

2022 MRS[®] SPRING MEETING & EXHIBIT

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May 23-25, 2022 | Virtual

Big Data for Li-Ion Battery Diagnosis and Prognosis

M. Dubarry and D. Beck

matthieu@hawaii.edu



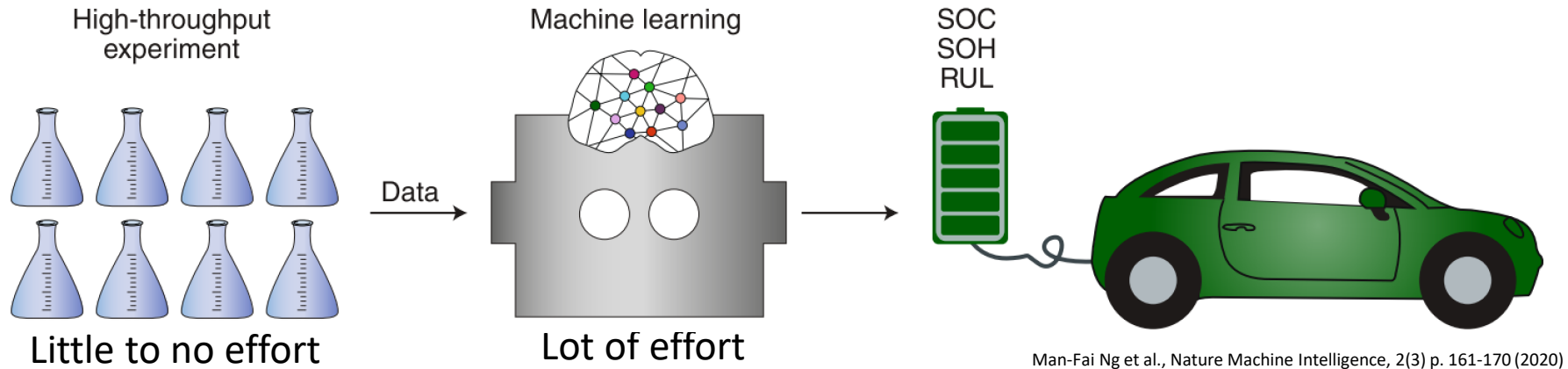
1680 East West Road, POST 109,
Honolulu, HI 96822
Ph: (808) 956-2349 • Fax: (808) 956-2336



Big Data for Li-Ion Diagnosis and Prognosis

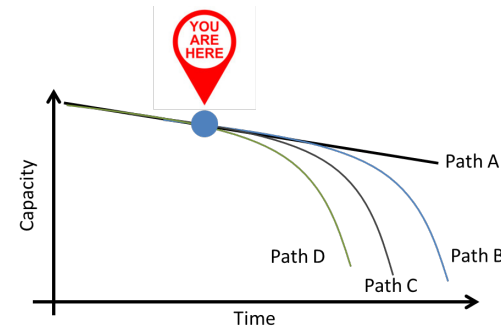
Artificial Intelligence

Objective/Significance

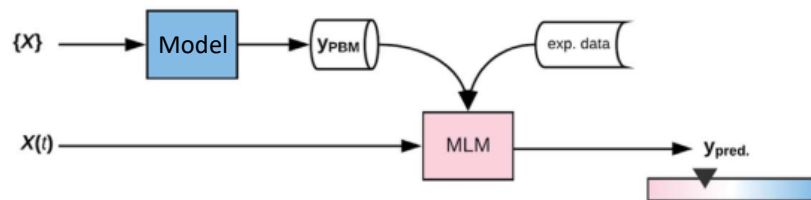


Experimental data is costly and time consuming,
Most studies only test a couple batteries,
Biggest dataset: 124 batteries with only charge varying

Problematic because of path dependence.



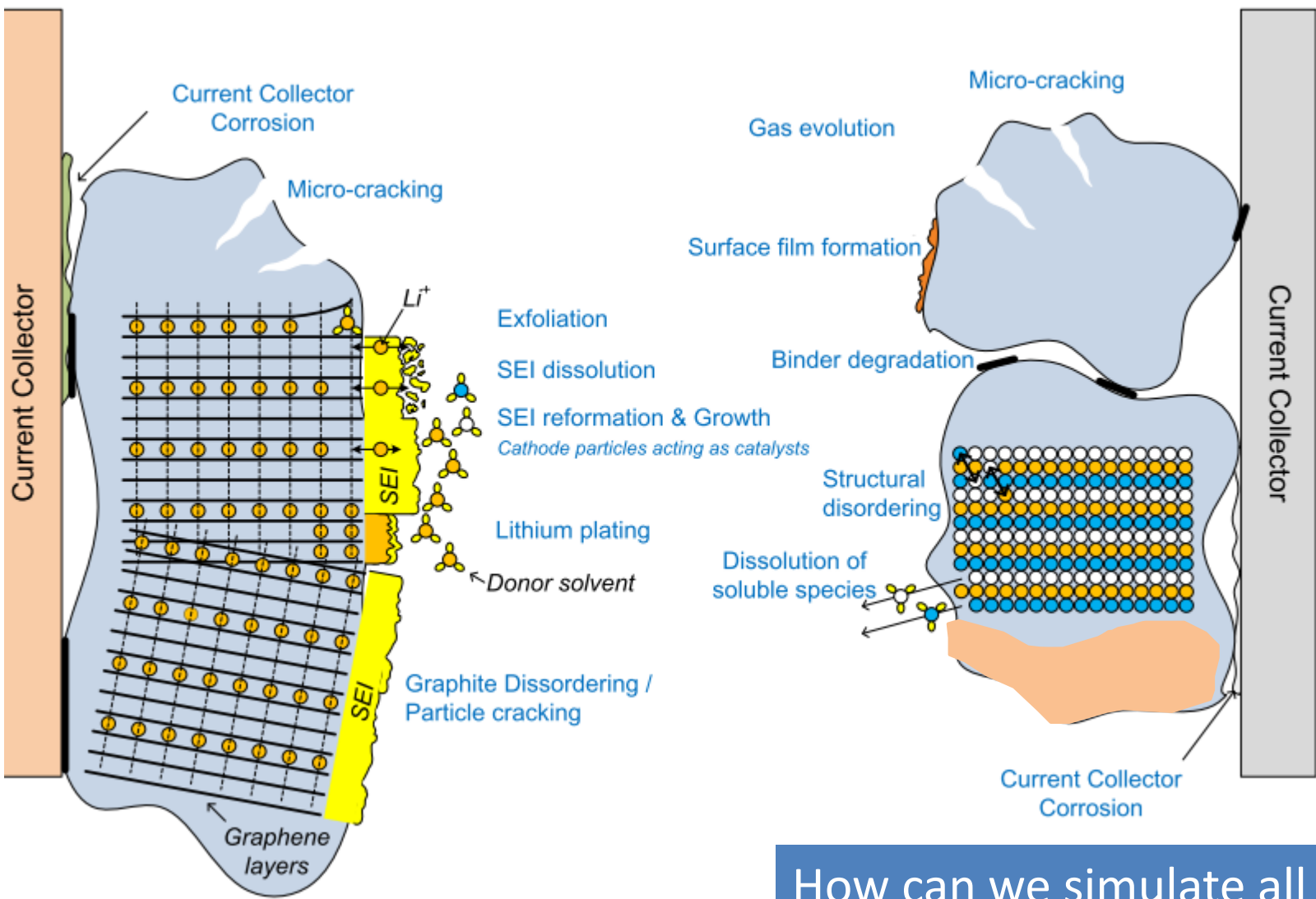
Current state of the art is far from the big data needed to make AI work



