Big Data for Li-Ion Battery Diagnosis and Prognosis

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Synthetic Training Data for AI Li-Ion Diagnosis and Prognosis

Path dependence of battery degradation

Objective/Significance

Traffic

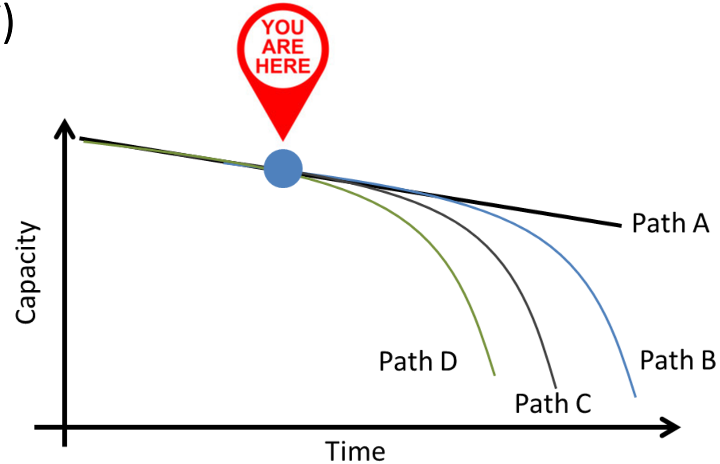
Road type

Driving habits

Charging habits

Temperature

Grid ties (V2G / G2V)



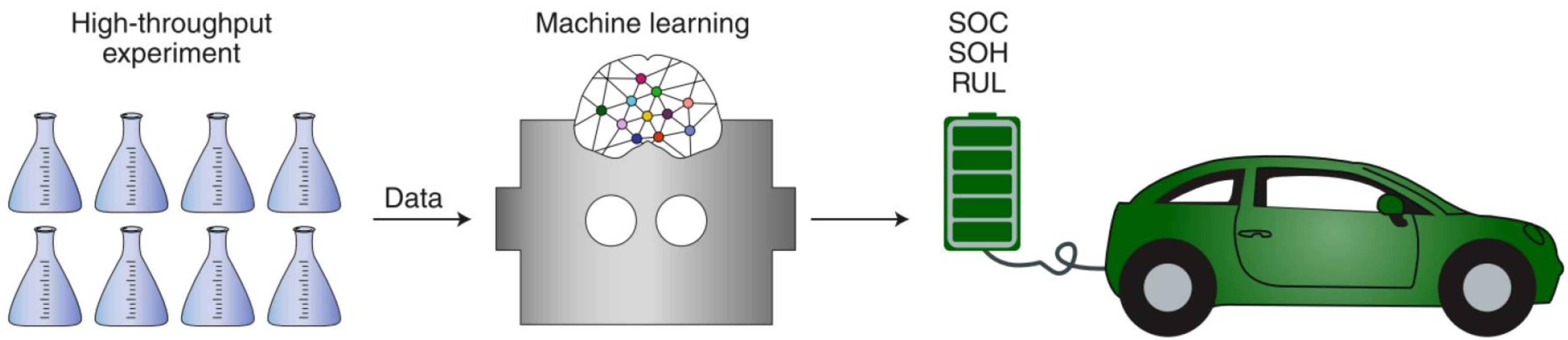
Different paths will lead to different degradation

Every battery is different

Need to test prognosis tools on wide array of scenarios

Artificial Intelligence

Objective/Significance



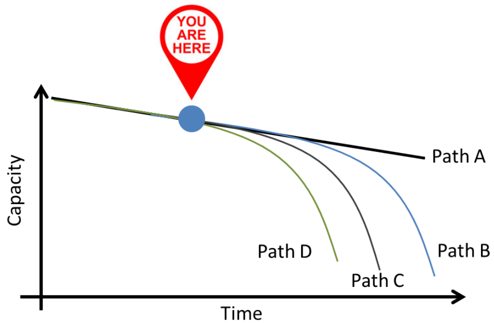
Little to no effort

Lot of effort

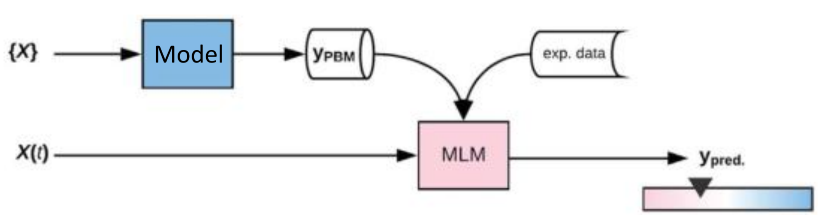
Man-Fai Ng et al., Nature Machine Intelligence, 2(3) p. 161-170 (2020)

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



Aylol et al., Journal of The Electrochemical Society, 2021 168 030525

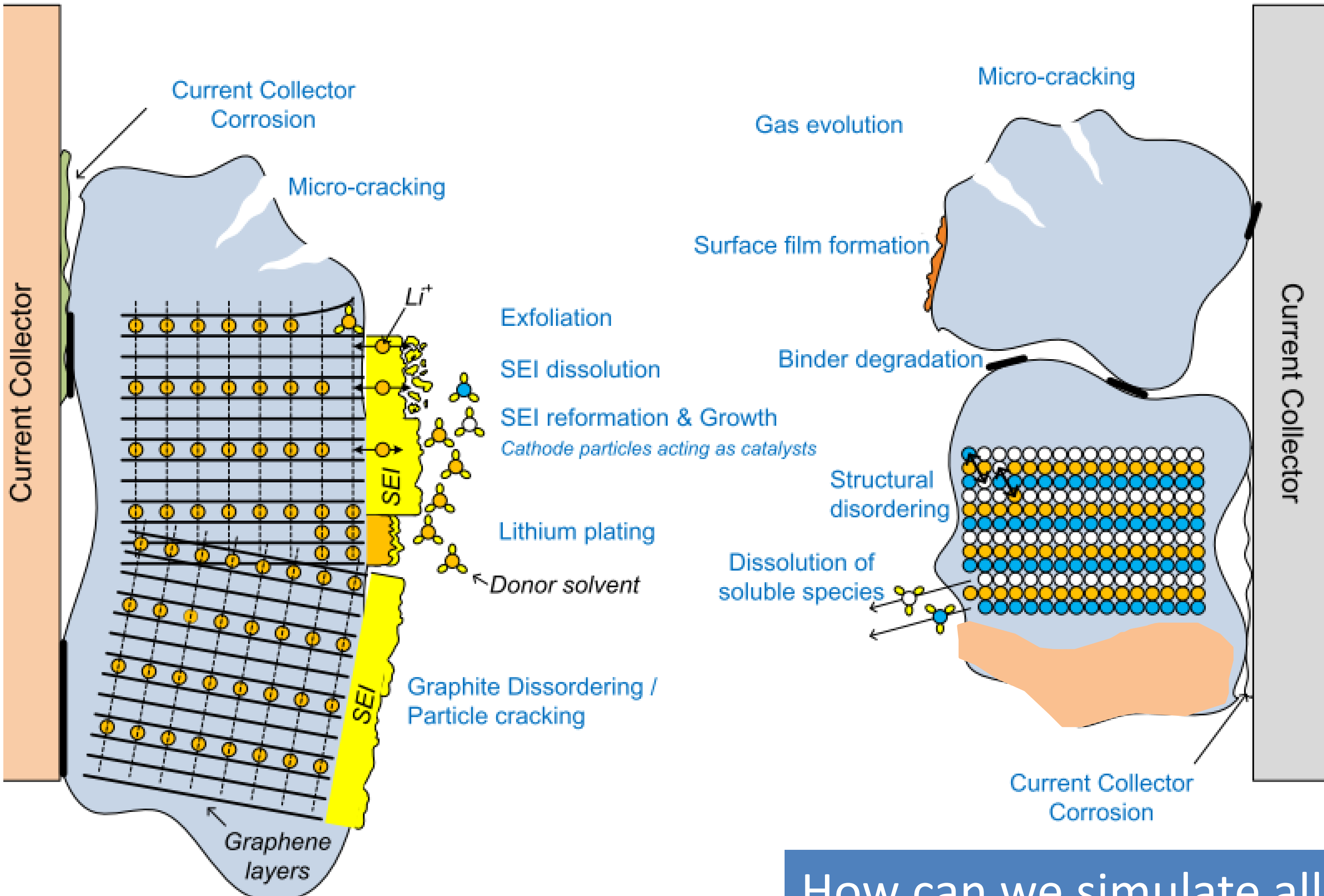
Solution: Transfer Learning
Create synthetic training datasets

