The Digital Edge:
How Data Drives Battery Breakthroughs

Dr. Simon Clark, Senior Researcher, SINTEF

ElectRObatt – Bucharest, Romania – Nov 1, 2024

Teknologi for et bedre samfunn

'Godfather of AI' shares Nobel Prize in physics for work on machine learning

OPINION

Did AI just win the Nobel prizes in physics and chemistry?

Opinion | When AI looked at biology, the result was astounding

The Nobel Prize in chemistry honored a real-world example of how AI is helping humans.

Embracing digital tools and workflows
~~can help give you an edge in your research~~
is becoming an essential part of research

Digital Optimization Workflows
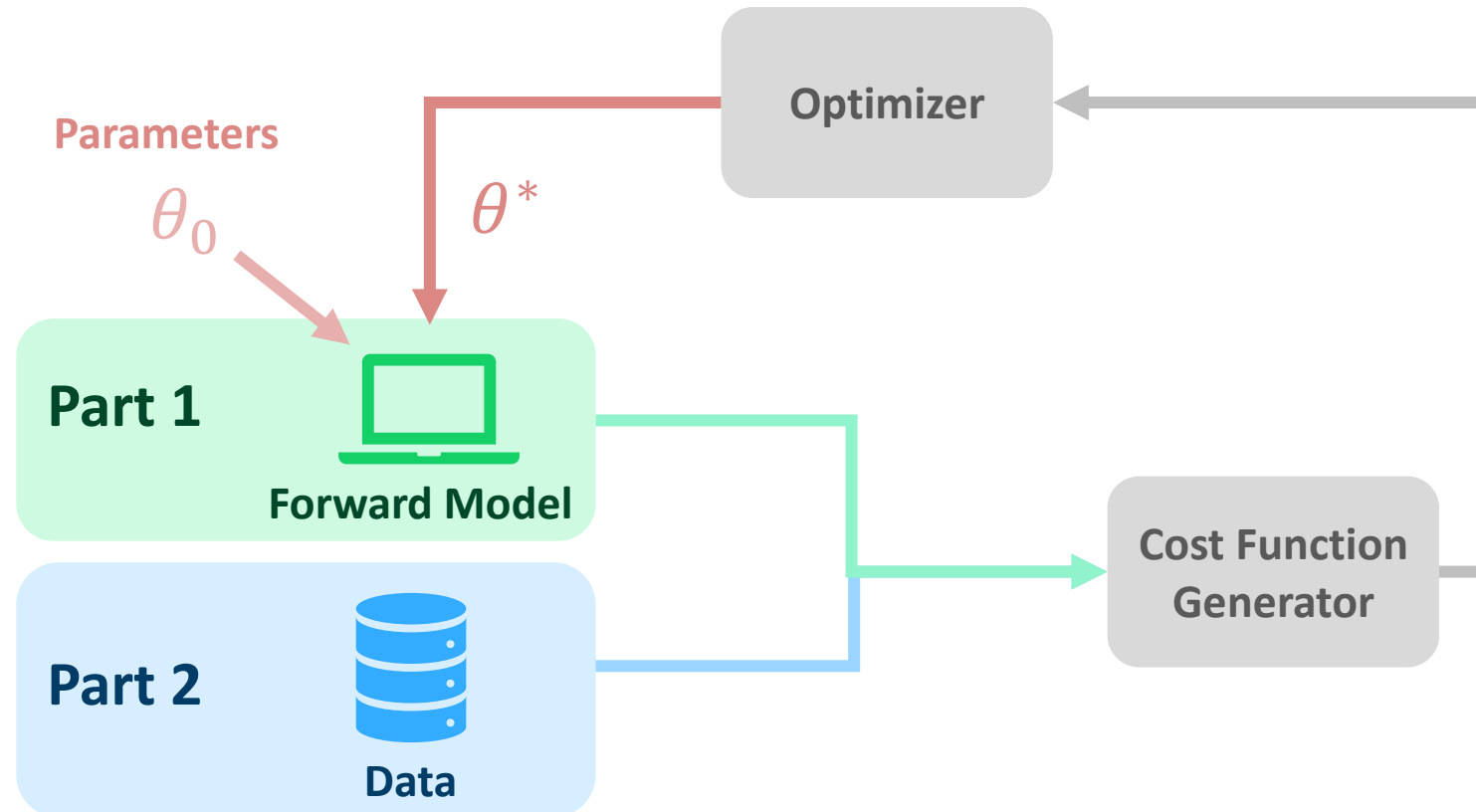
Example: Parameter Calibration

What is BattMo?