Solution: Transfer Learning
Create synthetic training datasets

Li-ion batteries are complex systems

Lithium ion battery degradation mechanisms

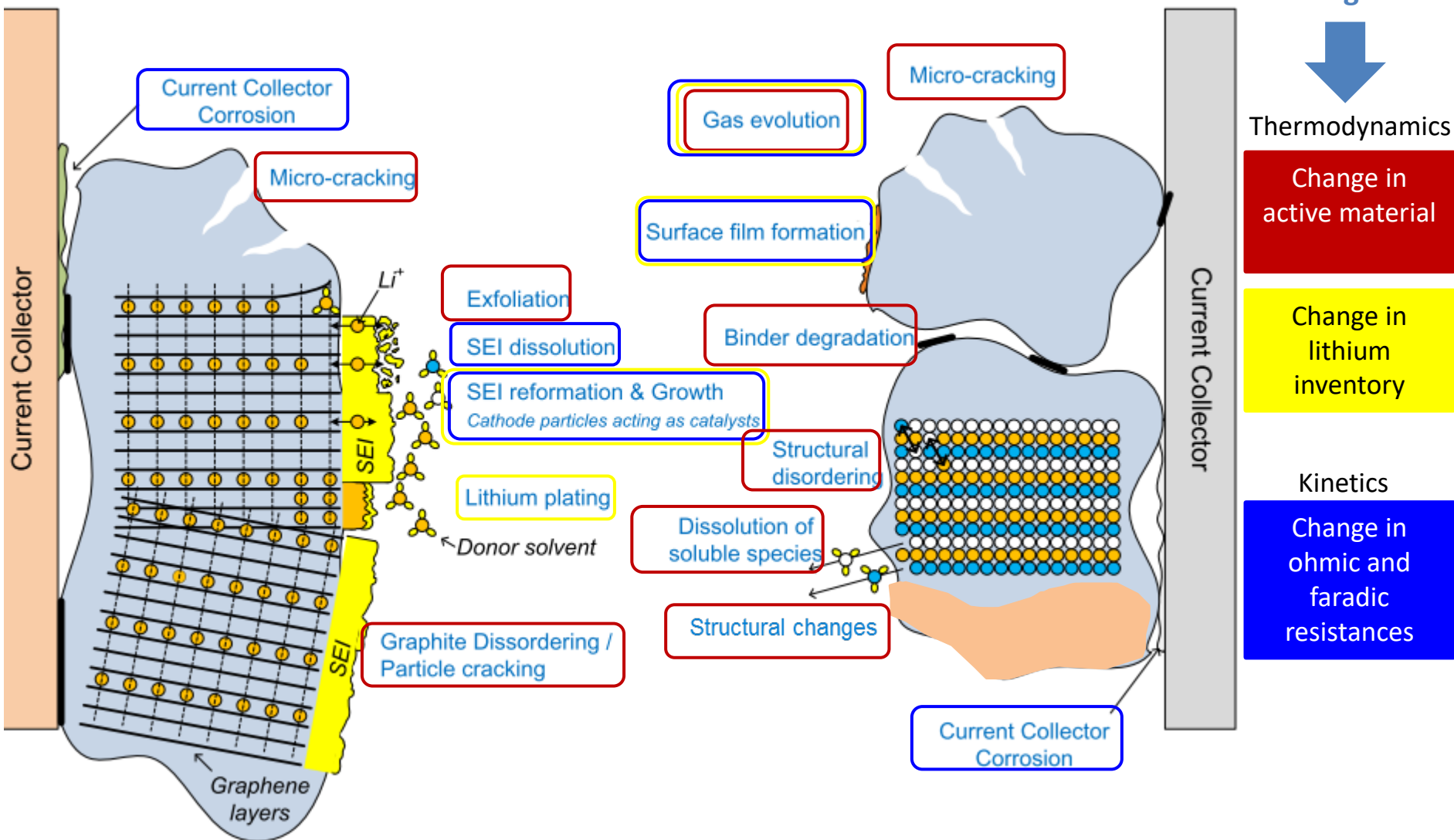


How can we simulate all of them?

