Ageing analysis on secondary use of Li-ion battery MegaPacks

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Outline

- Motivation
- Degradation mechanisms
- Pack level simulations
- Modeling Results
- Software Release
- Next Steps/Conclusions

Motivation

- Increased renewable integration is installing larger centralized lithium-ion battery packs (i.e., Megapacks, containerized cells supporting 1MWh total energy rating) to provide utility-scale services to grid operators
- Daily cycling of standalone lithium-ion grid storage will reduce the battery cells' capacity, where an end of life is marked when the cells have an 80% rated capacity
- Comprehending the strategies for secondary use of lithium-ion cells in grid-connected energy storage
- Reliable estimates of the end of life of these MegaPacks are necessary for accurately estimating lifecycle costs and benefits.

Objective: Develop computational framework and conduct the mechanistic modeling of ageing processes and large scale physics based hpc simulations of lithium-ion Megapacks

Degradation Mechanisms for Lithium-Ion Batteries

Governing Equation:

$$\frac{\partial c_i(r,t)}{\partial t} = \frac{D_i}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial c_i(r,t)}{\partial r}\right)$$

Boundary Conditions:

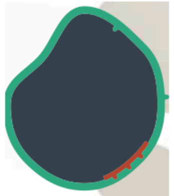
$$D_i \frac{\partial c_i(r,t)}{\partial r}\bigg|_{r=0} = 0$$

$$D_i \frac{\partial c_i(r,t)}{\partial r}\bigg|_{r=R_i} = -j_i$$

$$j_T = j_i + j_{sei} + j_{pl}$$

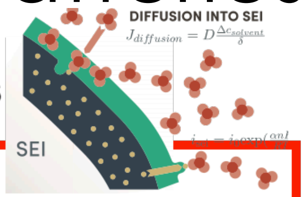
$$j_T = \frac{I}{V_i a_i n F}$$

$$a_i = 3\frac{\epsilon_i}{R_i}$$



Electrode Particle Kinetics

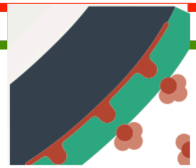
Physical Degradation Mechanisms



SEI Growth Kinetics:

$$j_{sei} = -\frac{i_{sei}}{nF} = -\frac{i_{o,sei}}{nF}\exp\left(-\frac{\alpha n F \eta_{sei}}{RT}\right)$$

$$\frac{\partial \delta_{sei}}{\partial t} = \frac{i_{sei} M}{\rho n F} \qquad \eta_{sei} = \eta_i + \phi_{OCV} - \phi_{o,sei} + \rho_{sei}\delta_{sei} I$$



Plating Kinetics:

$$j_{pl} = -\frac{i_{pl}}{nF} = -\frac{i_{o,pl}}{nF}\left(\exp\left(\frac{(1-\alpha)nF\eta_{pl}}{RT}\right) - \exp\left(\frac{-\alpha n F \eta_{pl}}{RT}\right)\right)$$

