, S, NE	7.1	36	Similar performance, relatively unaffected by individual Exp or Int
PE, M, S, NE, Exp	6.8	40	
PE, M, S, NE, Int	6.6	37	
PE, M, S, NE, Exp, Int	3.5	41	Improved via both EXP, Int
PE, M, S, Exp, Int	**0.02**	**26**	**Improved by removing NE**

Data Resampling Study

- Test changes in model performance (RMSE) when developed with data sampled at different rates
- Range of sampling rates: 50 [ms] to 1000 [ms]
  - Limits selected based on EPA drive cycles (1s) and commercially available battery testers
- Data corresponds to the UDDS drive cycle

Test 1

- Examined **varying sampling rate** while **preserving initial and final SOC levels** (varying sample size)
- Datasets of varying sample sizes from 1,800 samples (1s) to 36,000 samples (50ms)

Test 2

- Examined **varying sampling rate** while **preserving consistent sample sizes**
- Datasets were under-sampled from large set of sequential charging\discharging cycles
  - Large set based on a 50 ms sampling rate

Goal: Identify optimal sampling rate for modeling lithium-ion batteries

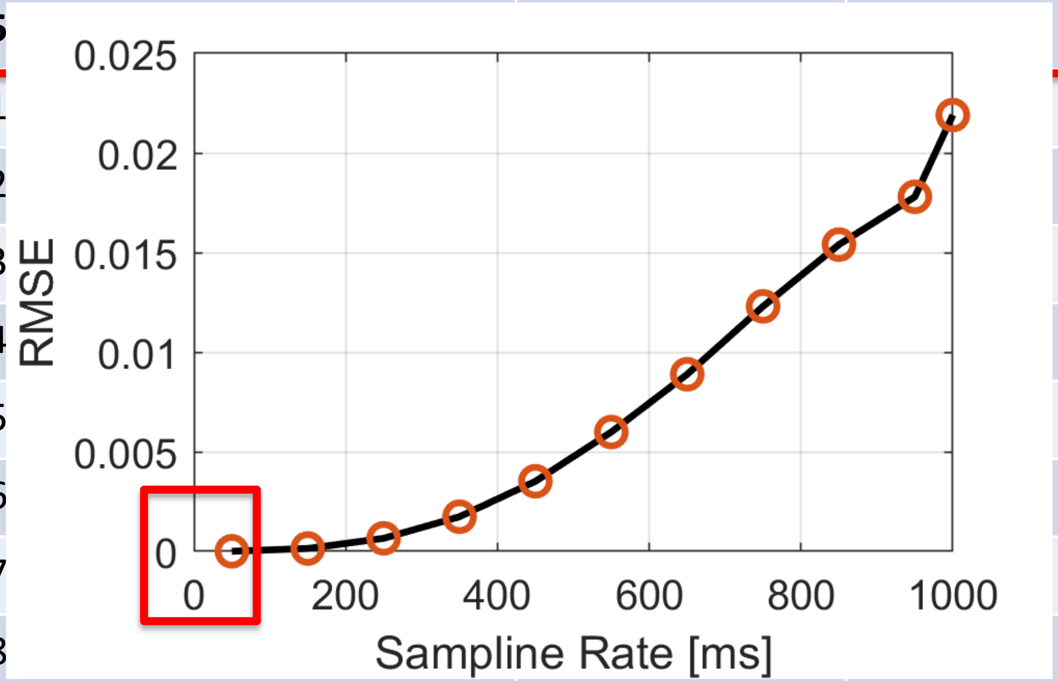
- Assess source of changes in performance:
  - Variations in sample size = more data (Test 1)
  - Ability to capture detailed battery dynamics with faster sampling rates (Test 2)
  - Combination of both factors

Summary of Data Resampling Study

Test 1: Varied sample rates, varied sample size

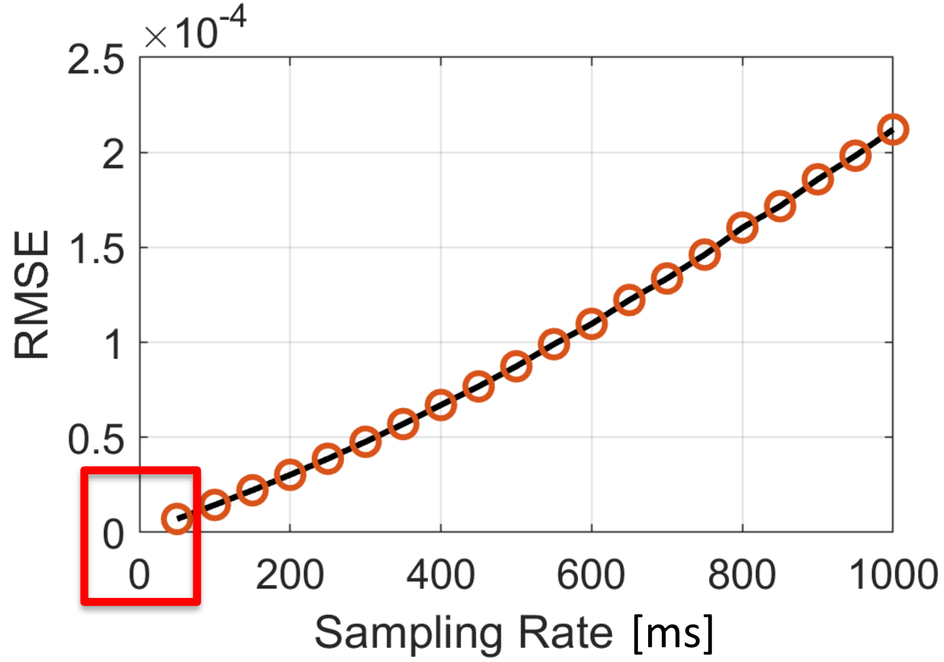
- Best performance achieved 50ms

Sampling Rate	RMSE	Terms
5		
1		
2		
3		
4		
5		
6		
7		
8		
950 [ms] (1900 samples)	1.78e-2	26
1000 [ms] (1800 samples)	2.19e-2	26