Big Data for Li-Ion Diagnosis and Prognosis

Li-ion batteries are complex systems

Lithium ion battery degradation mechanisms

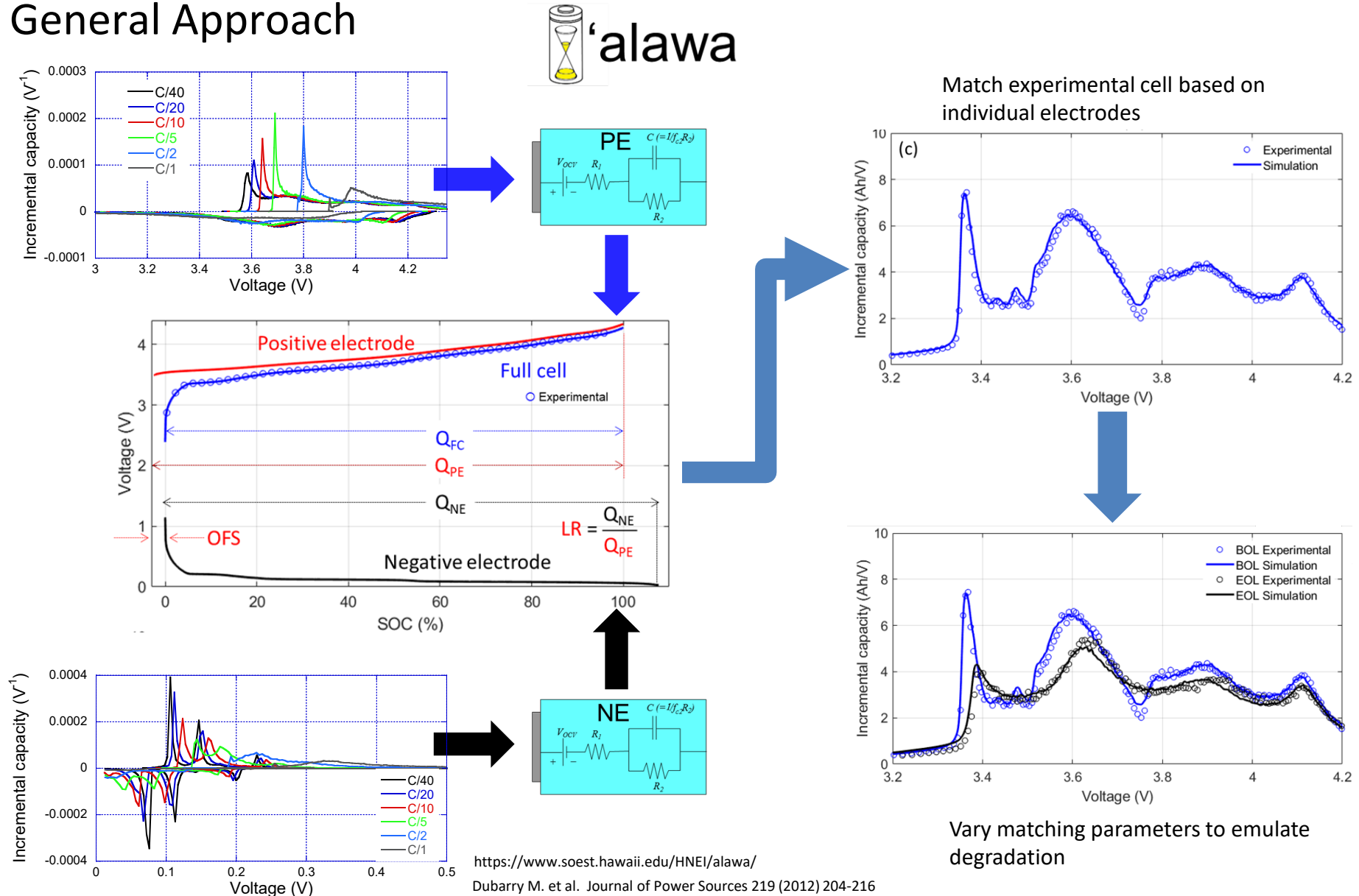


Big Data for Li-Ion Diagnosis and Prognosis

Building a Digital Twin: Mechanistic modeling



General Approach

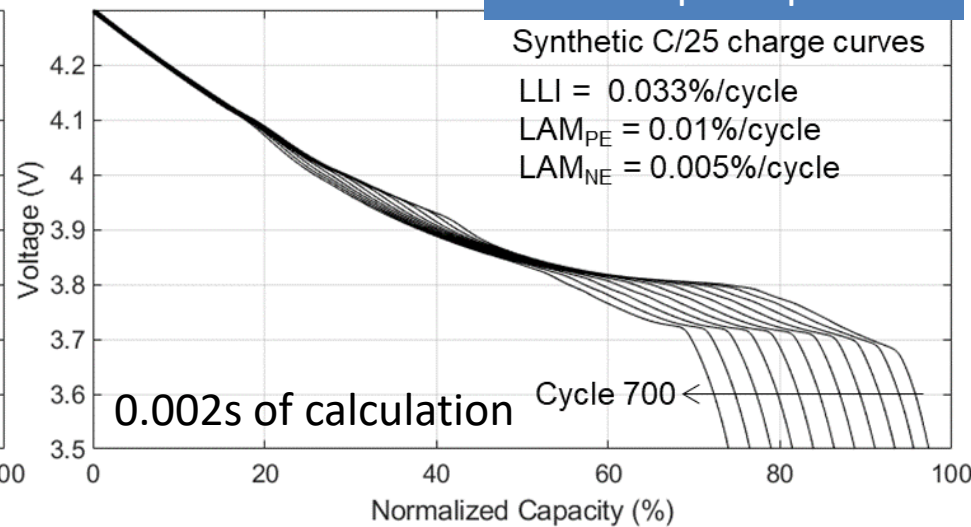
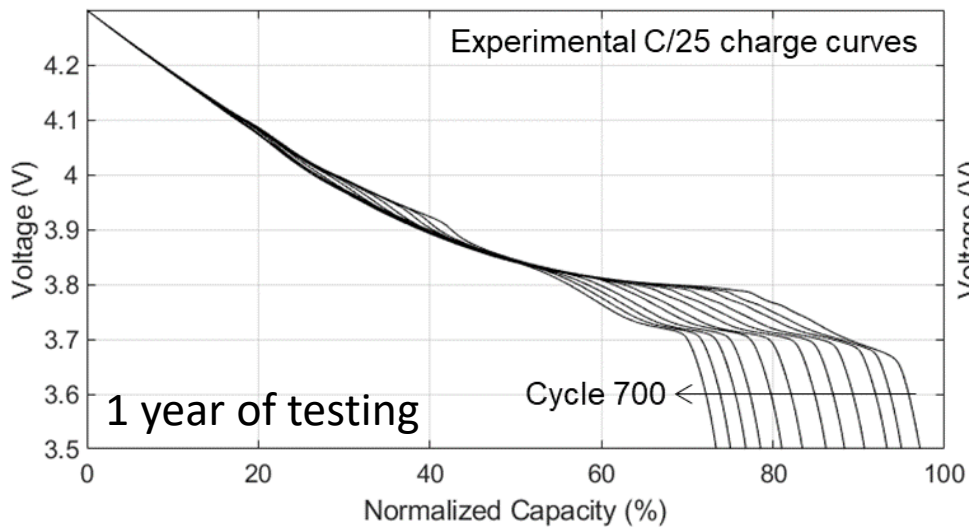