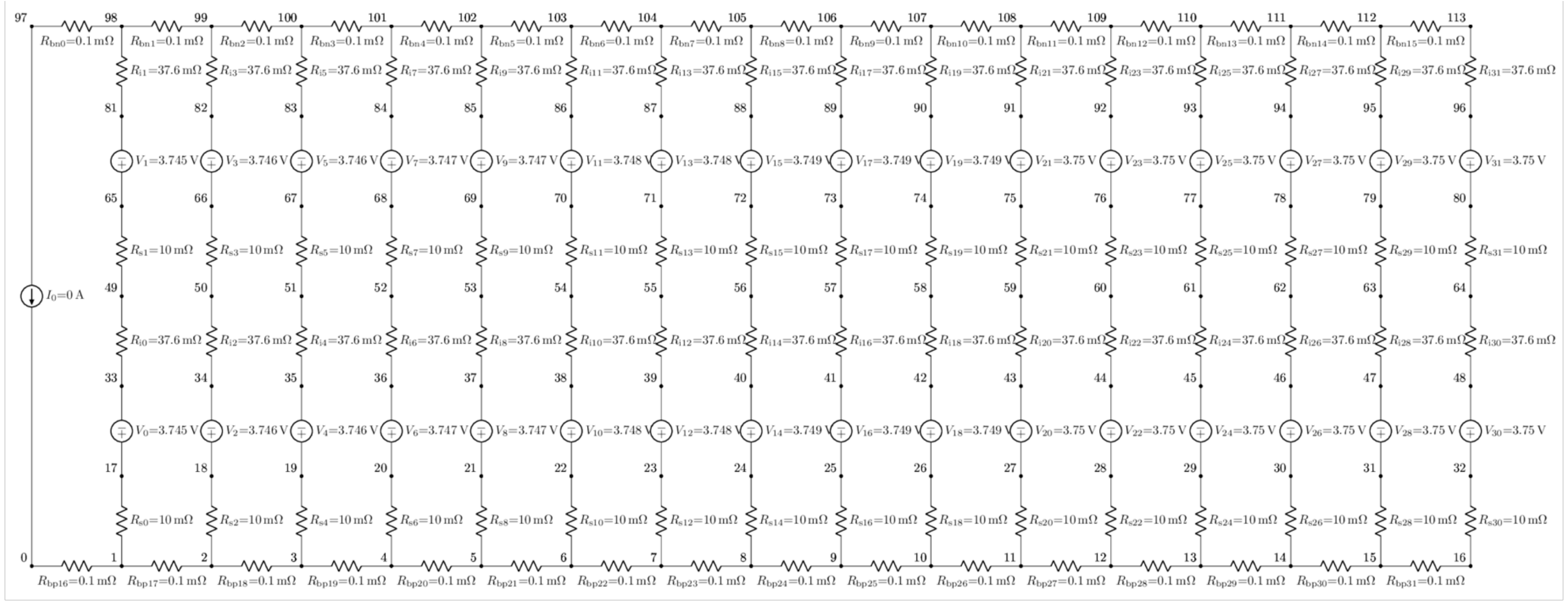
$$\frac{\partial \delta_{pl}}{\partial t} = \frac{i_{pl} M}{\rho n F} \qquad \eta_{pl} = \eta_i + \phi_{OCV} + \rho_{sei}\delta_{sei} I$$

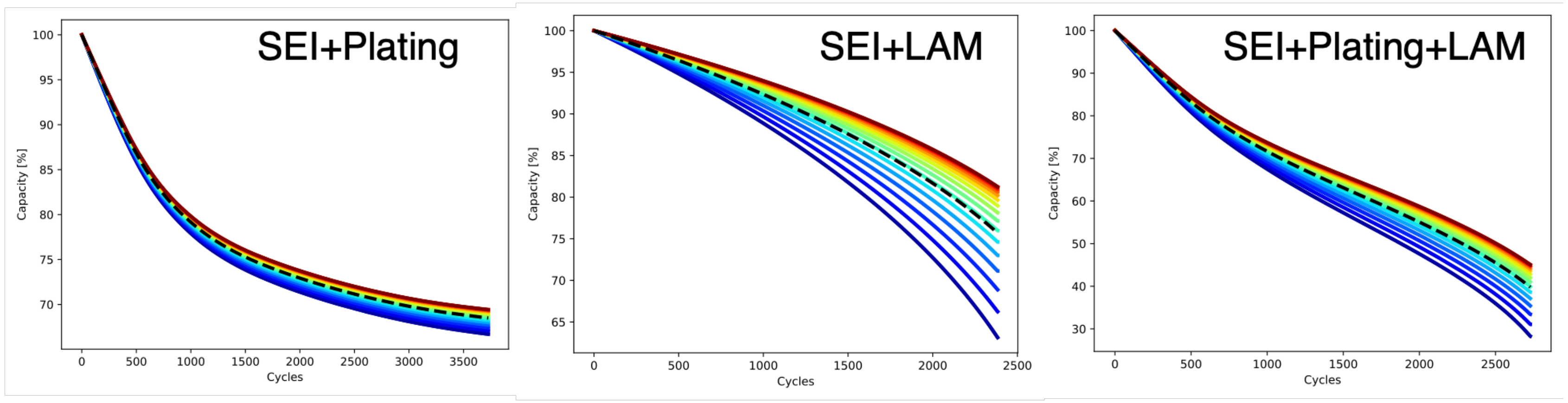
Loss of Active Material:

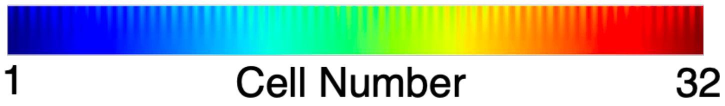
$$\frac{\partial \epsilon_i}{\partial t} = \beta\left(\frac{\Delta\sigma_h}{\sigma_y}\right)^m \qquad \Delta\sigma_h = E\alpha_{c_i}\Delta c_i$$

J. M. Reniers, G. Mulder, D. A. Howey, "Review and Performance Comparison of Mechanical-Chemical Degradation Models for Lithium-Ion Batteries," *J. Electrochem. Soc.*, **166**, pp. A3189–A3200, (2019).

