This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

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Sandia National Laboratories

Open-source software to accelerate the development of energy storage systems

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U.S. DEPARTMENT OF ENERGY   NNSA

Battery development takes time – 10 + years
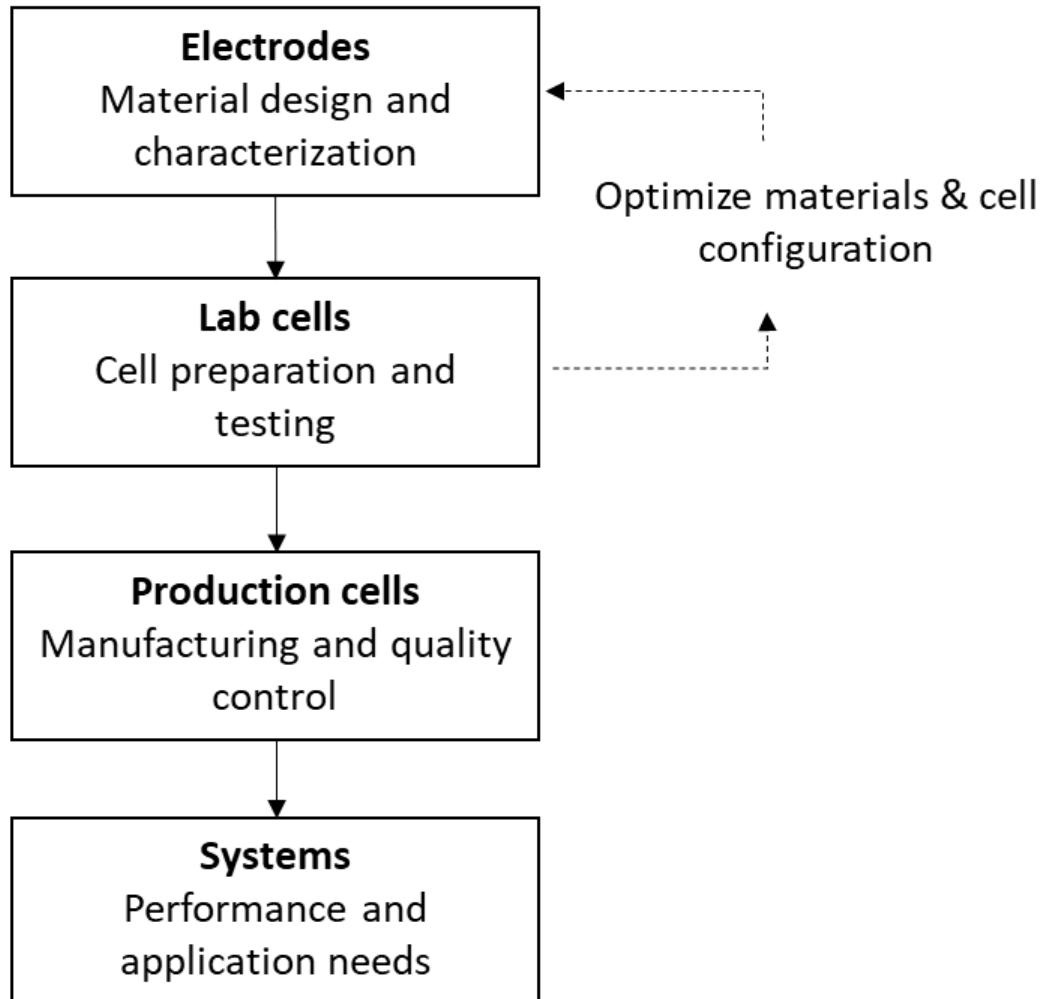
… But lab test conditions are different from field conditions

System operation
16 cells in series
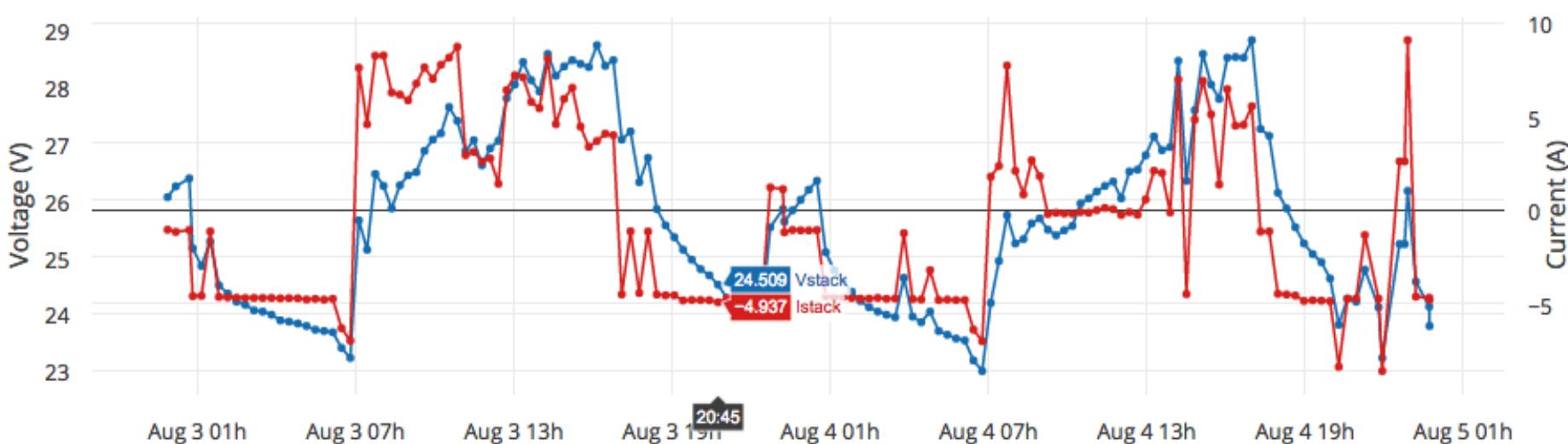
Single-cell testing
Red is current and green is voltage

4
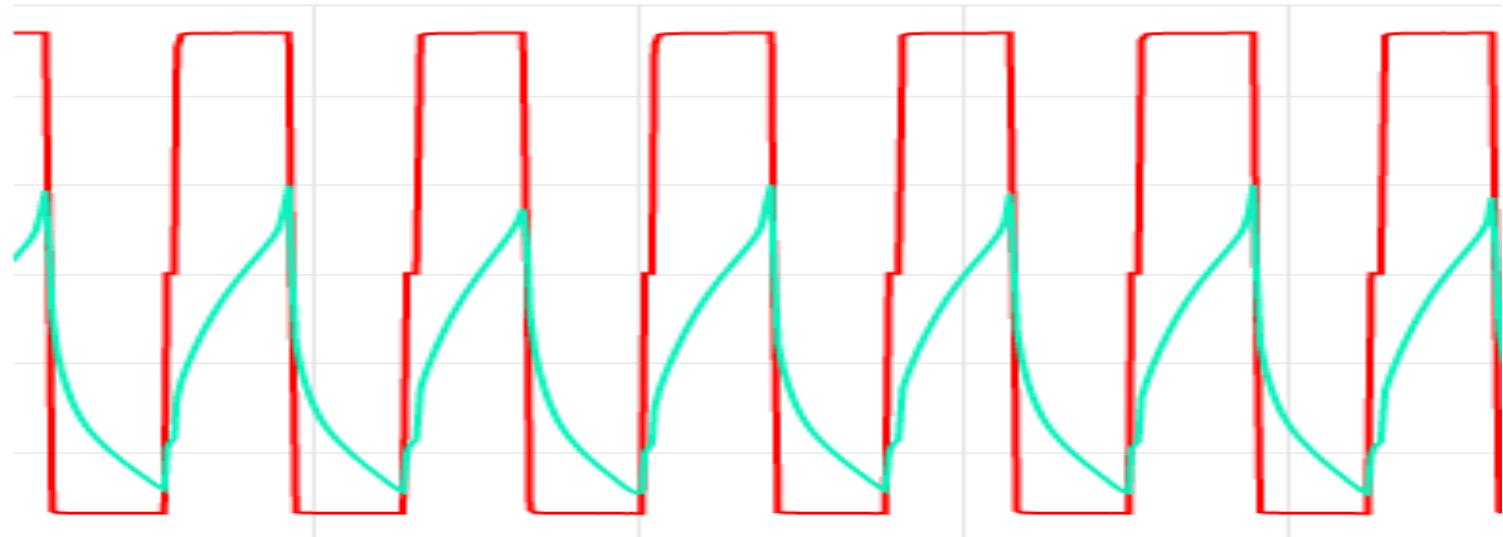
.. And sometimes, even mature commercial cells fail without warning

