PyBOP: Python Battery Model Optimisation and Parameterisation

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Battery Intelligence Lab

A framework for parameterisation and design optimisation

- Parameterise, optimise, and export your parameter sets within a single framework
- Any PyBaMM model, across various cost functions and optimisation algorithms

Model	DFN	SPMe	SPM
Time	4.5s	1.5s	1.3s

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- Parameterise, optimise, and export your parameter sets within a single framework
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Data quality   Excitation   Data points

Motivation: Battery models are useful for

Physical Insights

How does the model predict future evolution?

How sensitivity is the battery to manufacturing variations?

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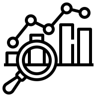

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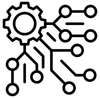
State Estimation

What is the current SoX of the cell?

How fast can I charge the cell?



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Physical Insights
How does the model predict future evolution?
How sensitivity is the battery to manufacturing variations?

State Estimation
What is the current SoX of the cell?
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Design Optimisation
How energy dense can the cell be?
What is the best design for this operation?

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Parameter values

Parameter uniqueness is unknown
(in principle or in practice).

Conventionally requires cell teardown

Excitation signals are not obvious from
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Domain expertise

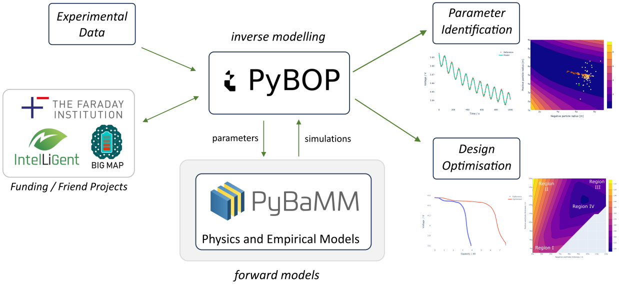
Is a more complex model needed?

Where should the complexity be added?

PyBOP is a platform to solve these challenges

Provides workflows for parameter identification and exploitation:

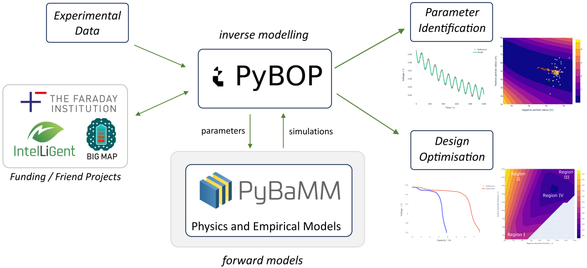
- Physics-based and empirical parameter identification
- Design optimisation capabilities
- Gradient & non-gradient optimisers
- Frequentist and Bayesian methods
- Multi-threaded computing



Multiprocessing enables this to be performant

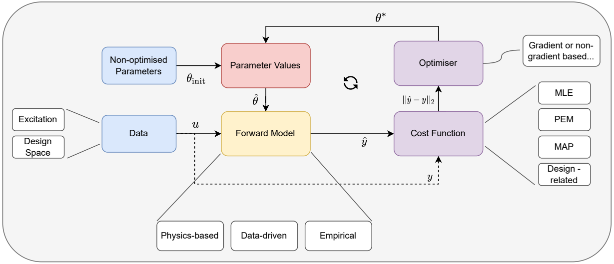
Multiprocessing is built into the package to speed up large parameter space optimisation

- $\sim$1.7x improvement for 4 cores
- $\sim$6.6x improvement for 12 cores



This is achieved through concise, intuitive design

```python
# Generate problem, cost function, and optimisation class
problem = pybop.Problem(model, parameters, dataset)
cost = pybop.SumSquaredError(problem)
optim = pybop.Optimisation(cost, optimiser=pybop.GradientDescent)
x, final_cost = optim.run()
```



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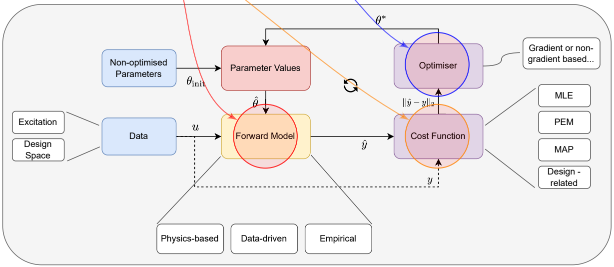
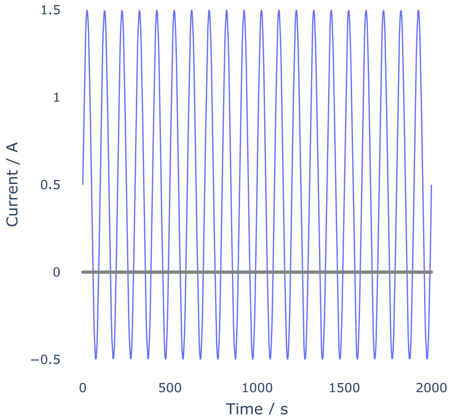


