PyBOP

The PyBOP Team

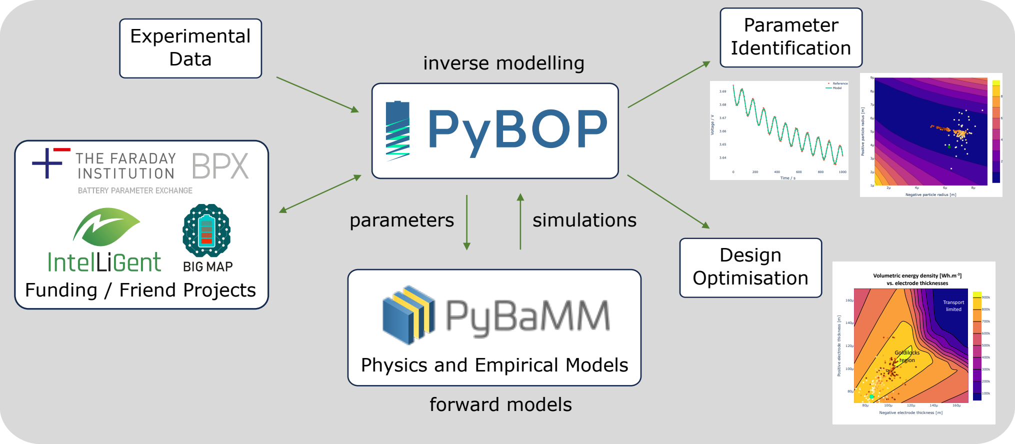
Online Developer Meetings
on the third Thursday, every other month

Agenda

- Recap of recent updates to PyBOP (10 min)
- Quick update from everyone (10 min)
- Discussion of open issues (30 min)
- Planning and assignment of tasks (10 min)

Introductory slides are available at the end of this presentation.

PyBOP project map



Experimental Data

inverse modelling

PyBOP

Parameter Identification

Design Optimisation

THE FARADAY INSTITUTION BPX BATTERY PARAMETER EXCHANGE

IntelLiGent BIG MAP

Funding / Friend Projects

parameters

simulations

PyBaMM

Physics and Empirical Models

forward models

Latest release

Aiming for a new release every 3 months.
https://pypi.org/project/pybop/

The Changelog is updated with new **features**, **bug fixes** and **breaking changes**.
https://github.com/pybop-team/PyBOP/blob/develop/CHANGELOG.md

Discussion of open issues

Kick-off questions:

- What issue are you working on/would you like to work on?
- Do you have any blockers?

Open issues: https://github.com/pybop-team/PyBOP/issues
Project board: https://github.com/orgs/pybop-team/projects/

Triage new issues

Other open items?

End of meeting

Below:

1. Introductory slides
2. Feature highlights

Introduction

With thanks to:

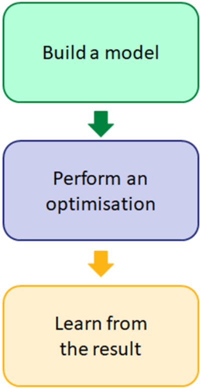
- the PyBaMM developers PyBaMM
- the PINTS developers

Aims

1. Parameter estimation from cell data
   - How will my battery respond to different excitations?
   - How is degradation affecting my battery performance?