Cell voltage deviation pattern triggered as battery misbehavior

Reference: https://ieeexplore.ieee.org/document/9228907
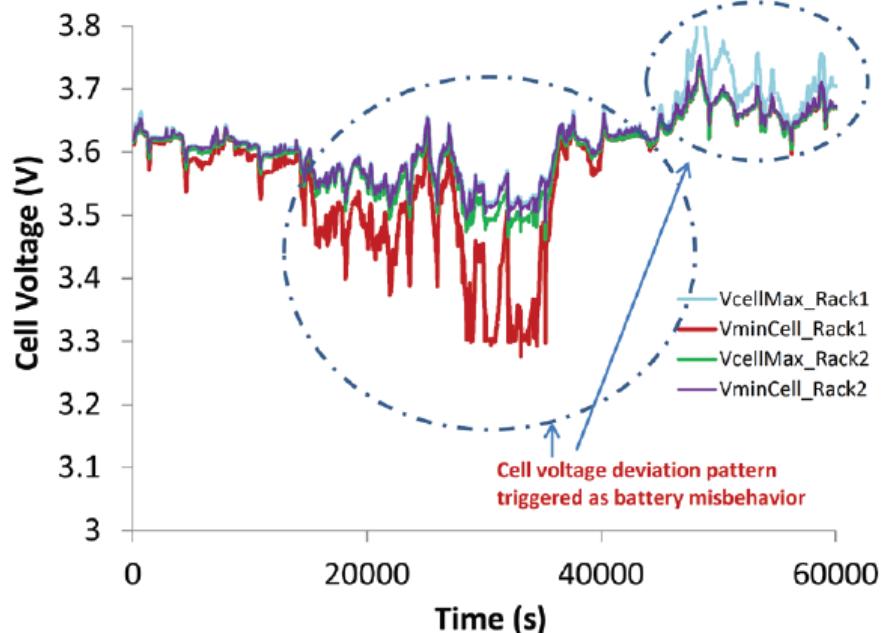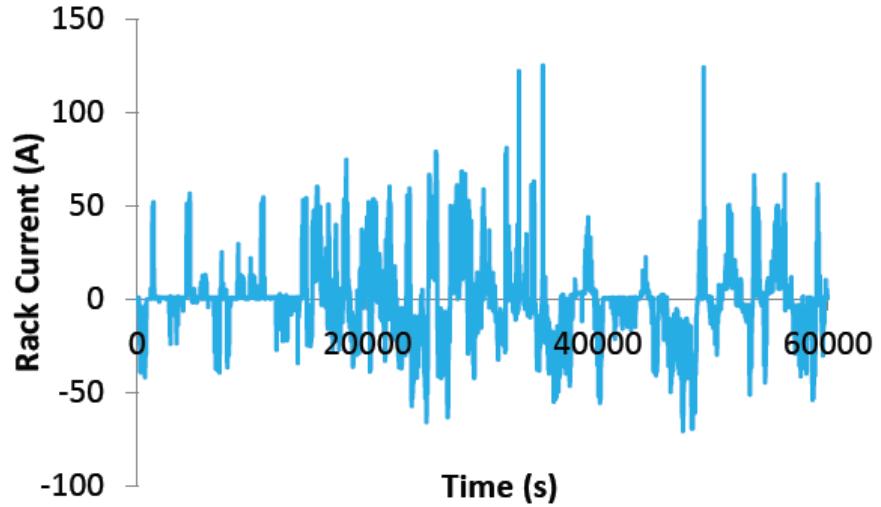
Software and data could help uncover and address problems early on

Aggregate data from different stages of development

Access existing cycling and system data

Standardize system data logging
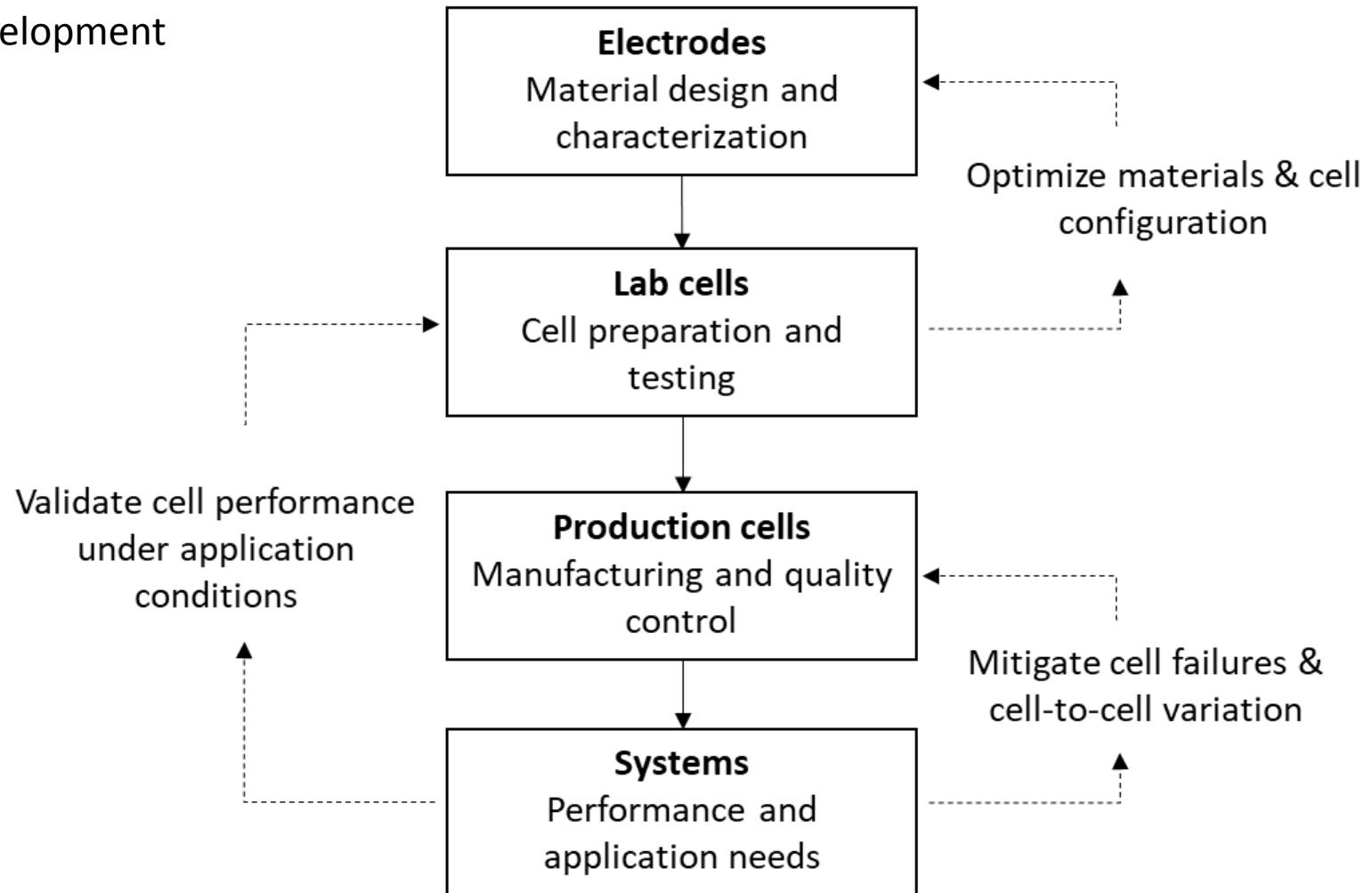
… But no commercial package includes all the tools needed by the battery industry