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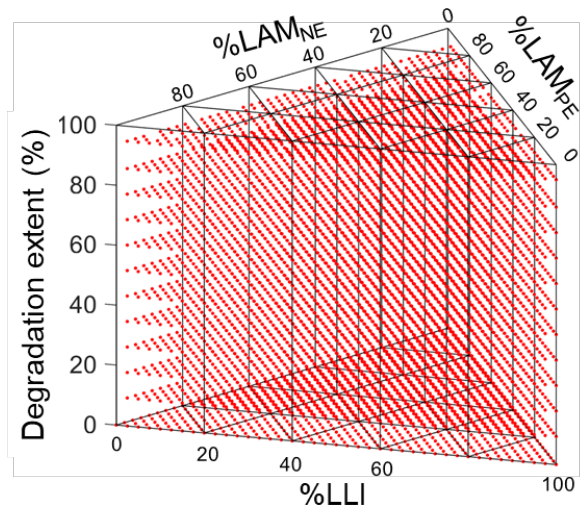
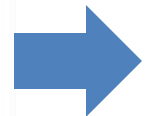
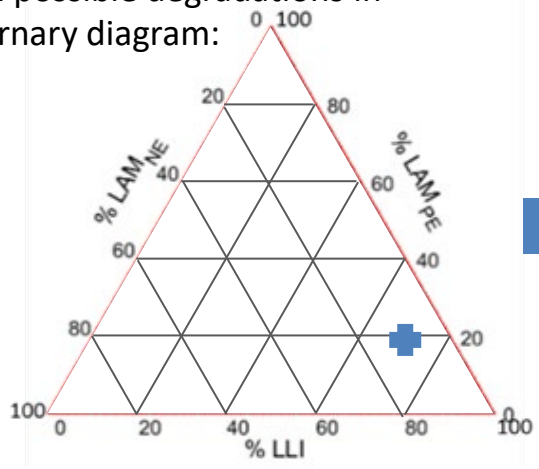
Use the mechanistic modeling approach

Emulation of battery electrochemical response

Aging reconstructed from simple equations



All possible degradations in ternary diagram:



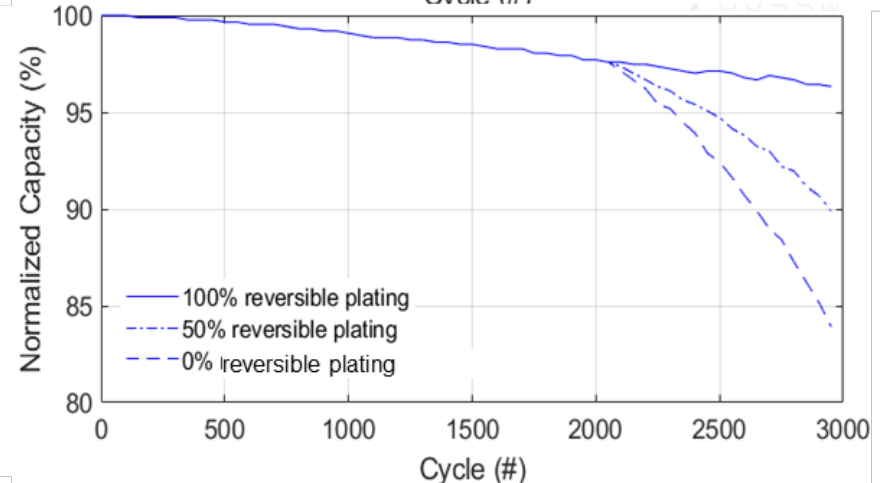
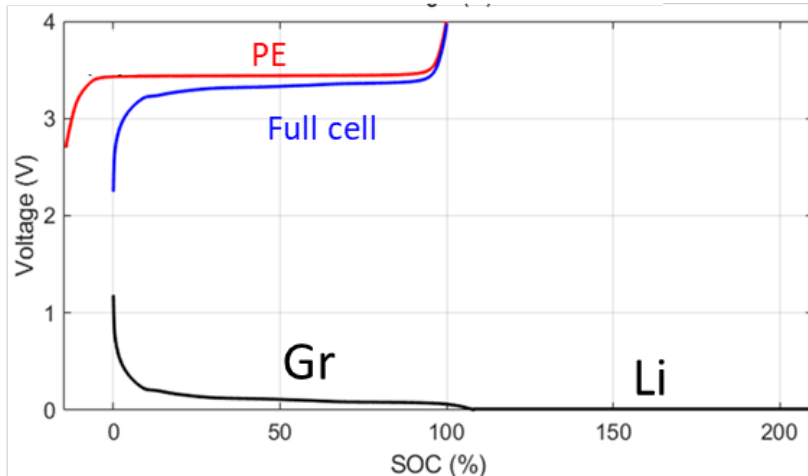
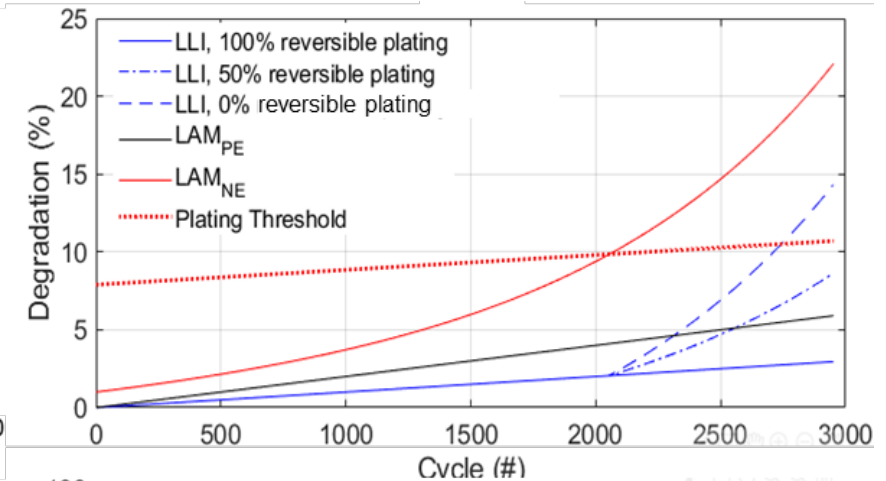
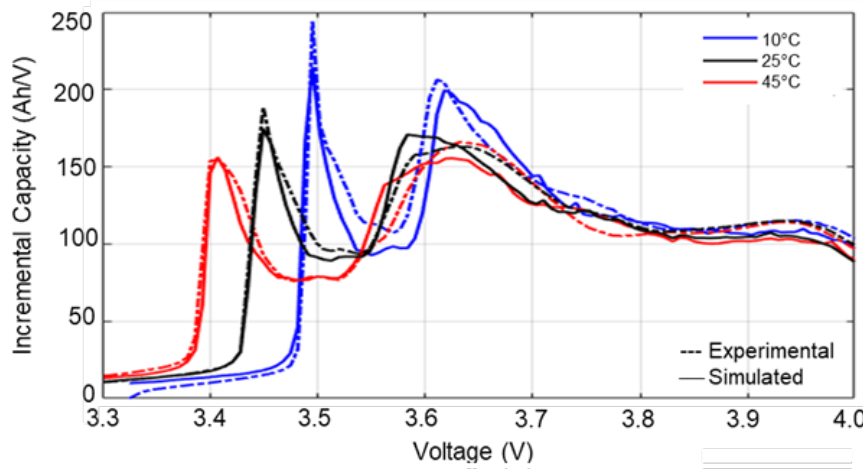
Infinite training data for diagnosis AI algorithms