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

Synthetic Training Data for AI Li-Ion Diagnosis and Prognosis

Li-ion batteries are complex systems

Lithium ion battery degradation mechanisms



J. Groot, State of Health Estimation of Li-ion batteries cycle life test methods

How can we simulate all of them?

Synthetic Training Data for AI Li-Ion Diagnosis and Prognosis

Model framework considerations

Electrochemical models

"Balance of plant"

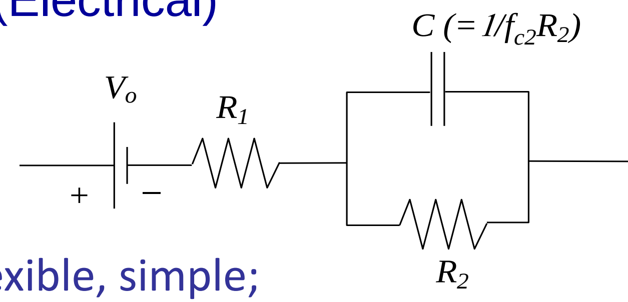
$$\frac{\partial i_l}{\partial x} - A_{max} i_{0,ref}\left(\frac{c}{c_{ref}}\right)^{\gamma} SOC^{\zeta}\left(\exp\left(\frac{(1-\alpha)nF}{RT}(\Phi_s-\Phi_l-U)\right) - \exp\left(-\frac{\alpha nF}{RT}(\Phi_s-\Phi_l-U)\right)\right) - A_{max}C_{dl}\left(\frac{\partial \Phi_s}{\partial t}-\frac{\partial \Phi_l}{\partial t}\right)=0$$

Use conservation principles to solve kinetic and mass transport equations

Computation intensive; very challenging with path dependence; difficult for diagnosis

Use mechanistic descriptions with system topology for analysis

Equivalent circuit models (Electrical)



Universal, flexible, simple; mechanistic for diagnosis
Difficult for path dependence

Different flavors with "forward looking" approach

What about a backward looking model?

Empirical models

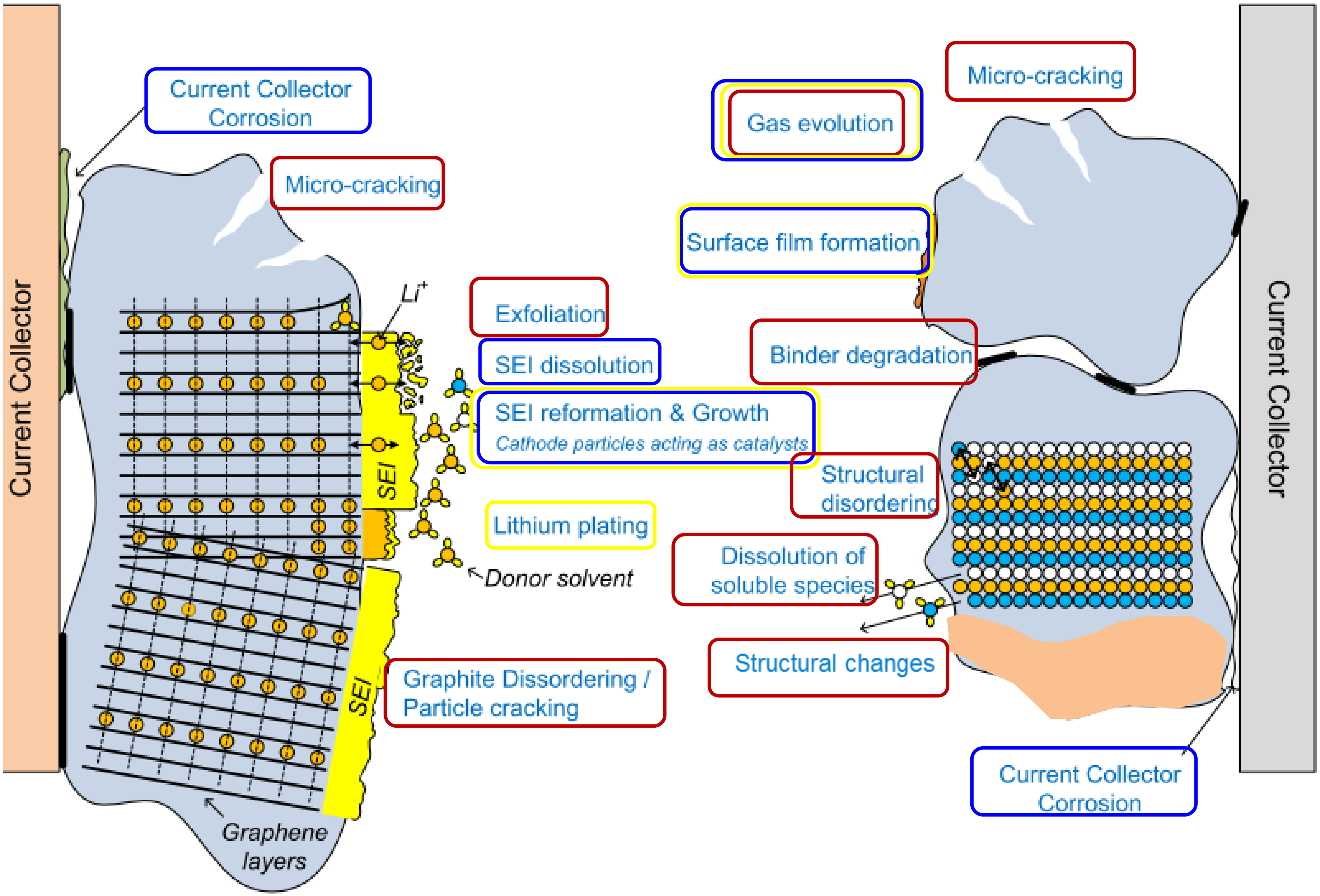
Need a large amount of training data to derive fitting parameters and algorithms