Test 2: Varied rates, same sample size

- Best performance achieved 50ms



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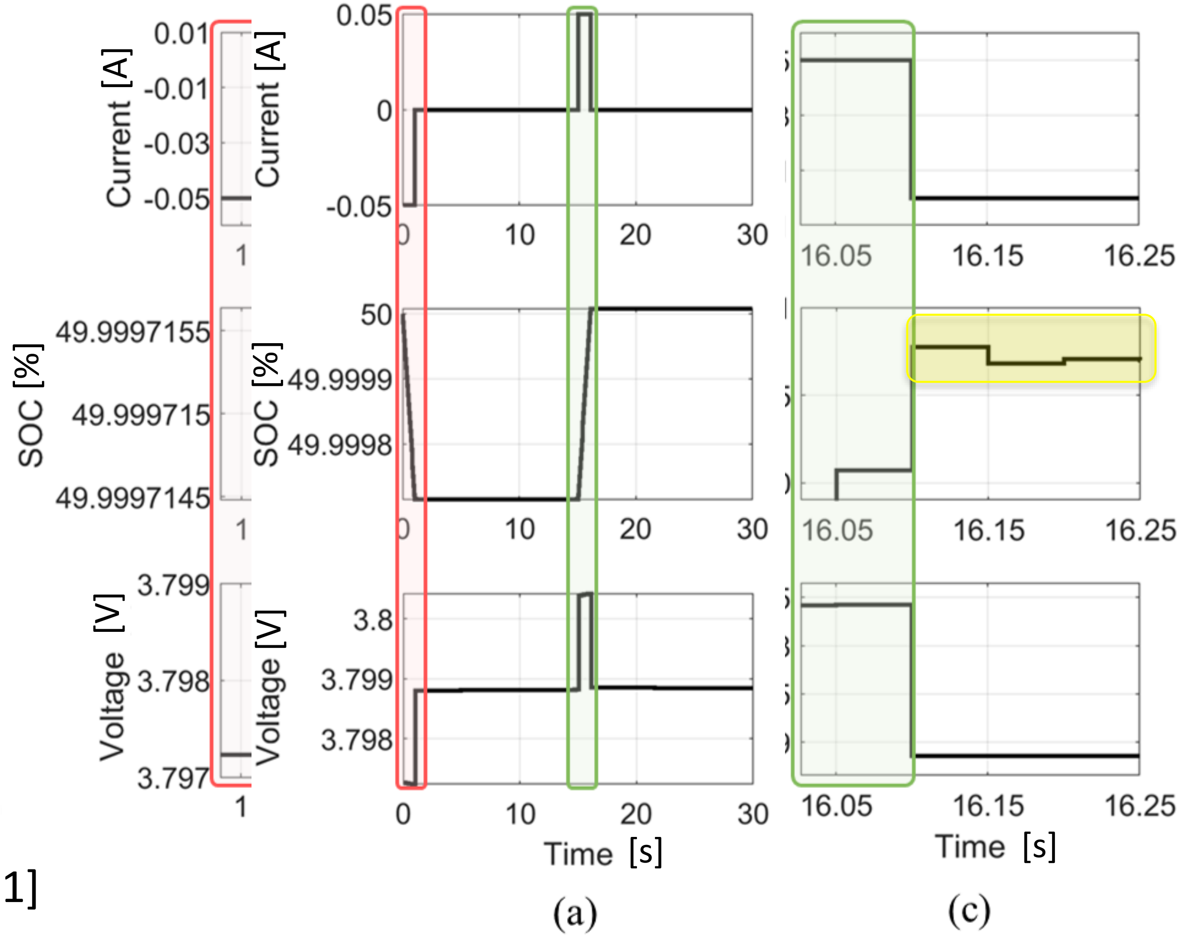
Pulse Relaxation Study

- Validation of empirical sampling rate optimization
- Examination of response to pulse-relaxation tests

- 2-part study: charging / discharging
- Initialize battery at 50% SOC
- Apply pulse followed by rest until steady-state (SOC)

- Part-1: Discharging
  - Discharge Pulse: $I = -0.05A$ for 1 second
  - Rest Period: $I = 0.0A$ for 14 seconds
- Part-2: Charging
  - Charge Pulse: $I = 0.05A$ for 1 second
  - Rest Period: $I = 0.0A$ for 14 seconds

- Analyzed response at rest to find SOC time scale
- Dynamics evolve in the order of milliseconds
- Aligns with time scale for charge transfer kinetics [10]
- Follow Butler–Volmer eq., exhibits **high SOC dependency** [11]
- Sampling rates of milliseconds are needed to capture SOC dynamics from measurement data



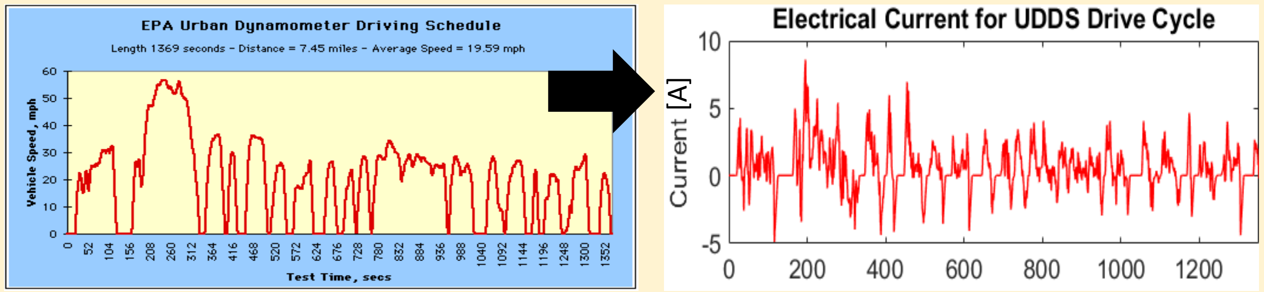
Pulse Relaxation Study: (a) Full Input/Output, (b) Discharge Pulse (red), (c) Charge Pulse (green)

[10] Derakhshan, M et al. Detecting mechanical indentation from the time constants of Li-ion batteries.
[11] Tsai, P. C., et al. Single-particle measurements of electrochemical kinetics in NMC and NCA cathodes for Li-ion batteries.