Capacity Fade of the Battery Pack







- Pack configurations with cells in series and parallel
- Several combinations of ageing mechanisms
- Impact of Bus bar element impedance on the cell heterogeneity
- Capturing cell-2-cell variability and its impact on the life cycle
- Allowing for rebalancing currents during variable drive cycles.

Chen, C.H., et.al., Journal of The Electrochemical Society, 167(8), p.080534.

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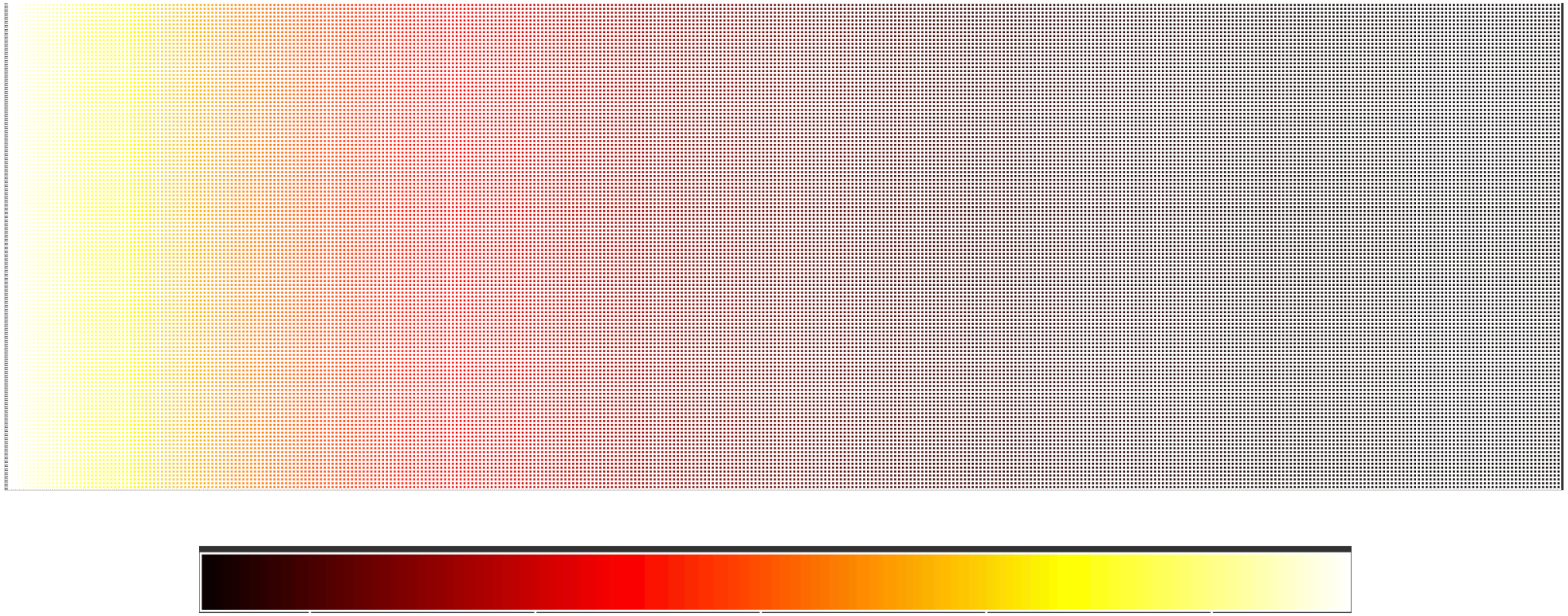
Computational profiling for the Battery Pack simulations