Open-source software can help: Innovation, Freedom, Integrity, Continuity, Sharing

There are over 2M open source projects on Github, and many contain the building blocks that we need

Open-source software powers smartphones around the world, supercomputing centers, and web servers

World-Wide Smartphone Sales (Thousands of Units)
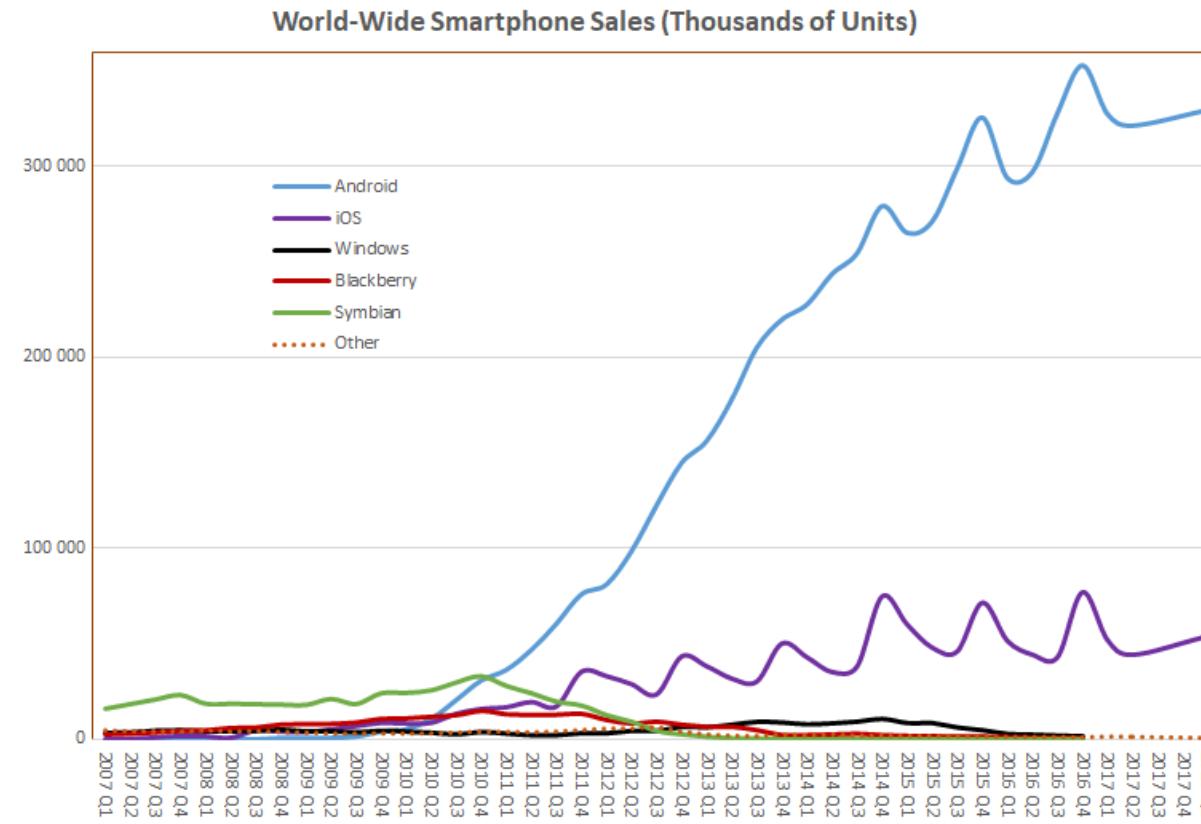
Not even apple can compete with open-source software!

# Large datasets have opened areas of research and software innovation

Fei-Fei Li: "Map the entire world of objects" (2009)
Allowed object classification ability to reach 97.3% (higher than human abilities)
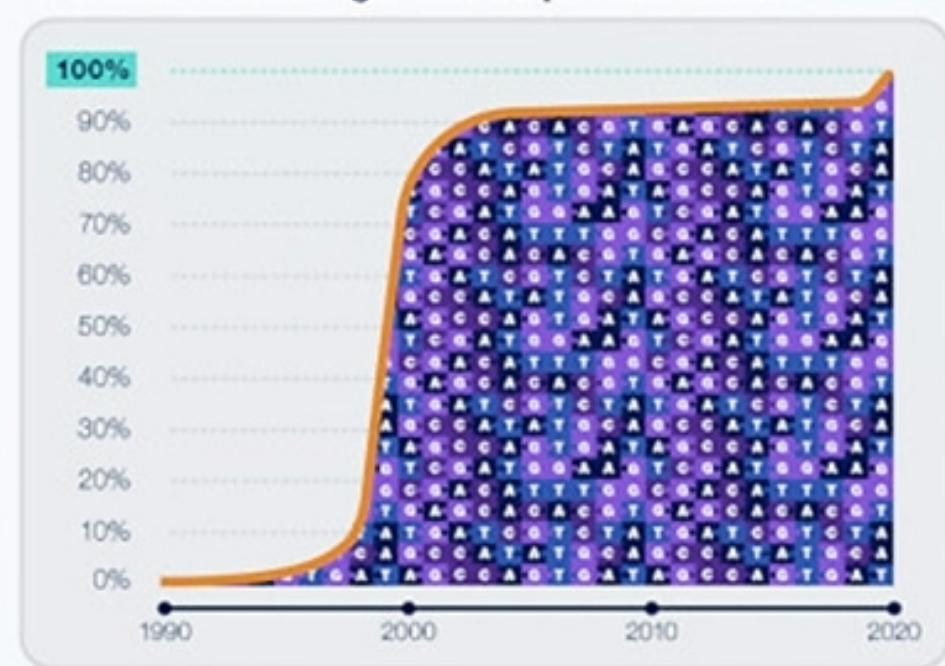
Deeper knowledge of human sequence variation has begun to alter the practice of medicine

We are learning what data and tools are also needed through our research activities

Field Application Data (ESTP, Demonstrations)
Collect normal & abuse data and environmental effects (T, humidity) from field systems (EPRI/SNL Report)

DC-Rack Data with Power Electronics (ESCAL, APEX)
Determine the impact of DC power quality (pulses and harmonics) on cell behavior

Module-Level Data (BEST, BATLab)
Assess the effect of cell-to-cell variation on safety and performance

Lab Cells Data (BTF, BATLab)
Design industry-relevant performance & abuse testing and quality assurance checks using data from all layers

