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TUM

Physics-informed Modeling Framework for AI-based Battery Pack Design, Operation and Diagnostics Optimization

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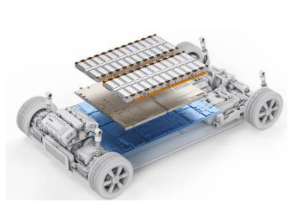
Motivation and Introduction

- Pack-level optimization necessitates the coupling of **electrical**, **electrochemical**, and **thermal** dynamics.
- **High number of variables** and **cross-interactions** complicates systematic analysis.
- We provide a precise and flexible **physics-informed** simulation framework to enable **AI-assisted optimization** on pack-level.



Main findings

- **Explicit pack topology and cooling** modeled under fully configurable boundary conditions.
- **DFN-level internal states at ECM-level speed** via adaptive discretization (SPMe → DFN).
- **Validated** against measurements on physical cells using Virtual Parallel Connection (RMSE(I) < 1%).
- Enables optimization of **system design, operation and diagnostics** based on BMS-observable and cell-level hidden states.

Inputs

Topology
- *msnp*
- contacting network
- terminal position

Heterogeneities
- Intrinsic: $\Delta Ci, \Delta Ri, \Delta SoHi$
- Extrinsic: $\Delta R_c, \Delta R_{int}, \Delta T, \Delta Q_{cool}$

Physicochemical cell parameter set
- NCA | Si-Gr
- C_N = 4.5 Ah
- $I_{ch,max}$ = 3C, $I_{dch,max}$ = 10C

Molicel P45b INR21700

Fidelity vs. Complexity on single-cell level
- Adaptive discretization in through plane: 1…N
- Adaptive discretization in solid domain: 3…N