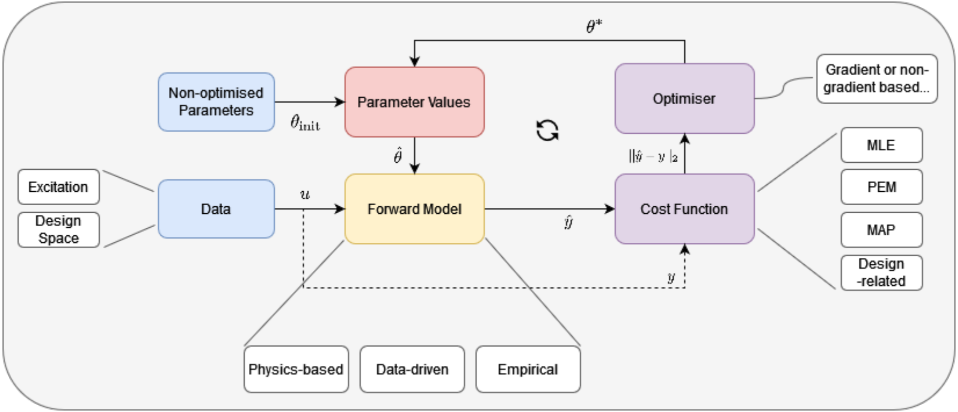
2. Model comparison
   - What can I learn from a more detailed model?
   - Is it worth the extra computational effort?

3. Design optimisation within practical constraints
   - How energy dense can I make my battery (at some rate)?



Icons made by Uniconlabs, RaftelDesign and Freepik from www.flaticon.com

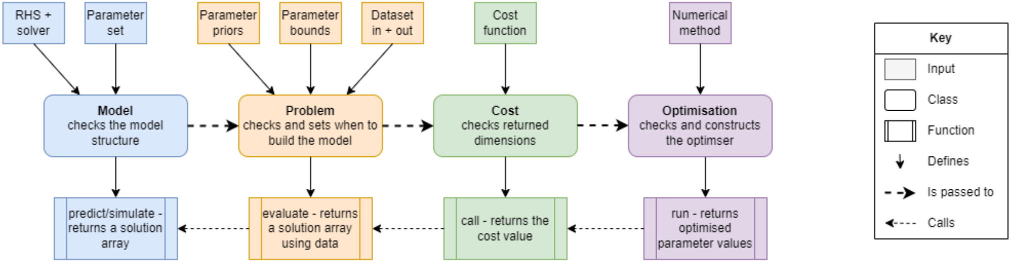
Architecture



Python objects

PyBOP

Main optimisation workflow:



RHS + solver

Parameter set

Parameter priors

Parameter bounds

Dataset in + out

Cost function

Numerical method

Model checks the model structure

Problem checks and sets when to build the model

Cost checks returned dimensions

Optimisation checks and constructs the optimser

predict/simulate - returns a solution array

evaluate - returns a solution array using data

call - returns the cost value

run - returns optimised parameter values

Key

Input

Class

Function

Defines

Is passed to

Calls

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Demo/examples

- Parameterisation
- Design optimisation

Parameterisation

PyBOP

1. Define a model (PyBaMM's SPM) and fitting parameters

```python
import pybop
import numpy as np

# Define model
parameter_set = pybop.ParameterSet.pybamm("Chen2020")
model = pybop.lithium_ion.SPM(parameter_set=parameter_set)

# Fitting parameters
parameters = pybop.Parameters(
    pybop.Parameter(
        "Negative particle radius [m]",
        prior=pybop.Gaussian(6e-06, 0.1e-6),
        bounds=[1e-6, 9e-6],
    ),
    pybop.Parameter(
        "Positive particle radius [m]",
        prior=pybop.Gaussian(4.5e-06, 0.1e-6),
        bounds=[1e-6, 9e-6],
    ),
)
```

Parameterisation

2. Generate synthetic data and define problem, cost and optimisation

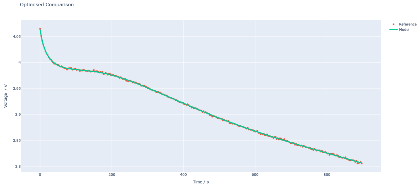
```python
# Generate data
sigma = 0.001
t_eval = np.arange(0, 900, 3)
values = model.predict(t_eval=t_eval)
corrupt_values = values["Voltage [V]"].data + np.random.normal(0, sigma, len(t_eval))

# Form dataset
dataset = pybop.Dataset(
    {
        "Time [s]": t_eval,
        "Current function [A]": values["Current [A]"].data,
        "Voltage [V]": corrupt_values,
    }
)

# Generate problem, cost function, and optimisation class
problem = pybop.FittingProblem(model, parameters, dataset)
cost = pybop.SumSquaredError(problem)
optim = pybop.CMAES(cost, max_iterations=100)
```