Name: Battery Modelling Toolbox

Created: 2019

Language: Julia / MATLAB

Version: 0.3.0-beta

Base Model: PXD Newman Model with Concentrated Solution Theory

Method: Finite Volume Method

Chemistry: Li-ion, Metal-Air, AEM Electrolyzer

Features: 3D cell geometries, Fast solutions
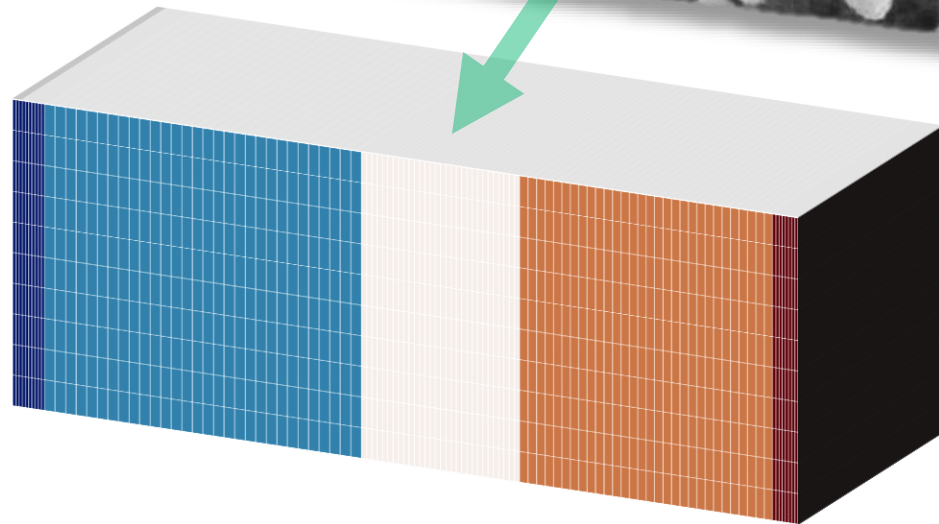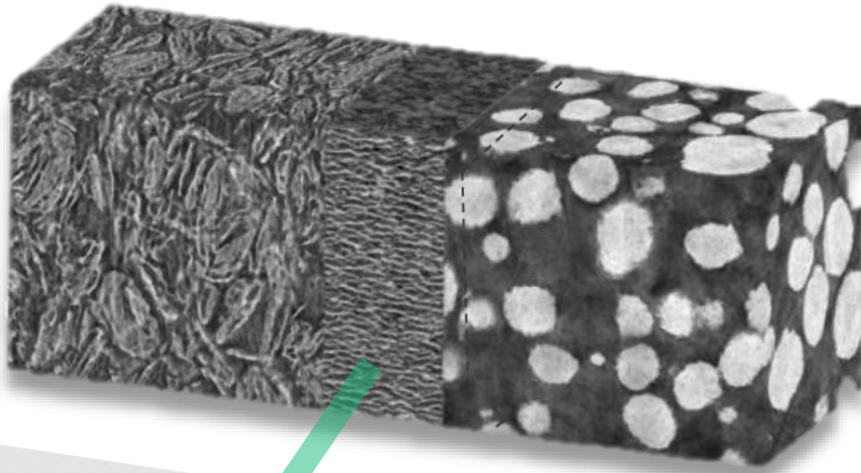Friendly web-app user interface

BattMo

What is BattMo?

BattMo simulates battery performance

BattMo **discretizes battery geometry** into a set of **finite volumes**, where it can solve **physics-based DFN equations for material transport, kinetics, and thermodynamics**

- negative electrode current collector
- negative electrode coating
- separator
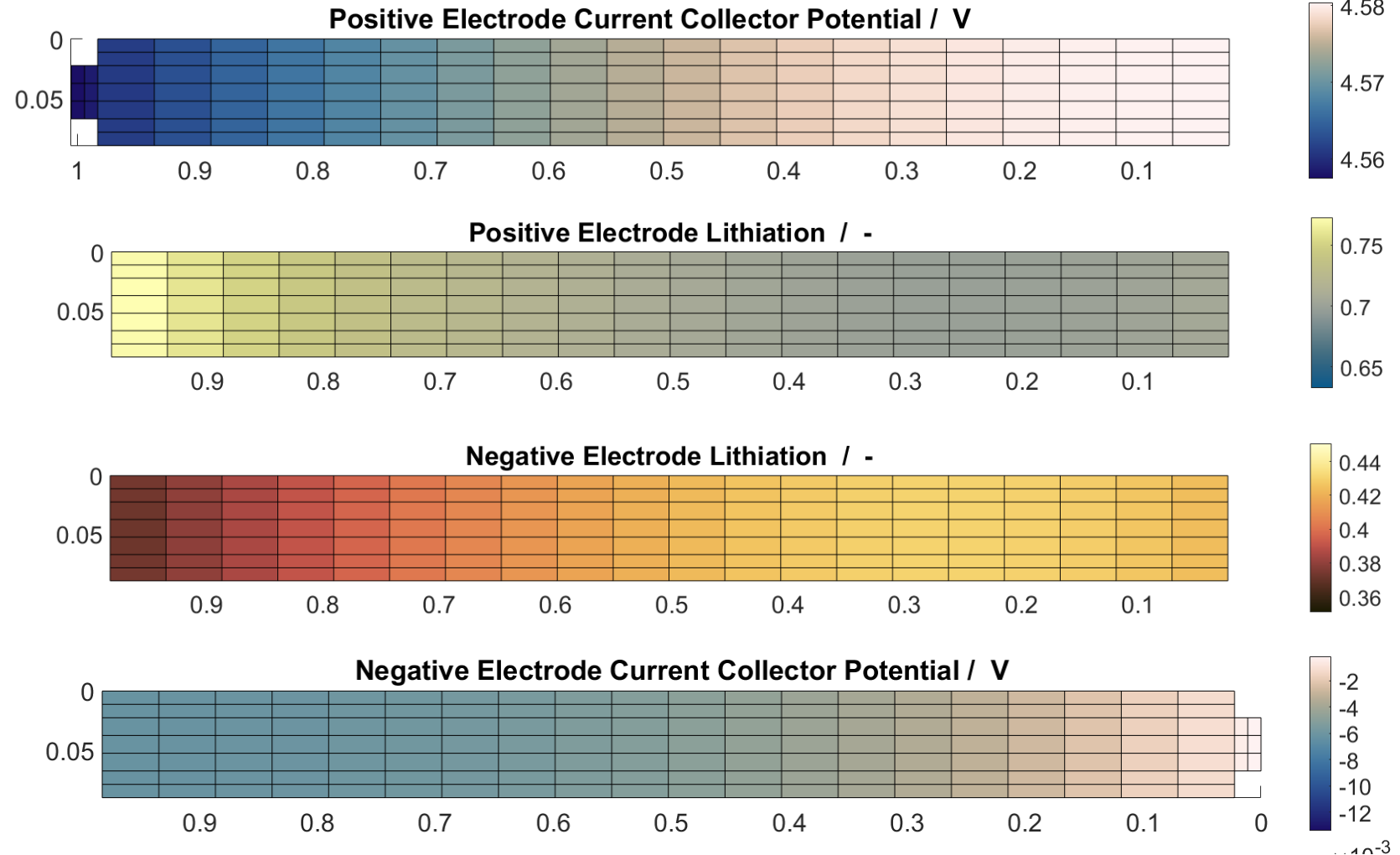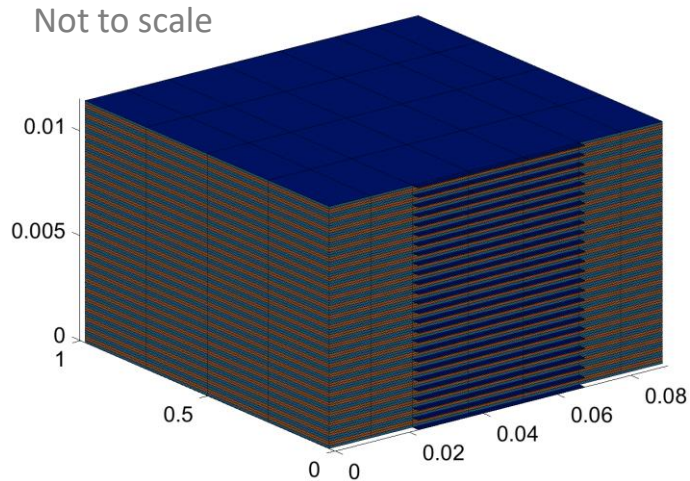- positive electrode coating
- positive electrode current collector