Parameterisation operating conditions

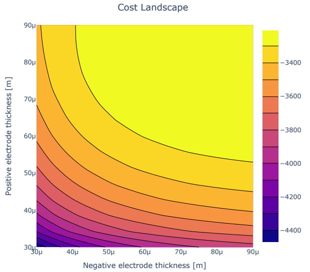
For the upcoming parameterisation examples,

- Biased Sinusoid Applied Current
- Synthetic data from Many-Particle DFN
- $T_0 = 298.15$ K, $SOC_0 = 100\%$
- NMC811–Gr/SiOx Chemistry

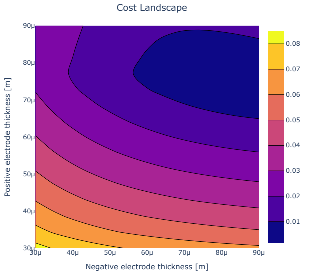


PyBOP provides multiple cost functions for parameter inference

Likelihood-based



Root Mean Squared Error



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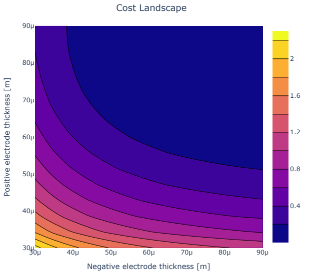

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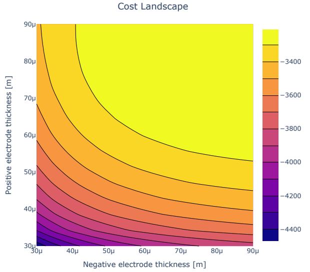

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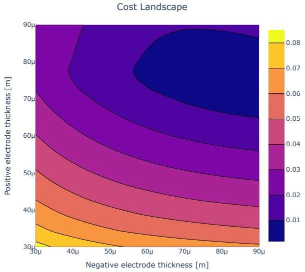

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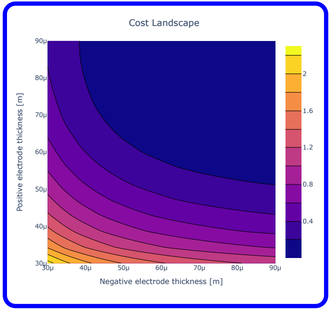


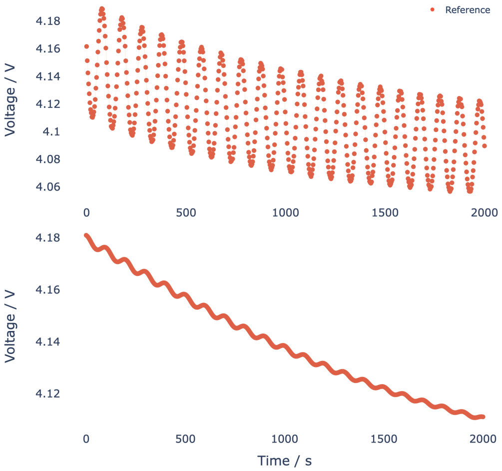
Example: Multi-signal parameter identification

Active Material Volume Fractions (Mass Loading) for each electrode[a] are identified from synthetic MP-DFN data.

- Fitting signals: Terminal voltage and predicted OCV
- Initial conditions $\sim \mathcal{N}(\mu, \sigma^2)$
- Maximum iters: 150

Ground truth parameter values:

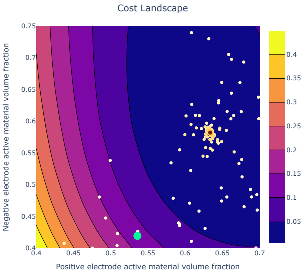
$$[\varepsilon_\mathrm{n} = 0.75, \ \varepsilon_\mathrm{p} = 0.665]$$



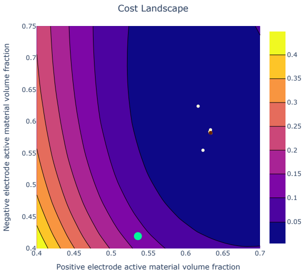
[a]All models are tested daily on the cloud!

