3rd Online Developer Meeting

The PyBOP Team

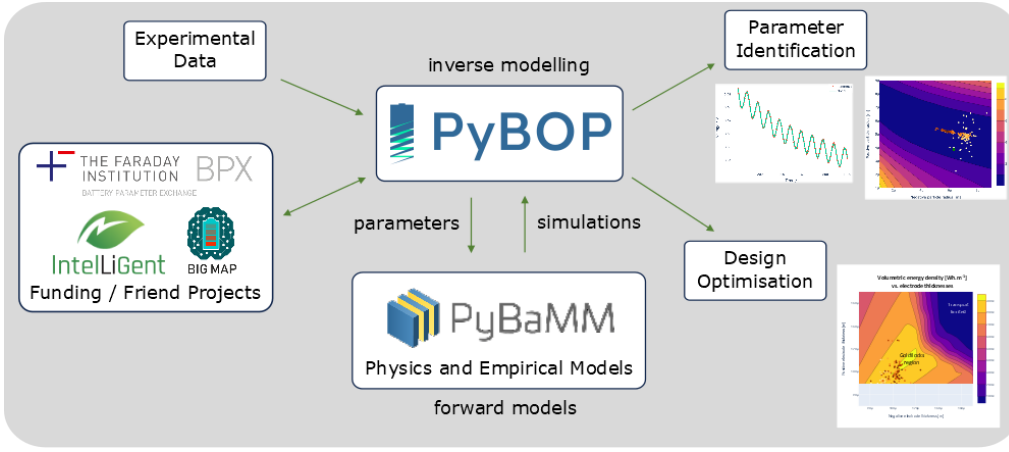
18th July 2024

Agenda

- Presentation on recent updates to PyBOP (Nicola, 10 min)
- Quick introduction/update from everyone (5 min)
- Discussion of open issues (30 min)
- Planning and assignment of tasks (15 min)

Introductory slides are available at the end of this presentation.

PyBOP project map



Recent updates

We released PyBOP v24.6 on 8th July.

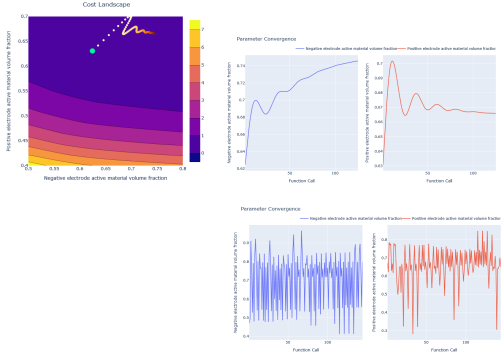
https://github.com/pybop-team/PyBOP/blob/develop/CHANGELOG.md

The Changelog is divided into new **features**, **bug fixes** and **breaking changes**.

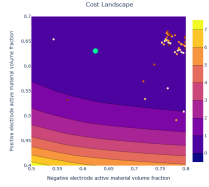
New in v24.6: Additional optimisers

#319 - Adds CuckooSearch optimiser with corresponding tests. #316 - Adds Adam with weight decay (AdamW), deprecates pints.Adam.

Adam with weight decay (AdamW)



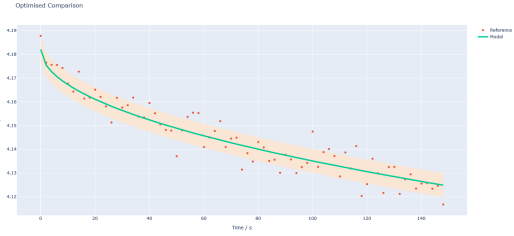
Cuckoo search

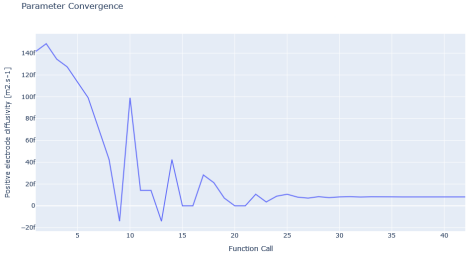


New in v24.6: GITT fitting example

PyBOP

#249 - Add WeppnerHuggins model and GITT example.