Number of Cells	MWh	Numerical Steps	Mesh Size (No of elements)	Time to Solution for 1Cycle (min)	Time to Solution for 1000Cycles (days)
500(4p125s)	0.01	180	20000	1.5	1.04
5000(40p125s)	0.1	180	200000	9.35	6.49
50000(400p125s)	1	180	2000000	82.62	57.28

- Run on 64 Core node
- Constant Current charge/discharge cycling with rest periods
- Coupled electrochemical model (SPM) with the thermal transport (no cell-cell thermal distribution)



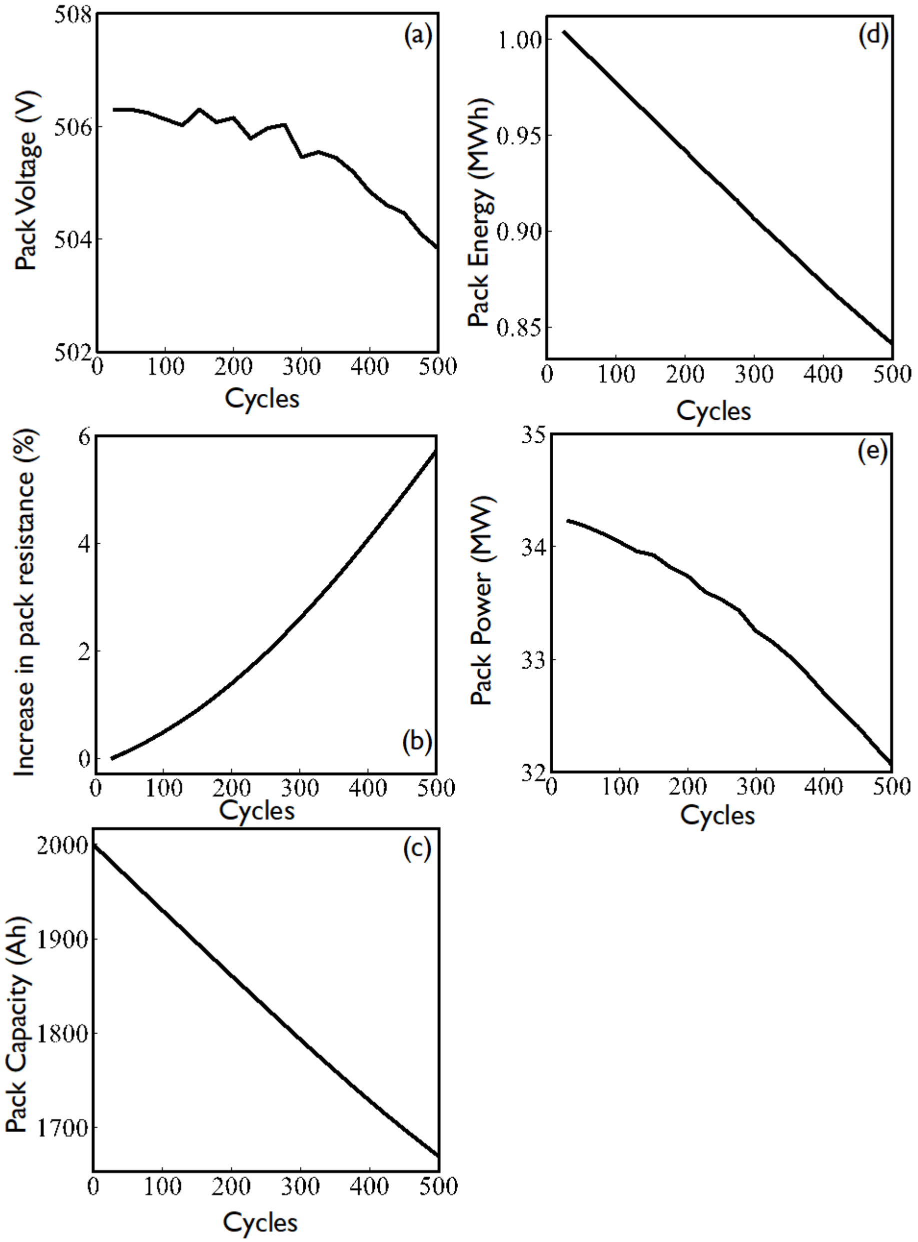
Pack level characteristics

- MWh system was constructed to understand pack level dynamics
- All the cell were assumed to have same initial state and have identical properties
- Assumed no busbar/interconnect resistances with SEI/plating/LAM degradation mechanisms