bstantial resources to develop; limited applicability & less practical

Dubarry, M., et al. (2012). Journal of Power Sources **219**: 204-216.

Li-ion batteries are complex systems

Lithium ion battery degradation mechanisms



Useful categorization for diagnostics

Thermodynamics

- Change in active material
- Change in lithium inventory

Kinetics

- Change in ohmic and faradic resistances

J. Groot, State of Health Estimation of Li-ion batteries cycle life test methods

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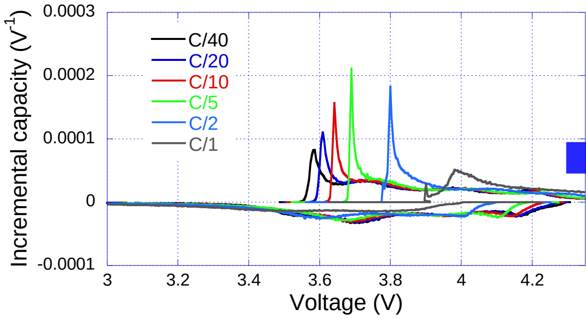
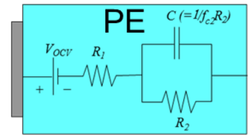
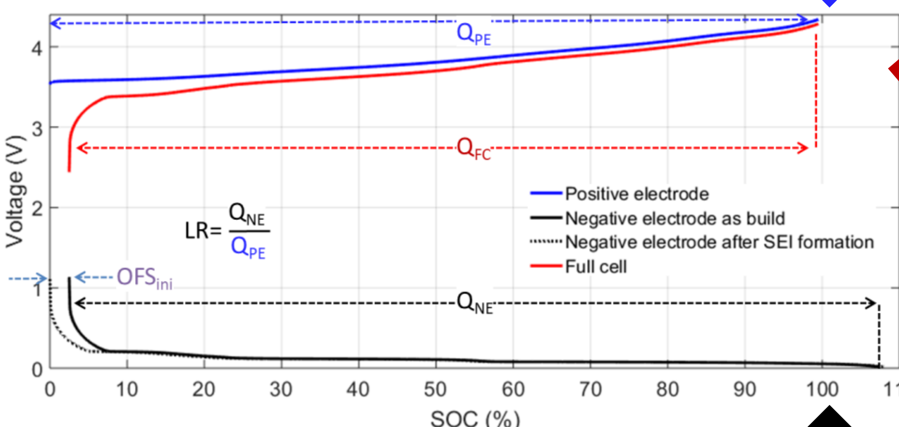
Mechanistic modeling