Dubarry M. et al., Journal of Power Sources 479 (2020) 228806
Dubarry, M., et al. (2017). "State of health battery estimator enabling degradation diagnosis: Model and algorithm description." *Journal of Power Sources* 360: 59-69.

Big Data for Li-Ion Diagnosis and Prognosis

More complexity for real scenarios

More than LLI and LAMs... Kinetics, blends and plating



Dubarry M. et al., Journal of Power Sources 479 (2020) 228806

Baure, G. and M. Dubarry (2019). "Synthetic vs. Real Driving Cycles: A Comparison of Electric Vehicle Battery Degradation." *Batteries* 5(2).

Dubarry, M., et al. (2020). "Perspective on State-of-Health Determination in Lithium-Ion Batteries." *Journal of Electrochemical Energy Conversion and Storage* 17(4): 1-25.

Schindler, S., et al. (2019). "Kinetics accommodation in Li-ion mechanistic modeling." *Journal of Power Sources* 440: 227117.

Computed datasets: Replicate complexity of real scenarios

Open access synthetic datasets : LFP, NCA, NMC811 vs. Graphite

V vs. Q datasets

>5,000 $\{LLI, LAM_{PE}, LAM_{NE}\}$

At least 0.85% resolution

> 700,000 V vs. Q curves

Duty cycle datasets

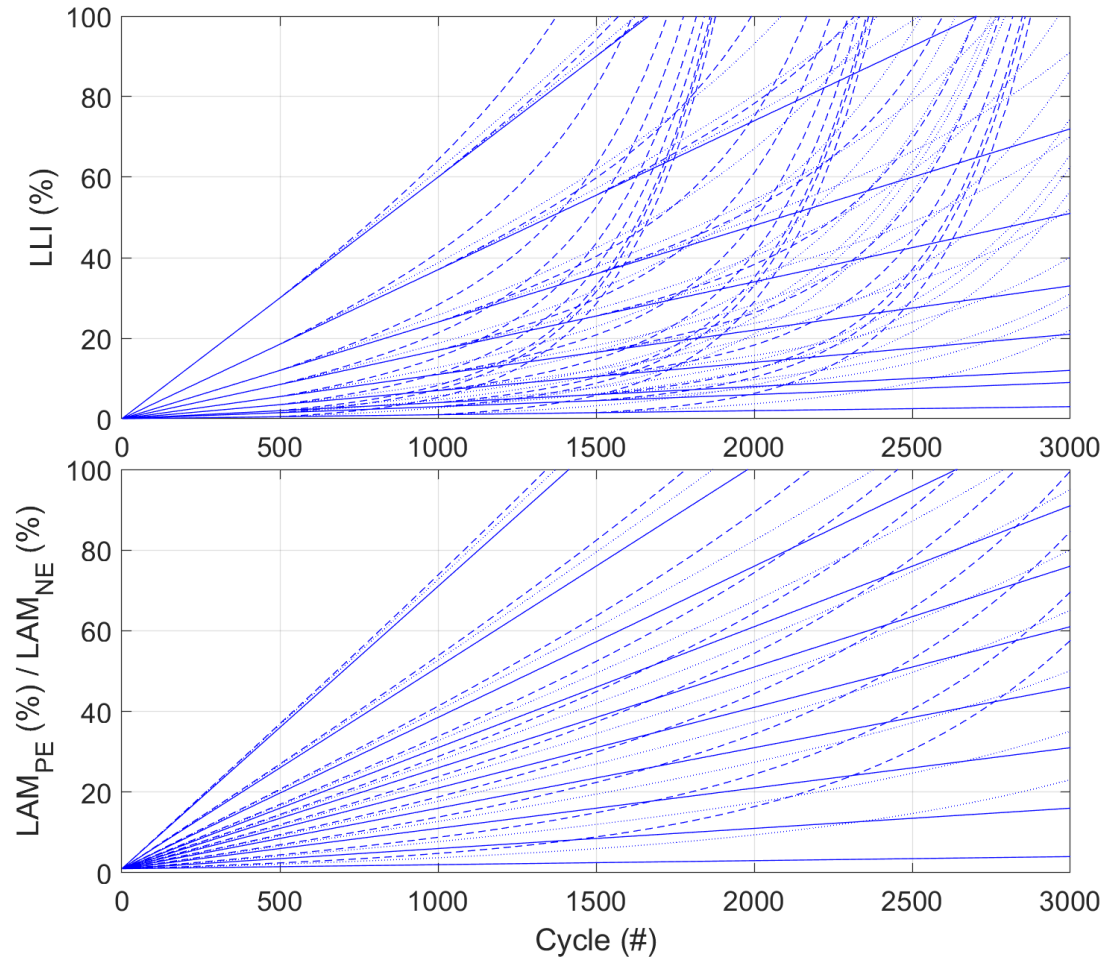
> 125,000 unique LLI/LAM evolution

> 3,000,000 V vs. Q curves

8 parameters varied

$$\%deg = a \times cycle + e^{(b \times cycle) - 1}$$

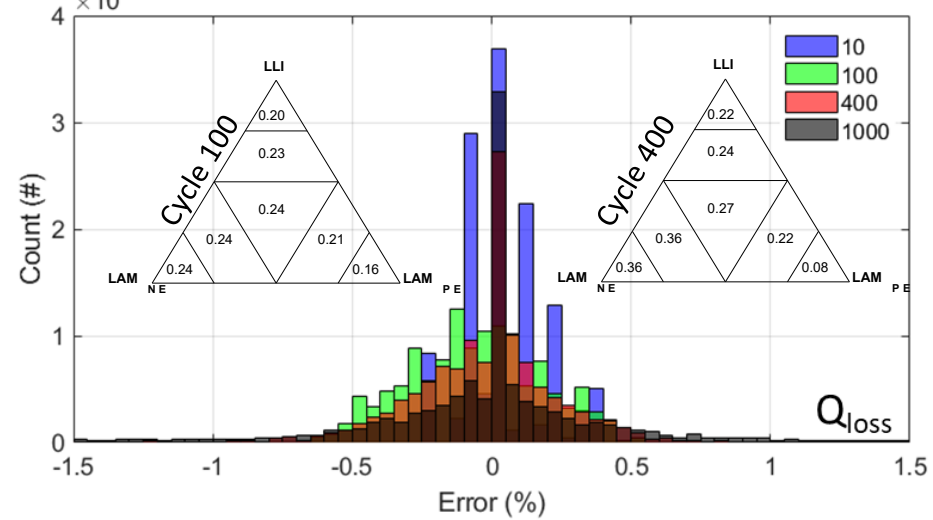
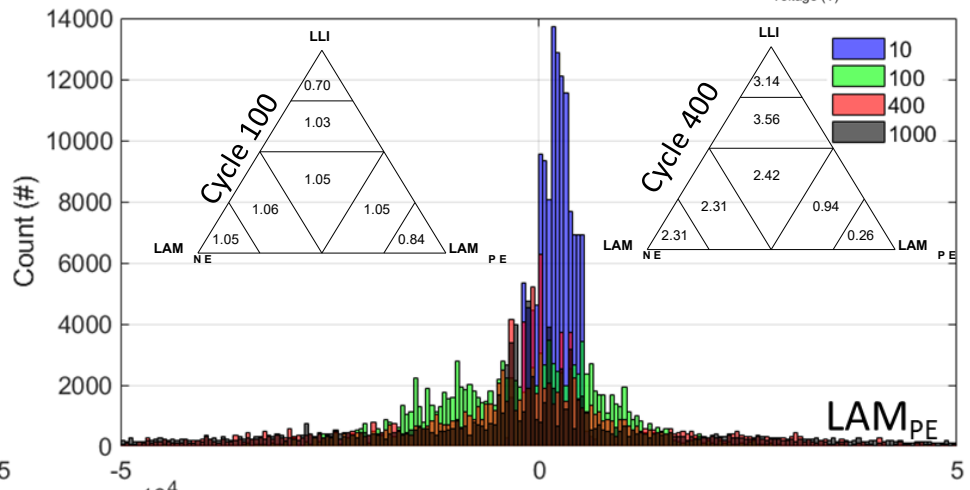
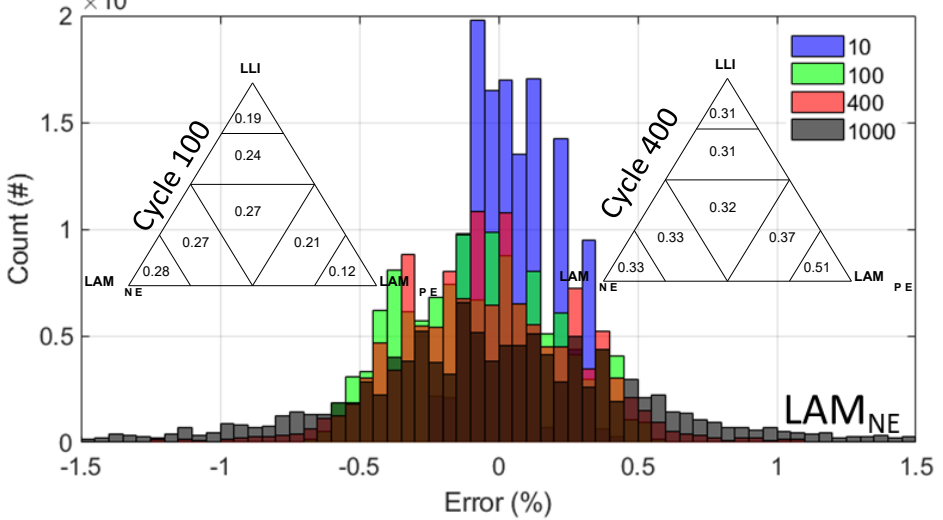
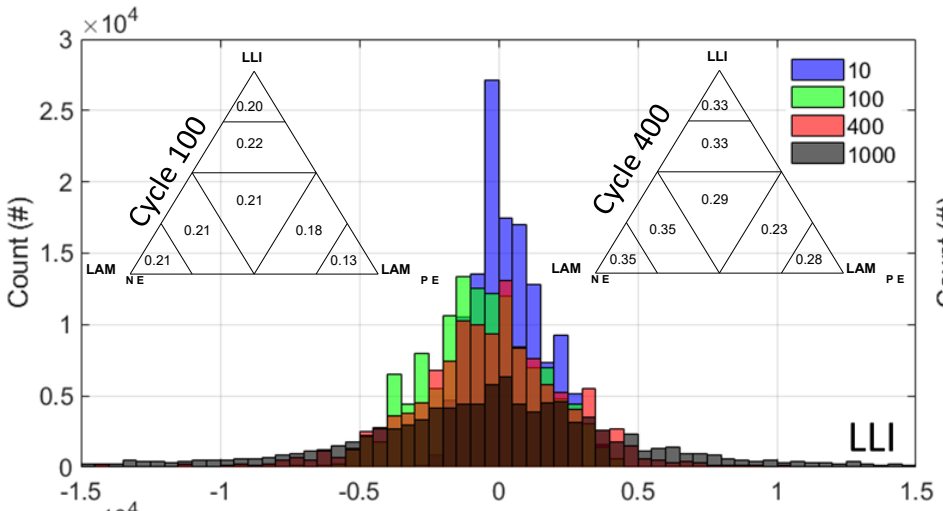
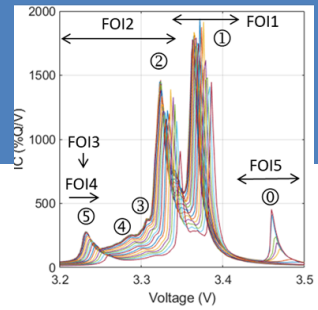
for LLI , LAM_{NE} , & LAM_{PE}
plus delay and plating rev.