Battery Digital Twin of SOC Dynamics (PhITEDD)

- Developed SOC model using battery input/output data
  - Training/Validation data: Stochastic drive cycle
  - Cross-Validation data: US06 (highway driving) cycle
- Initialization: model development
  - Baseline physics-informed library
  - Optimal sampling rate: 50 [ms]
  - Standard operating temperature: 25°C

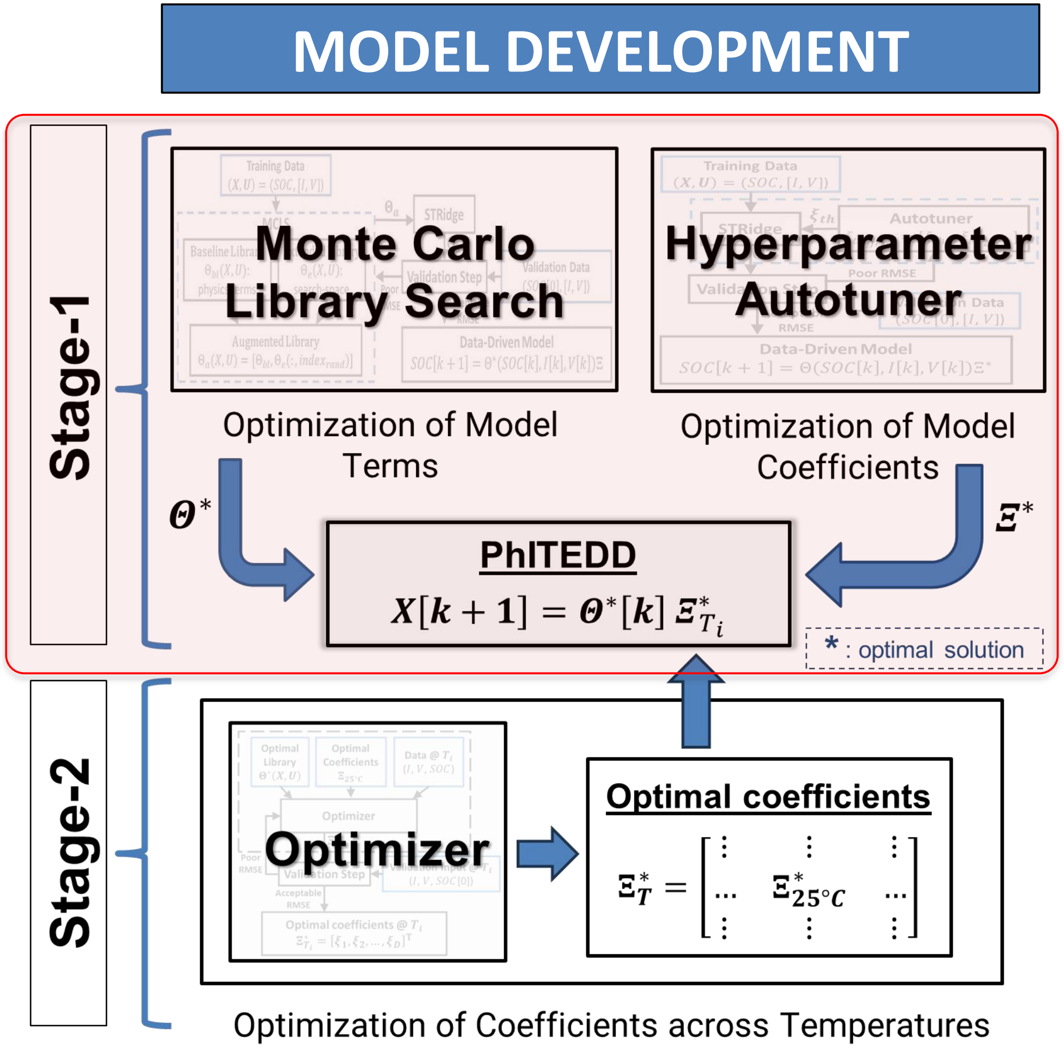
Battery Input



epa.gov/sites/default/files/2015-10/us06col.txt

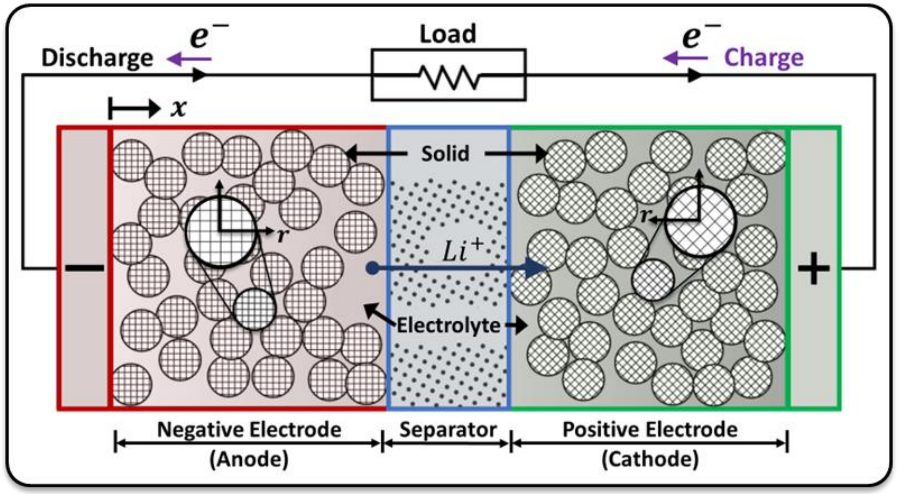
Battery Outputs

Voltage (V)	State-of-Charge (SOC)	Temperature (T)



Physics-Informed Library Terms

- Incorporated physics-informed terms derived from electrochemical (DFN) model
  - Enhance interpretability, generalizability, and computational efficiency
- Lithium transport is a diffusion process with trigonometric and exponential terms
  - $\mathbf{exp}(\cdot), \boldsymbol{sin}(\cdot)$
- Charge transfer follows the Butler-Volmer equation has hyperbolic functions
  - $\mathbf{sinh}(\cdot), \boldsymbol{cosh}(\cdot)$
- Electrolyte's electric potential is a combination of current and electrolyte concentration
  - $\boldsymbol{I}$
- Voltage is the difference in the solid potential between the cathode and anode
  - $\boldsymbol{V}$
- SOC relates to initial values and the solid concentration
  - $\boldsymbol{SOC}$
- Time history of current is captured with integral term
  - $\int \boldsymbol{I}$
- **Polynomials** & **mixing** included for other nonlinearities