Teknologi for et bedre samfunn

What can BattMo do?
BattMo has a library of common materials and formats

SINTEF

BattMo developers are leaders in battery research and keep updated libraries of material and cell design parameters

Not to scale

Positive Electrode Current Collector Potential / V

Positive Electrode Lithiation / -

Negative Electrode Lithiation / -
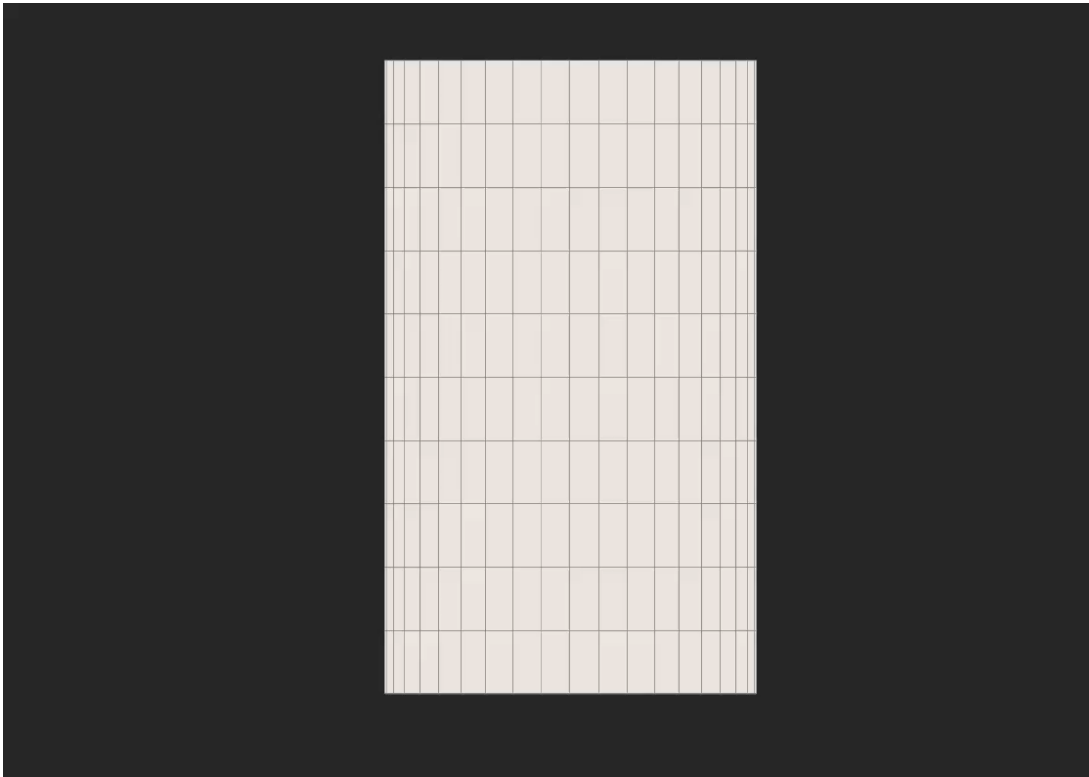
Negative Electrode Current Collector Potential / V

What can BattMo do?
BattMo simulates big batteries in 3D+

Industry is moving towards large format battery cells (Tesla 4680, BYD Blade, etc.)

Large cells are difficult to simulate! You need to solve millions of coupled partial differential equations. Most battery simulation frameworks rely on simplifying reductions.