$$Q_{pack} = \min\left(\sum_{i=1}^{N_p} Q_i\right)_{N_s}$$

$$E_{pack} = Q_{pack}V_{pack}$$

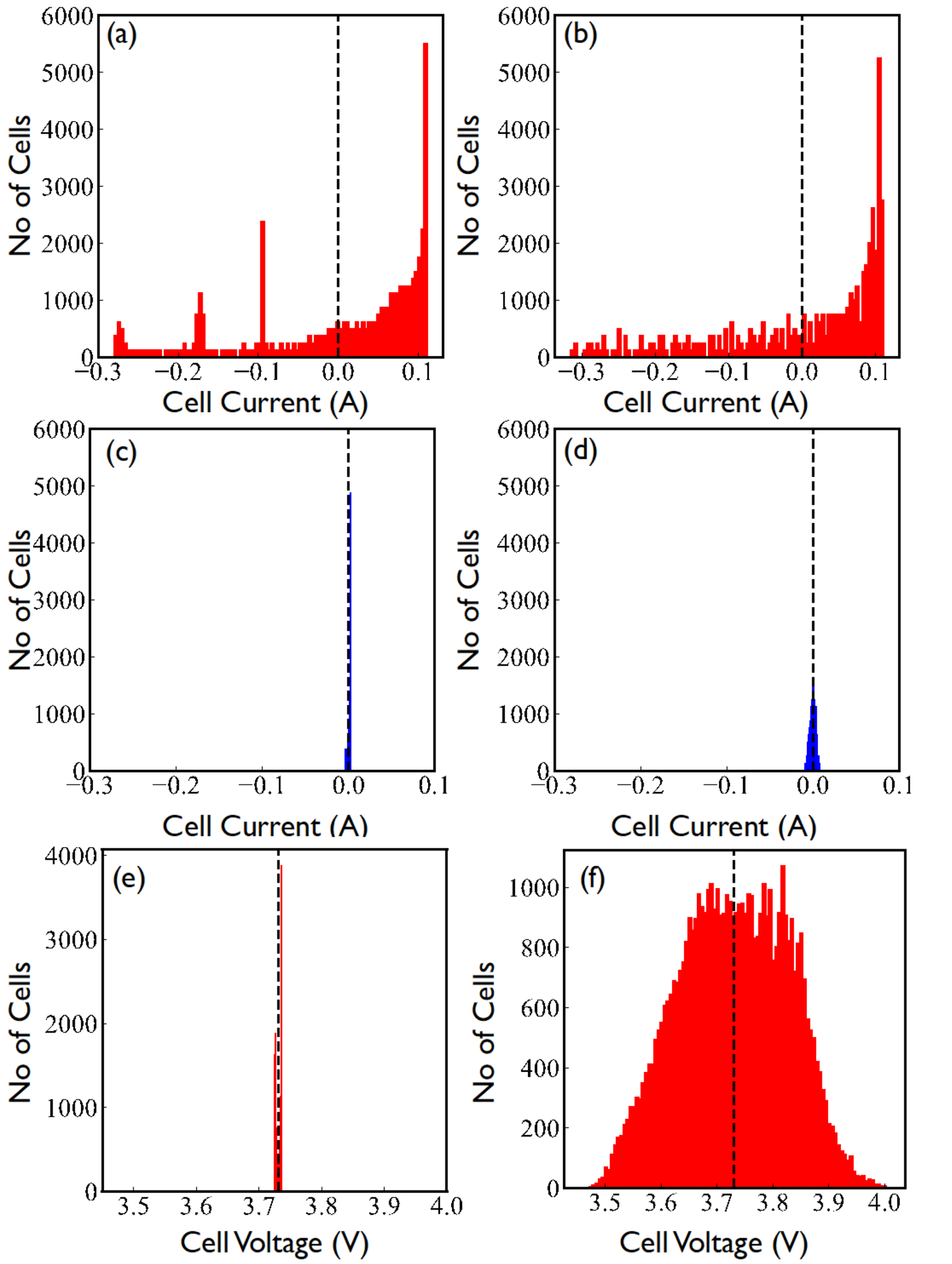
$$P_{pack} = \frac{V_{pack}^2}{R_{pack}}$$



