Oak Ridge National Laboratory

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OE Storage, FY25 : Computational Framework for BESS

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U.S. DEPARTMENT of ENERGY

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Project Team

ORNL Team

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Acknowledgements

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Project Overview

Project Goal: Develop a physics based multiscale framework for large scale ageing and degradation simulation for Battery Energy Storage Systems (BESS).

i. We prioritized Li-ion system to reduce (≈99% of deployed BESS) today's dominant operational and financial risk.

ii. Design the computational architecture to be chemistry-portable, seeding rapid extensions to VRB physics and plant models.

Current Practices: Typical system scale models for Li-Ion or Vanadium Flow BESS uses (a)simplified equivalent circuit models, (b) limited by the number of cells, chemistry and formfactors, and/or (c) lack the ability to resolve degradation and aging features at the cell scale.

Why ORNL: We are well positioned with the HPC computing facilities for efficient design and performance analysis of Li-BESS. While also aiding in generating significant long-term cycling synthetic data for AI/ML efforts.

Innovation: Our current approach is (a) computationally efficient for design, and analysis of BESS even with >10000 cells, (b) utilizes fully physics based model at the cell scale with resolved degradation and aging mechanisms, (c) applicable to any cell chemistry and formfactor with right parameter identification, and (d) accelerate simulation of thousands of cycles of these large BESS systems in a matter of days.

Impact: This work is valuable for grid-scale BESS deployments, as the framework enables analysis of high-voltage systems, which age more reliably than equivalent low-voltage/high-current, designs and operational conditions, including grid use cases like frequency regulation (FR), energy arbitrage (EA), and their combinations. This work supports analysis for improved Li-BESS design, long-term operation, and development of aging-informed BMS control algorithms.

Alignment: This aligns well with the DOE-OE mission, through aiding the development of grid scale BESS to improve safe and reliable power delivery

Lithium-ion battery systems

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Project Overview

- Develop physics-based pack level simulation framework.
  - Accelerating life cycle simulations is of utmost importance.
  - Speed up identification of optimal battery pack construction parameters.
  - Identify strategies/control algorithms to minimize aging/degradation of pack due to current imbalance.

- Tasks:

Cell level:
- Identification of physics-based parameters, specific to the individual cells used in the pack construction.
  - Obtained using parameter optimization algorithms (computational limitation)
  - Experimental characterization data is limited.

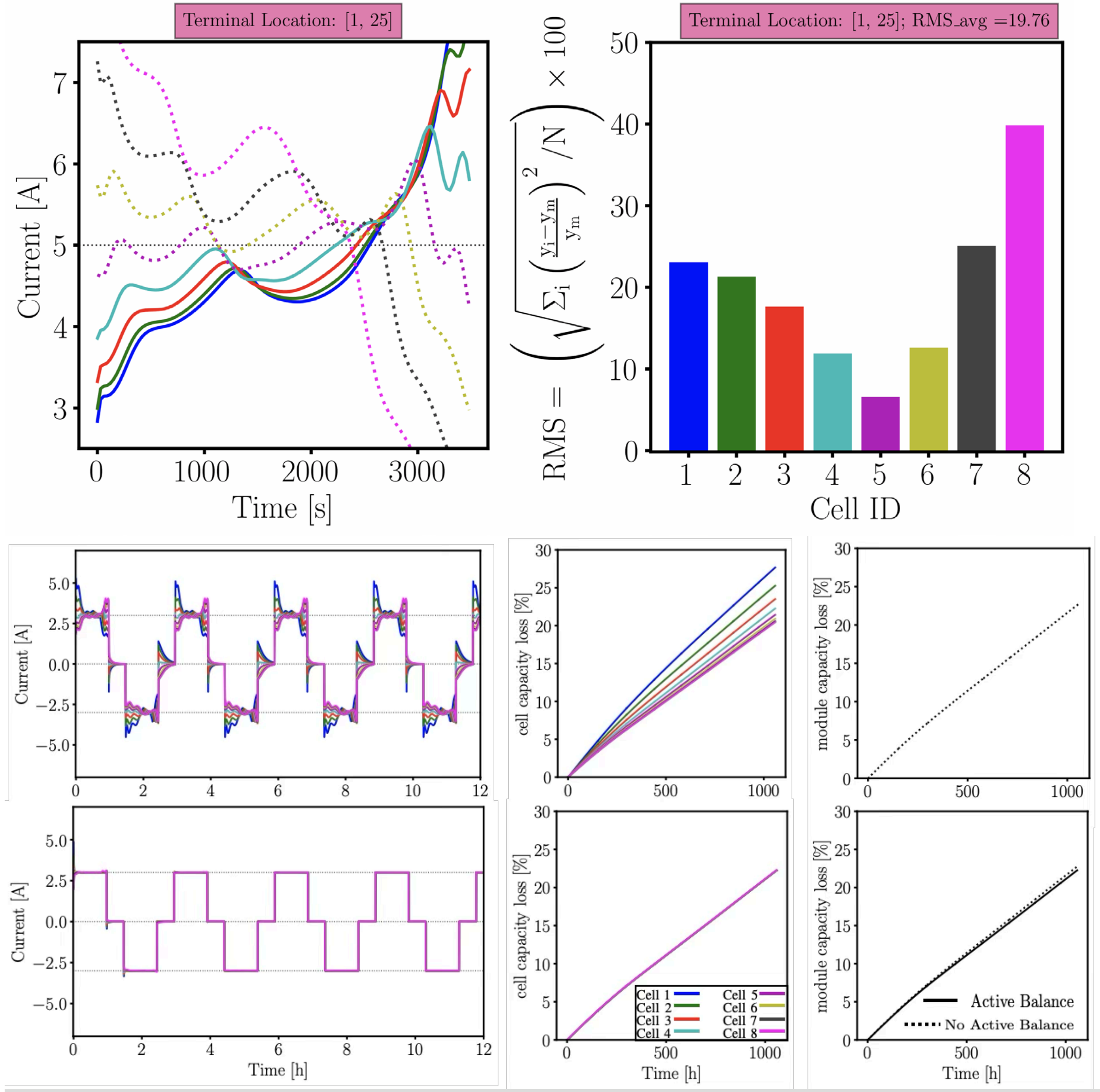
Module/pack level:
- Develop the module/pack scale physics-based simulation framework.
  - Improve implementation of active control elements.
  - Identify strategies to minimize degradation.
  - Module validation study.
  - Optimize module construction parameters.

Grid / MegaPack level:
- Improve the computational efficiency of the framework (Parallel and GPU based solvers).
- Test multiple pack designs and realistic load cycles to minimize degradation while ensuring safe operation

Previous Improvements and Progress: Overview

1. Cell level and module level physics-based parameters were identified utilizing experimental data provided by Sandia National Lab.
2. Imbalance cause aging heterogeneity within the cells, which make the module/pack life estimations(experiments) or predictions (simulations) unreliable.

- ➢ Identified strategies to minimize imbalances:
  (a)Adjusting the passive resistive elements or adding more cells in series (b)Terminal choice (c)Active balancing strategies.
- ➢ Efficient module/pack design optimization, and improving performance and life cycle analysis, are achievable utilizing the framework.



A. Surya Mitra, Yuliya Preger, Jacob Mueller, Srikanth Allu, “Physics-Based Analysis of Cell Imbalances and Aging in Lithium-Ion Battery Modules and Packs”, Accepted 2025, JES.