👉 BattMo solves the **full set of equations** on detailed **3D grids in minutes** – not hours. This gives **better insights with fewer assumptions**
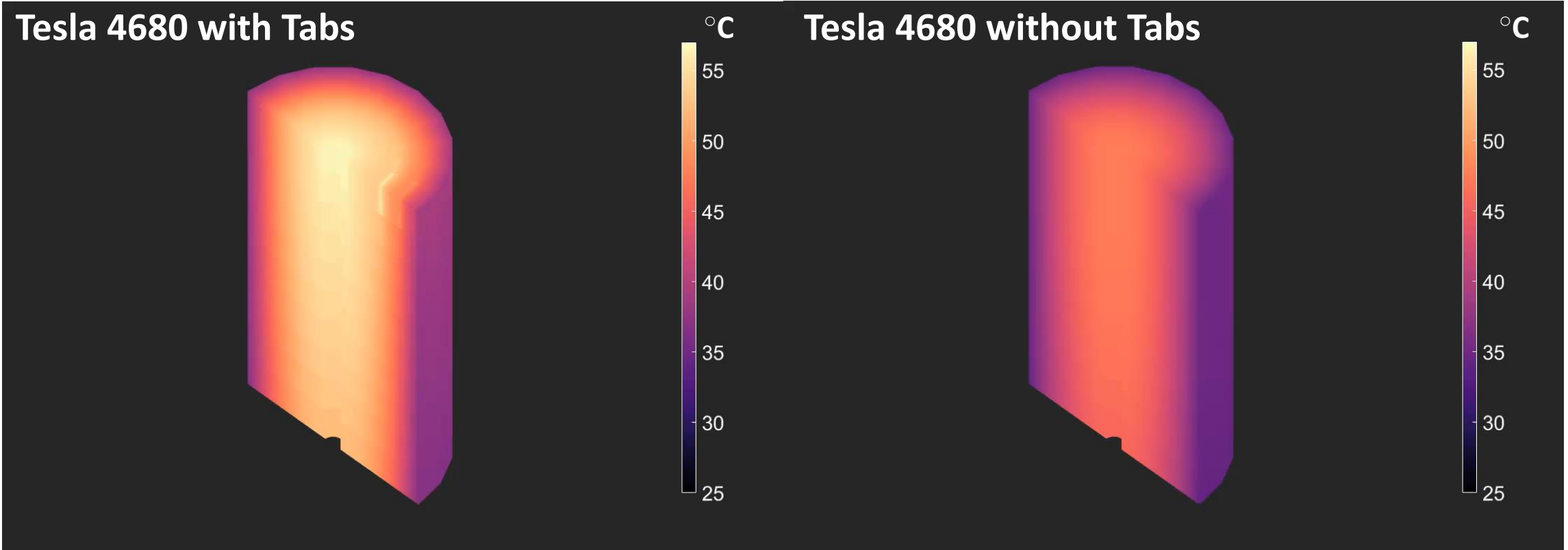
What can BattMo do?

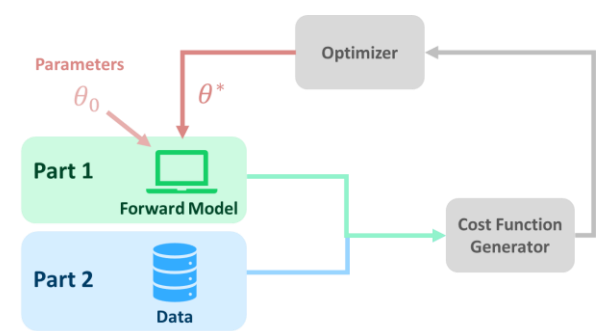## BattMo couples thermal and electrochemical performance