SMPe ↔ DFN

Cooling Scenario
- Active / Passive
- Air, liquid, PCM
- $T_{ambient}$

Load Profile
- CC, CCCV, Fast Charge Profile
- Dynamic Profile

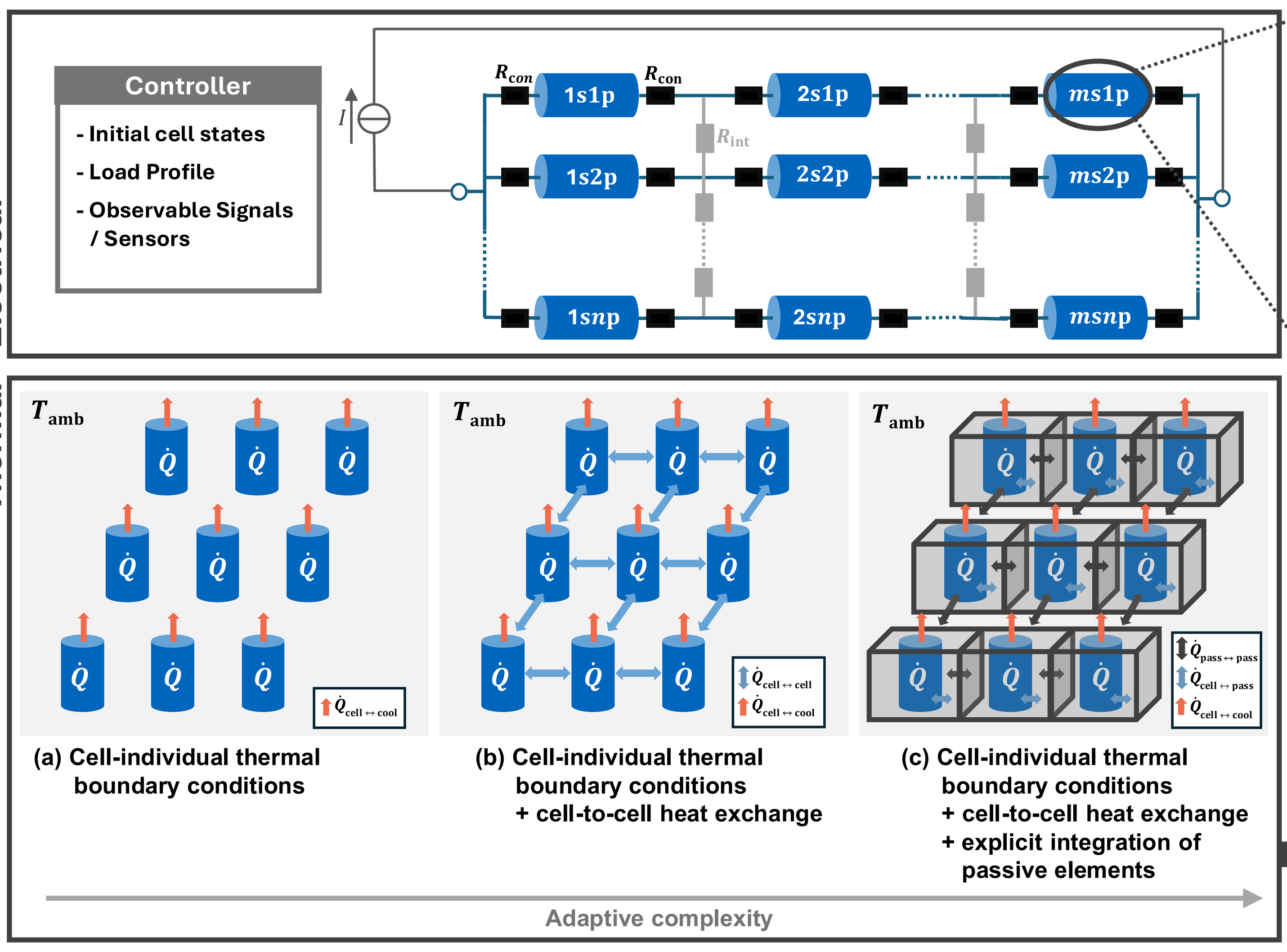
Outputs

System-level states (BMS-observable): U_{sys}, U_{module}, I_{sys}, T_{sensor}

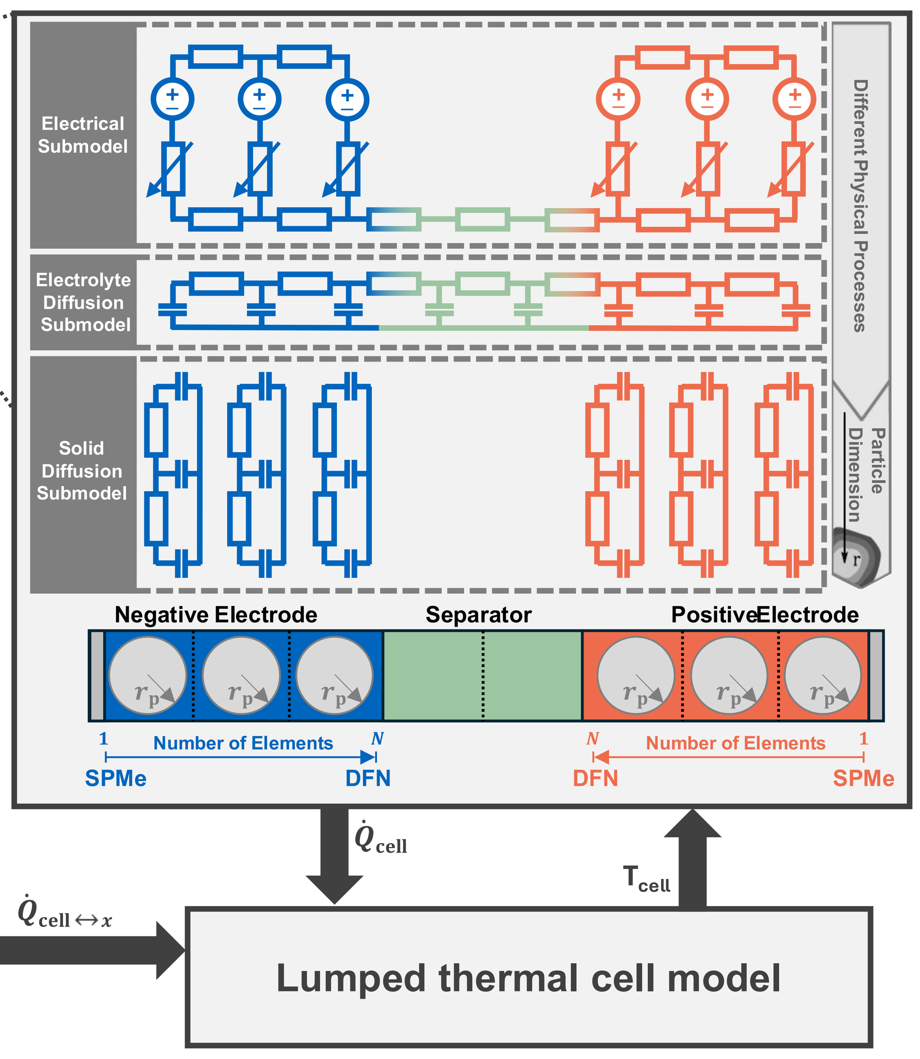
Cell-level states (hidden): U_{cell}, I_{cell}, $T_{cell,0D}$, SoC_{cell}, η_{anode}, c_s, c_l, Q_{gen}