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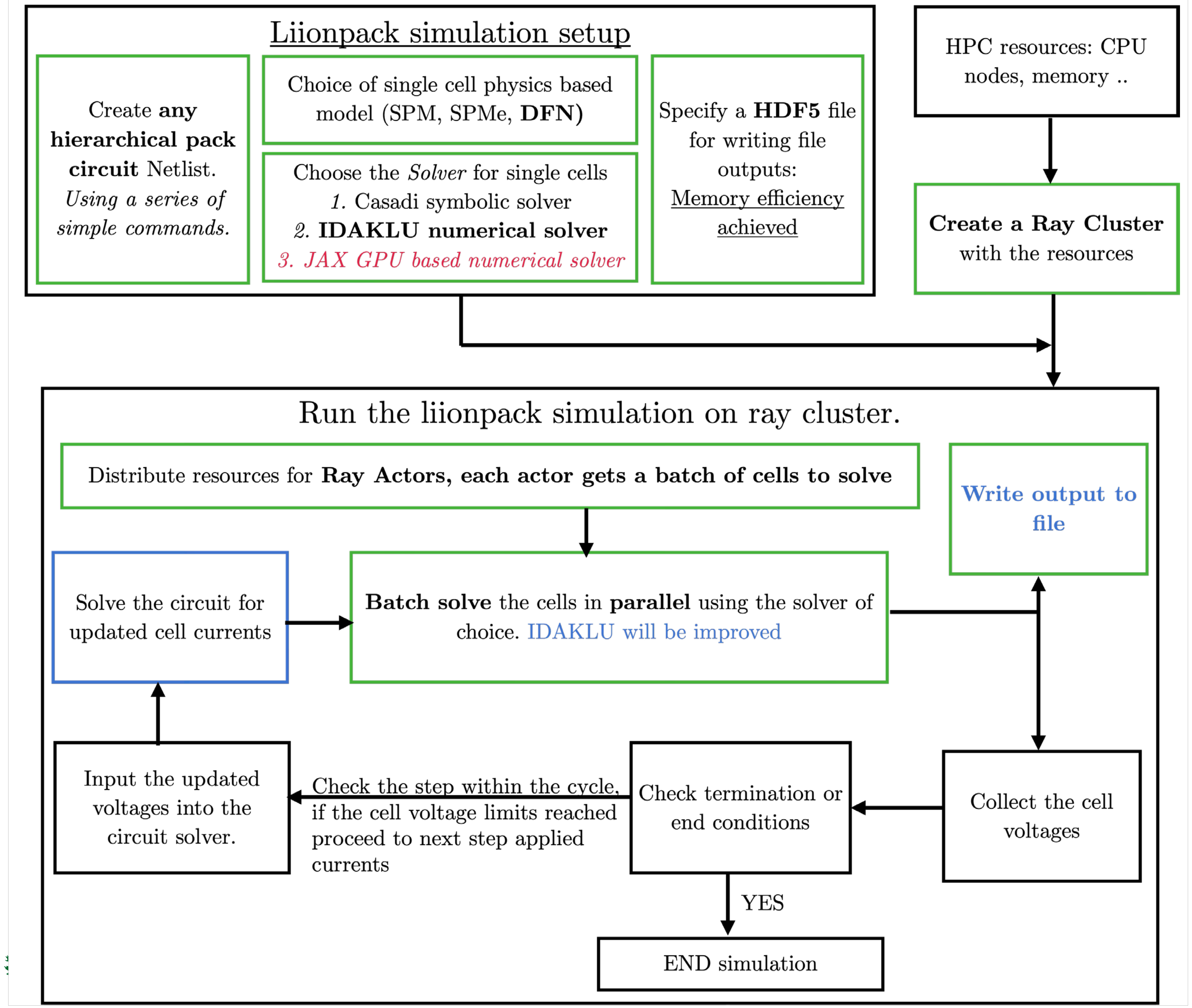
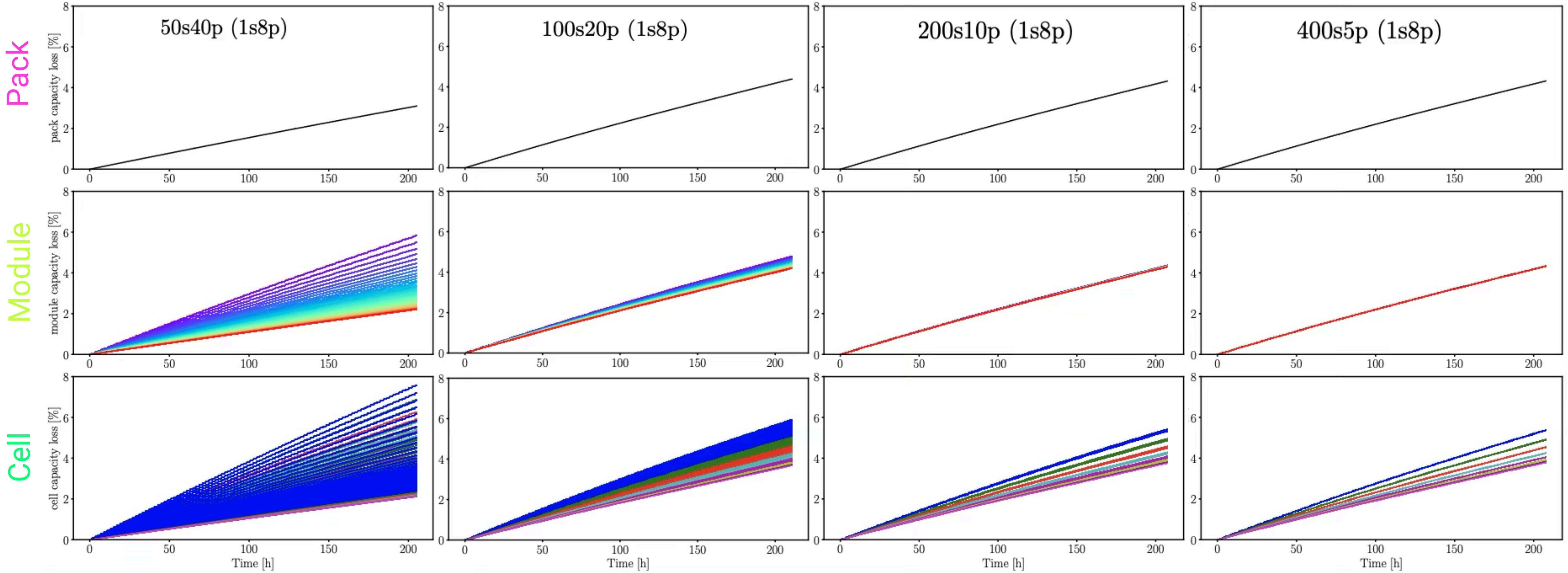
Updates and Progress on Technology: June 2025



- List of improvements:
  1. Ease of hierarchical pack construction
  2. DFN model for single cells
  3. Numerical solvers
  4. Memory efficiency
  5. Parallel batch solve orchestration on HPC
- The best achieved wall time per time step is 4.1s, for a megapack with 16000 cells run on hpc cluster utilizing 512 cpu cores.
  - The serial processes like file I/O, circuit solve will be improved, to get nearly 10x speed up.
  - A 100x speedup in solver is achievable by optimizing numerical solvers.
  - Further speed up can be expected with GPU based solvers
- **Improve the system scale synthetic data generation capabilities for performance and life cycle analysis. Also aid in ML efforts. (ROVI)**

