PyBaMM - Python Battery Mathematical Modelling

A flexible, open-source python package for development, comparison, and fast solutions of physics-based battery models.

The PyBaMM Team

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ABSTRACT

As the worldwide battery modelling community grows, there is a clear need for software that uses modern software engineering techniques to facilitate cross-institutional collaboration on battery research. The Python package PyBaMM addresses this need by being

- Open-source and freely available
- Flexible with a modular design
- Well-tested by employing test-driven software development practices

PyBaMM allows users to easily:

- Change model parameters
- Run **drive cycles**/standard **experimental routines** (CCCV, GITT, etc)
- Simulate **degradation mechanisms** such as SEI formation, lithium plating, and particle cracking, including **coupling between mechanisms**
- Add additional physics (model equations entered symbolically)
- Achieve fast simulation times (Doyle-Fuller-Newman model with ~3000 states solved in **under 200ms** for a 1C constant current discharge)

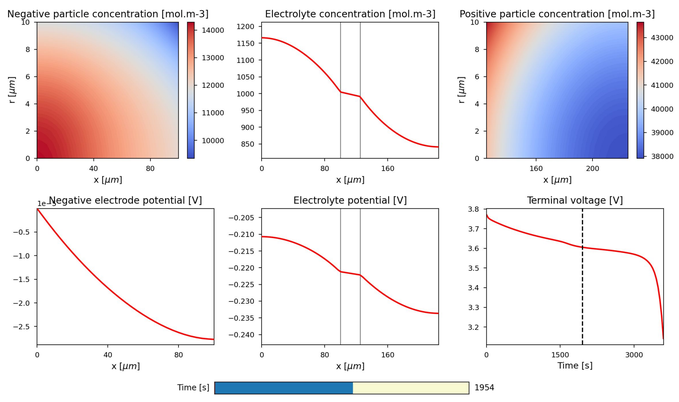
SIMPLE INSTALLATION

Just like other python packages, PyBaMM can be easily installed on **Windows, Mac, and Linux** with just one command:

```
pip install pybamm
```

Then run a 1C discharge of the Doyle-Fuller-Newman Model:

```
import pybamm
model = pybamm.lithium_ion.DFN()
sim = pybamm.Simulation(model)
sim.solve([0,3600])
sim.plot()
```



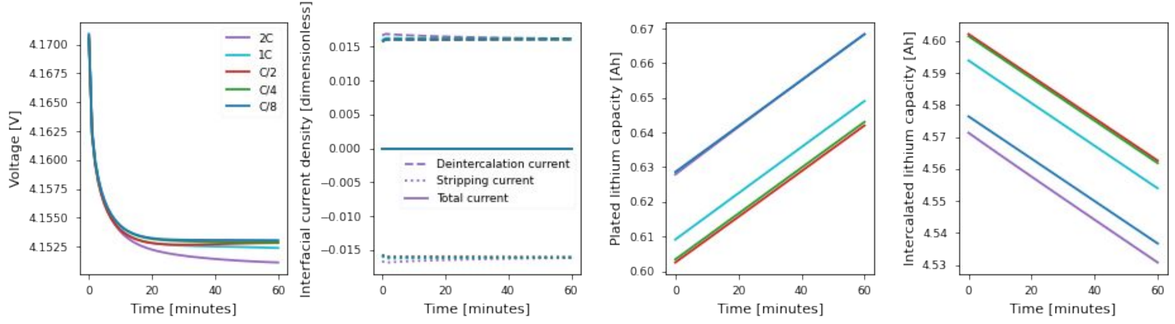
FAST SOLUTIONS

Millisecond solve times for a 1C discharge using the CasADi solver (n grid points per domain)

Single particle model (SPM)			Doyle-Fuller-Newman (DFN)		
Grid points	**States**	**Time (ms)**	**Grid points**	**States**	**Time (ms)**
10	21	1.8	10	281	35
40	81	1.9	40	3521	190
80	321	3.6	80	13441	870