Multi-Cell Transmission Line Model

Electro-thermal multi-cell model

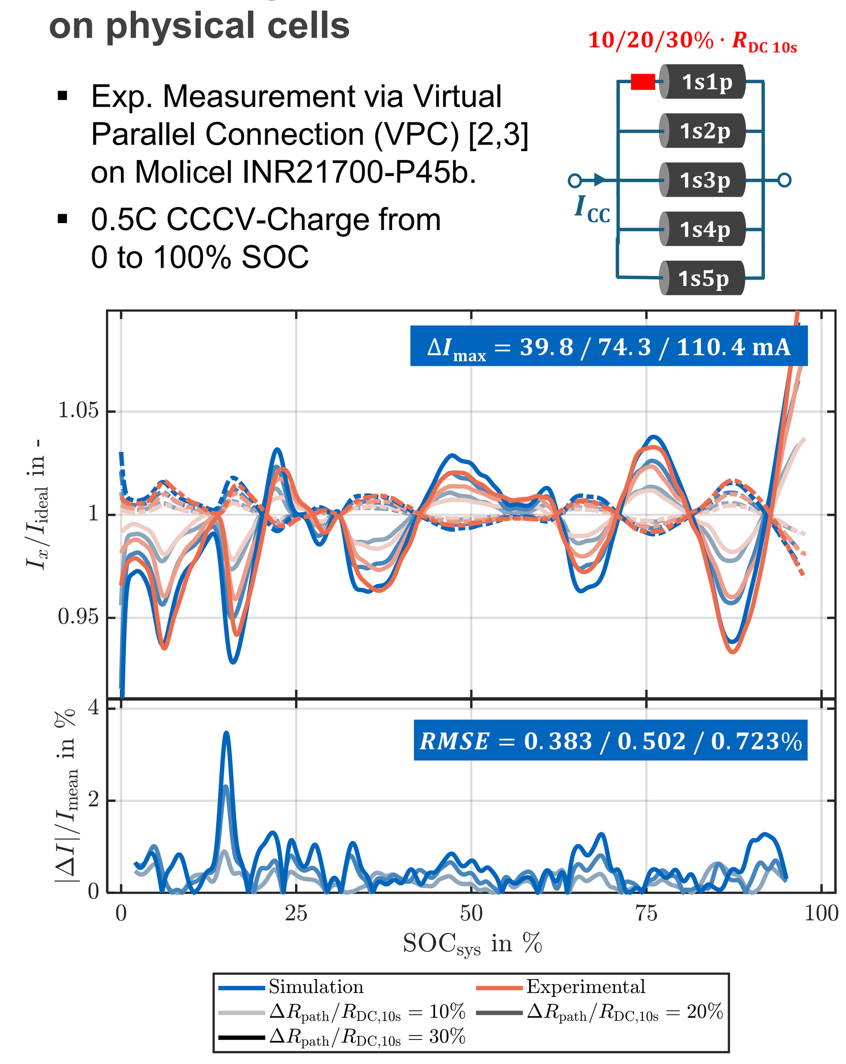


Physicochemical single-cell model [1]