Temperature strongly affects electrochemical reactions and transport. BattMo solves them together, on the same grid. No need for co-simulation. Even for very large grids.
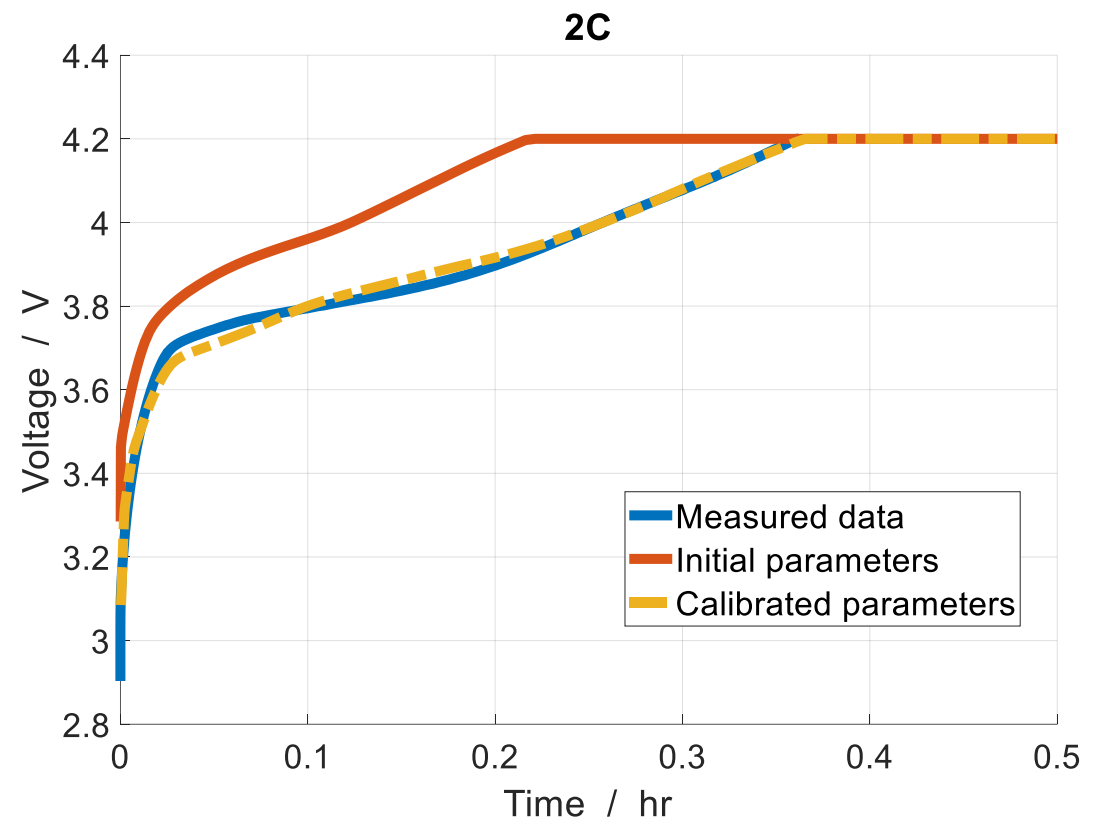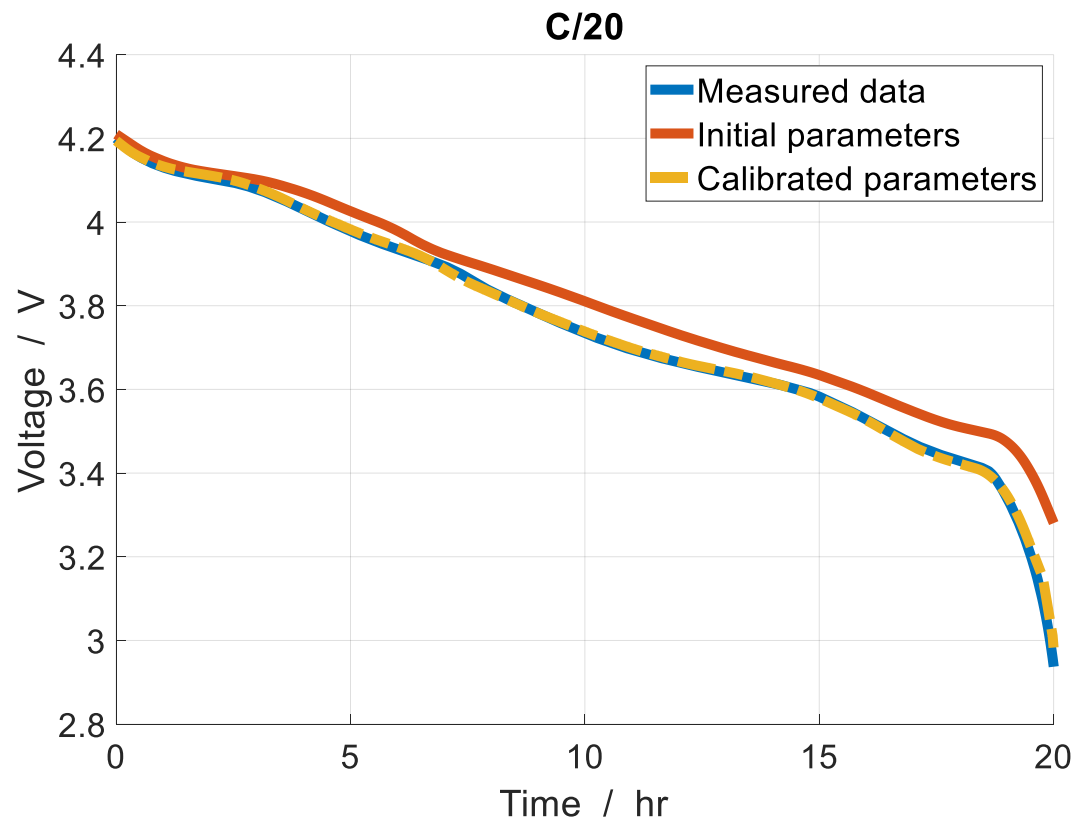
What can BattMo do?
BattMo does parameter calibration

Parameter calibration under low-rate and high-rate conditions help give robustness under different conditions