CC cycling of 175kWh pack configurations:

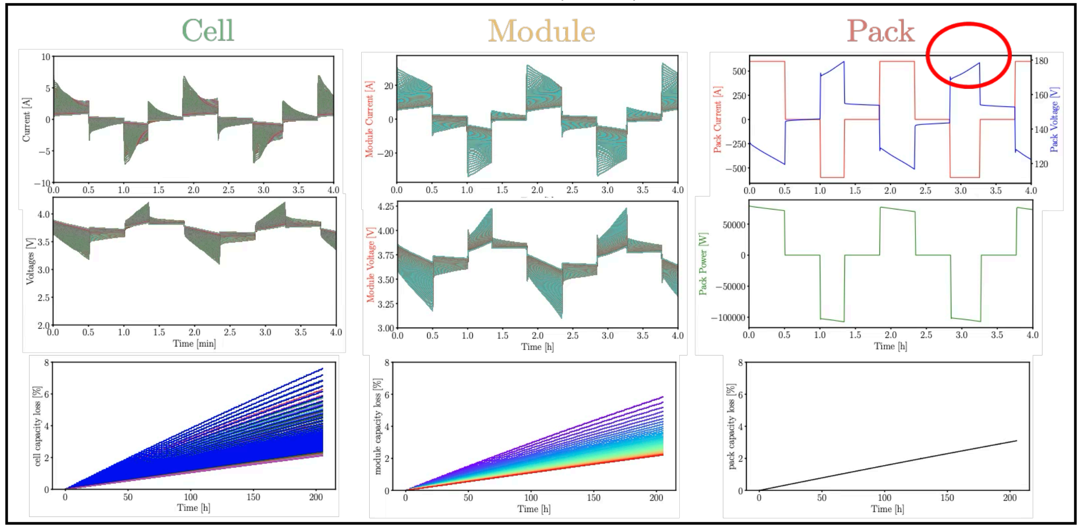
Pack Configuration	Capacity (Ah)	Maximum Voltage (V)	Operating Condition
100s20p (1s8p)	480	420V	CC (240A charge 1800s—rest 1800s—240A discharge 1800s—rest 1800s)
200s10p (1s8p)	240	840V	CC (120A charge 1800s—rest 1800s—120A discharge 1800s—rest 1800s)
50s40p (1s8p)	960	210V	CC (480A charge 1800s—rest 1800s—480A discharge 1800s—rest 1800s)
400s5p (1s8p)	120	1680V	CC (120A charge 1800s—rest 1800s—120A discharge 1800s—rest 1800s)



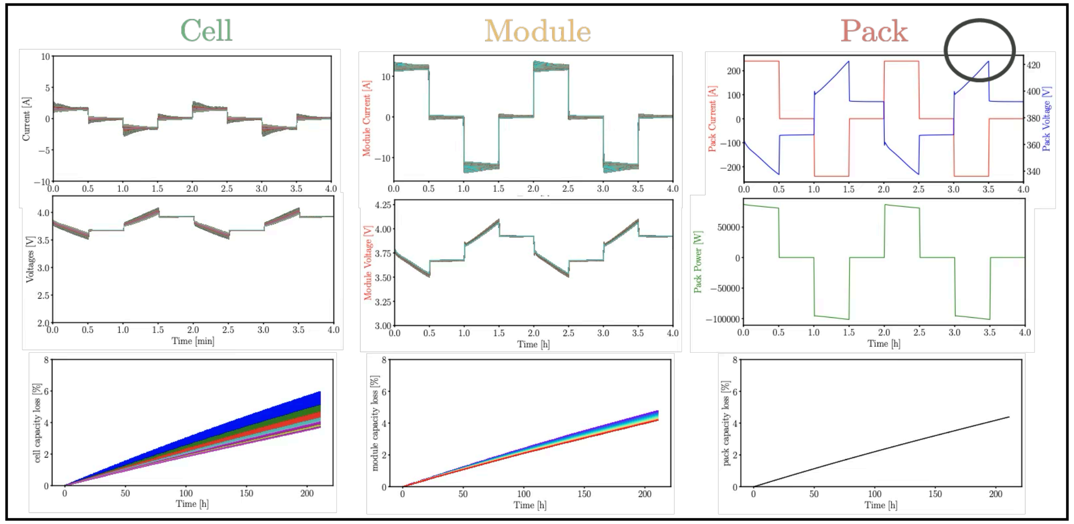
- The predicted pack cycle life for high voltage system is more reliable in comparison to a low voltage system, due to less aging variations at the cell scale.

Analysis of CC cycled packs

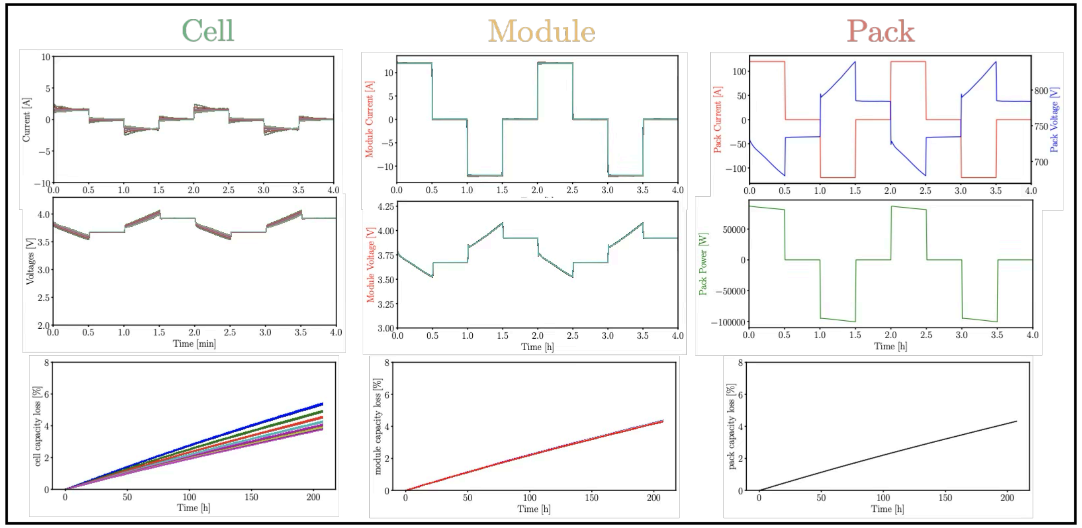
50s40p (1s8p)