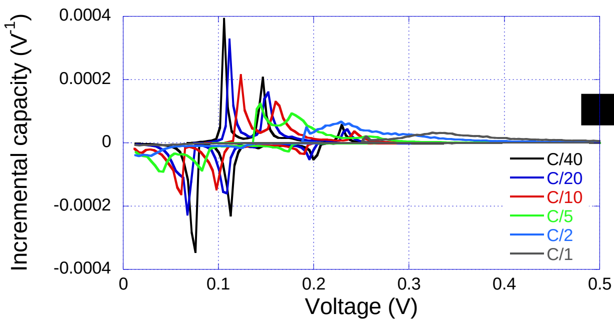
General Approach

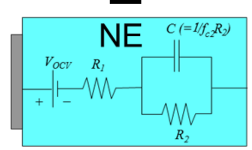
'alawa

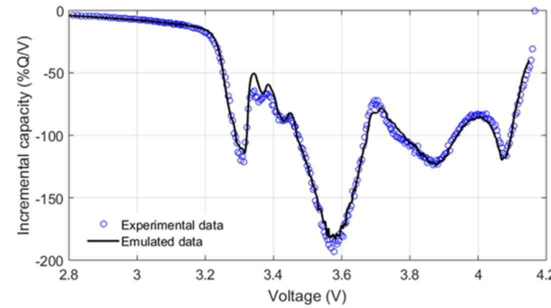


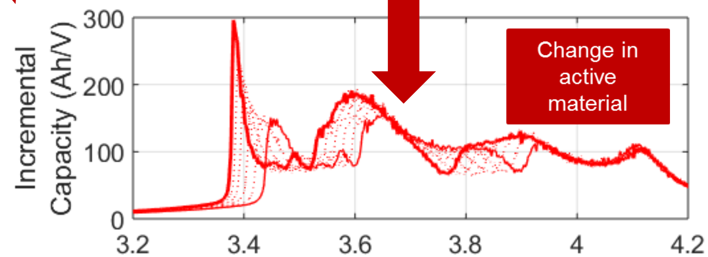


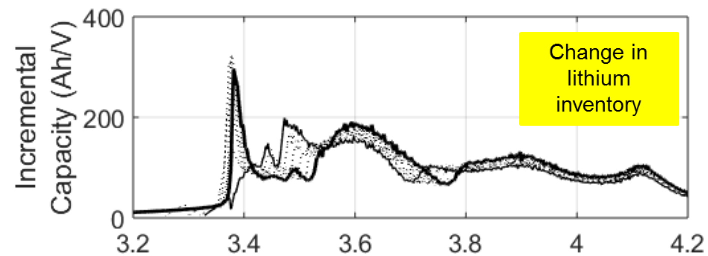


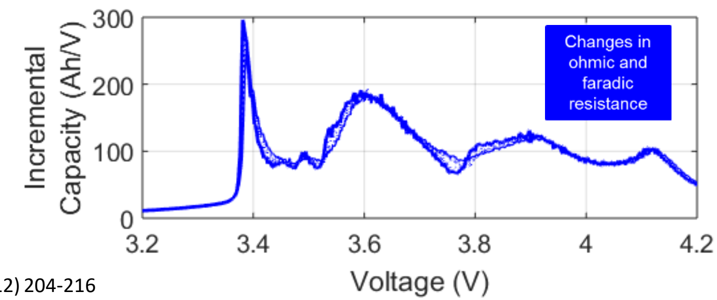










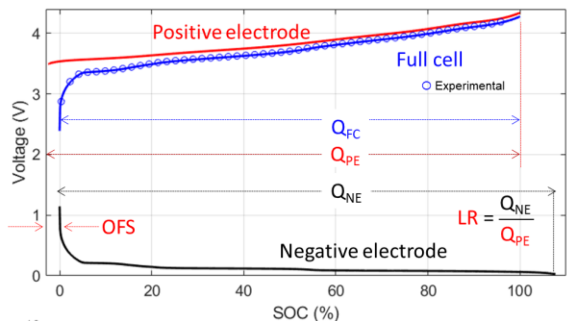


https://www.soest.hawaii.edu/HNEI/alawa/

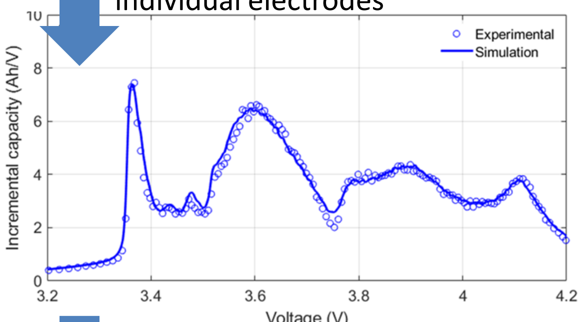
Dubarry M. et al. Journal of Power Sources 219 (2012) 204-216