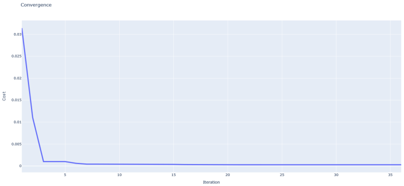
Parameterisation

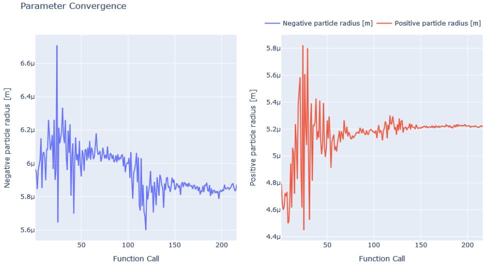
3. Run the optimisation and plot the results

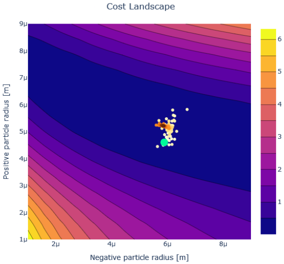
```python
# Run the optimisation
x, final_cost = optim.run()
print("True parameters:", parameters.true_value())
print("Estimated parameters:", x)

# Plot the timeseries output
pybop.quick_plot(problem, problem_inputs=x, title="Optimised Comparison")

# Plot convergence and parameter traces
pybop.plot_convergence(optim)

# Plot the parameter traces
pybop.plot_parameters(optim)

# Plot the cost landscape with optimisation path
pybop.plot2d(optim, steps=15)
```

Parameterisation results


Optimised Comparison


Convergence


Parameter Convergence


Cost Landscape

Design optimisation

1. Define a model (PyBaMM's SPMe) and design parameters

```
import pybop
import numpy as np

# Define parameter set and model
parameter_set = pybop.ParameterSet.pybamm("Chen2020", formation_concentrations=True)
model = pybop.lithium_ion.SPMe(parameter_set=parameter_set)

# Fitting parameters
parameters = pybop.Parameters(
    pybop.Parameter(
        "Positive electrode thickness [m]",
        prior=pybop.Gaussian(7.56e-05, 0.05e-05),
        bounds=[65e-06, 10e-05],
    ),
    pybop.Parameter(
        "Positive particle radius [m]",
        prior=pybop.Gaussian(5.22e-06, 0.05e-06),
        bounds=[2e-06, 9e-06],
    ),
)
```

Design optimisation

2. Set the target experiment and define problem, cost and optimisation

```
# Define test protocol
experiment = pybop.Experiment(
    ["Discharge at 1C until 2.5 V (5 seconds period)"],
)
init_soc = 1  # start from full charge
signal = ["Voltage [V]", "Current [A]"]

# Generate problem
problem = pybop.DesignProblem(
    model, parameters, experiment, signal=signal, init_soc=init_soc
)

# Generate cost function and optimisation class:
cost = pybop.GravimetricEnergyDensity(problem, update_capacity=True)
optim = pybop.PSO(
    cost, verbose=True, allow_infeasible_solutions=False, max_iterations=15
)
```