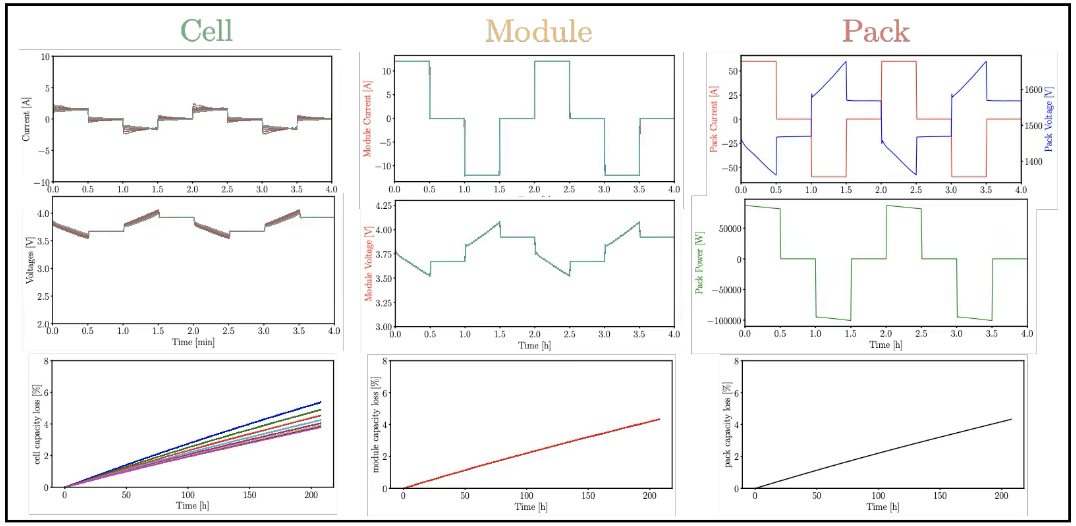
100s20p (1s8p)



200s10p (1s8p)

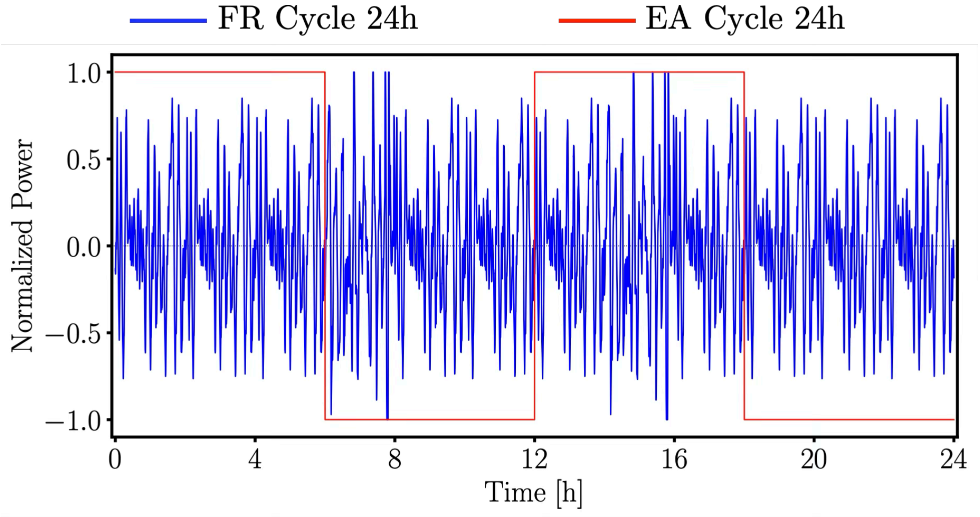


400s5p (1s8p)



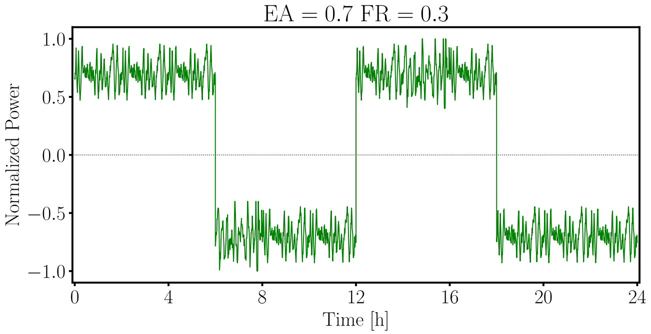
- High level of imbalances cause, cells to hit voltage limits earlier → The actual maximum voltage of the pack without overcharging the cells is < expected maximum voltage

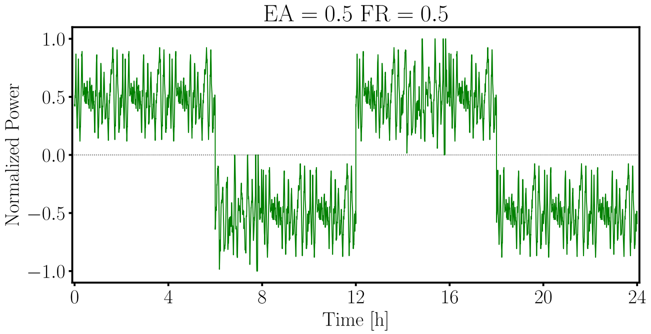
Power cycling of 175kWh, 200s10p(1s8p) pack

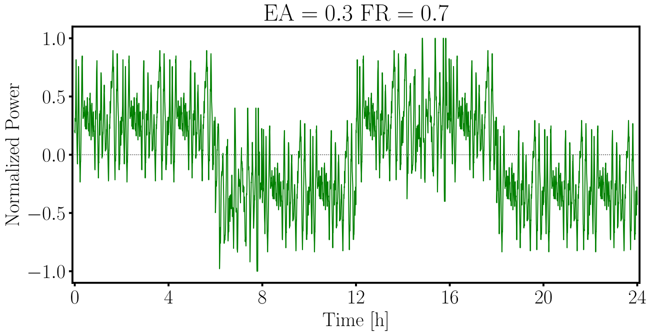


- Realistic power cycles (24h), with energy arbitrage (EA), frequency regulation (FR), and combinations of both are simulated.
- The normalized FR cycle was obtained from the PNNL report "*Protocol for Uniformly Measuring and Expressing the Performance of Energy Storage Systems*", Figure 5.3.2. *The total energy of the cycle = integral of power with time; is ensured to be zero at 24hrs.*
- The EA cycle was chosen, based on available literature.

- For a combination of x% EA and y% FR, the 24h power cycle is determined by ensuring the ratio of energy contributions from EA and FR is fixed to x/y.
- Nominal power = pack capacity * cell nominal voltage) *(No.of series connections) → Nominal Power = 240 x 3.6 x 200 x1 = 172.48 kWh
- The applied power cycle for pure EA or pure FR is: (Nominal power) x (normalized power cycle) .