Mechanistic modeling

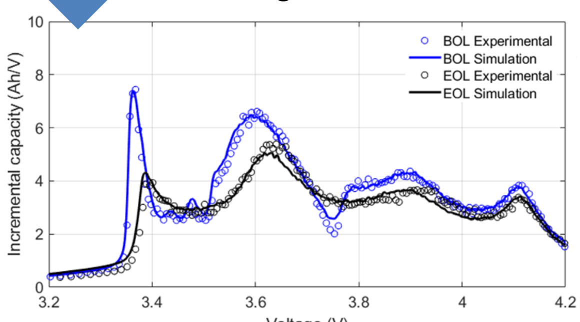
Simulation of duty cycles and prognosis

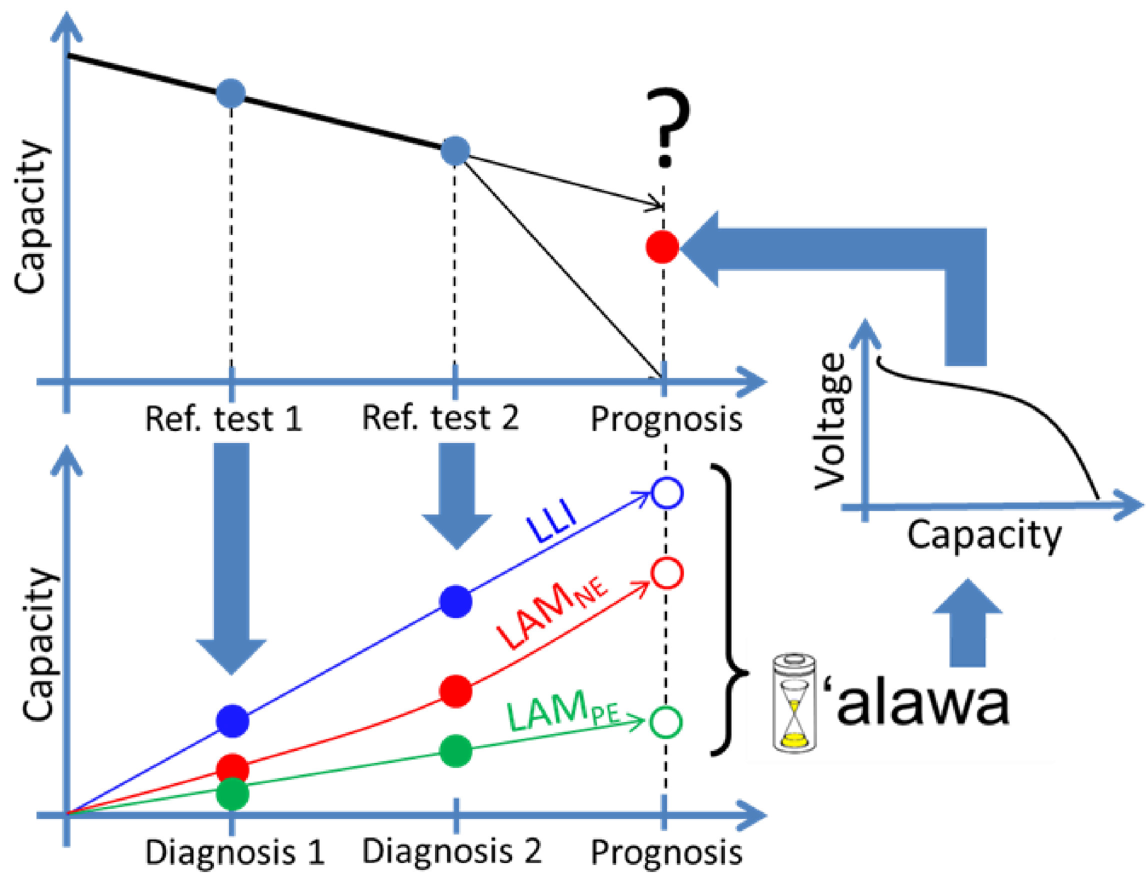


Match experimental cell based on individual electrodes



Vary matching parameters to emulate degradation



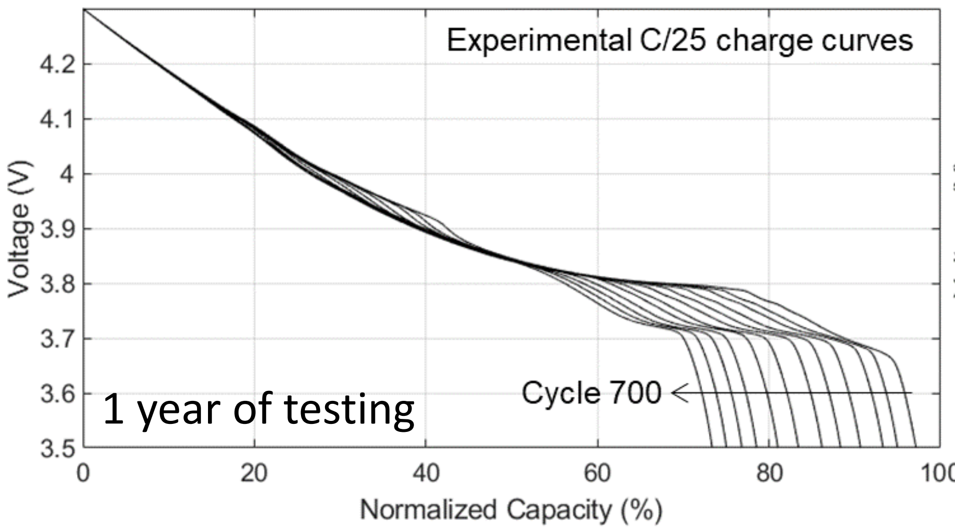


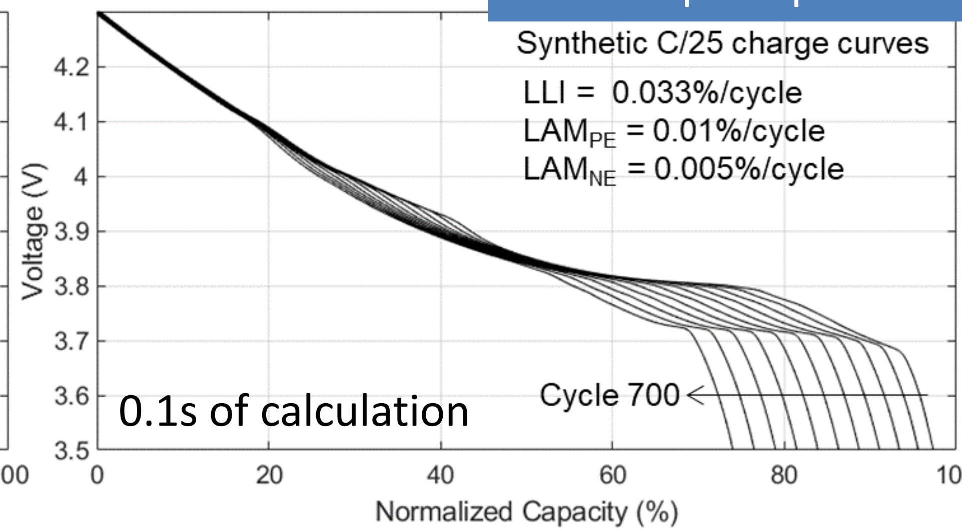
Dubarry M. et al., Journal of Energy Storage, 29, 101391 (2020); doi: 10.1016/j.est.2020.101391

Use the mechanistic modeling approach

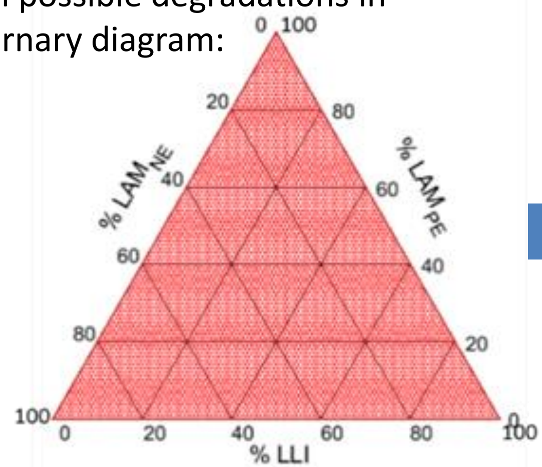
Emulation of battery electrochemical response

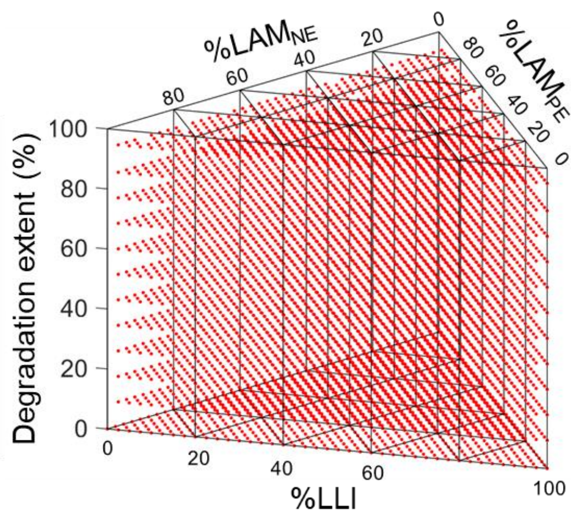
Aging reconstructed from simple equations





All possible degradations in ternary diagram:





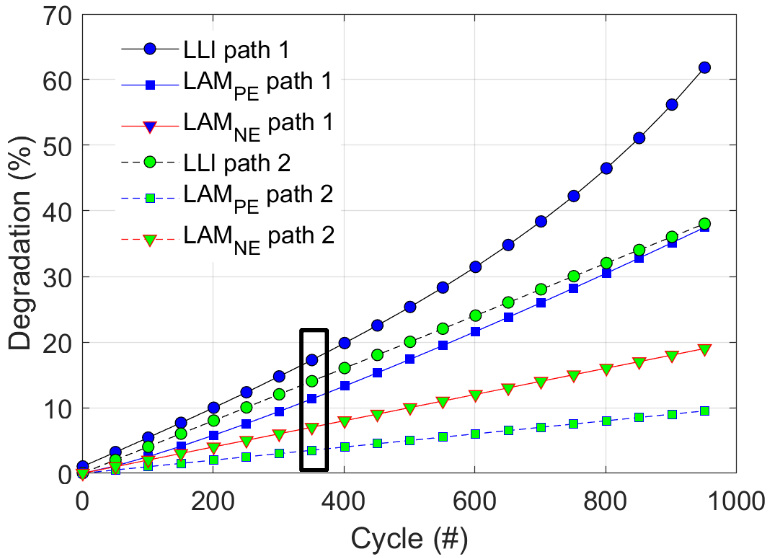
Infinite training data for diagnosis AI algorithms

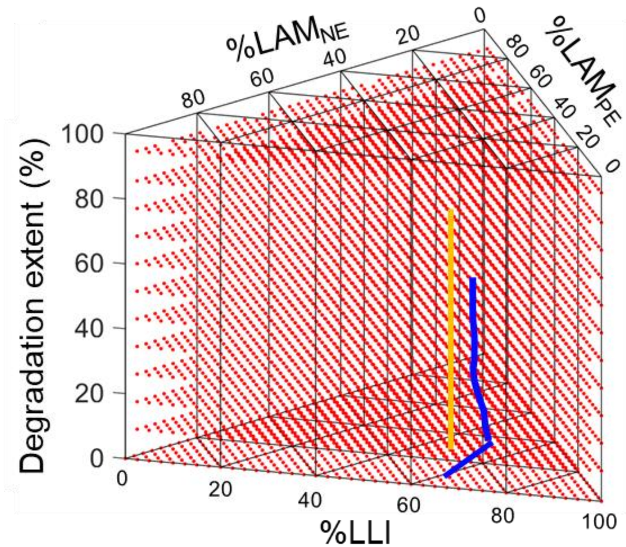
Dubarry M. et al., Journal of Power Sources 479 (2020) 228806