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Diagnosis

Apply to entire dataset



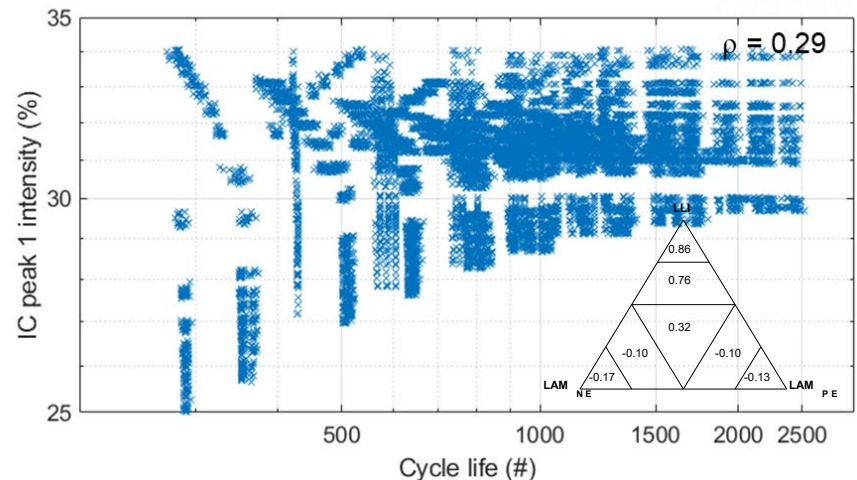
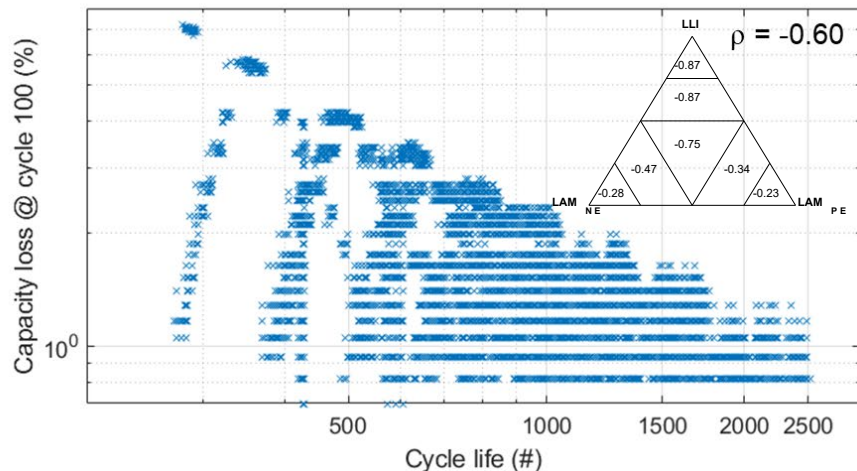
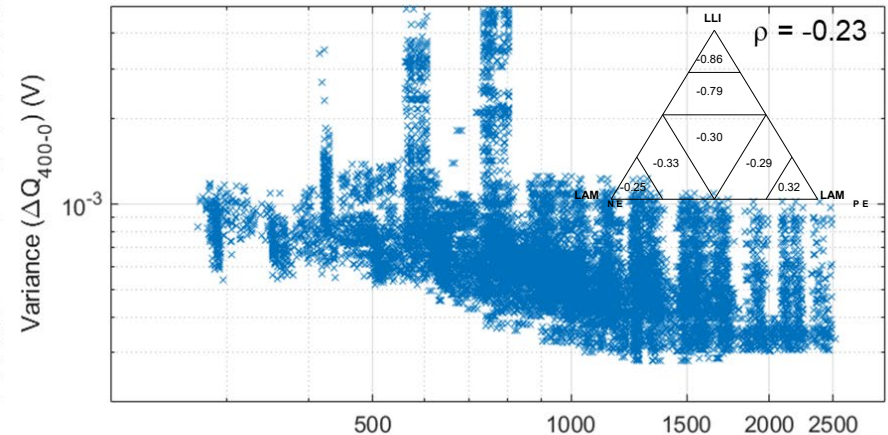
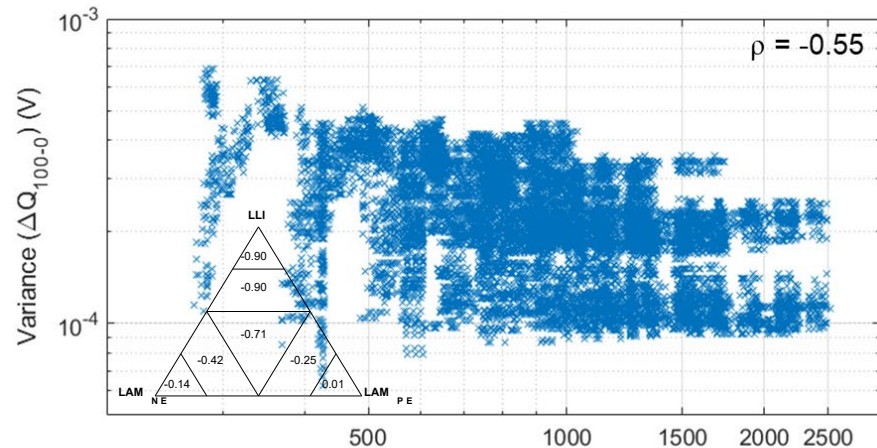
|Diagnosis error| < 1% @ 4 cycles and for > 125,000 duty cycles

Big Data for Li-Ion Diagnosis and Prognosis

Prognosis

Datasets can be used for training or for sensibility analysis.

What parameters can be used for early prognosis?