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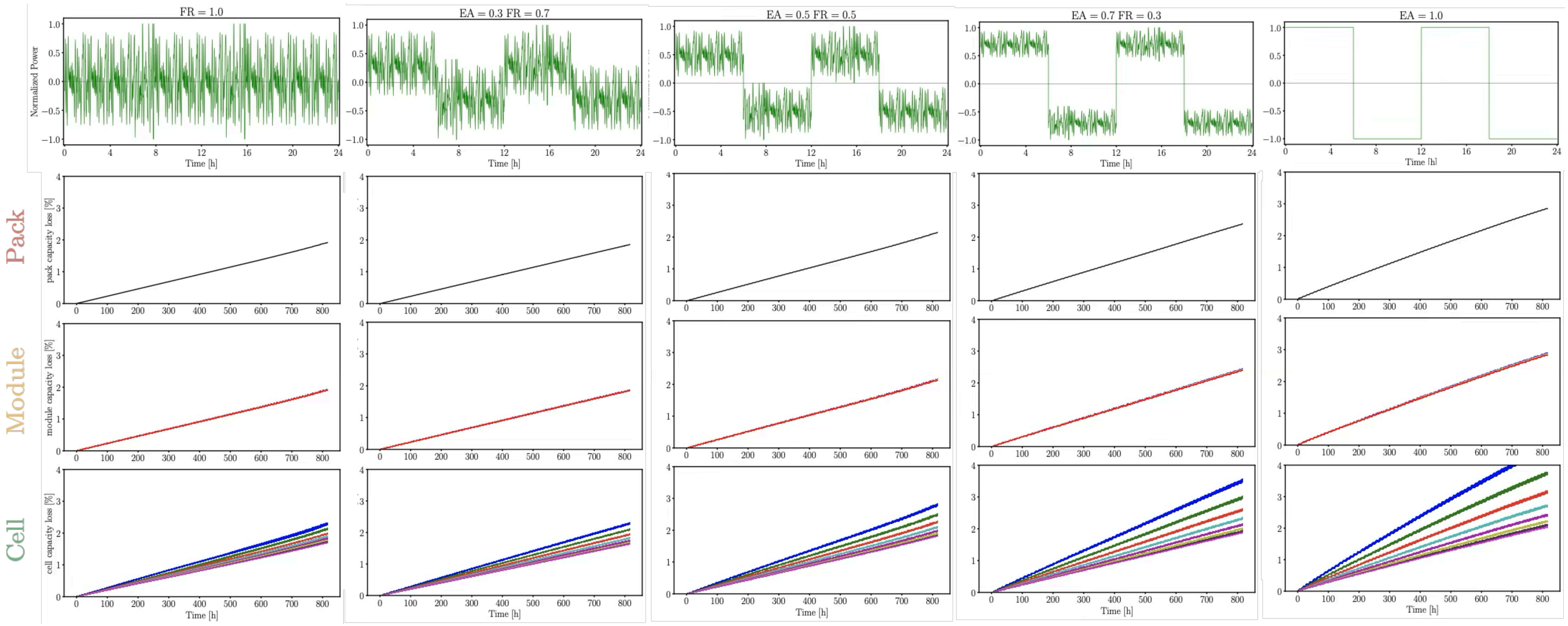
Frequency regulation and Energy arbitrage cycles



- Pure EA cycle causes most aging as expected due to a deeper charge and discharge, in comparison to a pure FR cycle which operates within a narrow range of SOC.

- Particle mechanics could play an important role with FR upon long term cycling, while other mechanism such as lithium plating could be significant with EA cases.

Summary of Progress: FY 2025

- ❖ Improved the HPC scalability of the framework to test multiple pack designs and operating conditions in a matter of days.
- ❖ Aging heterogeneity among the cells implies, that the characteristic aging observed at the system scale has a variation with respect to individual cells.
  - ➢ The predictability of long-term aging of the system is expected to vary largely due to few cells hitting the EOL faster.
  - ➢ Aging disparity cause potential risks in long-term cycling, when only pack level features are monitored.
- ❖ Constant current cycling shows that a high voltage system age more reliably than a low voltage high current system with the same power rating and same number of cells.
- ❖ Demonstrated a realistic power cycles with energy arbitrage, frequency regulation, and combinations of EA + FR. Show expected results for a 34 days worth of 24h cycle data.

Publications:

- **Vikrant, K.S.N., Tranter, T.G., Wiggins, G.M., Brett, D.J. and Allu, S., 2024, January. "Ageing Studies of Mega Battery Packs for Grid Storage Applications Using Physics Based Modeling". In *2024 IEEE Electrical Energy Storage Application and Technologies Conference (EESAT)* (pp. 1-6). IEEE.**
- A. Surya Mitra, Yuliya Preger, Jacob Mueller, Srikanth Allu, "Physics-Based Analysis of Cell Imbalances and Aging in Lithium-Ion Battery Modules and Packs", Accepted 2025, JES.
- Preger, Yuliya, Jacob Mueller, Armando Fresquez, Srikanth Allu, and Chaz Rich. "Impact of Module Configuration on Lithium-Ion Battery Performance and Degradation: Part I. Energy Throughput, Voltage Spread, and Current Distribution." *Journal of The Electrochemical Society* 172, no. 5 (2025): 050540
- A. Surya Mitra, Michael Starke, Srikanth Allu. "From Cell to System: Accelerated hpc Simulations of BESS Aging under Frequency Regulation and Arbitrage Usecases", in preparation, IEEE EESAT 2026.

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System-scale Vanadium Redox Flow Batteries

Johnson Dhanasekaran

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Project Overview

- Develop physics-based system-level simulation framework.
  - Scaling up Vanadium Redox Flow Batteries (VRFB) is a critical step in its deployment and widespread adoption.
  - Simulation route can greatly accelerate identification challenges in the scale up and long term cycling.
  - Tackle capacity fade in conjunction with ancillary system components, such as pumps and rectifiers.
- Tasks:

VRFB model:
- High fidelity model with low computational demand.
  - 1-D cells expected to provide sufficient accuracy.
  - Important degradation mechanisms included.
  - Validate against available experimental data.

System level simulation:
- Incorporate VRFB model into system-scale simulation.
  - Include pumps and rectifiers.
  - Identify appropriate input parameters for the system, such as flow rate and voltage window.

Optimal design:
- Resolve the effects of real-world operational conditions, such as blocked cell.
- Minimise levelized cost of energy storage
- Support digital twinning of a VRFB operation.

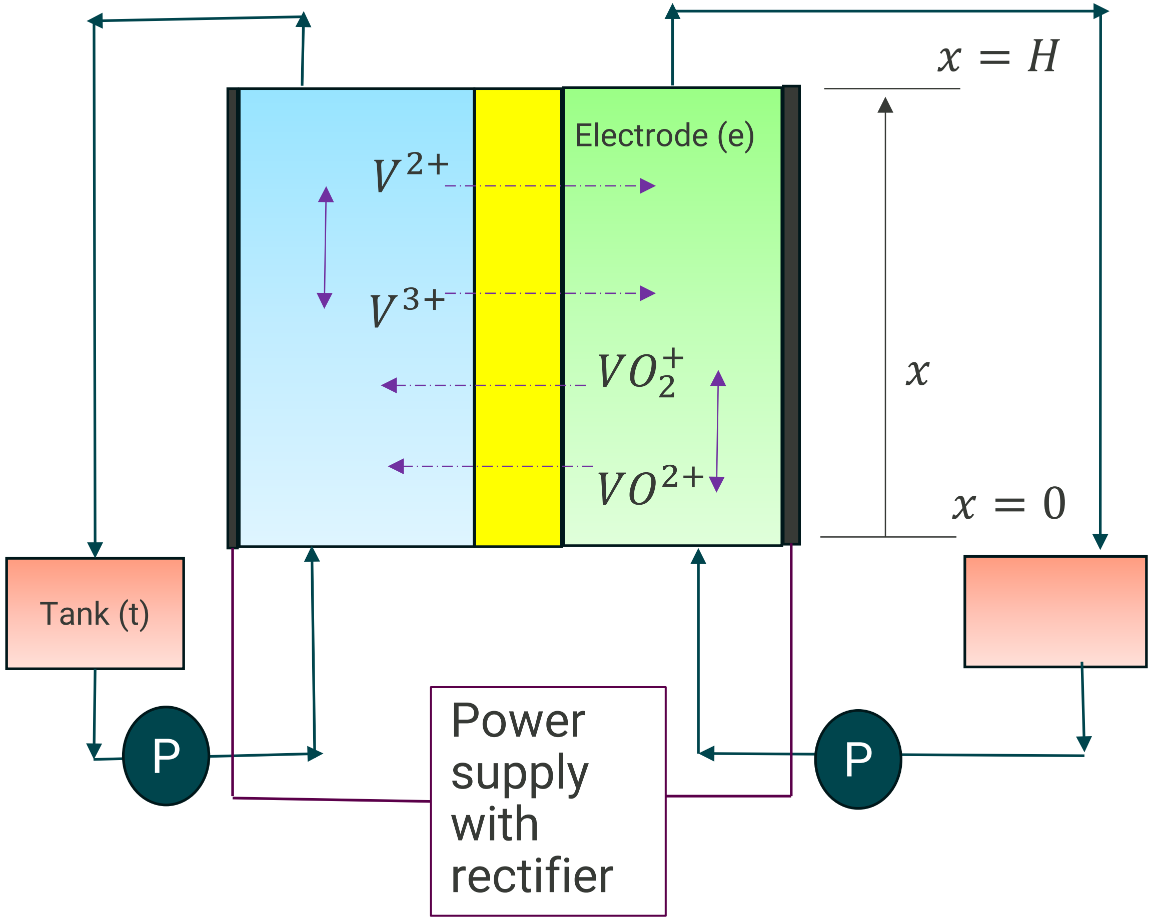
Pseudo 2-D system with independent cells implemented with capacity fade mechanisms