Verfiying optimality with convergence plots

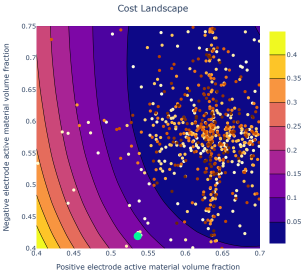
CMA-ES



Differential Evolution



Particle Swarm



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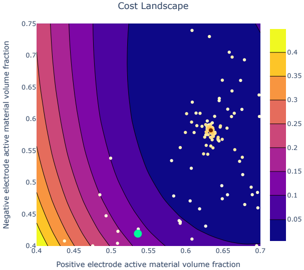

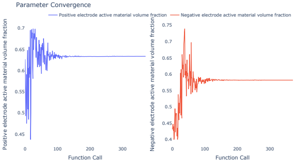

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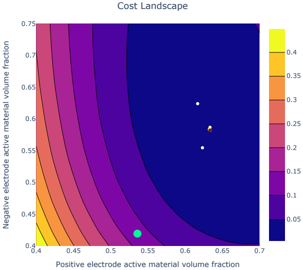

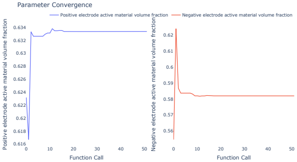

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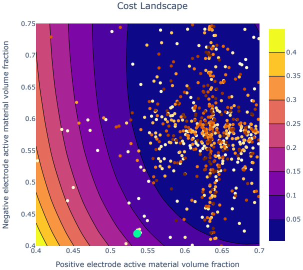

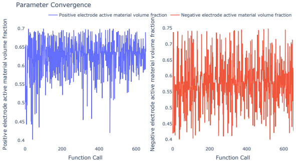

Gradient-based optimisers offer a deterministic solution

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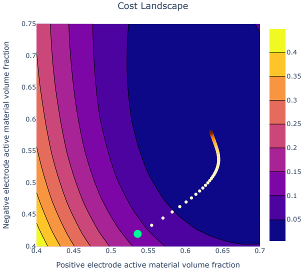
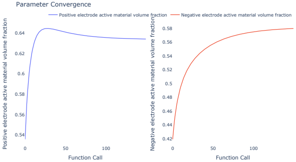
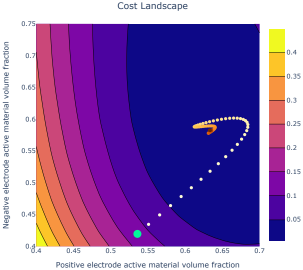
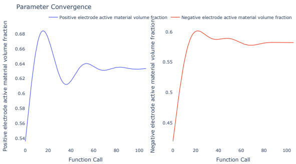
Gradient Descent



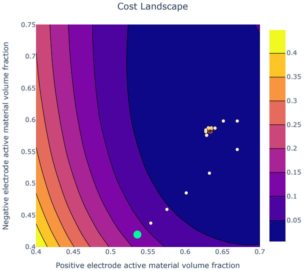


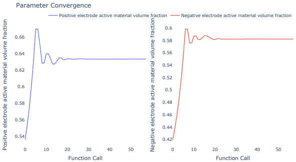
Adam





IRPropMin





Example: Multi-signal parameter identification

With the correct excitation, parameter identification can be fast and robust. However, challenges still exist,

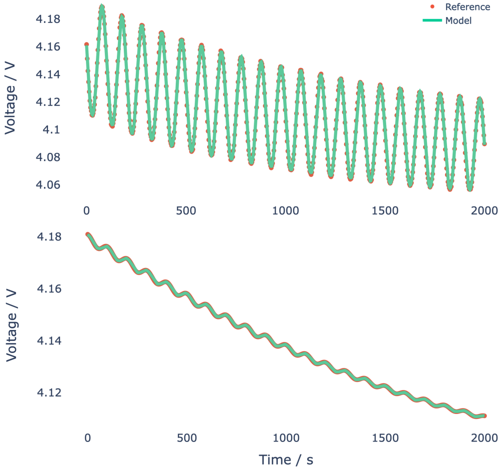
- Missing physics in forward model
- Metadata quality