C/20

Legend:
- Measured data
- Initial parameters
- Calibrated parameters

2C

Legend:
- Measured data
- Initial parameters
- Calibrated parameters

Experimental data: Manuel Ank *et al* 2023 *J. Electrochem. Soc.* **170** 120536
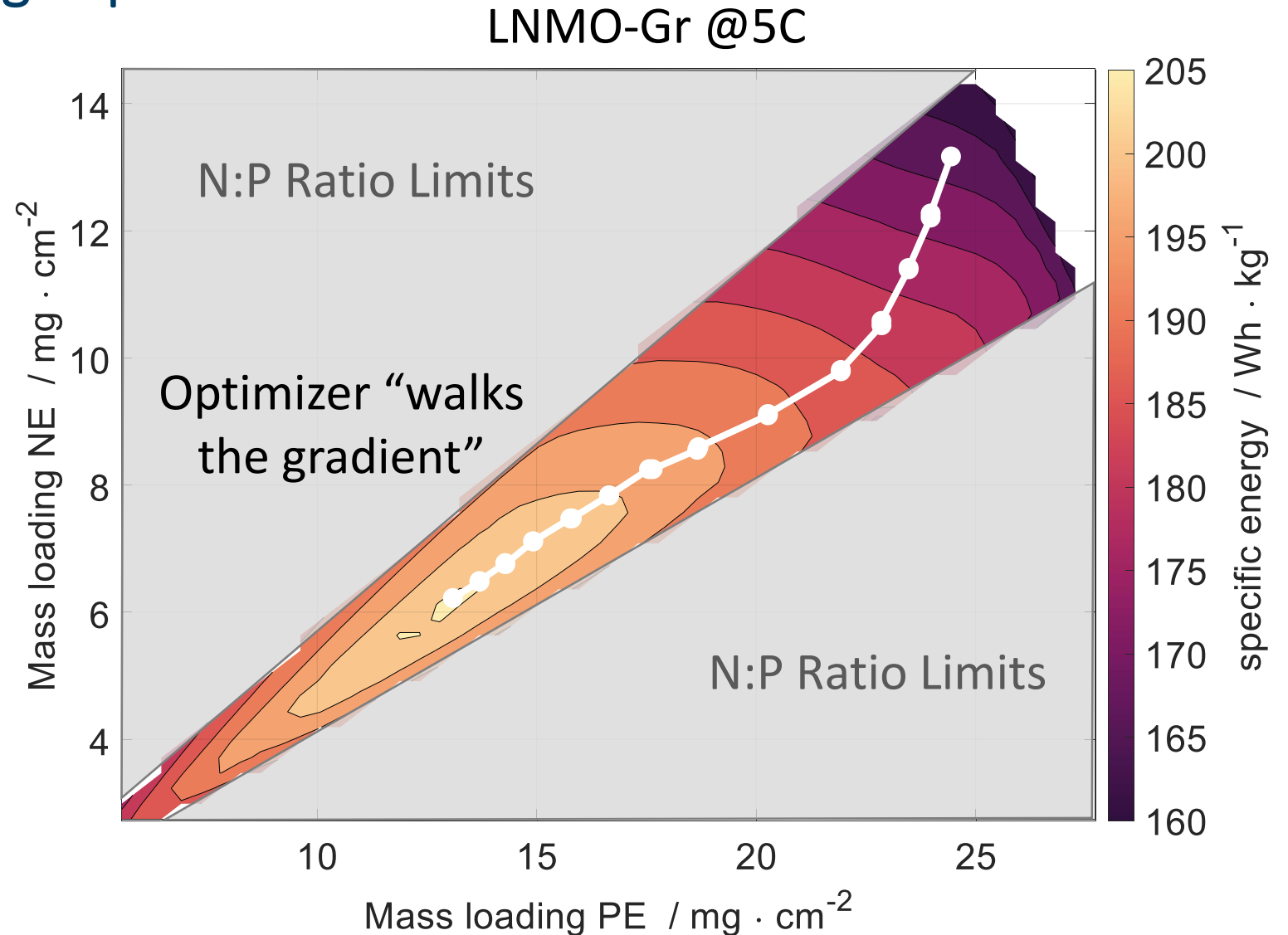
Teknologi for et bedre samfunn

What can BattMo do?
BattMo does design optimization

Gradient-Based Optimization

- Automatic Differentiation provides the gradients "for free"

- Gradient-based optimization can reduce the number of computations from hundreds to tens

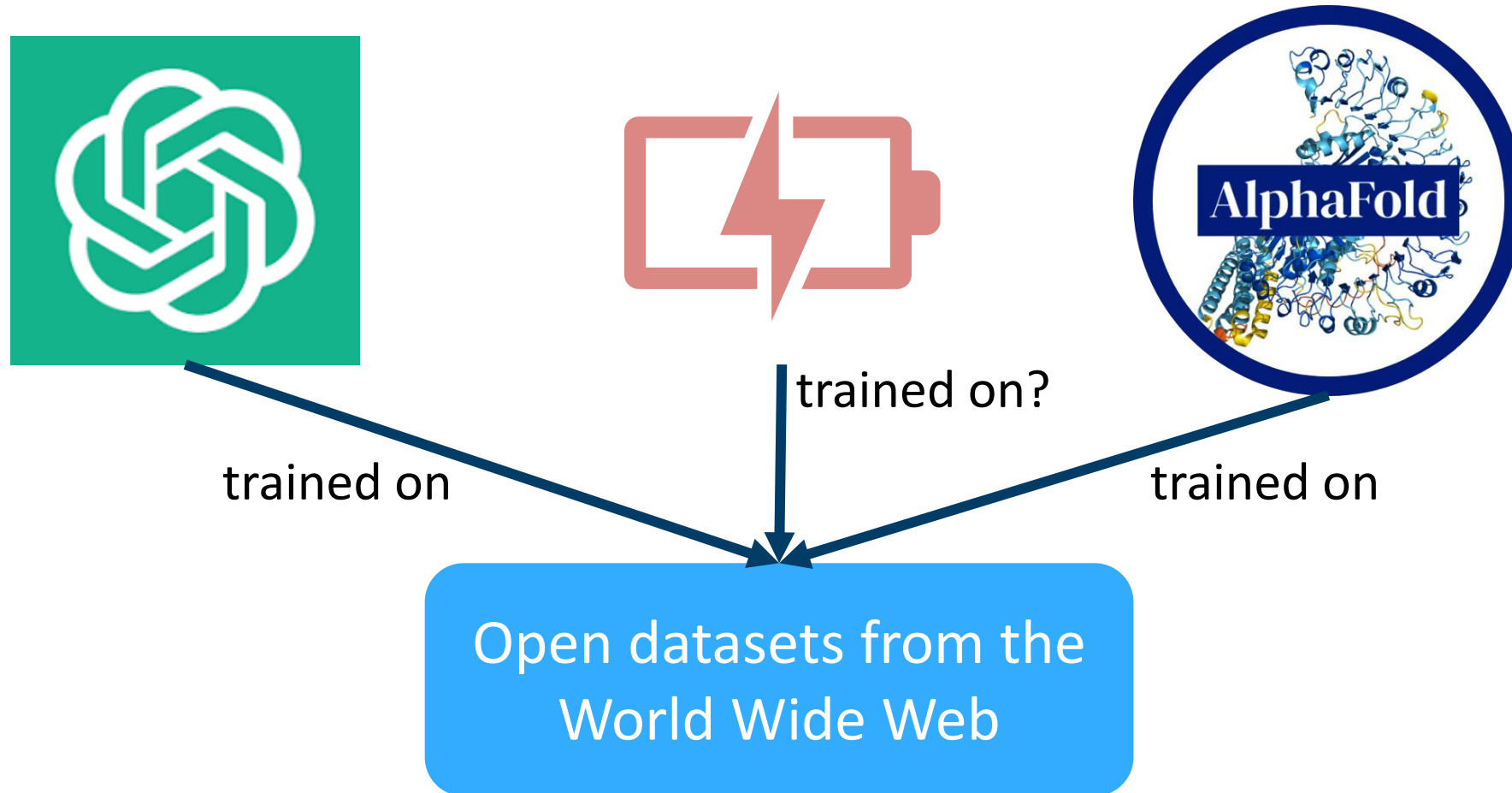- Good for design optimization and parameter calibration