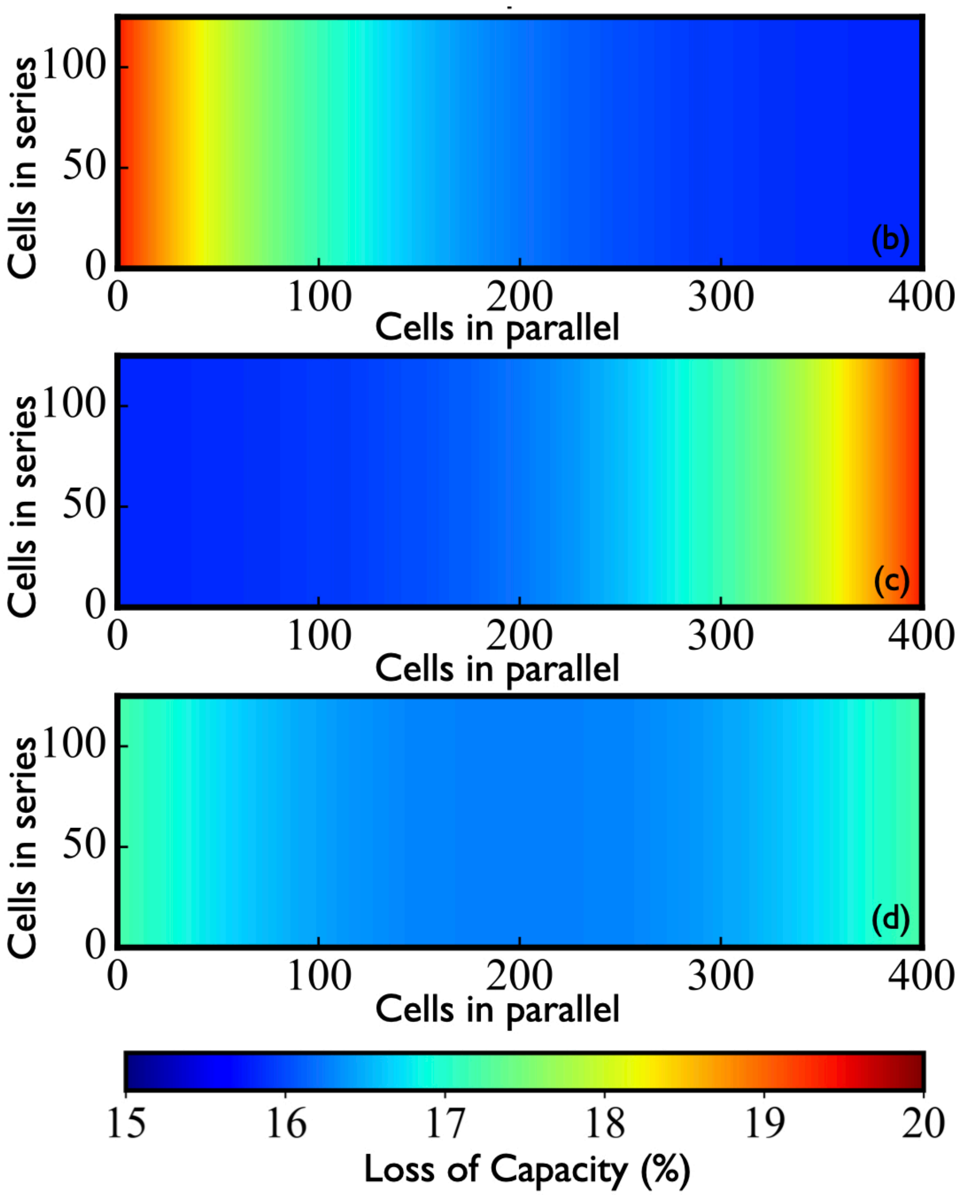
Balancing of currents

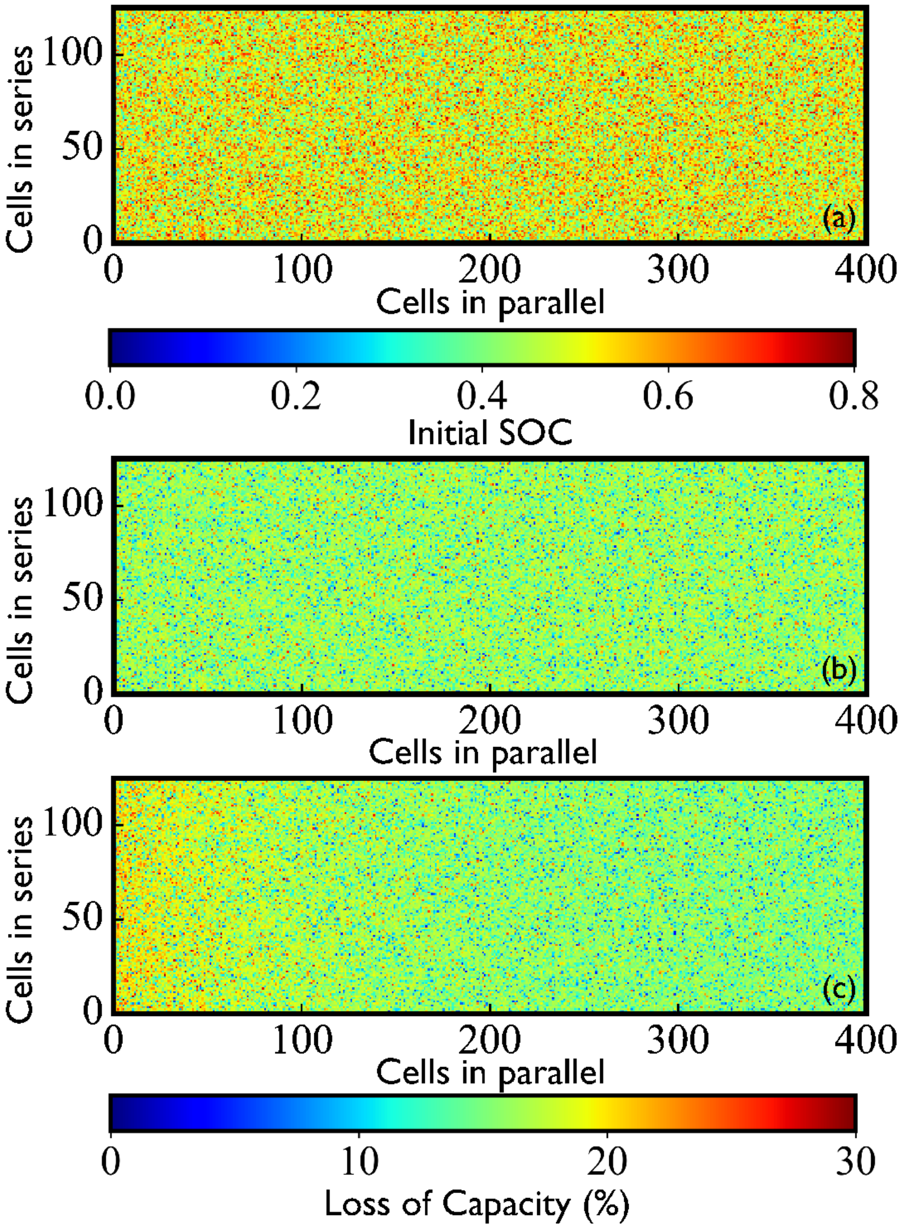
Immediately after discharge/charge during rest periods, we observed positive and negative currents in the busbar/connectors

- In absence of the internal resistances, we do not observe any relaxation effects and balance current are negligible in the circuit.
- With SOC distribution and internal busbar resistances, we observe different voltage response in the cells and subsequent positive and negative currents in the busbars and internal connectors
- These behaviors are important to consider at system design and integrating with power electronics components