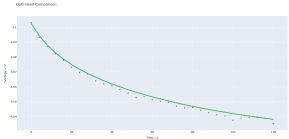


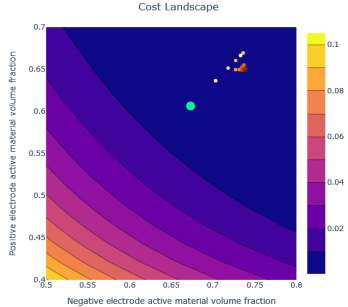


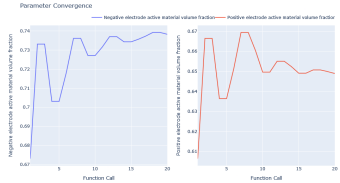
New feature (WIP): Multi-fitting problem class

PyBOP

#364 - Adds the MultiFittingProblem class and the multi_fitting example script.
#322 - Add Parameters class to store and access multiple parameters in one object.







Questions?

Discussion of open issues

Let's introduce everyone:

- Where are you joining from?
- What issue are you working on/would you like to work on?

Open issues: https://github.com/pybop-team/PyBOP/issues
Project board: https://github.com/orgs/pybop-team/projects/7

End of meeting

Below:

1. Introductory slides
2. Feature highlights

Introduction

With thanks to:

- the PyBaMM developers PyBaMM
- the PINTS developers

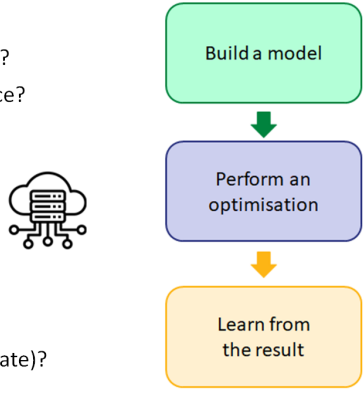
Aims

PyBOP

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?

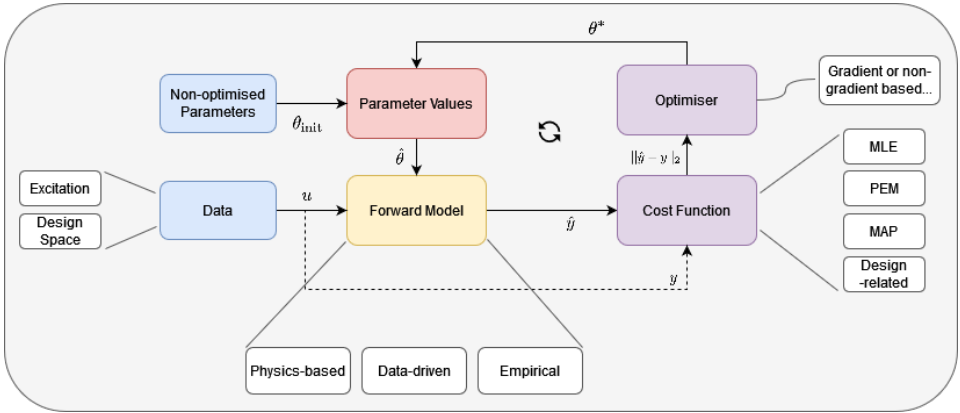
3. Design optimisation within practical constraints
   - How energy dense can I make my battery (at some rate)?



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

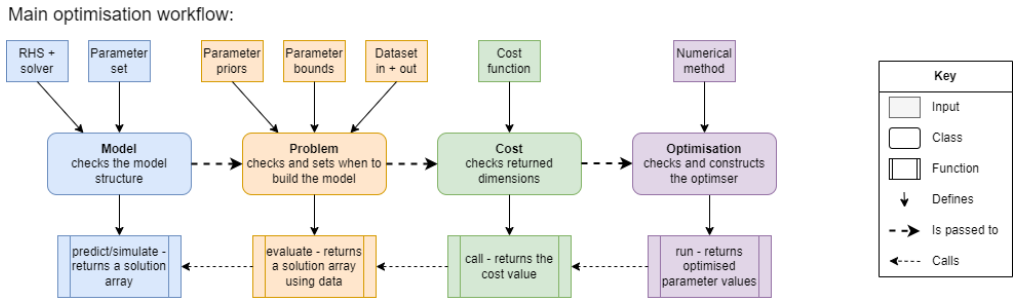
Architecture

PyBOP



Python objects

PyBOP



Demo/examples

- Parameterisation
- Design optimisation

PyBOP

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

```
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],
    ),
)
```

PyBOP

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

```
# 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)
```