Design optimisation

3. Run the optimisation and plot the results

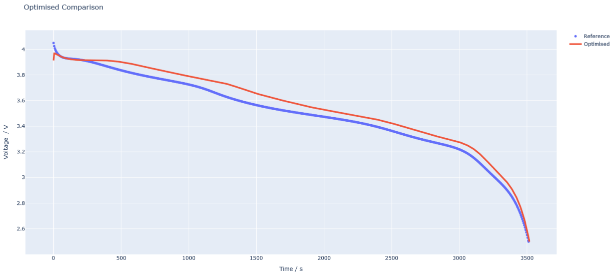
```python
# Run optimisation
x, final_cost = optim.run()
print("Estimated parameters:", x)
print(f"Initial gravimetric energy density: {cost(optim.x0):.2f} Wh.kg-1")
print(f"Optimised gravimetric energy density: {final_cost:.2f} Wh.kg-1")

# Plot the timeseries output
if cost.update_capacity:
    problem._model.approximate_capacity(x)
pybop.quick_plot(problem, problem_inputs=x, title="Optimised Comparison")

# Plot the cost landscape with optimisation path
pybop.plot2d(optim, steps=10)
```

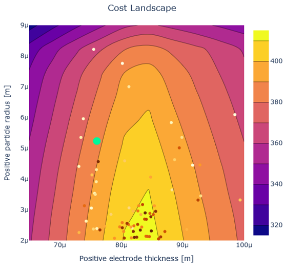
Design optimisation

Output

```
Estimated parameters: [6.51159429e-05 2.32340723e-06]
Initial gravimetric energy density: 386.31 Wh.kg-1
Optimised gravimetric energy density: 410.78 Wh.kg-1
```

Results

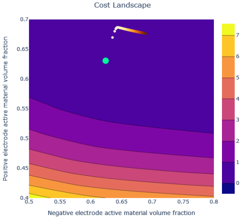


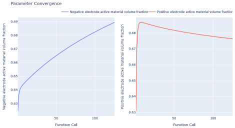


Choice of optimisers

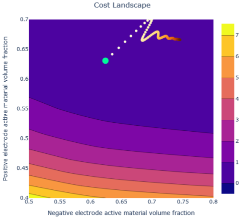
Gradient-based

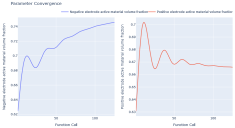
Gradient descent



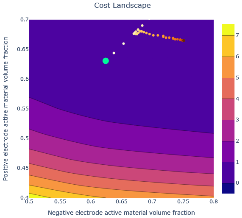


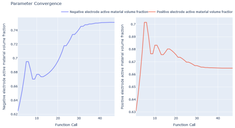
Adaptive moment (AdamW)





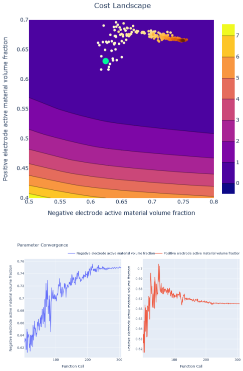
Resilient backpropagation (IRPropMin)



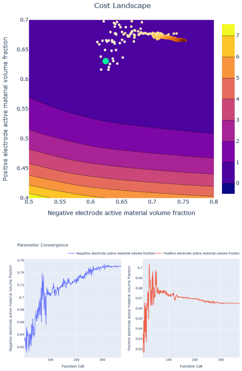


Evolution strategies

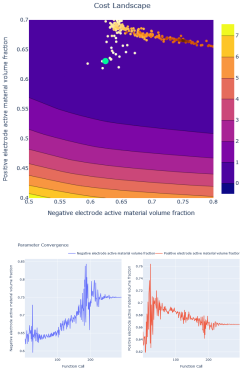
Stochastic natural evolution strategy (SNES)



Exponential natural evolution strategy (SNES)



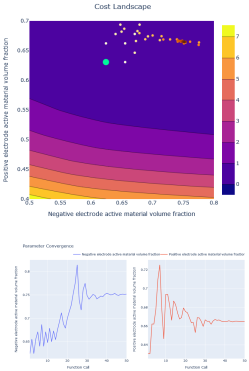
Covariance matrix adaptation (CMA-ES)