Linking datasets at Sandia

Central database

As a result, we launched the first web-based public battery cycling database
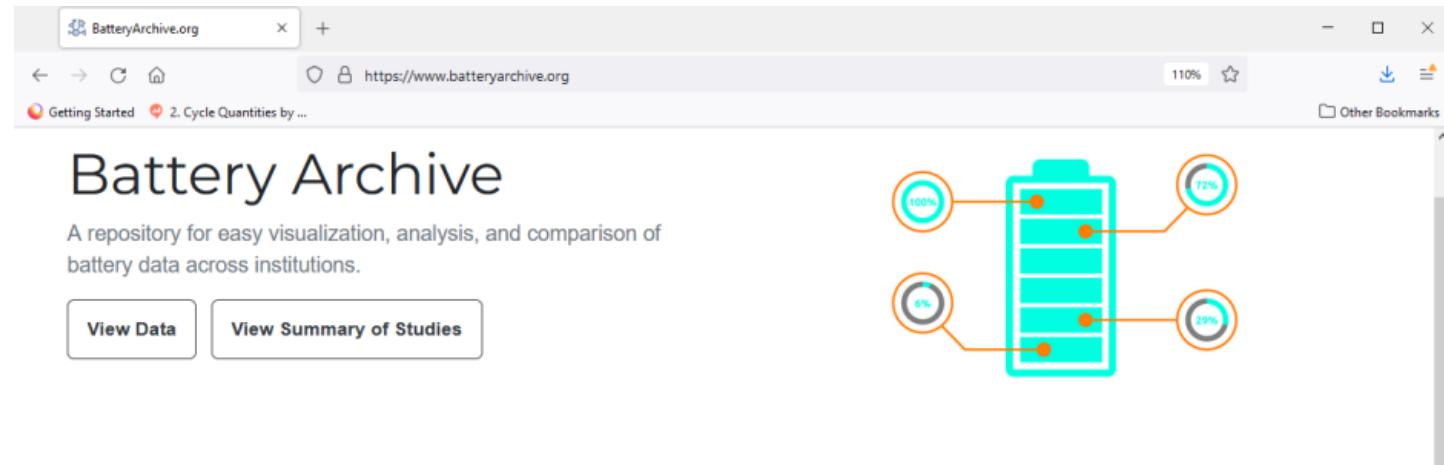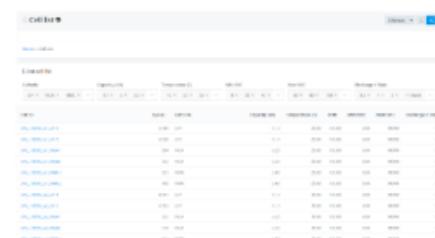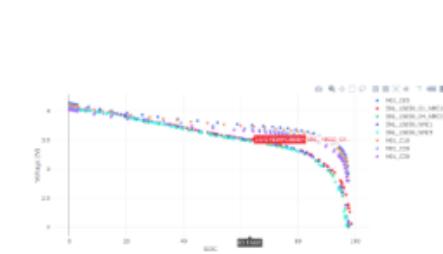
www.batteryarchive.org

Search by metadata or cycling conditions

Cell list

Cathode
LFP × | NCA × | NMC × | ∨

Capacity (Ah)
3.2 × | 1.1 × | 3 × | ∨

Temperature (C)
15 × | 25 × | 35 × | ∨

Min SOC
0 × | 20 × | 40 × | ∨

Max SOC
60 × | 80 × | 100 × | ∨

Discharge C Rate
0.5 × | 1 × | 2 × | +1 more | ∨

Home > Cell List

Li-ion cell list

Cell ID	Cycles	Cathode	Capacity (Ah)	Temperature (C)	DOD	MIN SOC	MAX SOC	Discharge C Rate
SNL_18650_G1_LFP5	3,545	LFP	1.10	25.00	100.00	0.00	100.00	1.00
SNL_18650_G1_LFP6	3,636	LFP	1.10	25.00	100.00	0.00	100.00	1.00
SNL_18650_G1_NCA1	654	NCA	3.20	25.00	100.00	0.00	100.00	1.00
SNL_18650_G1_NCA2	522	NCA	3.20	25.00	100.00	0.00	100.00	1.00
SNL_18650_G1_NMC1	521	NMC	3.00	25.00	100.00	0.00	100.00	1.00

Access standard quantities and download the data
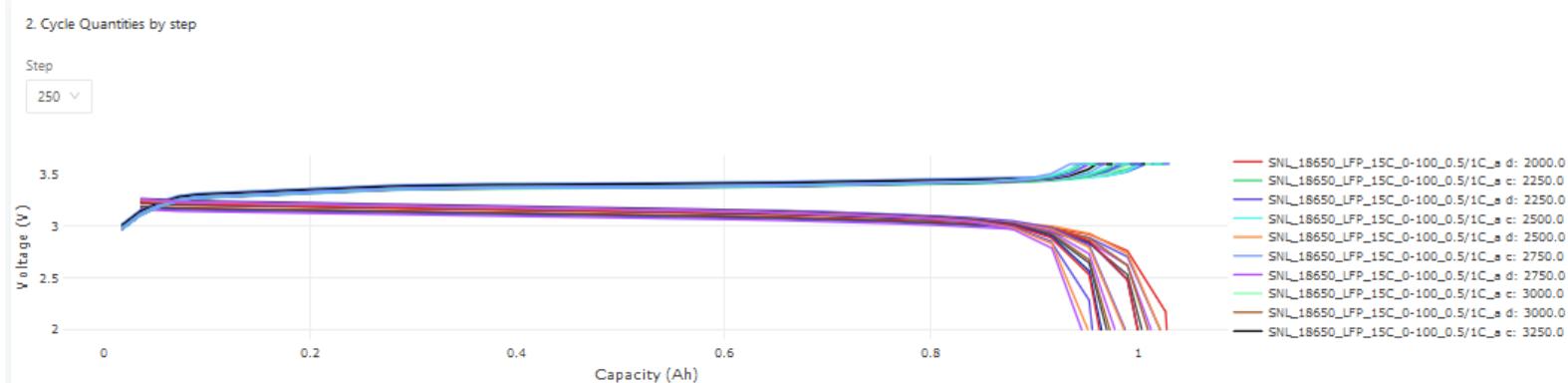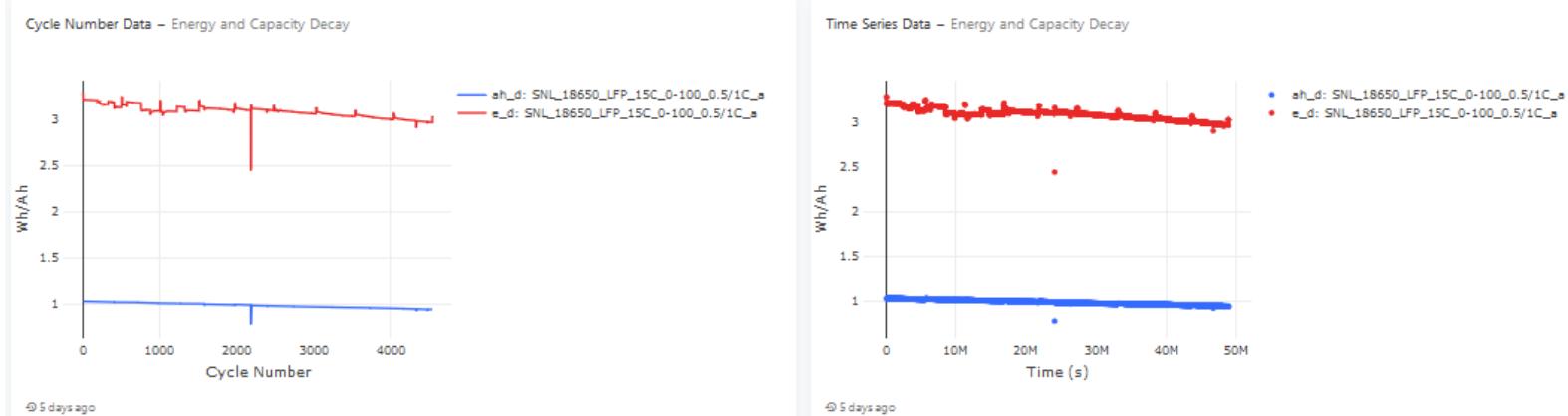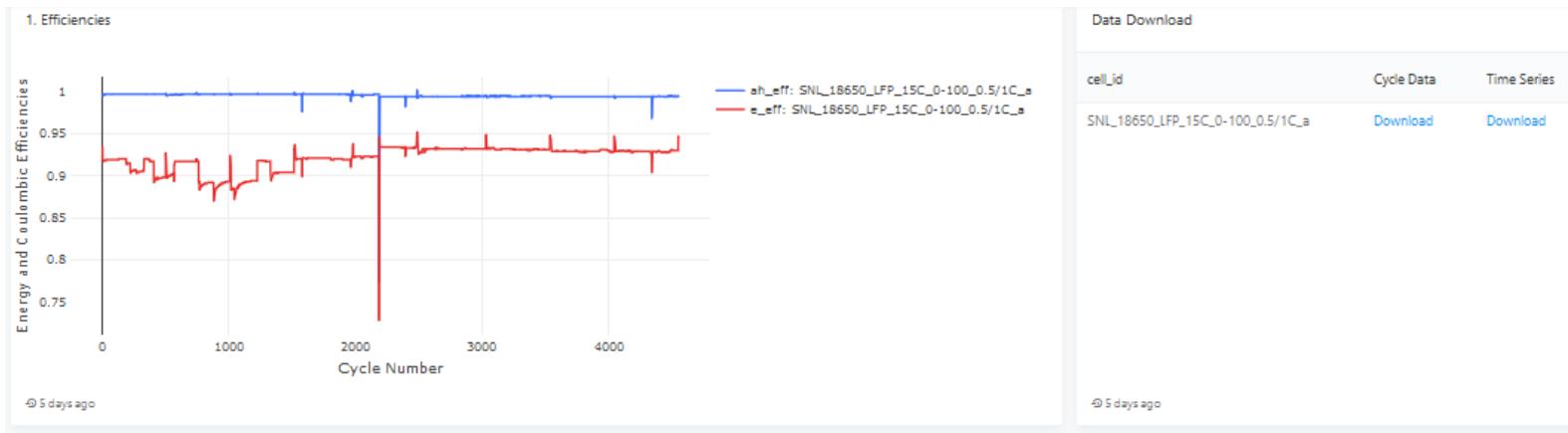
Many different motivations for using Battery Archive