Validation against measurements on physical cells

- Exp. Measurement via Virtual Parallel Connection (VPC) [2,3] on Molicel INR21700-P45b.
- 0.5C CCCV-Charge from 0 to 100% SOC

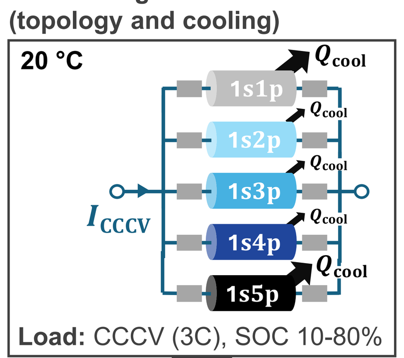


System Design

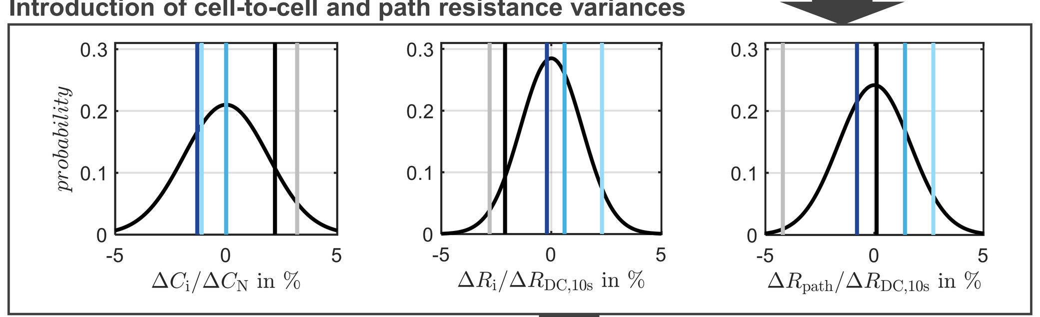
Inhomogeneity analysis for given pack configuration

- Quantify the impact of manufacturing and aging spread under topology and thermal constraints.
- Derive allowable tolerances and sensor placement.

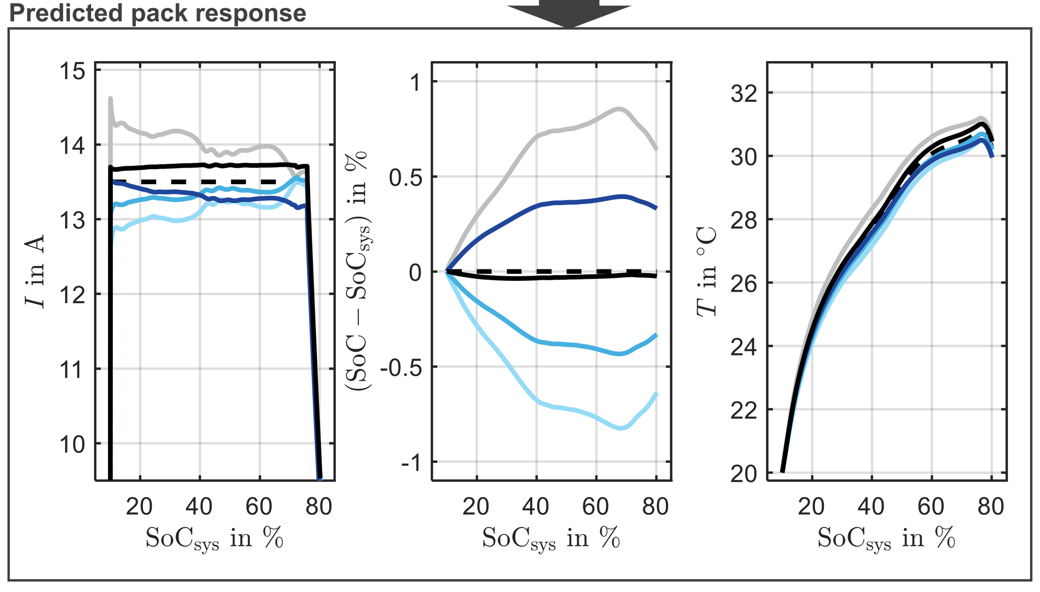
Pack configuration (topology and cooling)