SOC Prediction Results: Experimental data @25°C

- Trained & Validated model with stochastic cycle

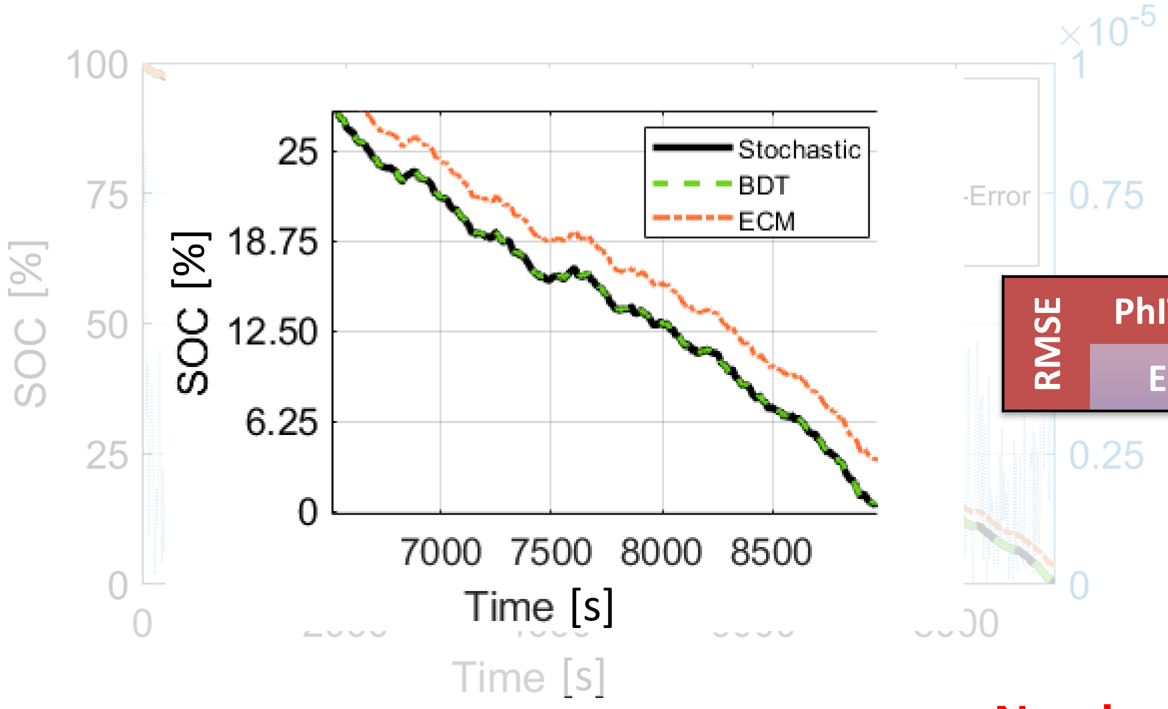
Prediction Error

- Training RMSE: 2.2e-6
- Validation RMSE: 4.8e-4
- ECM RMSE: 2.4e-2

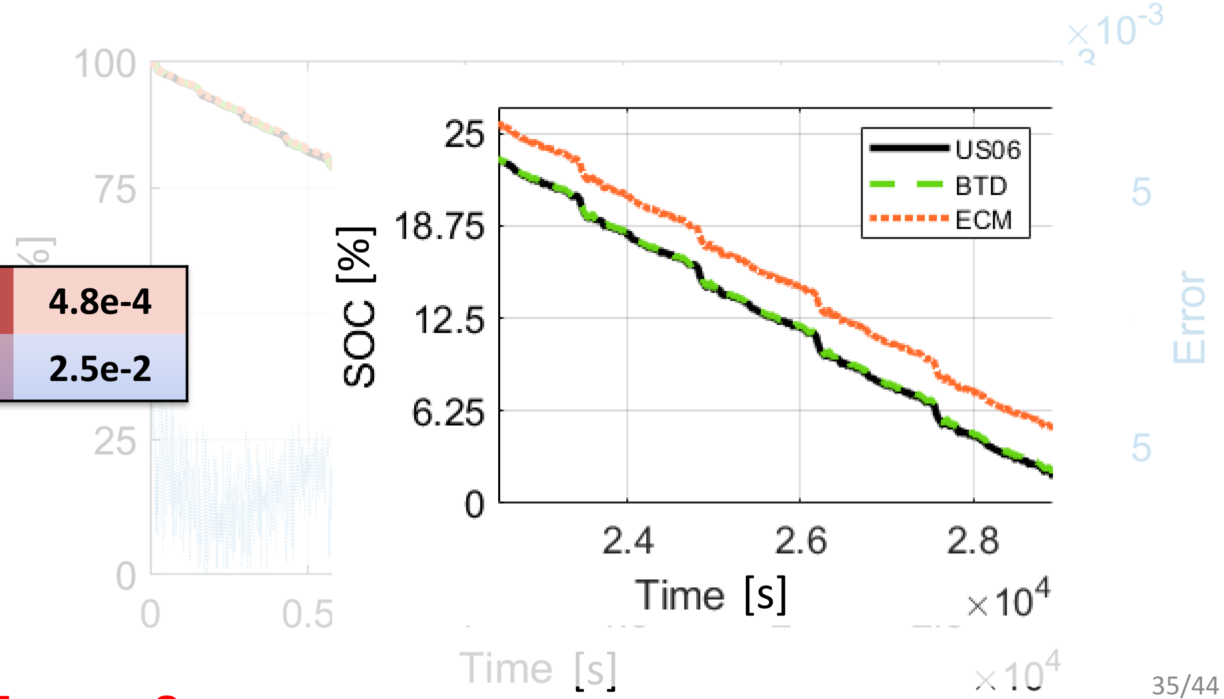
- Cross-Validated on unseen data US06 cycle
  – Input profiles (I, V) and **initial SOC** (100%)