Over 11,000 site users, many return visits, from over 50 countries, academia, and industry

- Representatives of utilities installing energy storage systems who are trying to get a better sense of what conditions exacerbate battery degradation

- Researchers in universities and companies who are trying to validate their battery degradation models with more data + class projects for undergrads

- Battery software start-ups which need data to test their algorithms and product (new data collection would be expensive)

- Individuals at companies that already have battery data and want to compare their results with available technologies

- And more…

More datasets will be made available

Make battery data easily available for general public use:

- Current data: single cell Li-ion cycling (UL, SNL, HNEI, Oxford …)

- In the works: single cell mechanical abuse data and calorimetry (SNL, ORNL)

- Next: module data and system data

Long term:

- Cell to system for cycling and abuse data for Li-ion and emerging technologies

Example of cell abuse data
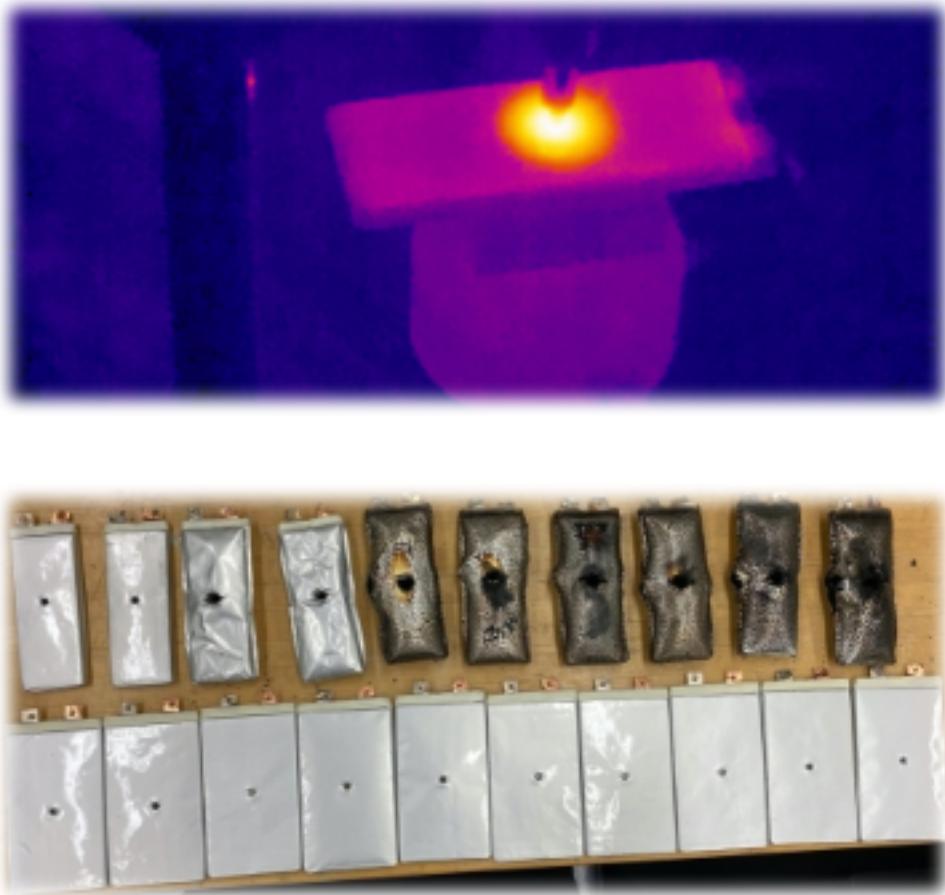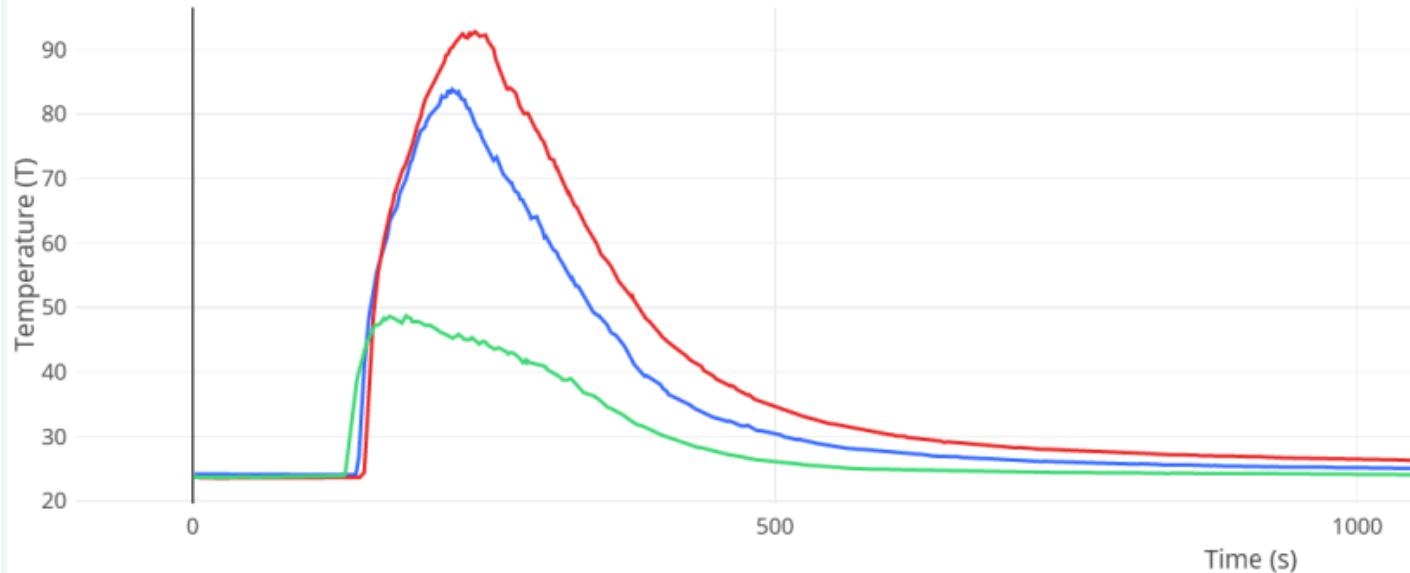
Aggregating data from a single standard protocol for battery abuse can enable the prediction of thermal runaway risks for new cells.