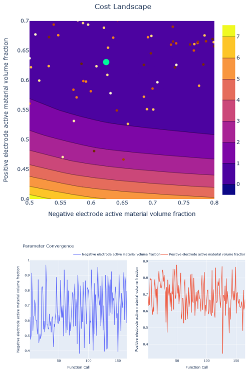
Other optimisers

PyBOP

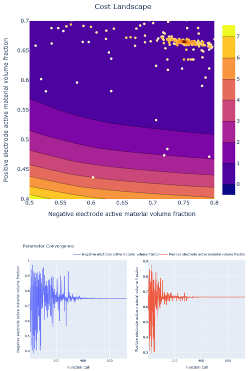
Nelder Mead



Particle swarm optimisation



SciPy differential evolution



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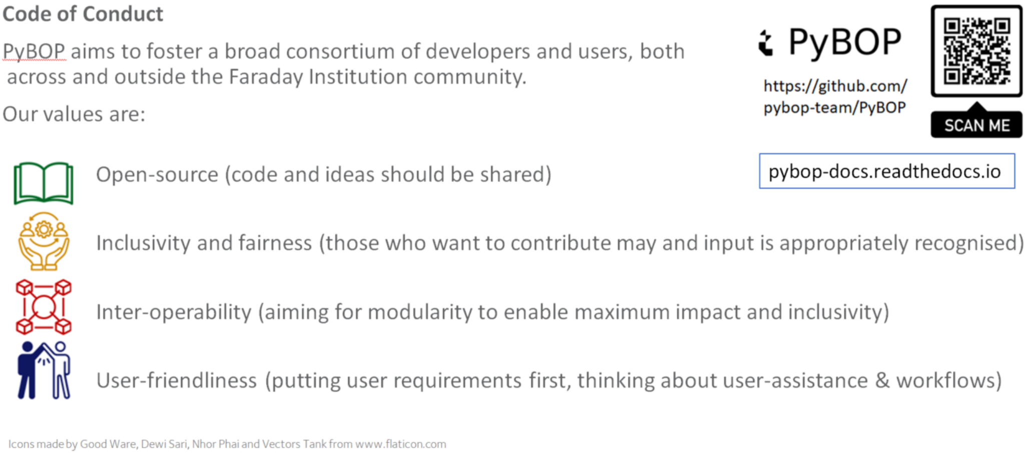
Collaboration



Code of Conduct

PyBOP aims to foster a broad consortium of developers and users, both across and outside the Faraday Institution community.

Our values are:

- Open-source (code and ideas should be shared)
- Inclusivity and fairness (those who want to contribute may and input is appropriately recognised)
- Inter-operability (aiming for modularity to enable maximum impact and inclusivity)
- User-friendliness (putting user requirements first, thinking about user-assistance & workflows)

PyBOP

https://github.com/pybop-team/PyBOP

SCAN ME

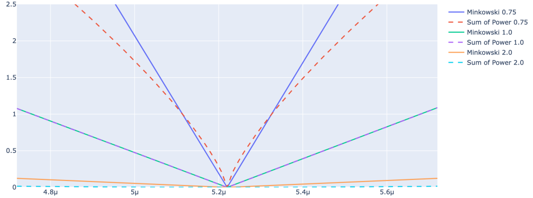
pybop-docs.readthedocs.io

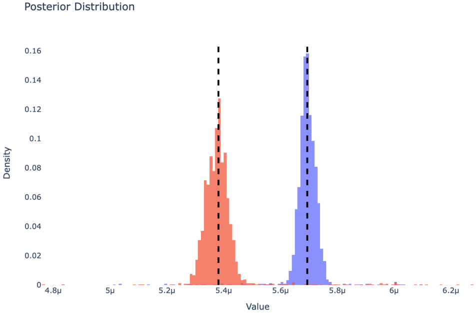
Icons made by Good Ware, Dewi Sari, Nhor Phai and Vectors Tank from www.flaticon.com