LNMO-Gr @5C

What can BattMo do?
BattMo has a Web App - app.batterymodel.com

No source selected   ⚙ Properties   ▤ Filters

Scenes

Scene

Sources
- Video Cap
- Audio Inp
- Window (
- Display C

Audio Mixer

Desktop Audio   -inf dB
-60 -55 -50 -45 -40 -35 -30 -25 -20 -15 -10 -5 0

Mic/Aux   -inf dB
-60 -55 -50 -45 -40 -35 -30 -25 -20 -15 -10 -5 0

Scene Transiti...

Fade

Duration   300 ms

Controls

Start Streaming

Start Recording

rt Virtual Cam ⚙

Studio Mode

Settings

Exit

LIVE: 00:00:00   REC: 00:00:00   CPU: 0.5%, 60.00 fps

European Union

Practices for Pu...   W3 Cool URIs for the Se...   Streamlit document...   »   📁 All Bookmarks

BattMo. BattMo is a framework for continuum modelling of electrochemical devices. It simulates

Simulation

Results

Materials and models

BatteryModel.com   DOI 10.5281/zenodo.6362783   ⓞ GitHub   Doc BattMo-app

Digital Optimization Workflows

Example: Parameter Calibration

AI Needs Data!

trained on

trained on?

trained on

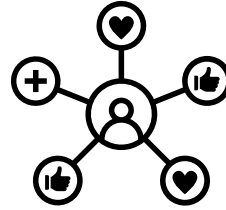Open datasets from the World Wide Web

World Wide Web (1989)

"Many of the discussions of the future at CERN end with the question - *Yes, but how will we ever keep track of such a large project?* This proposal provides an answer to such questions."

This was the beginning of the modern world-wide web, born from a need to improve research data management.