Not all the data can be shared: the need for private data repositories

Released the software that powers battery archive as an open-source project

https://github.com/battery-lcf
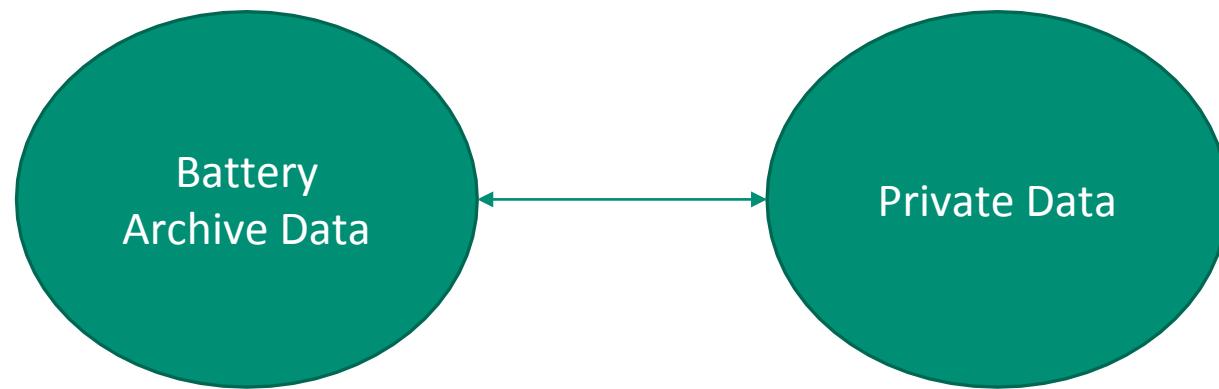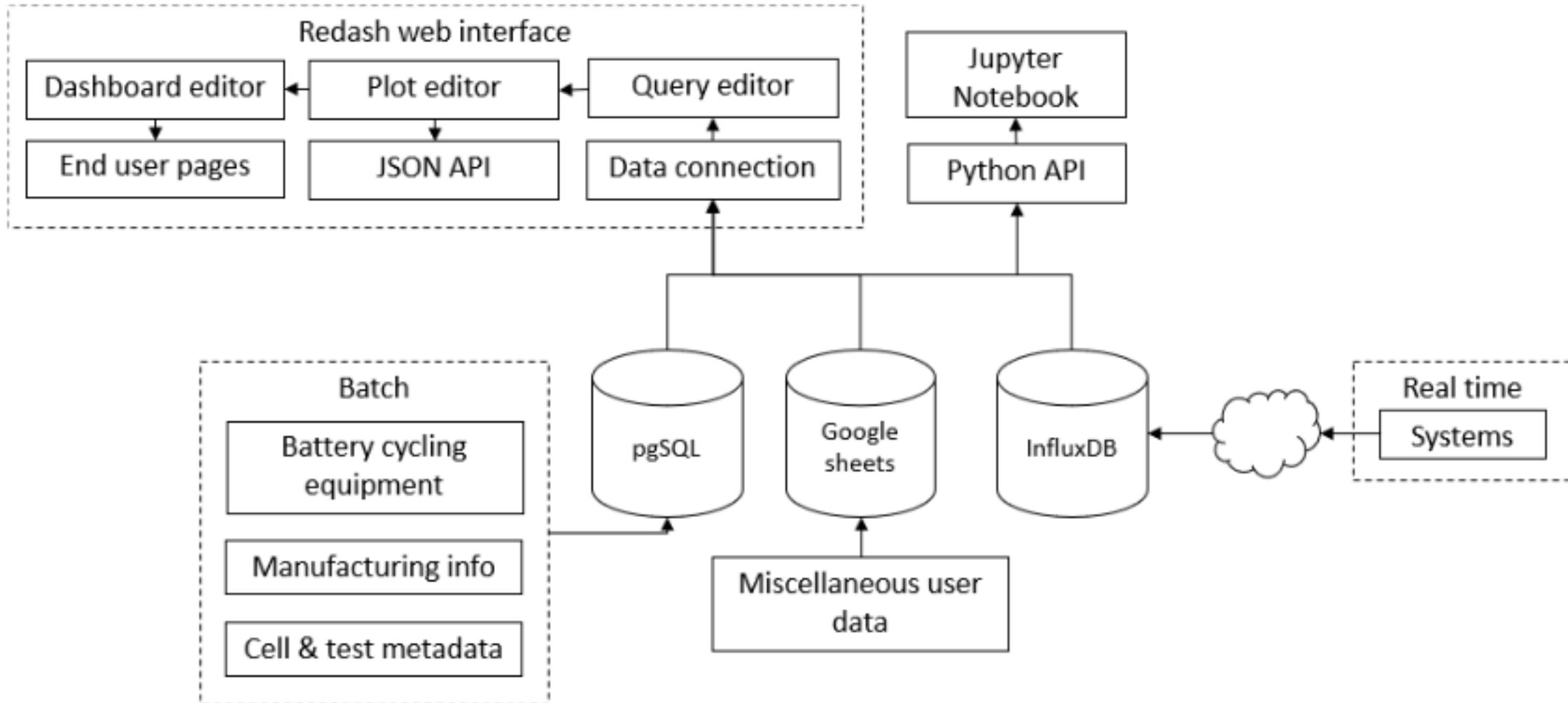
Researchers interact only with a web interface to browse and plot their data
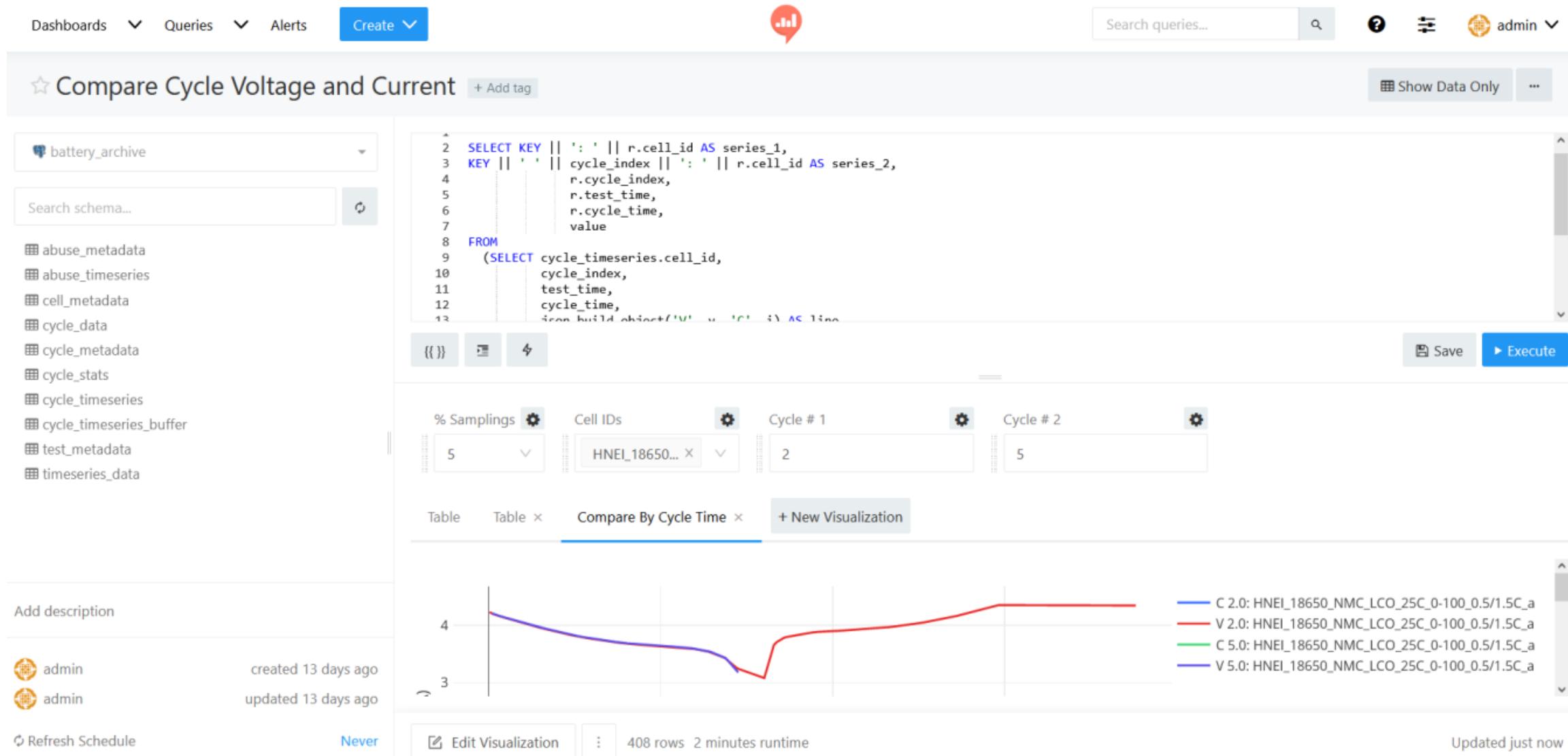
Consolidate data from manufacturing to systems