Effect of Terminals and initial SOC distribution



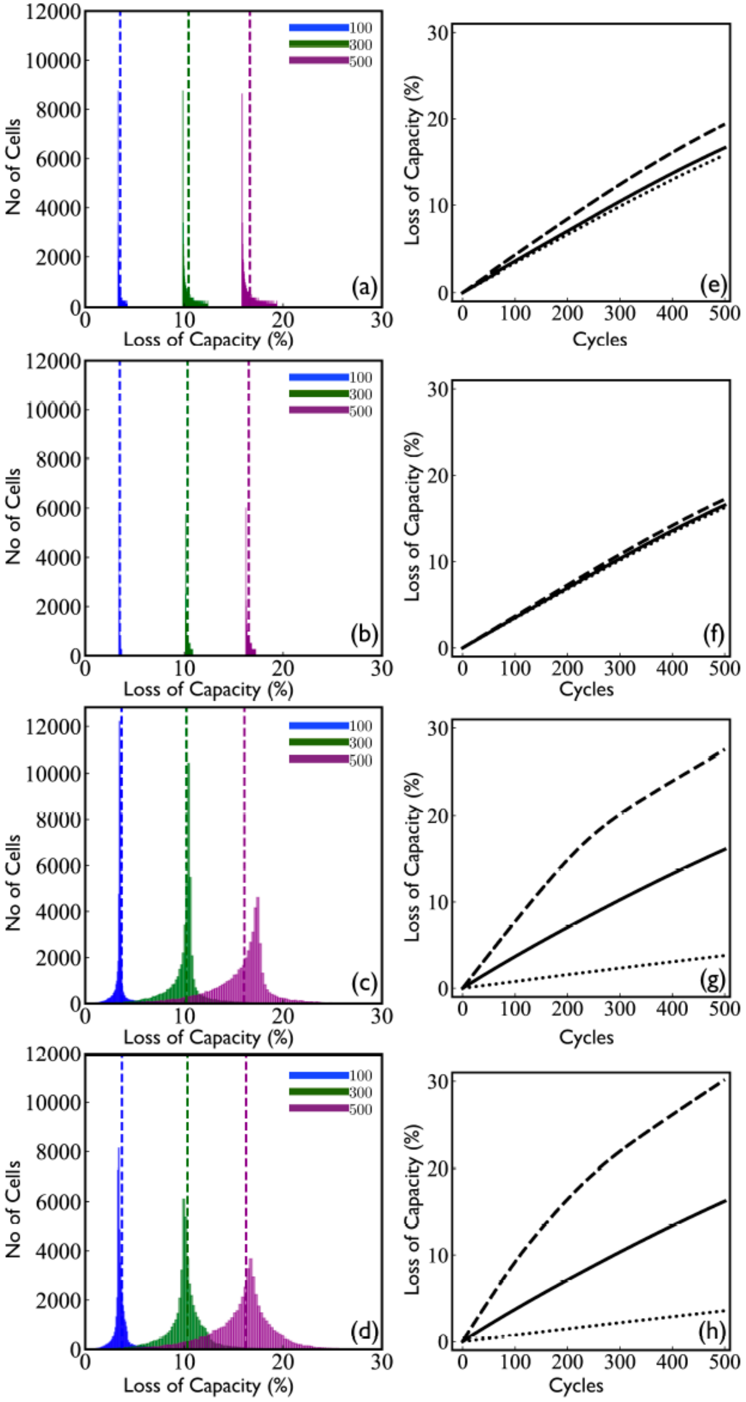


Studies of Pack capacity degradation

Understand variability due to

(a) Terminal connections (b) Busbar and connector resistances
(c) Initial SOC of cells.

- With same initial state, individual minimum cell capacity loss follows same pack loss trajectory
- With different terminal connections we do not see much difference between maximum and minimum degradation of cell to that of pack.
- With just initial SOC distribution and negligible bus bar resistances, the standard deviation of capacity loss increases with number of cycles. We observed that under these conditions, some cells reach 20% EOL and fail earlier than the pack capacity.
- Low initial SOC age linearly and large SOC show maximum degradation.



Software Release

- Software developed as part of Pack level simulations are made part of liionpack repository.
- Released this an open-source package in collaboration with UCL, liionpack has been submitted to the Journal of Open Source Software (JOSS).
- More information about the submission and its review process is available on the JOSS website.
- Open to public, new features are added regularly

Next Steps

- Integration of BMS control algorithms
- Conduct simulations of the MegaPacks under realistic load cycles
- Deploy the physical integrated Digital Twin
- Identify integrational challenges of MWh systems

Publications

Tranter, T., Timms, R., Sulzer, V., Planella, F., Wiggins, G., Karra, S., Agarwal, P., Chopra, S., Allu, S., Shearing, P. and Brett, D., 2022. liionpack: A Python package for simulating packs of batteries with PyBaMM. *Journal of Open Source Software*, *7*(70)

Vikrant, K.S.N., Tanter, T.G., Wiggins, G., Brett D.J.L, Allu S., Ageing studies of battery packs for large scale grid storage applications using physics based modeling, Applied Energy (under Review)

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