Introduction of cell-to-cell and path resistance variances



Predicted pack response

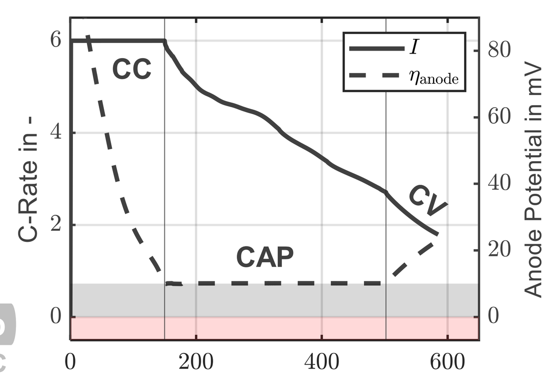


Fast Charging

Anode-potential aware fast charging (single-cell)

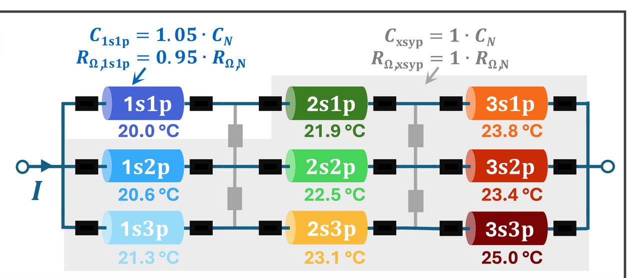
- Minimize charge time subject to $\eta_{anode} \geq 10$ mV
- CC → CAP → CV (CAP: constant anode pot.)