- $V^e \frac{dc_i^e}{dt} = -Q^e H \frac{c_i^e}{dx} \pm \frac{I}{zF} - A_m \left(\sum_i l_i n_i^{cross}\right)$

$$V^t \frac{dc_i^t}{dt} = Q^t \left(c_{i|_{x=\mathrm{H}}}^e - c_i^t\right)$$

- $n_i^{cross} = \frac{k_i c_i^e}{D} + c_i^e v_m + \frac{z_i F}{RT} k_i c_i^e \frac{\Delta\Phi_1}{D}$

Diffusion: $\frac{k_i c_i^e}{D}$; Convection (via electrolyte leakage): $c_i^e v_m$; Electro-migration: $\frac{z_i F}{RT} k_i c_i^e \frac{\Delta\Phi_1}{D}$



- Capacity fade mechanisms.
  - Ion crossover: n_i^{cross}
  - Side reactions: $l_i \neq 0$
    - All crossover ions are consumed.
  - Electrolyte leakage: $\frac{dV^t}{dt} = \pm N v_m A_m$
    - Includes osmotic and electro-osmotic contribution.

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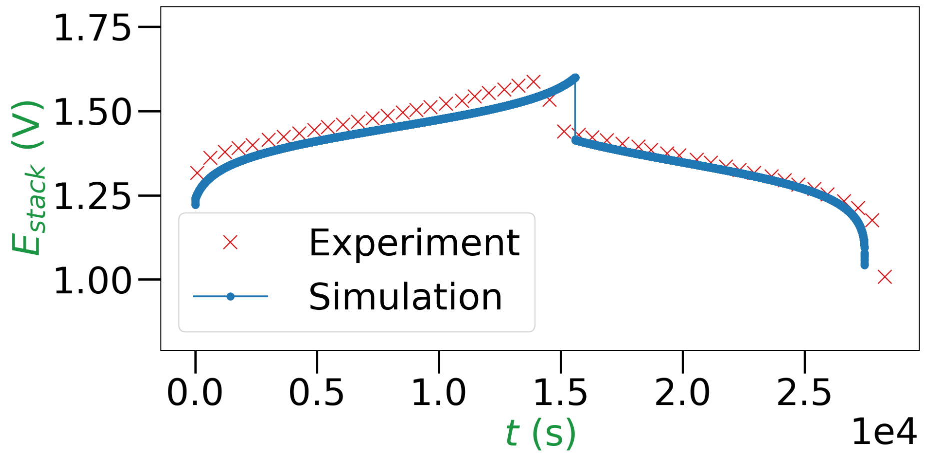
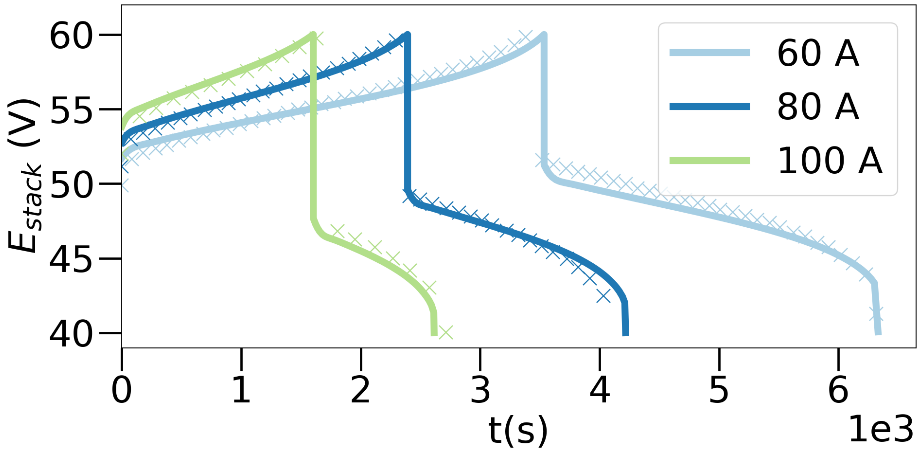
Wang, Hao, et al. "A new zero-dimensional dynamic model to study the capacity loss mechanism of vanadium redox flow batteries." *Journal of Power Sources* 603 (2024): 234428.

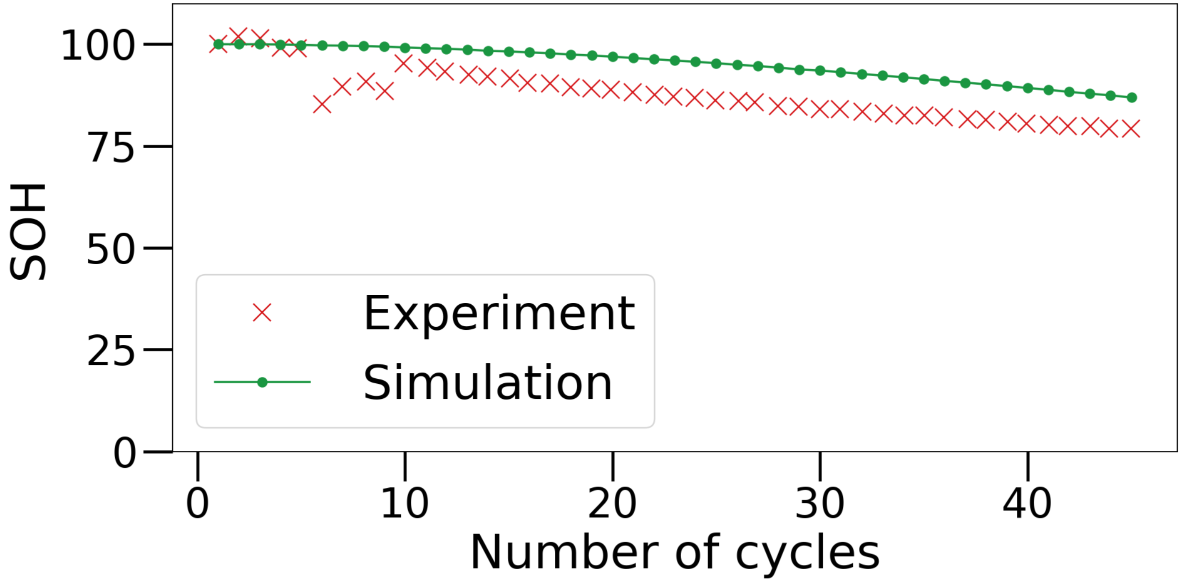
Model validated against diverse experiments