Production Data

cell_id ▲	study	Anode Batch ID	Cathode Batch ID	Anode Weight (kg)	Cathode Weight (kg)
C012320A-038	3-pulse+1-cycle-Battery 1-SBT	A - 011520	C - 110819	0.98	1.80
C012320A-041	3-pulse+1-cycle-Battery 1-SBT	A - 011520	C - 110819	0.98	1.80
C012320A-045	3-pulse+1-cycle-Battery 1-SBT	A - 012120	C - 110819	0.96	1.86
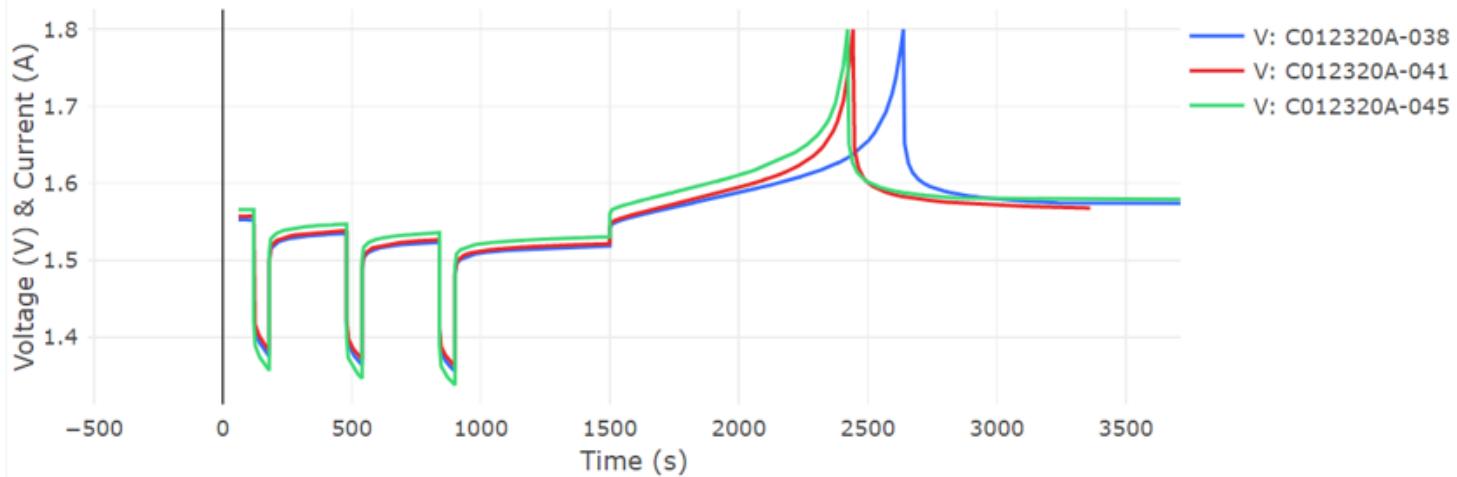
Cell Pulse Testing   System Data
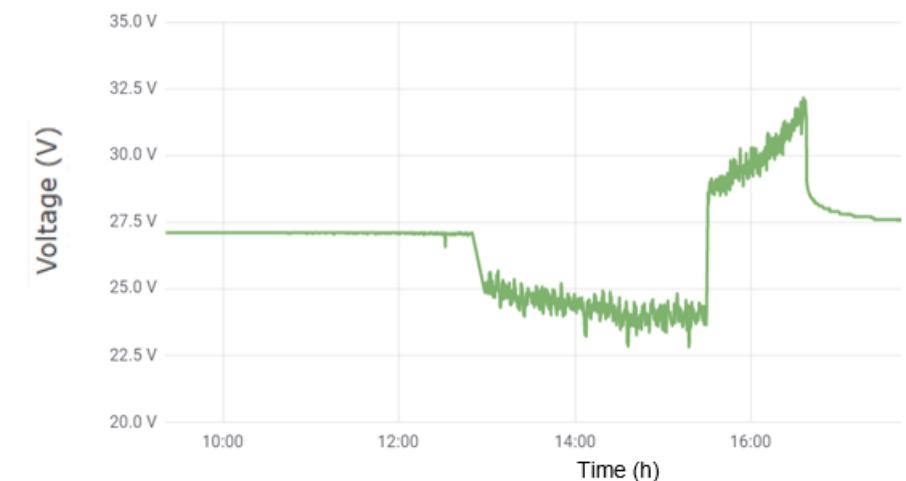
Linking different types of data across the battery lifecycle can accelerate the optimization of materials and cell configurations.