Prediction Error

- Cross-Validation RMSE: 8.5e-4
- ECM RMSE: 2.5e-2



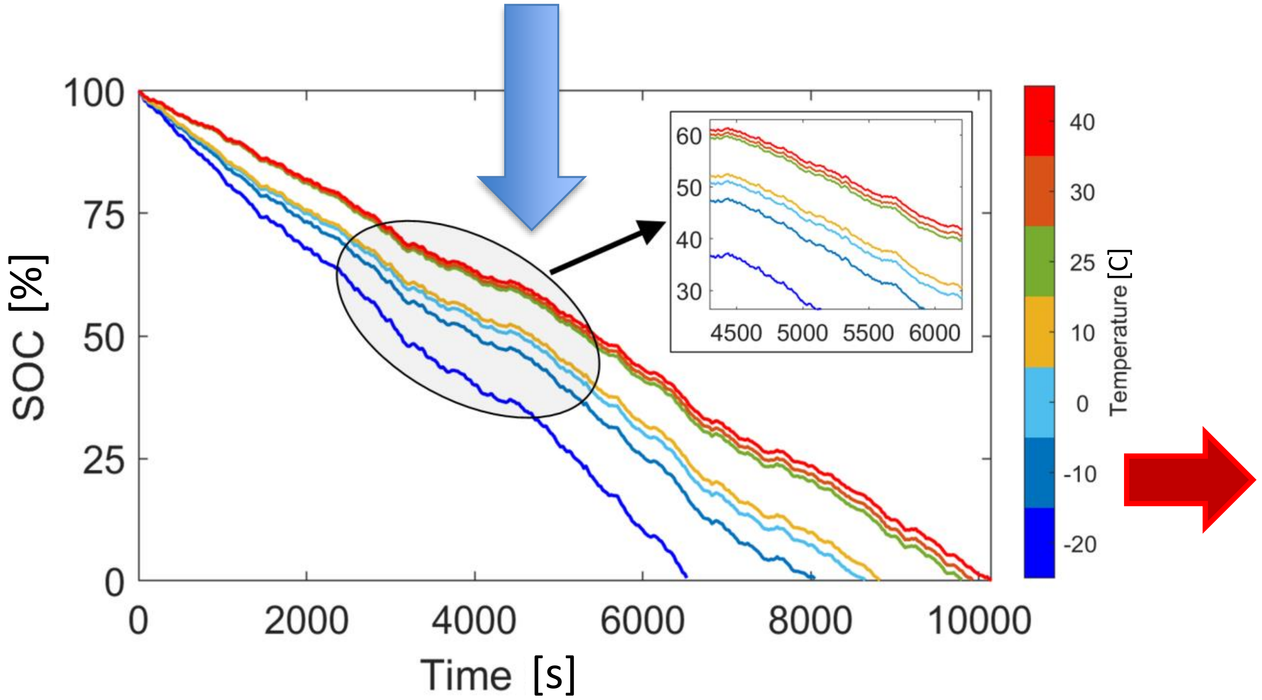
RMSE		
	PhITEDD	4.8e-4
	ECM	2.5e-2

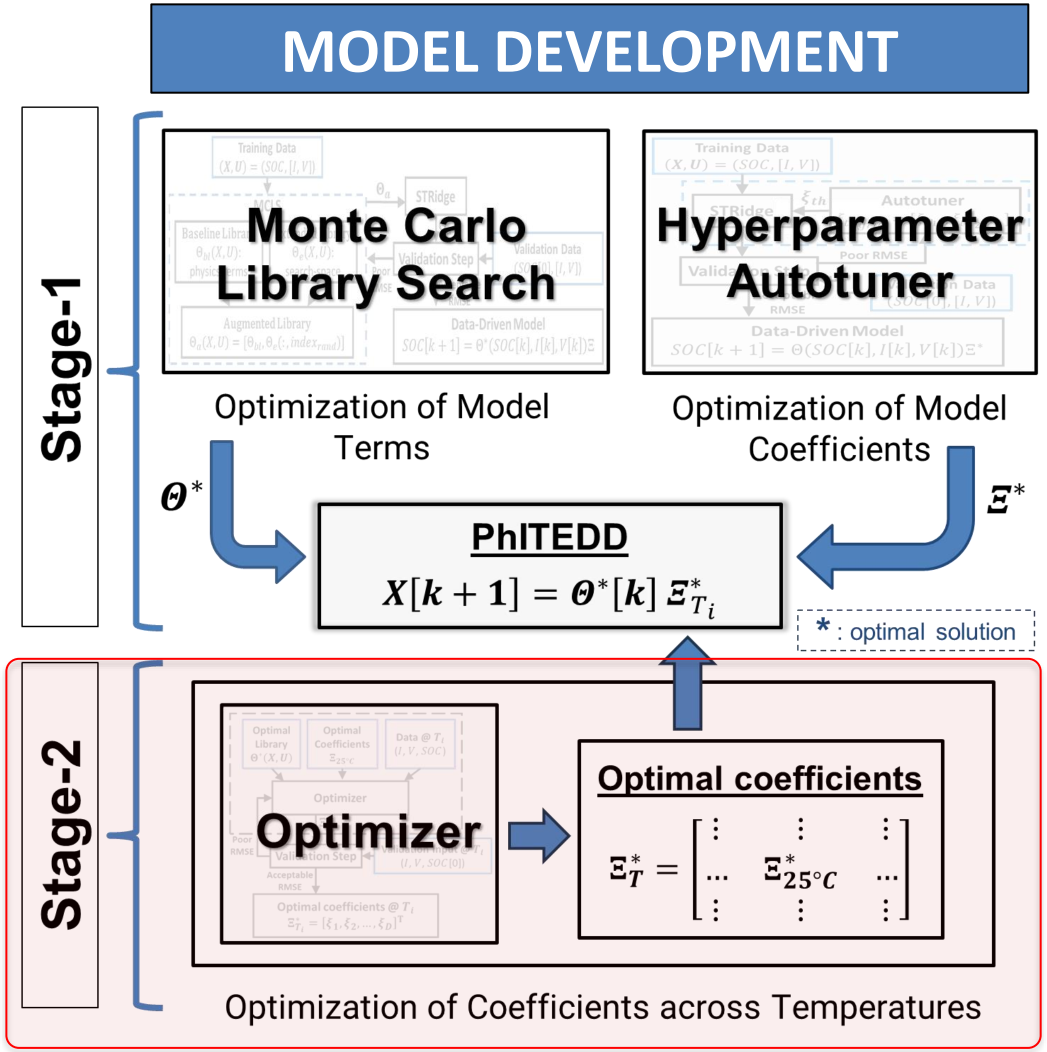


Number of Terms: 8

Physics-Informed Temperature Dependent Explicit Data-Driven (PhITEDD)

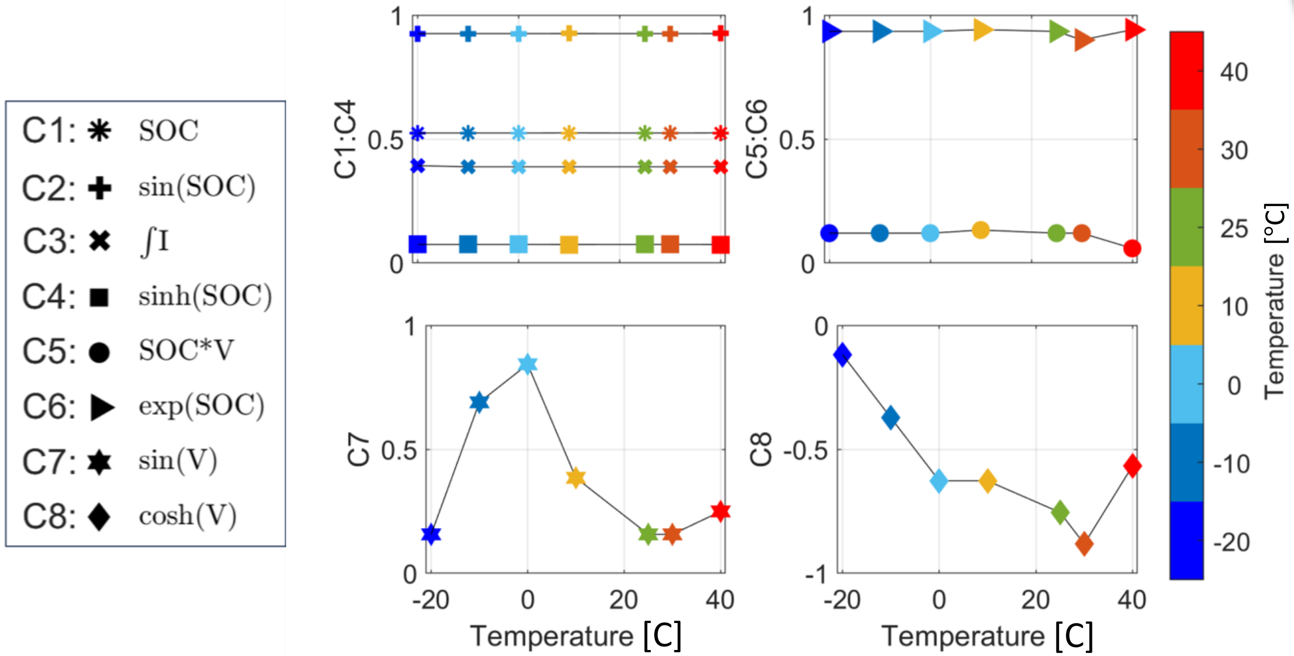
- LiB operational range includes:
  - SOC levels: 0% to 100%
  - Temperatures (T): $-20°C$ to $40°C$
- Battery capacity varies depending on T