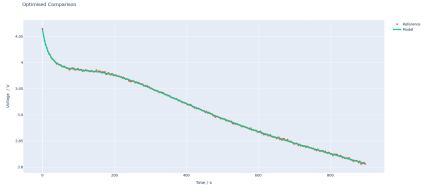
PyBOP

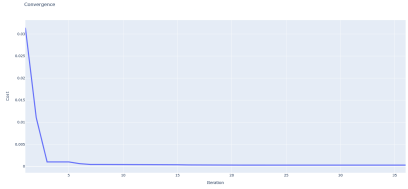
3. Run the optimisation and plot the results

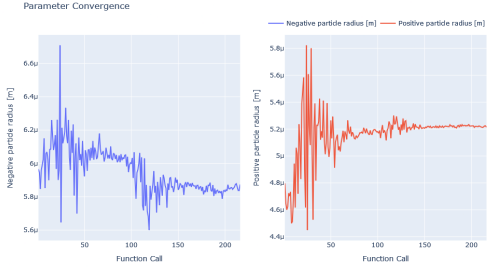
```
# Run the optimisation
x, final_cost = optim.run()
print("True parameters:", parameters.true_value())
print("Estimated parameters:", x)

# 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)
```

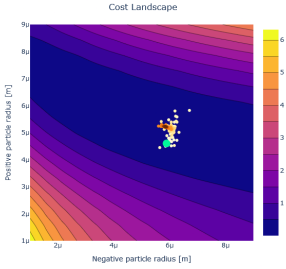
Parameterisation results

PyBOP









PyBOP

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

```python
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],
    ),
)
```

PyBOP

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
)
```

PyBOP

3. Run the optimisation and plot the results

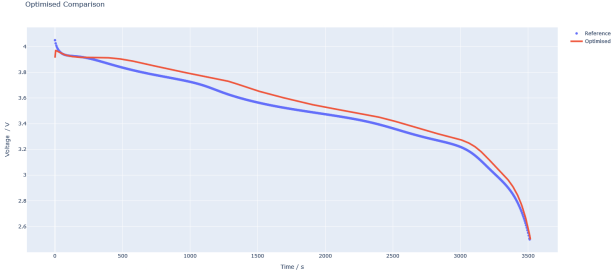
```
# Run optimisation
x, final_cost = optim.run()
print("Estimated parameters:", x)
print(f"Initial gravimetric energy density: {cost(optim.x0):.2f} Wh.kg-1")
print(f"Optimised gravimetric energy density: {final_cost:.2f} Wh.kg-1")