Single cell



Multiple cells





High predictive power (RMS error: 7%)

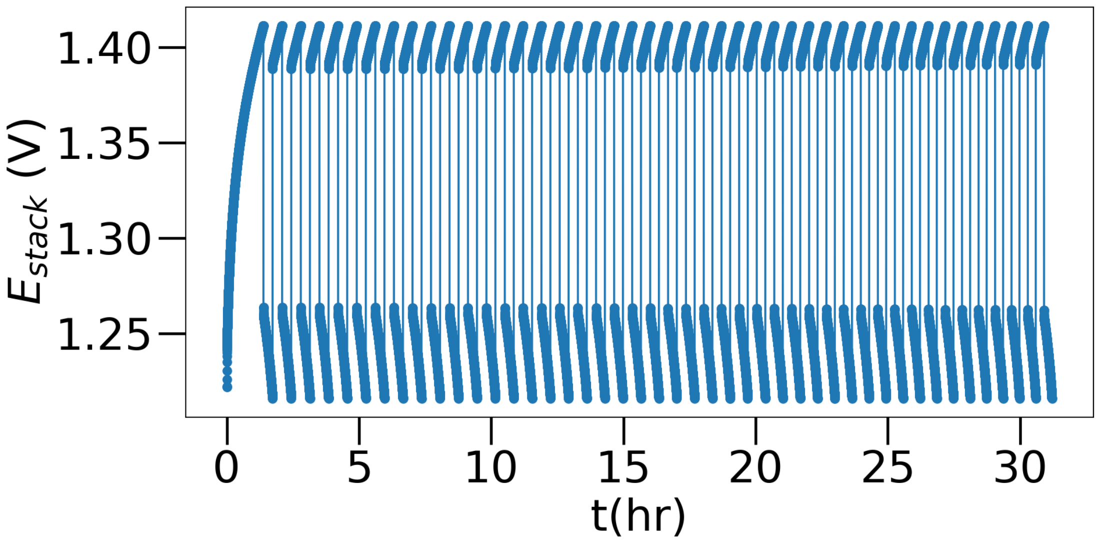
$$SOH = \frac{t_n}{t_1}$$

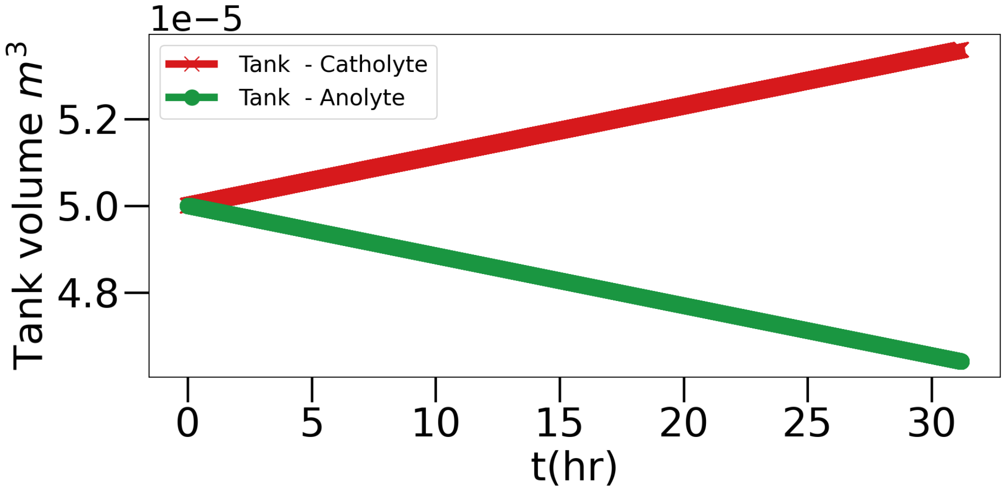
t_n: Time taken for n^{th} discharge cycle

Kim, Soowhan, et al. "Cycling performance and efficiency of sulfonated poly (sulfone) membranes in vanadium redox flow batteries." *Electrochemistry Communications* 12.11 (2010): 1650-1653.
Knehr, K. W., et al. "A transient vanadium flow battery model incorporating vanadium crossover and water transport through the membrane." *Journal of The Electrochemical Society* 159.9 (2012): A1446.
Wang, Hao, et al. "A new zero-dimensional dynamic model to study the capacity loss mechanism of vanadium redox flow batteries." *Journal of Power Sources* 603 (2024): 234428.

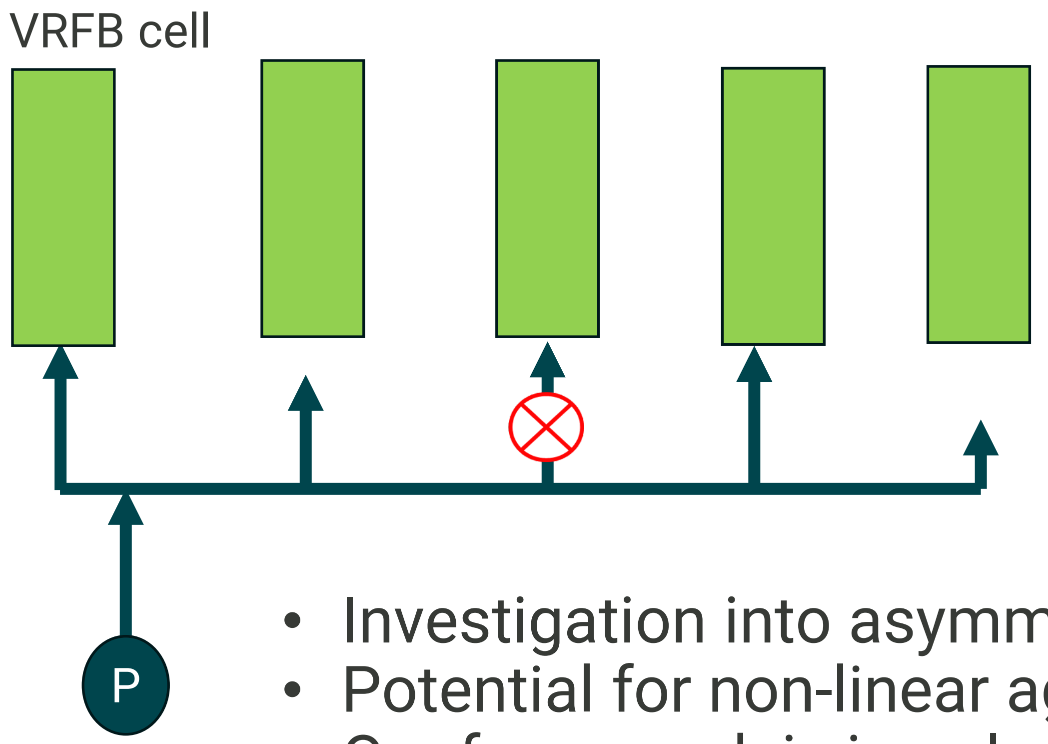
Preliminary results are promising

- Successful deployment of multiple cycles
  - Framework can pick up the small deteriorations per cycle.
  - Enables tracking of long-term health of VRFB.
- Volume of electrolyte in tank is a critical diagnostic tool.
  - Experimental team from Sandia team (Dr. **Reed Wittman** & Dr. **Sam Macchi**) believe this is aligns with expectations.
  - We are in talks to obtain experimental data for rigorous validation.
  - Predictions be leveraged to predict optimal rebalancing of electrolyte.