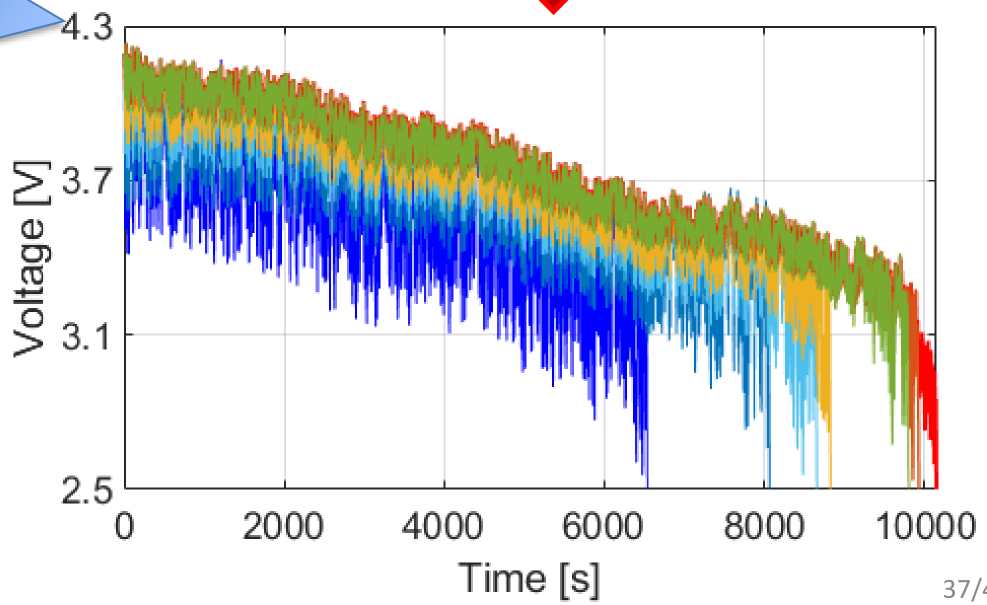




Physics-Informed Temperature Dependent Explicit Data-Driven (PhITEDD)

- Coefficients correspond to the 8 model terms (normalized coefficients)
- Coefficients C1 through C6 experience negligible changes with change in temperature
- Coefficients involving V (C7 and C8) display the highest temperature dependency
  - Temperature dependency of V terms is associated with changes in battery's voltage response
- The final model achieved an average RMSE of 1.1e[illegible] across $-20°C$ to $40°C$





PhITTED vs State-of-the-art

	Modeling Requirements	Computational Time (UDDS cycle = ~29,000 [sec])	Accuracy (RMSE)
PhITEED	• Dynamic Response data • Data across various temperatures		
ECM	• Charge/Discharge Profiles • OCV curves • Impedance data (EIS tests) • Data across various temperatures • Multiple models per SOC range		
DFN	Knowledge of battery composition • Physical properties • Material properties • Electrochemical parameters		