Load: CC (6C)→CAP→CV
SOC 10-80%

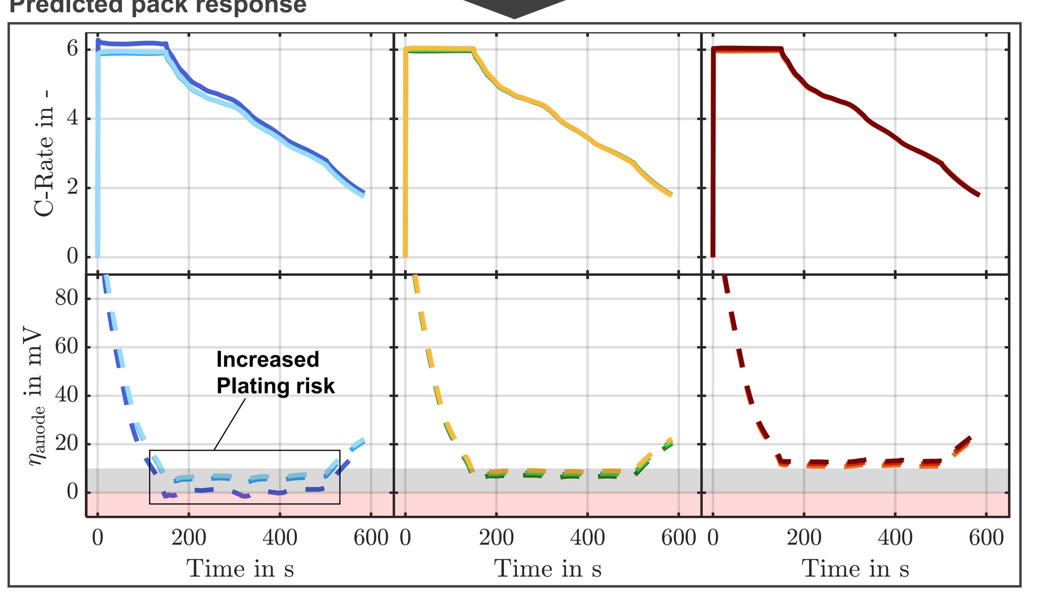


Application at pack level under thermal and cell-to-cell inhomogeneity

Identify limiting cell and its plating risk



Predicted pack response

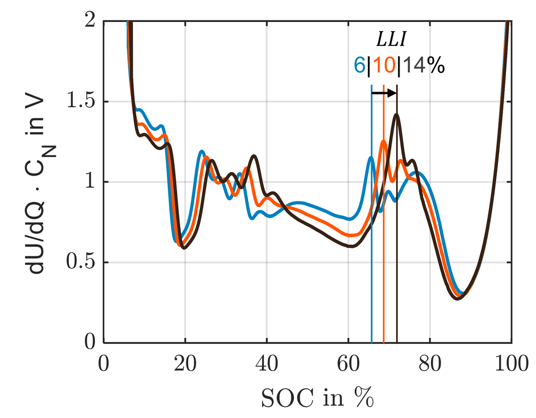


Differential Voltage Analysis

Peak analysis over cell aging (single-cell)

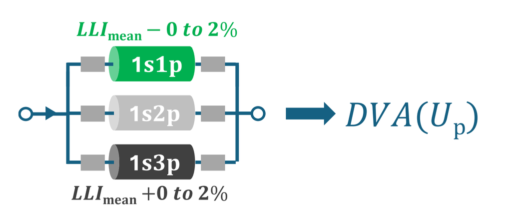
- Introduce Loss of Lithium Inventory (LLI): 6%, 10%, 14%
- Induces half-cell balancing shift
- Directly observable in single-cell DVA

Load: CC (0.05C)
SOC 0-100%

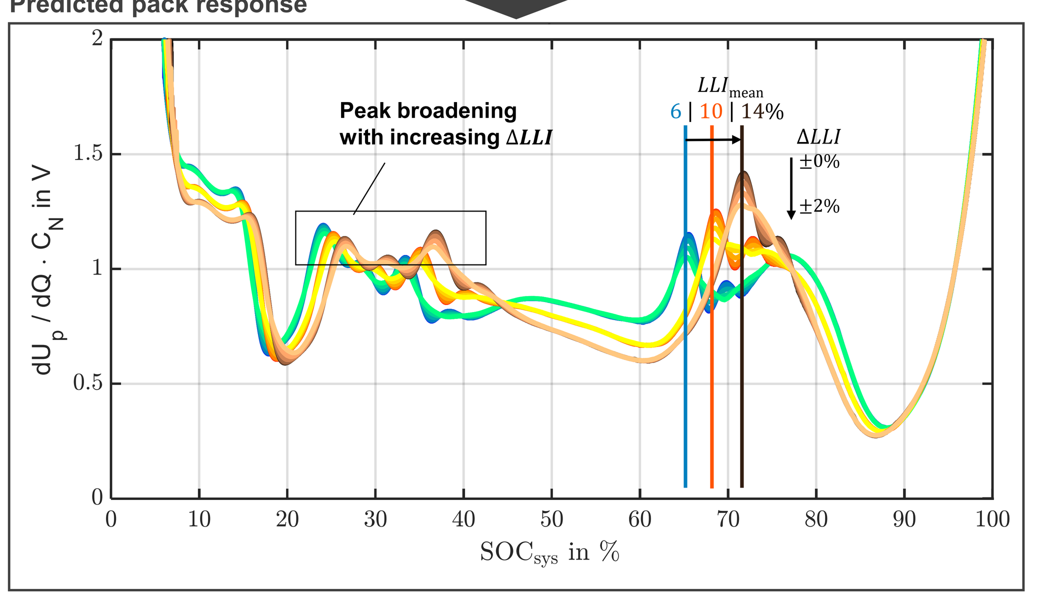


Application at pack level under SOH inhomogeneity

Observation of voltage signal of the parallel configuration U_p



Predicted pack response



Input for AI-assisted Optimization: pack design • operation • diagnostics

Acknowledgements

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