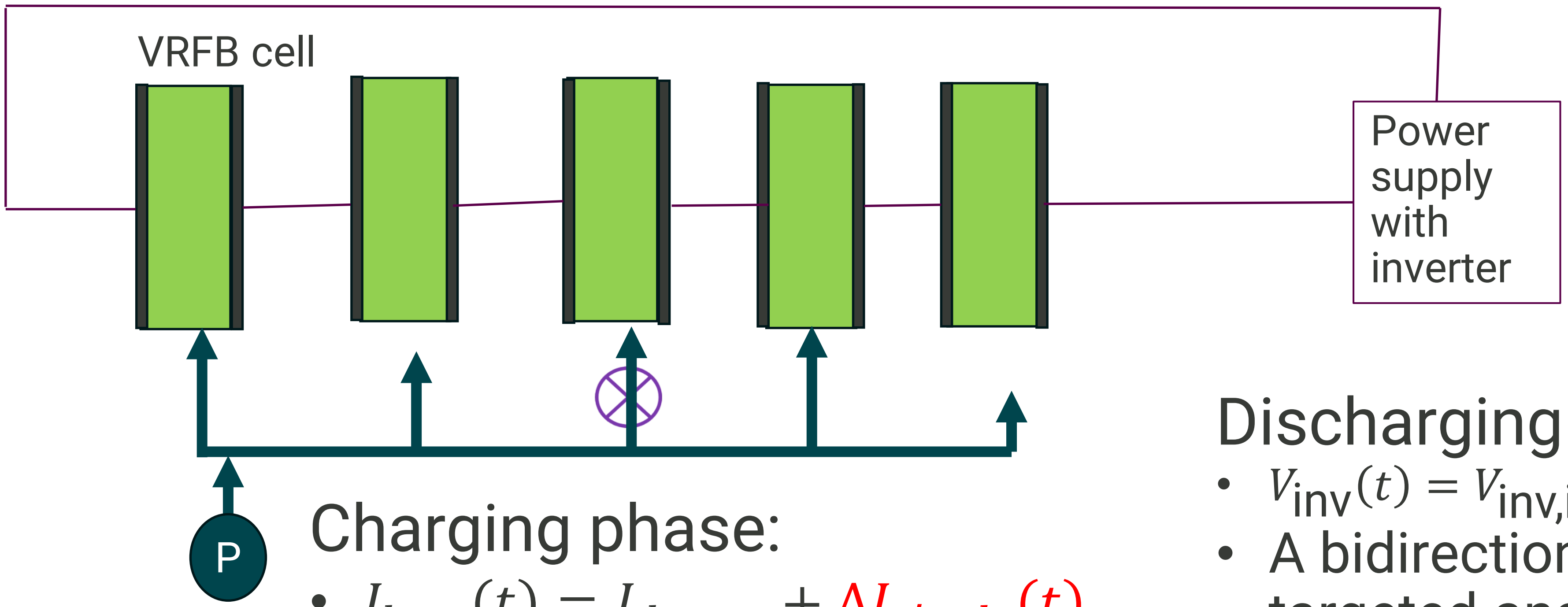
On system scale non-uniform flow and pump power



- Investigation into asymmetric flow and clogging.
- Potential for non-linear ageing.
- Our framework is in pole position to answer these questions.
- In the future this can be expanded to multiple stacks.

- Current literature on single and multiple stacks deal with pressure losses and transport delays but not asymmetric flow.

Non-linear currents from imperfect rectifier can compound issue



Charging phase:

- $I_{batt}(t) = I_{dc,avg} + \Delta I_{ripple}(t)$
- Oscillations will impact battery ageing
- Small degradation per cycle accumulate and can be resolved by our model

Discharging phase:

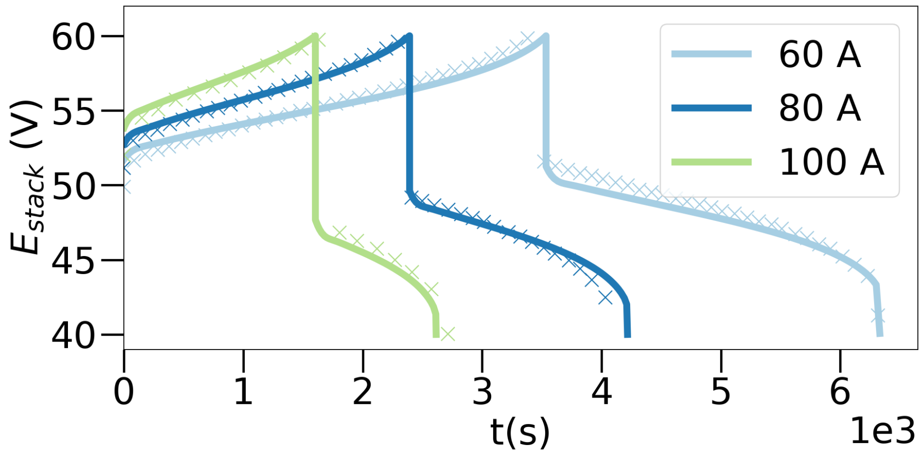
- $V_{\text{inv}}(t) = V_{\text{inv,ideal}}(t) + v_{\text{ripple}}(t)$
- A bidirectional inverter for targeted analysis.
  - $L \frac{dI_{ac}}{dt} + R\, I_{ac} = V_{inv}(t) - V_{grid}(t)$
- Dead time voltage can also be incorporated:
  - $V_{dt}(t) = D_{dt} \times I_{ac}(t)$

Ripple current & voltage: We will use the best available models

Gemmen, Randall S. "Analysis for the effect of inverter ripple current on fuel cell operating condition." *Journal of fluids engineering* 125.3 (2003): 576-585.
Jia, Xinyu, et al. "The degradation characteristics and mechanism of Li [Ni0. 5Co0. 2Mn0. 3] O2 batteries at different temperatures and discharge current rates." Journal of the Electrochemical Society 167.2 (2020): 020503.

Summary and Ongoing Efforts

- Physics based modelling framework can accurately predict experimentally observed voltage response and capacity fade.
  - Conduct simulations at the single electrode level (Completed)
  - Integrate the single cell with degradation mechanisms
- Incorporate pumps and pcs.
  - Include flow across the multiple cells and the pumps driving it. *(ongoing)*
  - Couple non-linear current supply due to rectifier. *(upcoming)*
- Identify strategies for performing the optimal design studies



Collaborations

- Monthly meeting with Reed Whitman team @SNL to gather data from the diagnostics and characterization experiments.
- Obtained single stack cycling data for different flow rates and electrode surface area
- Eventually understand the challenges of scaling up to multiple stacks and integrating with PCS systems.

Publications:

- **Srikanth Allu, Sam Macchi, Reed Wittman, "Understanding the Impact of Degradation Mechanisms on Scale up of Redox Flow Battery Systems", Accepted 2025, ECS Conference.**
- **Srikanth Allu, et.al., 'Development of Computational Framework to Study Vanadium Flow Battery Scale up of flow through and flow by systems', under preparation.**

Questions ?

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