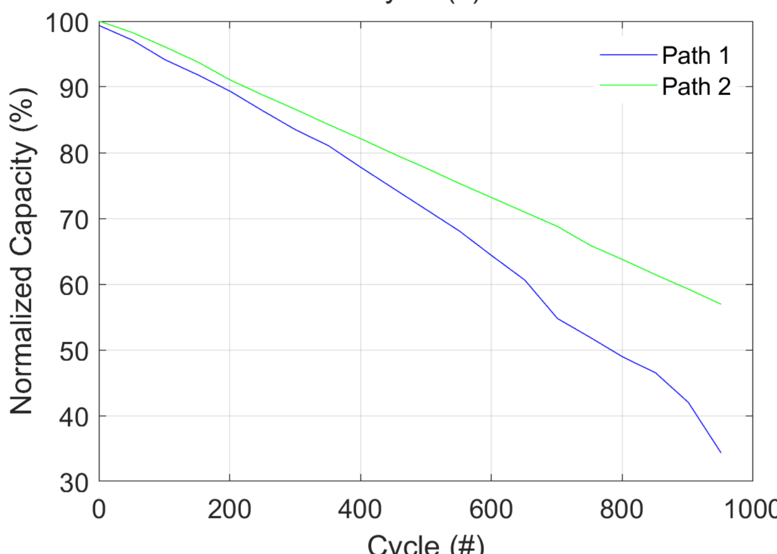
Dubarry, M., et al. (2017). "State of health battery estimator enabling degradation diagnosis: Model and algorithm description." Journal of Power Sources **360**: 59-69.

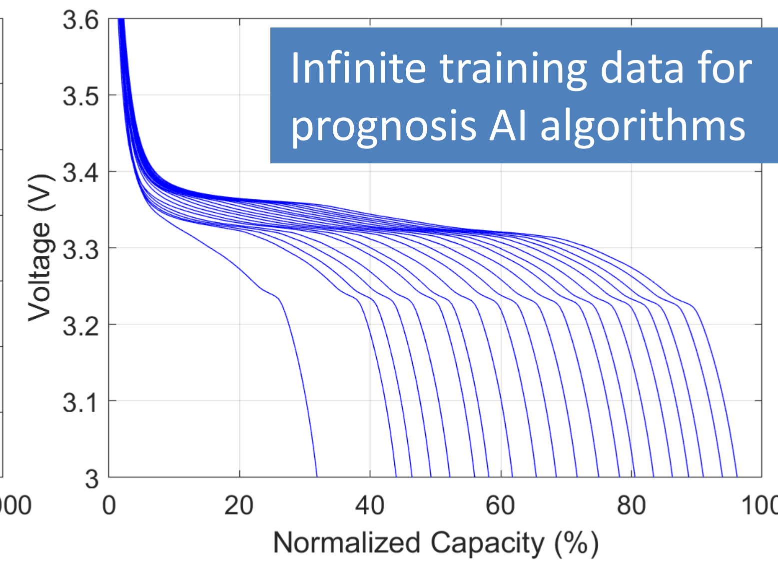
From diagnosis to prognosis

Prognosis: Needs to build full life-cycles









Infinite training data for prognosis AI algorithms

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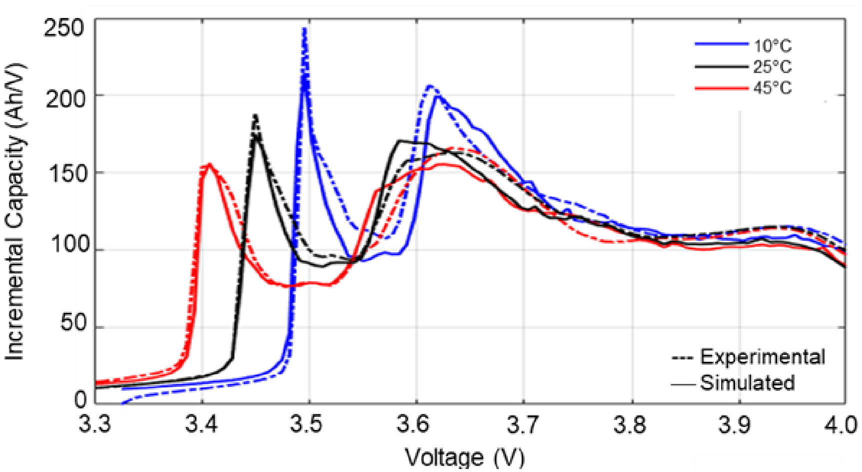
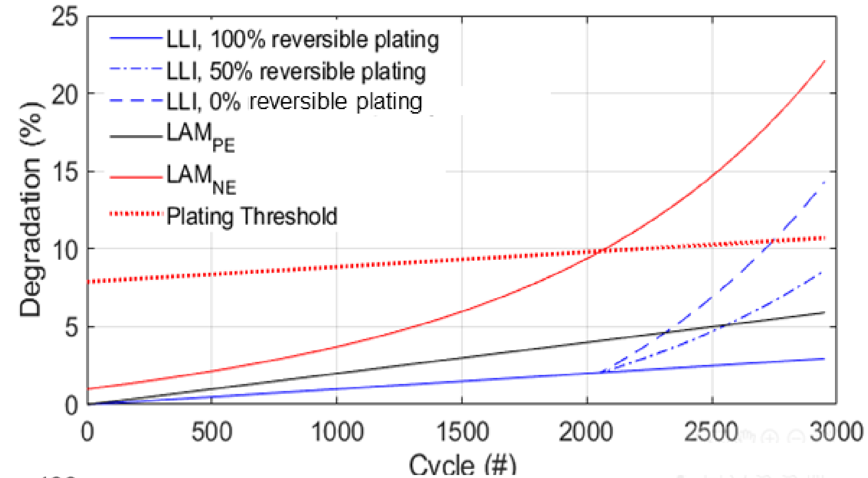
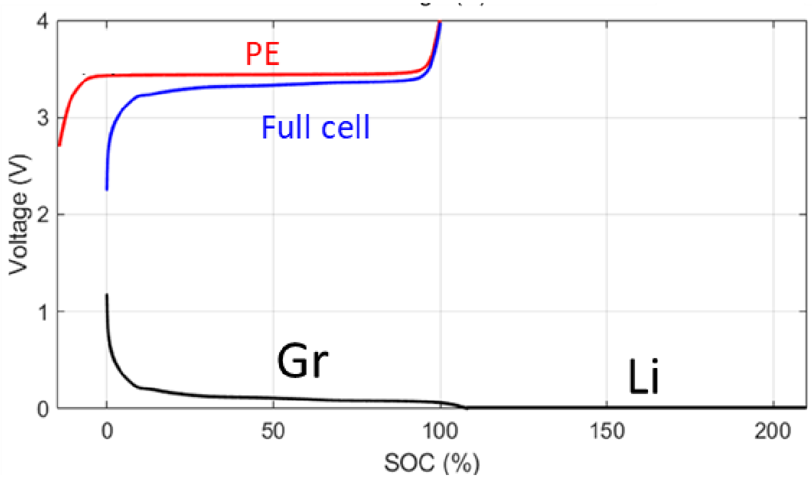
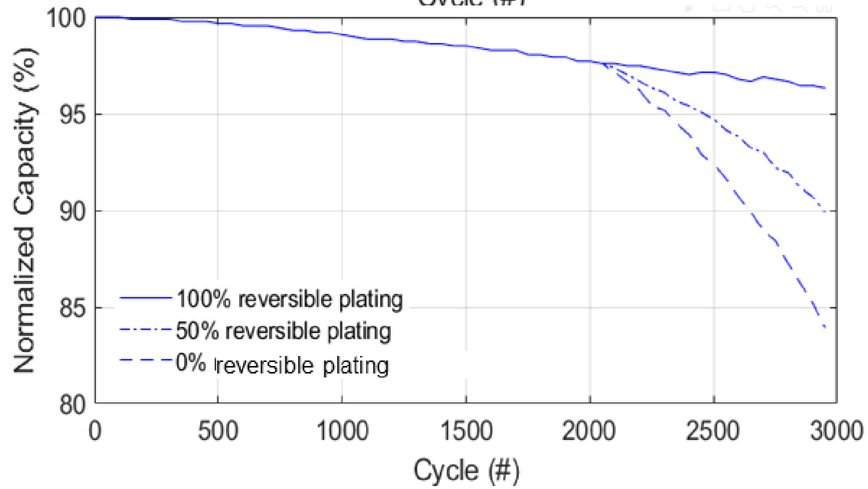
More complexity for real scenarios