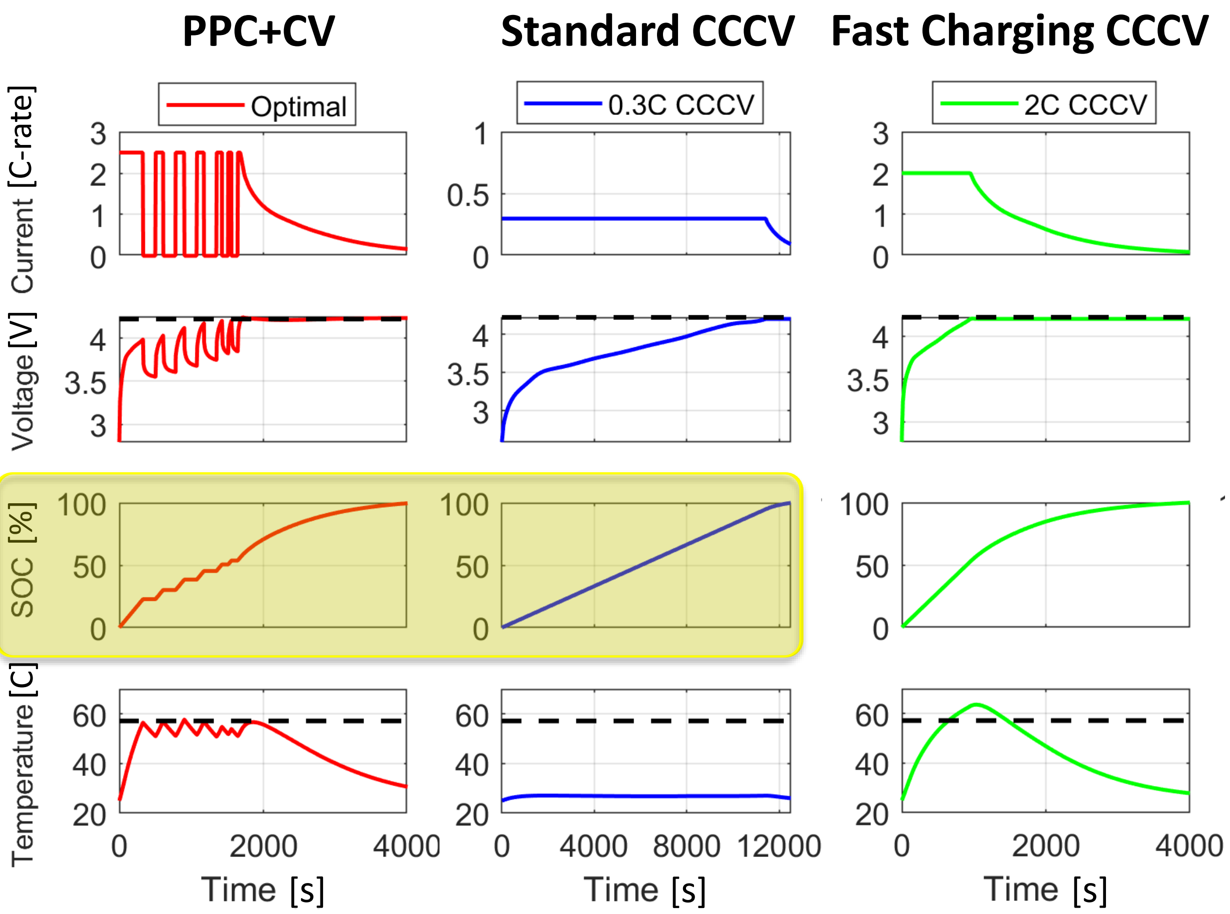
Optimal Charging Strategy

Optimal Strategy

- Charging-rate: 2.5C (12.5A) pulse
- Charging Time: 4,000s (1.1 hour)
  - SOC level: 0% - 100%
- **Satisfied safety constraints**
  - V of 4.2 or lower
  - T of 57°C or lower

Alternative strategies

- **Charged 66% faster than** standard strategy
  - Standard strategy: CCCV 0.3C (1.5A) charging rate
- **Lower temperatures** than fast charging CCCV
  - Fast charging CCCV: 2C (10A) charging rate
  - Temperature reached 64°C (7°C hotter)
  - Can lead to accelerated battery degradation



- t_f: 4,000s
- T_{max}: 57°C

- t_f: 12,000s
- T_{max}: 27°C

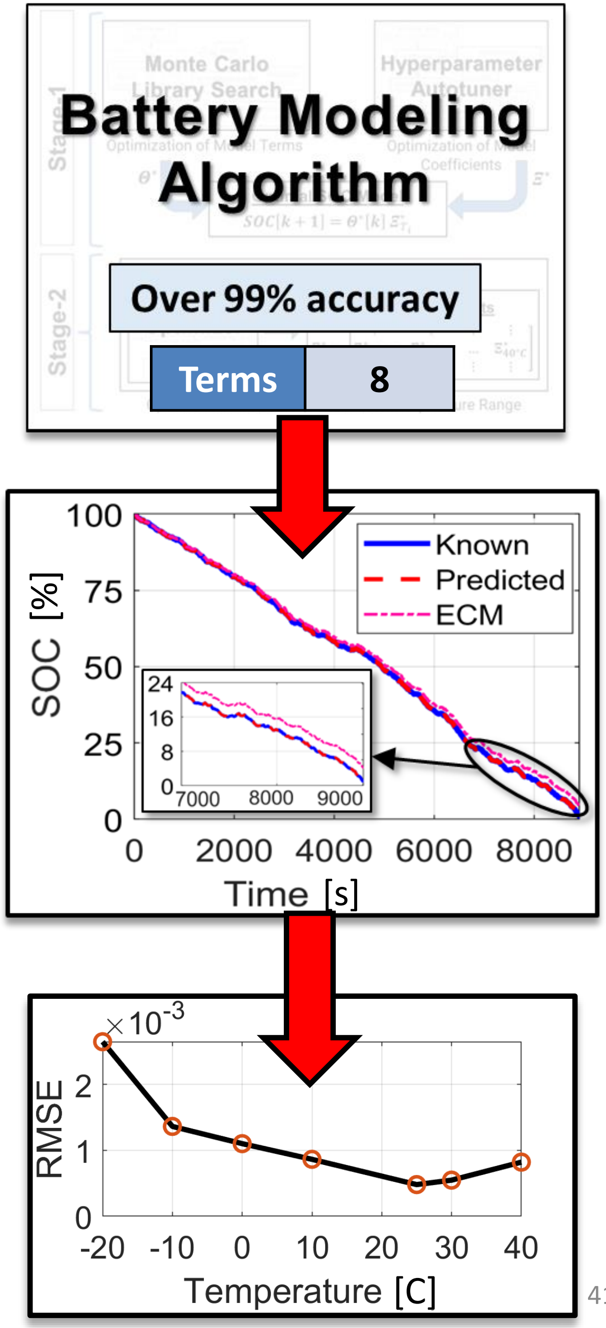
- t_f: 4,000s
- T_{max}: **64**°C

SUMMARY

Summary #1

- We tackle two major challenges in battery electric vehicles
  - range anxiety and slow charging times
- Develop high-accuracy physics-informed battery digital twin for real-time state forecasting, even in temperature extremes
  - Prediction error (RMSE) $< 1\%$
- Accurate and efficient model from operando data
- Model valid across operational range: error $< \mathbf{1}\%$
  - Temperature extremes ($-\mathbf{20}°\boldsymbol{C}$), low SOC ($0\%$)
  - Aggressive dynamic charging / discharging cycles
- Optimized library with physics inspired terms via Monte Carlo library search
- Optimal coefficients that balance accuracy and complexity via Autotunner

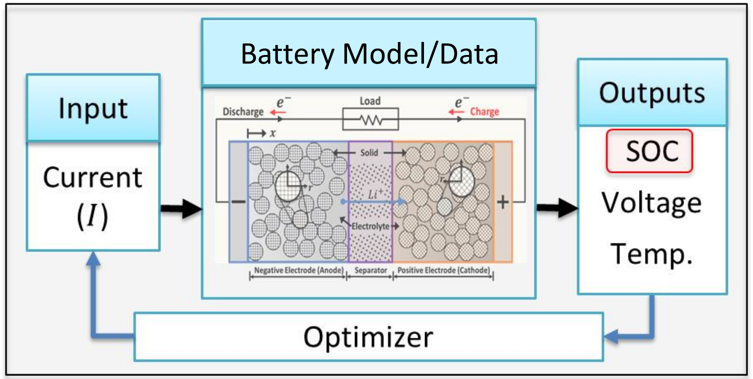
- Our method significantly reduced modeling cost
  - OCV method: requires many SOC curves, one per C-rate
  - ECM: requires multiple sets of coefficients for different SOC levels
- Without knowledge of the battery's composition, needed for physics-based methods