Semantic Technologies

Methods, standards and tools to attach meaning to data, and so enable *representation, integration and processing*
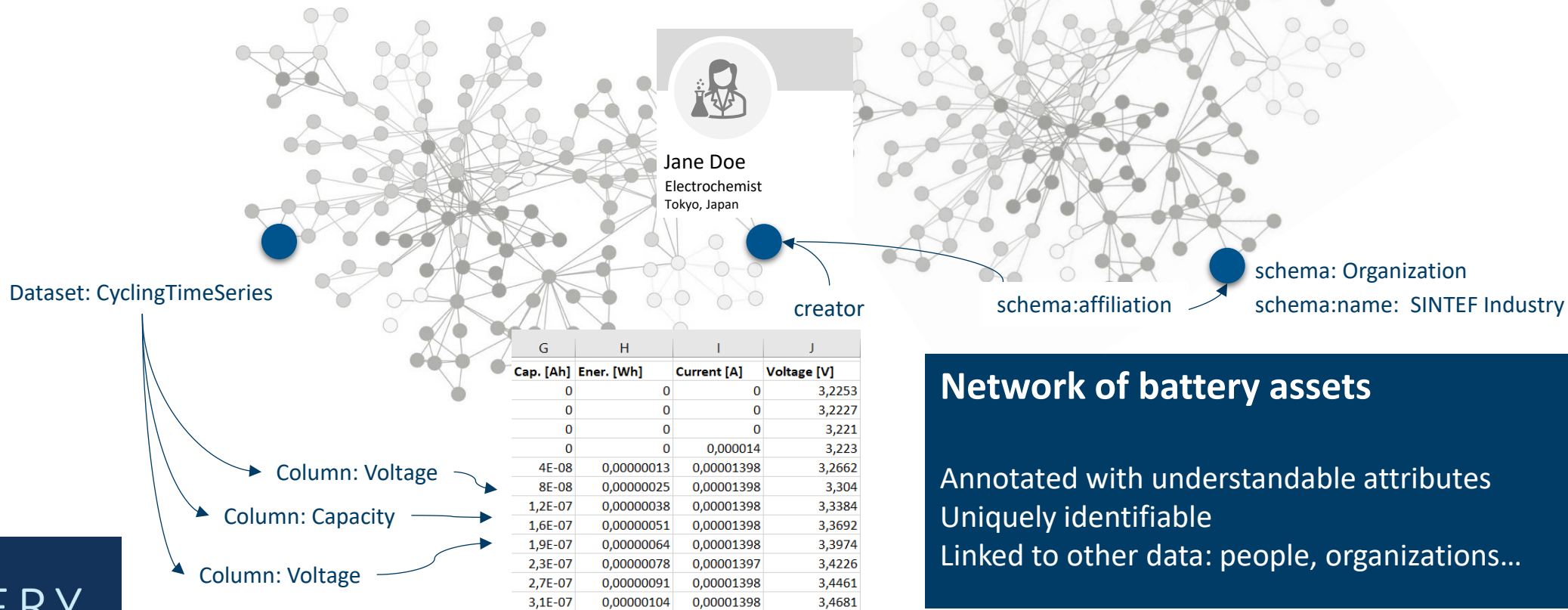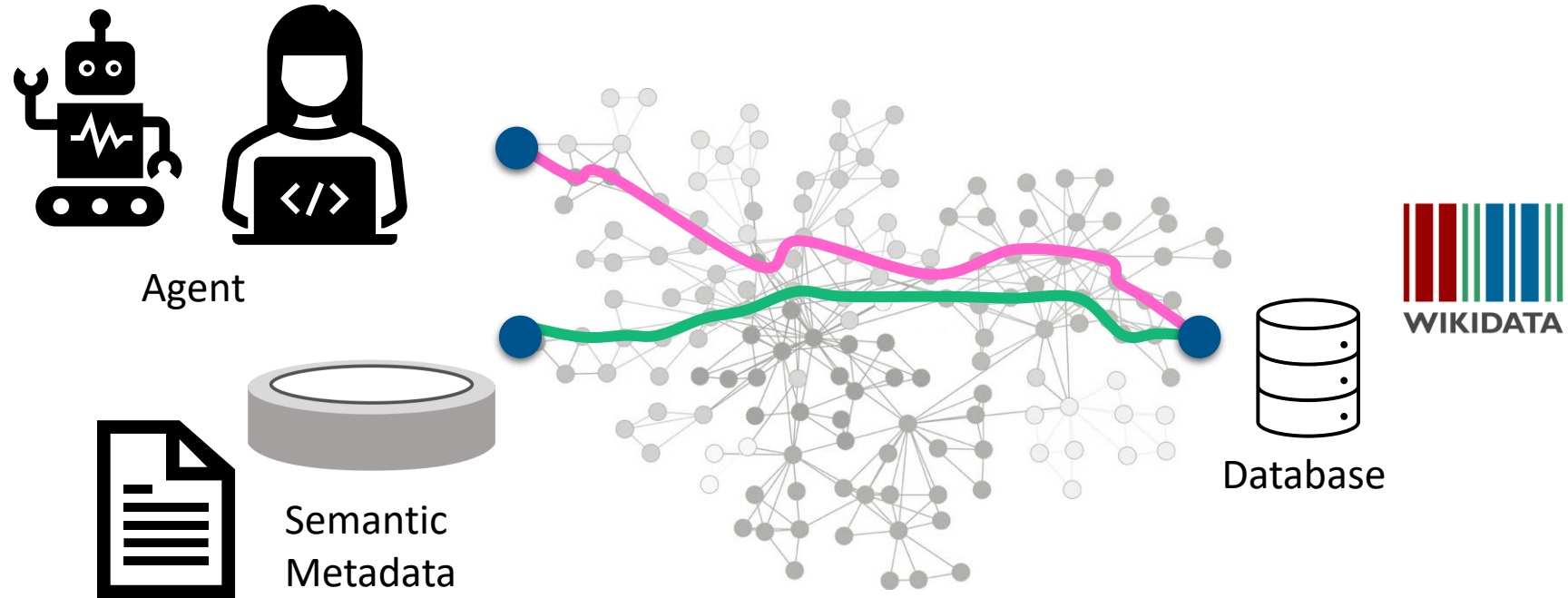
Semantic Technology

Battery Data Networks

Dataset: CyclingTimeSeries

Jane Doe
Electrochemist
Tokyo, Japan

creator

schema:affiliation

schema: Organization
schema:name: SINTEF Industry

Column: Voltage

Column: Capacity

Column: Voltage

G	H	I	J
Cap. [Ah]	Ener. [Wh]	Current [A]	Voltage [V]
0	0	0	3,2253
0	0	0	3,2227
0	0	0	3,221
0	0	0,000014	3,223
4E-08	0,00000013	0,00001398	3,2662
8E-08	0,00000025	0,00001398	3,304
1,2E-07	0,00000038	0,00001398	3,3384
1,6E-07	0,00000051	0,00001398	3,3692
1,9E-07	0,00000064	0,00001398	3,3974
2,3E-07	0,00000078	0,00001397	3,4226
2,7E-07	0,00000091	0,00001398	3,4461
3,1E-07	0,00000104	0,00001398	3,4681

Network of battery assets

Annotated with understandable attributes
Uniquely identifiable
Linked to other data: people, organizations…

Teknologi for et bedre samfunn

Semantic Technology

Agent

Semantic
Metadata

Database

```
{
    "@context": "https://w3id.org/emmo/domain/battery/context",
    "@type": "CR2032"
}
```

https://emmo-repo.github.io/domain-battery/examples/example_linked_data_battery_cell_metadata.html

Teknologi for et bedre samfunn

Semantic Technology

Summary

- Leveraging digital tools and methods is becoming more and more essential for researchers in all fields.

- In batteries, we have a lot of powerful digital tools already – but they are often difficult or unstable to use!
  - BattMo offers an open-source framework for continuum models of batteries (also for 3D grids) that is fast, flexible, and free!
  - BattMo includes tools for parameter calibration and design optimization
  - Battery2030+ data and ontology tools offer a way to integrate battery data with the Semantic Web!

- Digital tools help us to save time and get the most value from our data

www.digibattproject.eu

**Funded by
the European Union**

BATTERY
2030+

IntelLiGent

HYDRA

[/] digibatt