More than LLI and LAMs… Kinetics, blends and plating









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

Computed datasets

Open access synthetic datasets : LFP vs. Graphite

Diagnosis

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

0.85% resolution

> 500,000 V vs. Q curves

Prognosis

> 100,000 duty cycles

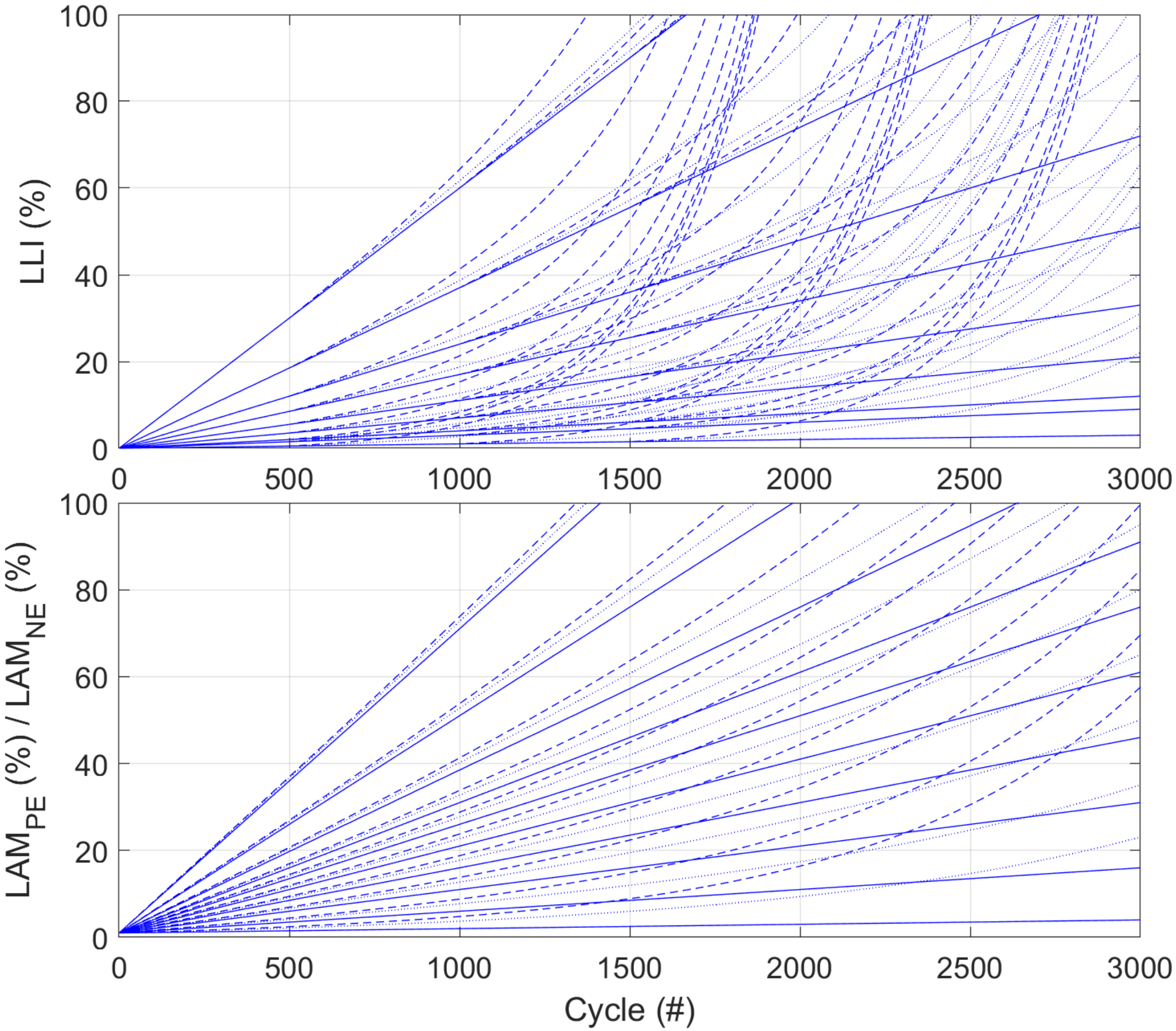
> 3,000,000 V vs. Q curves

8 parameters varied

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

For LLI, LAM_{NE}, & LAM_{PE}

Plus delay and plating rev.