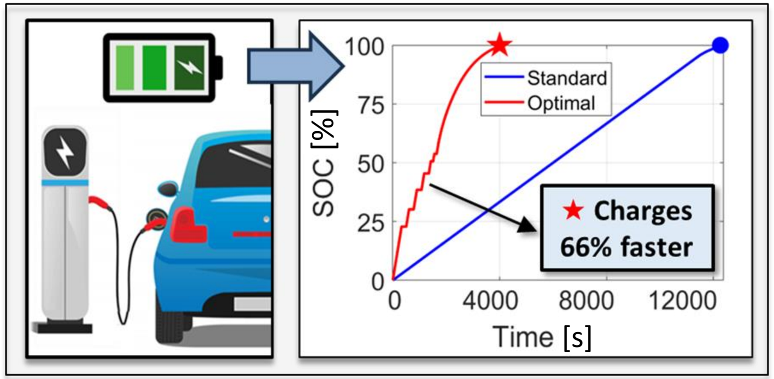
Summary #2

- Adaptive optimization for constraint-based optimal charging
- Incorporated full-order physics-based battery model (DFN/P2D)
  - Includes thermal effects
- Solution met fast charging demands while ensuring safe operation
  - Prevented over-heating: T of 57°C (90% of max 63 °C) or lower
  - Prevented over-charging: V of 4.2 or lower
  - Helped mitigate negative effects on battery health
- Charged 66% faster than standard 0.3C CCCV strategy
- Comparable 2C CCCV strategy subjected LiB to high temperatures
  - 7°C above limit, can lead to adverse effects on battery health

Adaptive Optimization Algorithm

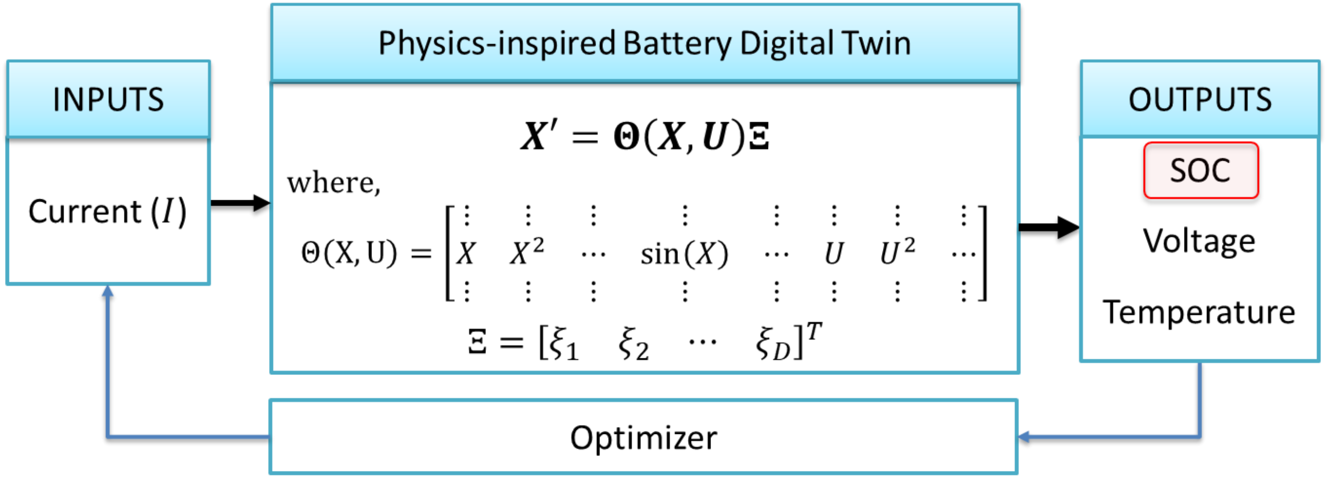


Solution



Future Work

- Expand optimization criteria to minimize damage to cyclable life of battery
  - Quantified by capacity fade
- Perform experiments on batteries with different chemistries and form factors
- Improve the efficiency of our optimization approach
  - Substitute electrochemical model with accurate physics-inspired battery digital twin



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- University Research Project

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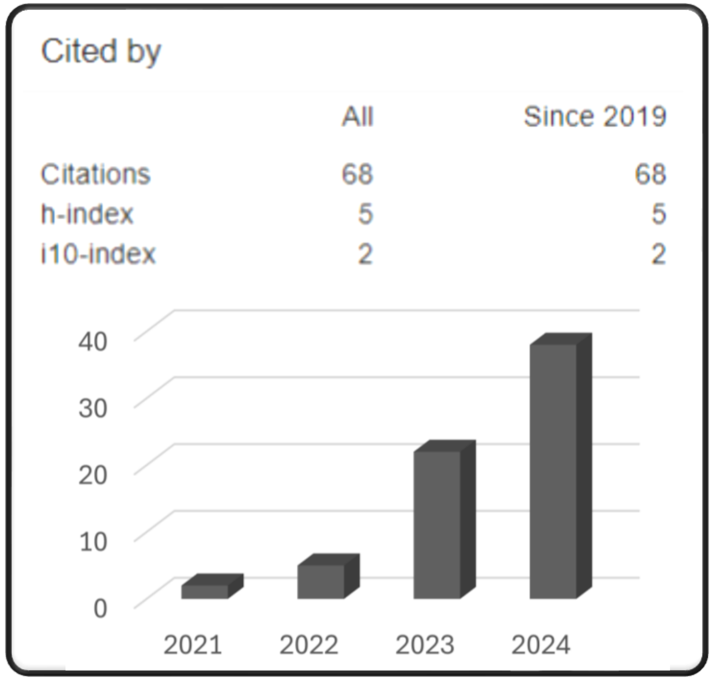
Physics-inspired and Control-Oriented Modeling of Lithium Batteries for Accurate State-of-Charge Prediction and Fast-Charging

Renato J. Rodriguez Nunez

Advisor: Damoon Soudbakhsh



Selected Publications

1) Fast Charging of Li-ion Batteries via Learning and Optimization. In ECC’24. IEEE
2) Physics-Informed & Temperature-Dependent Battery Digital Twin. Energy ’24 (rev.)
3) Impact of light-weighting & battery technologies on EV sustainability. EIA Review ’24
4) Data-driven Discovery of LiB SOC Dynamics. J. Dyn. Syst. Meas. Control ’24
5) Data-driven control: Theory and applications. In ACC’23. IEEE
6) Discovering governing equations of LiBs pertaining SOC. In ACC’23. IEEE
7) A physics-inspired machine learning nonlinear model LiB. In ACC’23. IEEE
8) Modeling of LiBs for real-time analysis and control. In ACC’22. IEEE
9) Adaptive takeoff maneuver optimization for America’s cup. J. Sail. Tech. ’22
10) On automating hyperparameter optimization for ML applications. SPMB ’21. IEEE

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