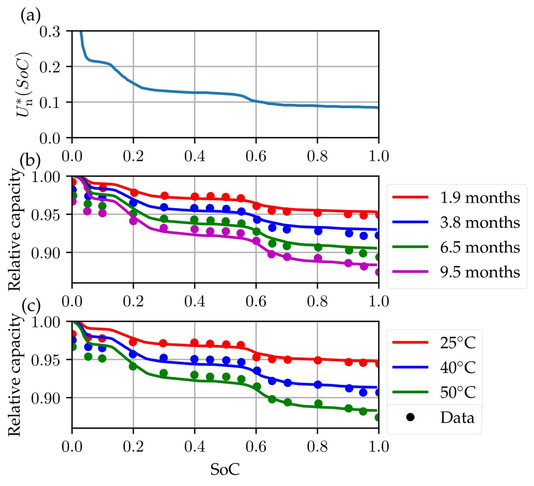
MODELLING LITHIUM PLATING [paper|code]

- Reversible and irreversible lithium plating models from O'Kane et al. 2020.
- PyBaMM's framework allows easy coupling with other degradation mechanisms.



MODELLING SEI LAYER GROWTH

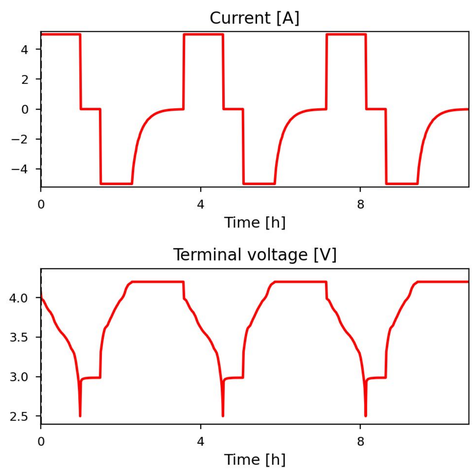
- Several models for SEI layer growth are available, including:
  - reaction limited
  - diffusion limited
  - electron-migration limited
- SEI layer resistance and pore clogging included
- Simulates calendar aging and cycle aging
- Can be coupled with other degradation mechanisms



CUSTOM EXPERIMENTAL PROCEDURES [code]

PyBaMM allows users to enter custom experimental procedures in text form using the **Experiment** object, e.g.:

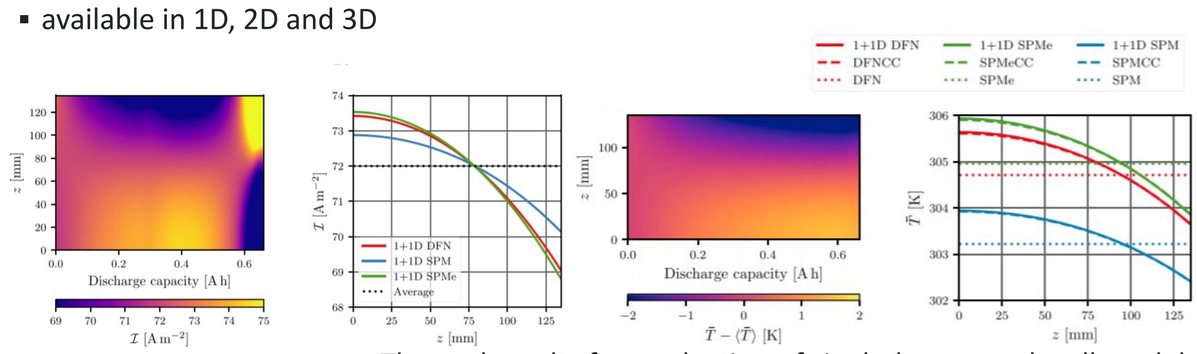
```
pybamm.Experiment(
    [
        ("Discharge at 1C until 2.5V",
        "Rest for 30 minutes",
        "Charge at 5A until 4.2V"
        "Hold at 4.2V until 10mA")
    ] * 3
)
```



THERMAL MODELLING OF LITHIUM-ION POUCH CELLS [paper|code]

PyBaMM includes:

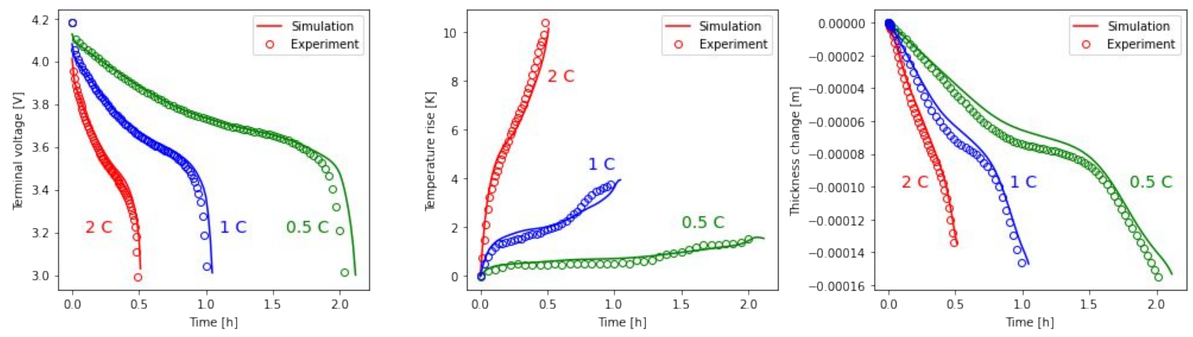
- fully-coupled full-order (e.g. Doyle-Fuller-Newman) and reduced-order (e.g. Single Particle Model) lithium-ion battery models
- available in 1D, 2D and 3D



Thermal results for a selection of single-layer pouch cell models

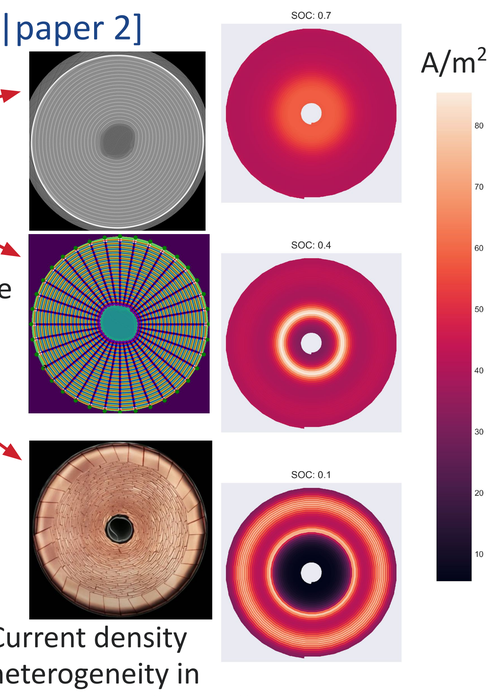
MODELLING STRESS RESPONSE IN ELECTRODE PARTICLES [paper|code]

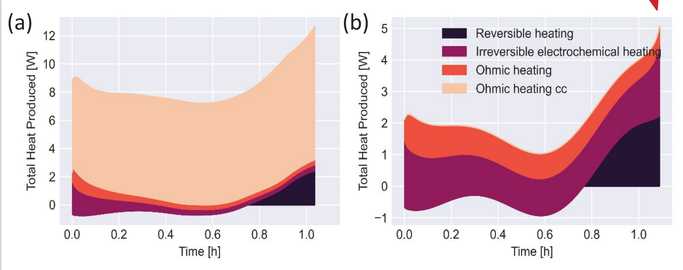
- Mechanically coupled diffusion physics from Ai et al. 2019
- Voltage, temperature and thickness change for a lithium cobalt oxide-graphite pouch cell agree well with experimental results



MODELLING OF JELLYROLL CELLS [paper 1|paper 2]

- PyBaMM can be used in circuits forming cells or packs. Jellyroll models are constructed from tomography or from geometric spirals with resistor networks representing current collector foils and 1000s of DFN models are computed in parallel representing electrochemistry in each section
- Tab locations and ohmic losses in cc's play major role in cell heating and current heterogeneity
- Standard tabs (a) are compared to Tesla's new 'tab-less' (b) design showing large differences





Current density heterogeneity in standard tabbed cells

REFERENCE

- V. Sulzer, S.G. Marquis, R. Timms, M. Robinson and S.J. Chapman (2020). "Python Battery Mathematical Modelling (PyBaMM)". *ECS ArXiv. February, 7.* [pdf]

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