# 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)
```

PyBOP

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

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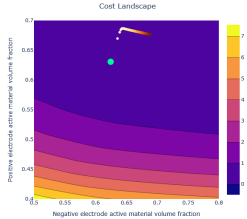
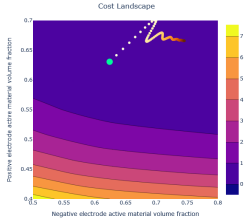
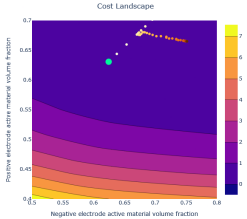
Gradient descent

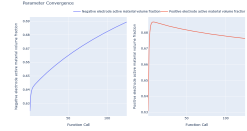
Adaptive moment (AdamW)

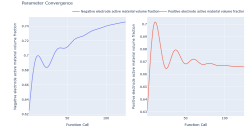
Resilient backpropagation (IRPropMin)

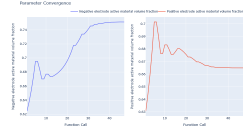












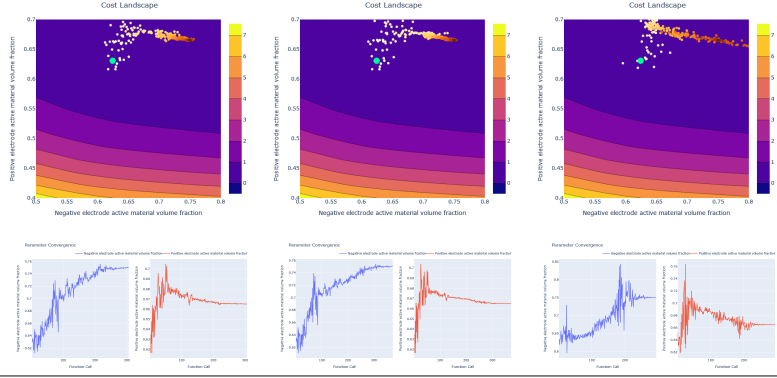
Evolution strategies

PyBOP

Stochastic natural evolution strategy (SNES)

Exponential natural evolution strategy (SNES)

Covariance matrix adaptation (CMA-ES)



Other optimisers

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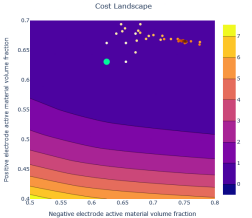
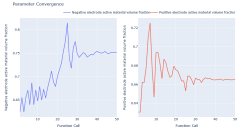
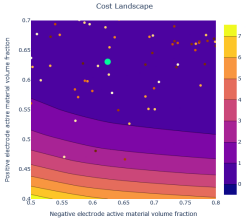
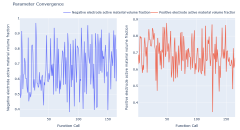
Nelder Mead



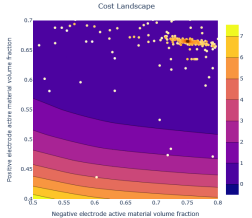


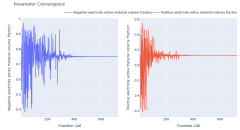
Particle swarm optimisation





SciPy differential evolution





Collaboration

PyBOP

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:

PyBOP

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

SCAN ME

pybop-docs.readthedocs.io

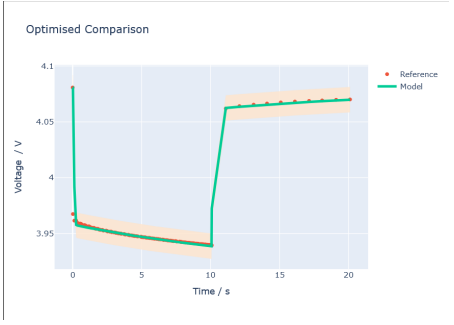
- Open-source (code and ideas should be shared)
- Inclusivity and fairness (those who want to contribute may and input is appropriately recognised)
- Inter-operability (aiming for modularity to enable maximum impact and inclusivity)
- User-friendliness (putting user requirements first, thinking about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

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

Feature highlights

PyBOP

#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

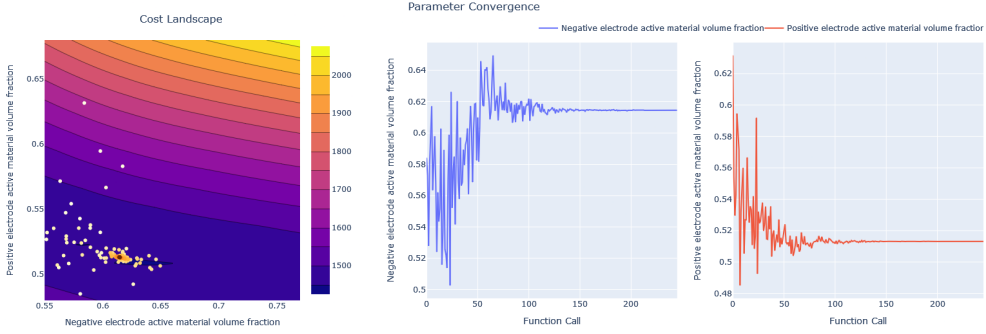
PyBOP

#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	

PyBOP

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



PyBOP

Credit and thanks to Agriya and Brady!

Features

#304 - Decreases the testing suite completion time.
#301 - Updates default echem solver to "fast with events" mode.
#251 - Increment PyBaMM > v23.5, remove redundant tests within integration tests, increment citation version, fix ex
#285 - Drop support for Python 3.8.
#268 - Fixes the GitHub Release artifact uploads, allowing verification of codesigned binaries and source distributi
#79 - Adds BPX as a dependency and imports BPX support from PyBaMM.
#267 - Add classifiers to pyproject.toml, update project.urls.
#195 - Adds the Nelder-Mead optimiser from PINTS as another option.

Bug Fixes

#317 - Installs seed packages into nox sessions, ensuring that scheduled tests can pass.
#308 - Enables testing on both macOS Intel and macOS ARM (Silicon) runners and fixes the scheduled tests.
#299 - Bugfix multiprocessing support for Linux, MacOS, Windows (WSL) and improves coverage.
#270 - Updates PR template.
#91 - Adds a check on the number of parameters for CMAES and makes XNES the default optimiser.