Feature highlights

New in v24.9: New costs and samplers

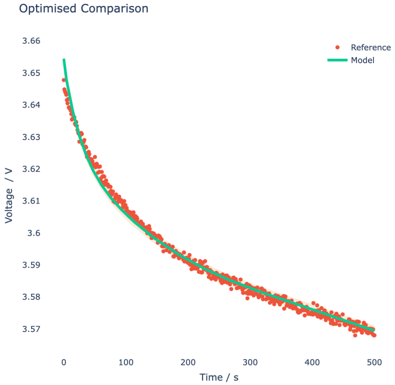
#462 - Adds Minkowski and SumofPower cost functions.
#6 - Adds Monte Carlo Sampling classes

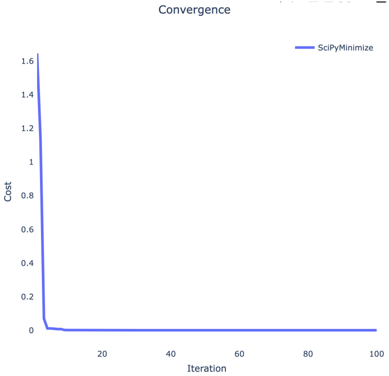




New in v24.9: Constrained optimisation

#353 - Allows user defined nonlinear constraints

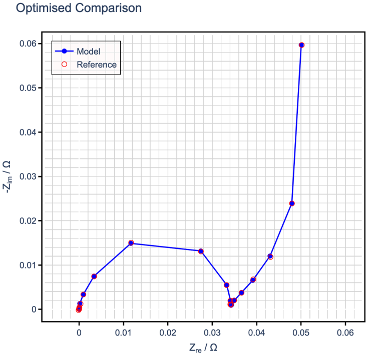


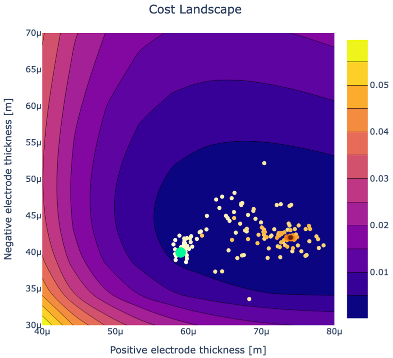


New in v24.9: Electrochemical impedance spectroscopy

PyBOP

#405 - Adds EIS prediction methods





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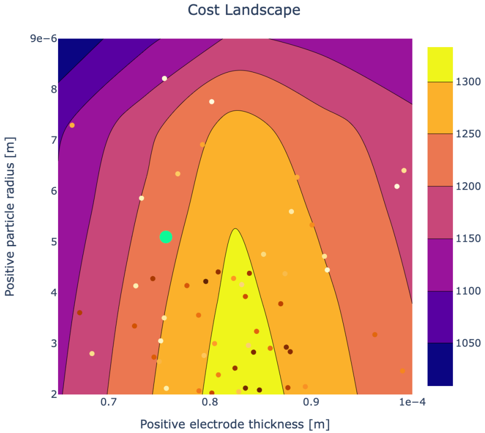
New in 24.9: Weighted costs

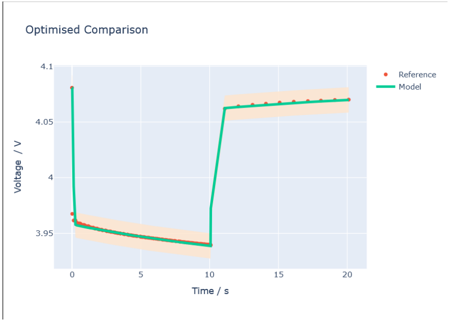
Combine costs with weighting:

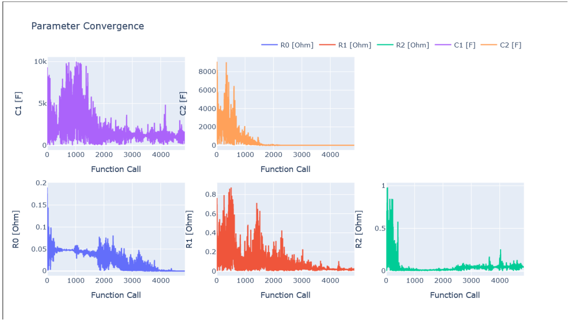
```
# Generate multiple cost functions and combine them
cost1 = pybop.GravimetricEnergyDensity(problem)
cost2 = pybop.VolumetricEnergyDensity(problem)
cost = pybop.WeightedCost(cost1, cost2, weights=[1, 1e-3])
```



New in v24.6: Experimental data fitting

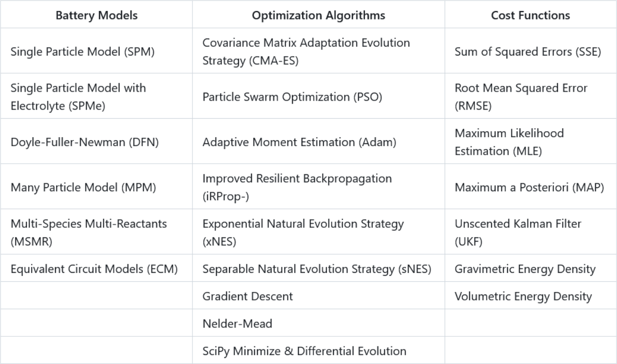
#241 - Adds experimental circuit model fitting notebook with LG M50 data from: https://github.com/WDWidanage/Simscape-Battery-Library/tree/main/Examples/parameterEstimation_TECMD/Data





New in v24.6: Additional PyBaMM models

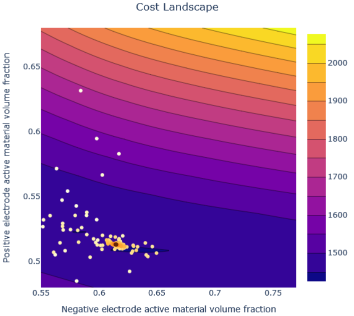
#250 - Adds DFN, MPM, MSMR models and moves multiple construction variables to BaseEChem. Adds exception catch on simulate & simulateS1.

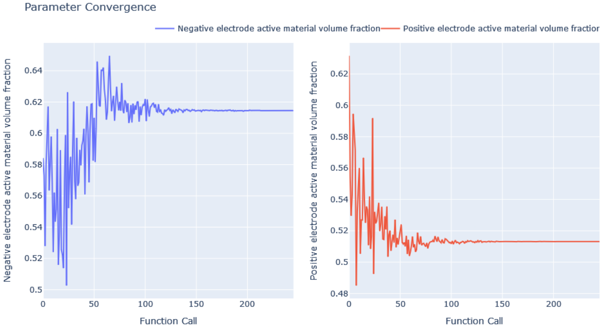


Battery Models	Optimization Algorithms	Cost Functions
Single Particle Model (SPM)	Covariance Matrix Adaptation Evolution Strategy (CMA-ES)	Sum of Squared Errors (SSE)
Single Particle Model with Electrolyte (SPMe)	Particle Swarm Optimization (PSO)	Root Mean Squared Error (RMSE)
Doyle-Fuller-Newman (DFN)	Adaptive Moment Estimation (Adam)	Maximum Likelihood Estimation (MLE)
Many Particle Model (MPM)	Improved Resilient Backpropagation (iRProp-)	Maximum a Posteriori (MAP)
Multi-Species Multi-Reactants (MSMR)	Exponential Natural Evolution Strategy (xNES)	Unscented Kalman Filter (UKF)
Equivalent Circuit Models (ECM)	Separable Natural Evolution Strategy (sNES)	Gravimetric Energy Density
	Gradient Descent	Volumetric Energy Density
	Nelder-Mead	
	SciPy Minimize & Differential Evolution	

New in v24.6: Maximum a Posteriori

#275 - Adds Maximum a Posteriori (MAP) cost function with corresponding tests and example script.


Cost Landscape


Parameter Convergence