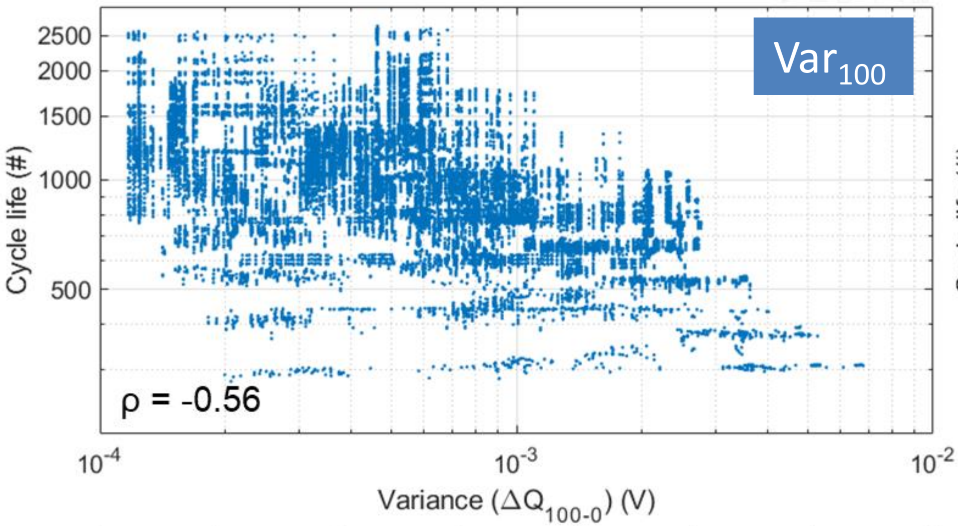


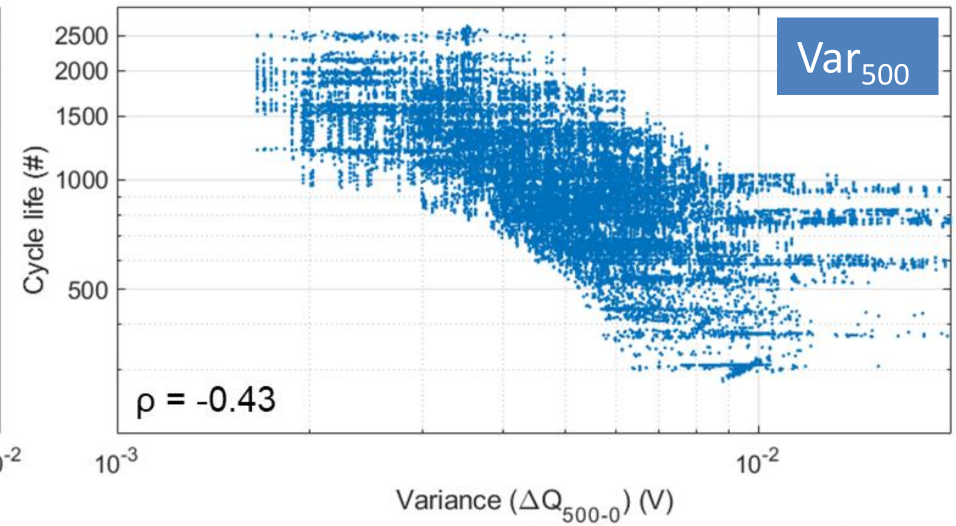
Graphite//LFP synthetic training diagnosis dataset, https://data.mendeley.com/datasets/bs2j56pn7y/1,
Graphite//LFP synthetic training prognosis dataset, https://data.mendeley.com/datasets/6s6ph9n8zg/1

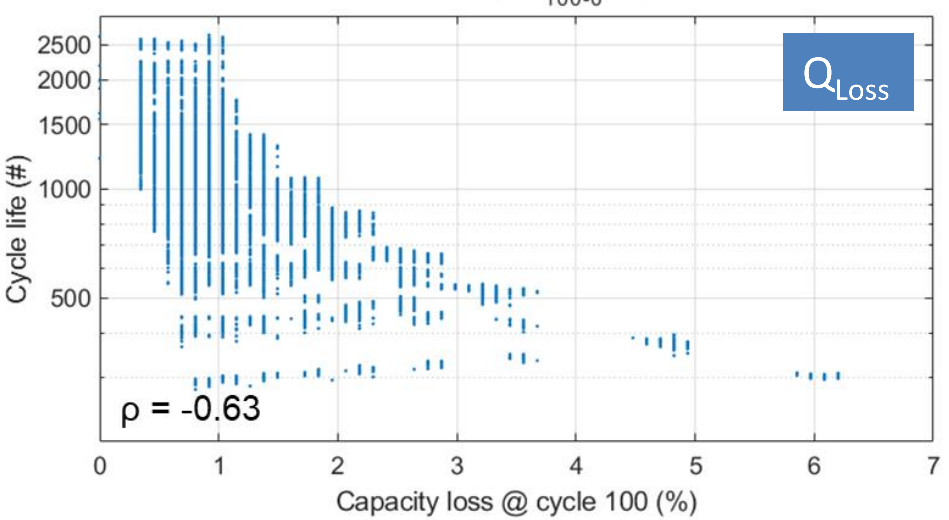
Sensibility analyses

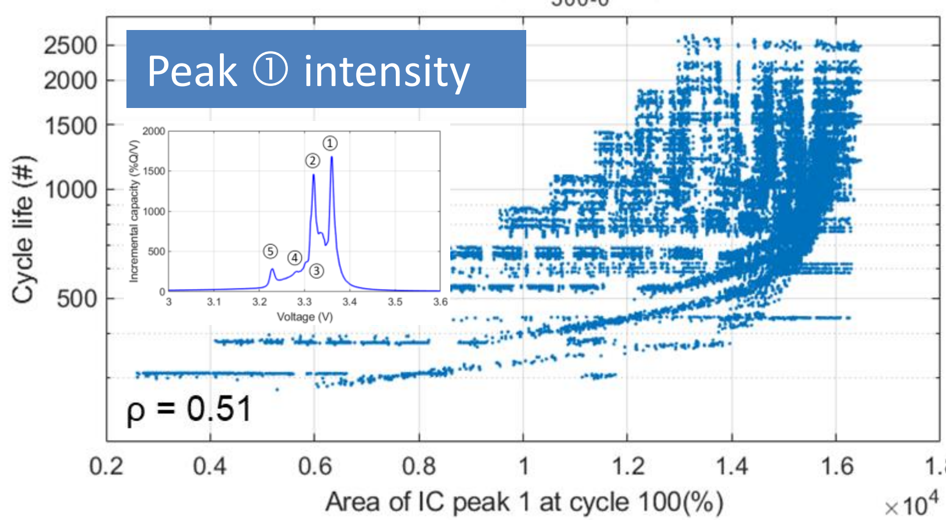
Datasets can be used for training or for sensibility analysis.

What parameters can be used for early prognosis?









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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

Broad applicability: cell chemistries, designs, and operating modes

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 **do not remove the need for experimental testing**
It is still essential, and the only way, to decipher which conditions cater to specific degradation.

More details: Dubarry M. et al., Journal of Power Sources 479 (2020) 228806
Dubarry M. et al., Energies, 2021, 14(9), 2371

Acknowledgments

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Thank you!

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