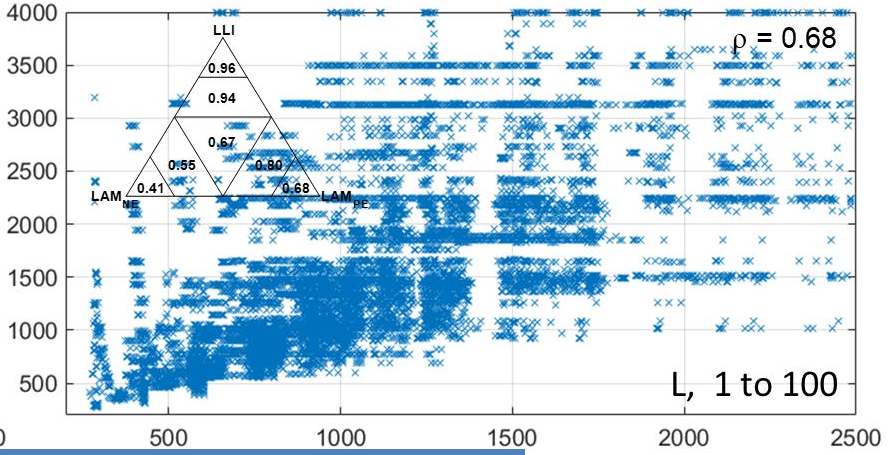
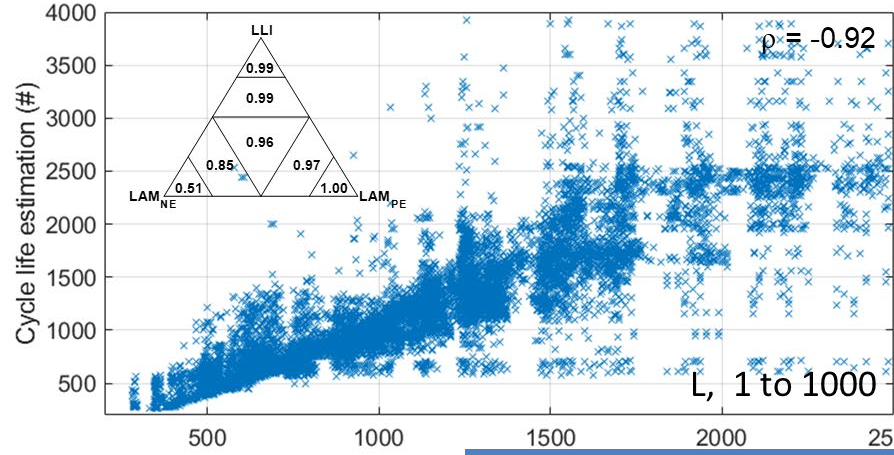
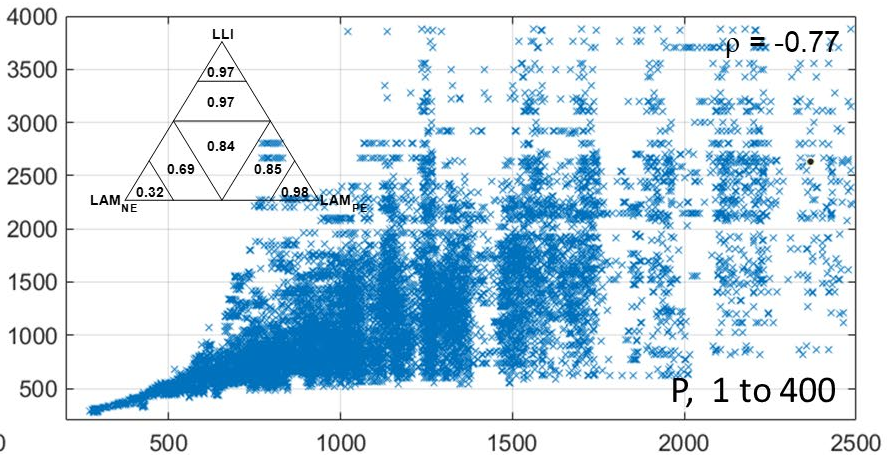
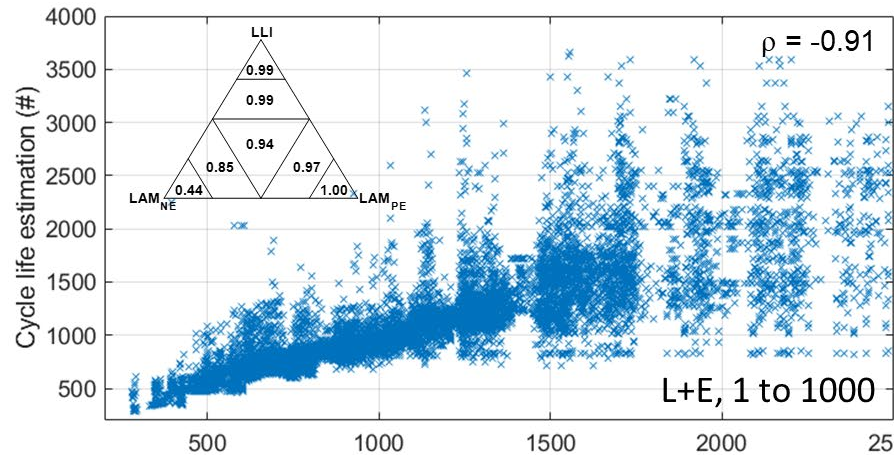
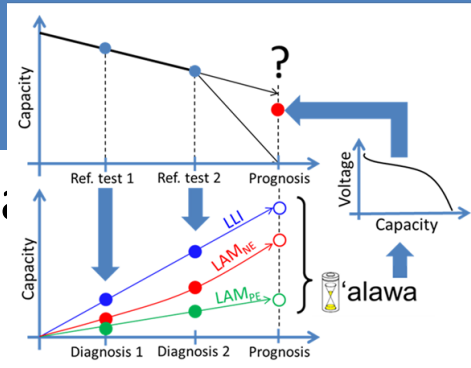


Single parameter early prognosis might be hard to get for complex degradations

Big Data for Li-Ion Diagnosis and Prognosis

Prognosis

Datasets can be used for training or for sensibility analysis
What parameters can be used for early prognosis?



Extrapolating from diagnosis is working better

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Conclusions

Proof-of-concept methodology to generate **big data training datasets**

Universal tool for creation of data indistinguishable from real one

Methodology could be **applied to different conditions** such as rate and temperature

Can handle **lithium plating with adjustable reversibility**

Ideal to **test validity** of different approaches for diagnosis or prognosis

The approach **does not remove the need for experimental testing**

It is still essential, and the only way, to decipher which conditions cater to specific degradation.

Big Data for Li-Ion Diagnosis and Prognosis

Acknowledgments

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Mahalo, questions?



matthieu@hawaii.edu