Use our open-source packages through standard REST APIs

Leverage existing resources from the community instead of redeveloping tools

Integrate with other software packages and systems
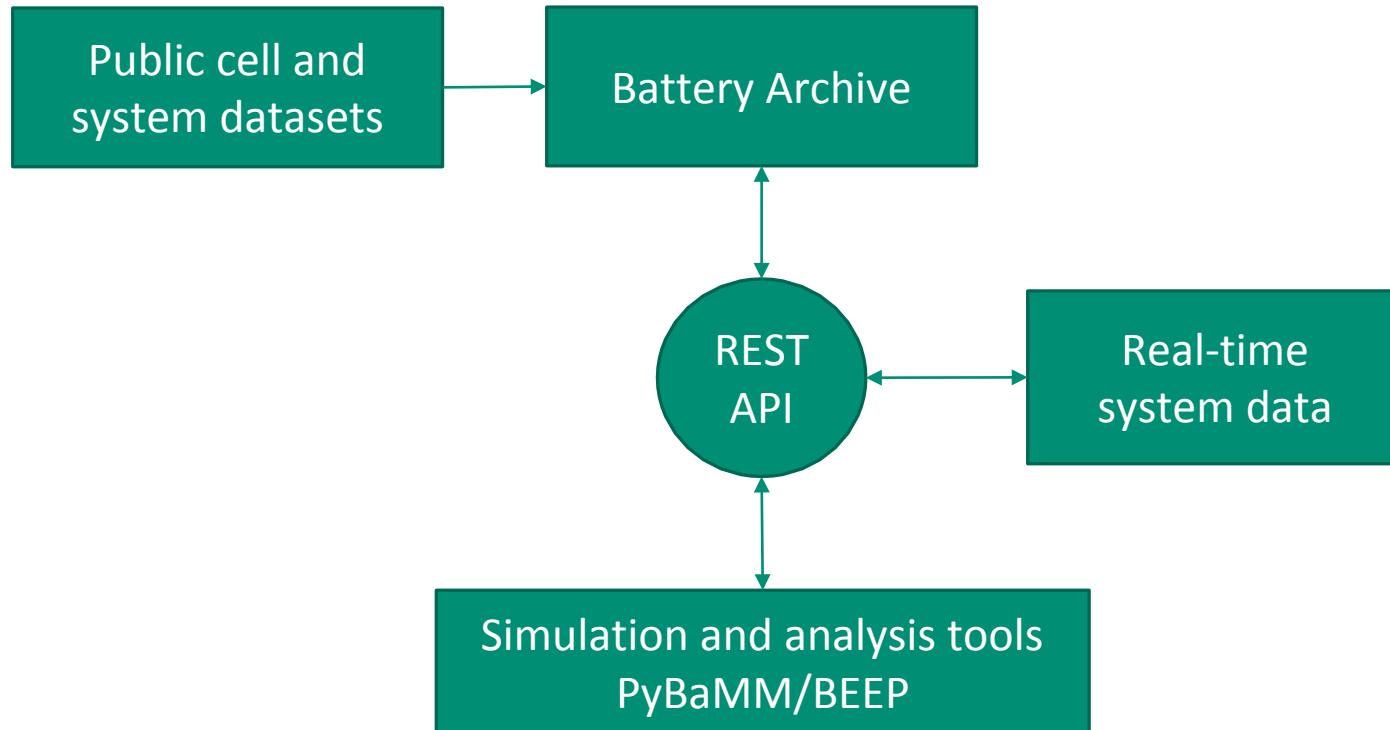
Comparison with simulation results from PyBaMM

Open source Python library (Faraday Institution) to solve physics-based electrochemical DAE models using DFN and SPM.

Run cycling protocols that match lab profiles.

```
[ ]  pybamm.set_logging_level("NOTICE")

     ncycle = 500 # total number of cycles to run

     experiment = pybamm.Experiment([
         (f"Discharge at 1C until {Vmin}V",
          "Rest for 1 hour",
          f"Charge at C/2 until {Vmax}V",
          f"Hold at {Vmax}V until C/50"
         )
     ] * ncycle,
     termination="80% capacity"
     )
```

Sulzer, V., et. al. (2021). Journal of Open Research Software, 9(1).
https://github.com/pybamm-team/PyBaMM

Cycle 50 (C/2 charge, 1C discharge)

Conclusions
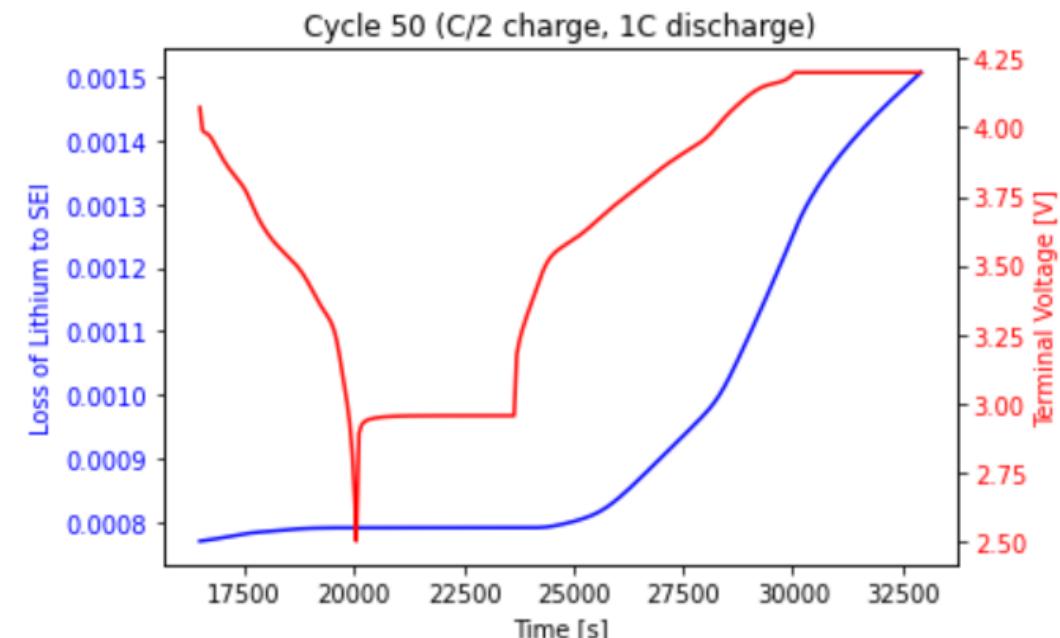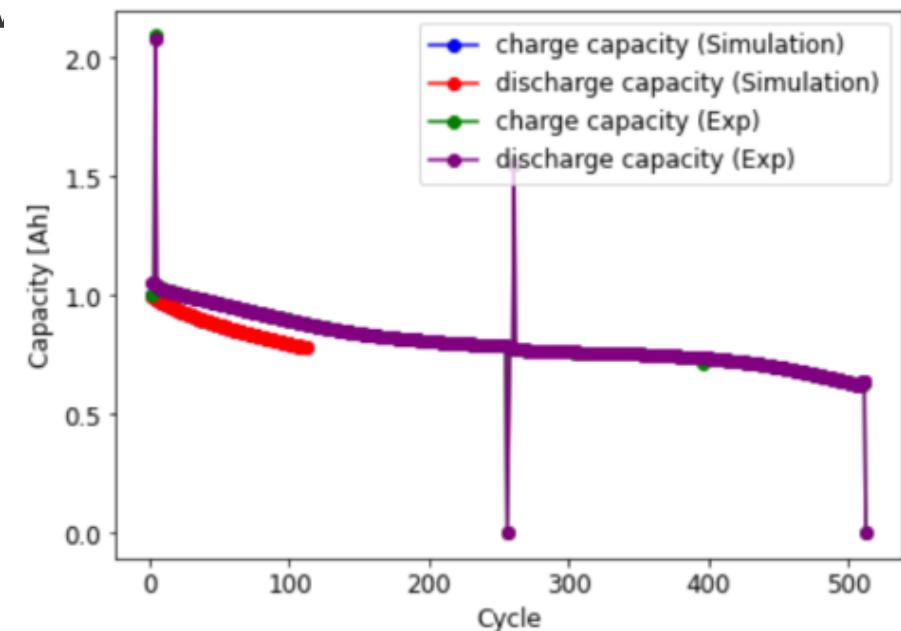
Provide data and tools to facilitate the progress of new battery technologies

- Starting a repository of public data and building a community of users

- Providing open source tools to maintain private datasets

- Linking data, models, and system control

To join the open-source projects or for more information on how to use the software systems, please contact vdeange@sandia.gov