Parameter values:

True: $[\varepsilon_{\mathrm{n}} = 0.75,\ \varepsilon_{\mathrm{p}} = 0.665]$

SPMe: $[\varepsilon_{\mathrm{n}} = 0.75,\ \varepsilon_{\mathrm{p}} = 0.656]$

SPM: $[\varepsilon_{\mathrm{n}} = 0.595,\ \varepsilon_{\mathrm{p}} = 0.631]$



Example: Physics-based design optimisation

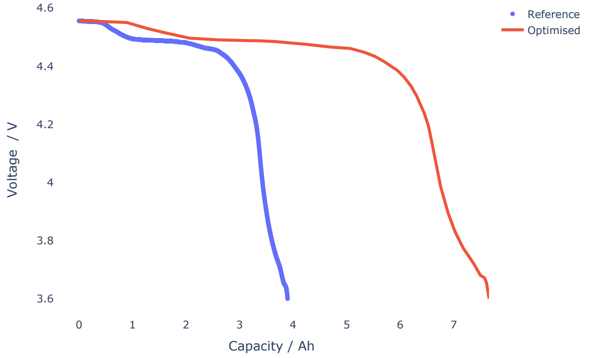
Chemistry: LNMO-Graphite/SiOx

Target: Maximize cell-level specific energy density

Parameters: Electrode coating thickness

Conditions: 1C cycling

Optimal:
$[L_n = 97\text{e-}06, \; L_p = 126\text{e-}06]$



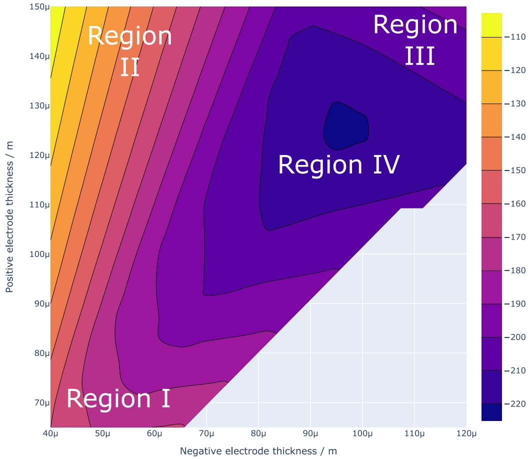
PyBOP enables physical insights into design optimisation

Region I: Electrodes too thin compared to inactive material

Region II: Poor N:P balancing

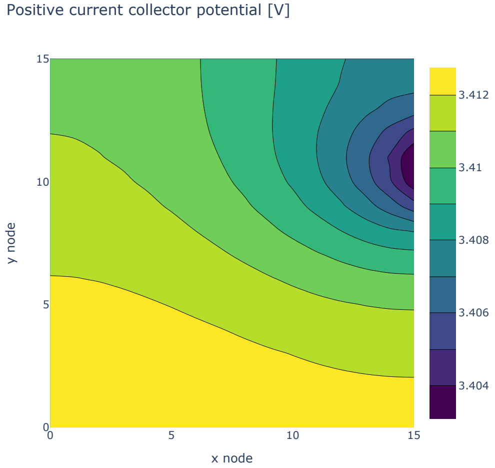
Region III: Electrodes too thick and cause transport limitations

Region IV: Ideal N:P balance and optimised wrt active material and transport



Spatial models enable larger-scale effects

- Spatial models[b] are available for application-specific design optimisation
- Enables design optimisation (tab placement, electrolyte composition, etc.) workflows from spatial variables (thermal, lithiation, etc.)



[b] Marquis et al. J. Electrochem. Soc., 2020

Conclusion and Outlook

- We presented a framework for optimisation and parameterisation of battery models
- This framework offers many optimisers, cost functions, and battery models
- Example workflows were presented covering parameterisation and optimisation

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Future Development:

- Monte Carlo and Bayesian Quadrature
- Integration of EIS predictions
- Improved workflows for battery relevant model optimisation
- v24.5 upcoming!

Get involved and become a developer and/or user!

GitHub Repository:

pybop-team/pybop

Installation:

```
pip install pybop
```

Examples **Docs** **Benchmarks**

Contact Info:

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