PyBaMM

an open-source Python library for battery modelling

University of Oxford · Carnegie Mellon University · UCL · Imperial College London · WMG, The University of Warwick · The Faraday Institution · MultiScale Modelling

Why PyBaMM?

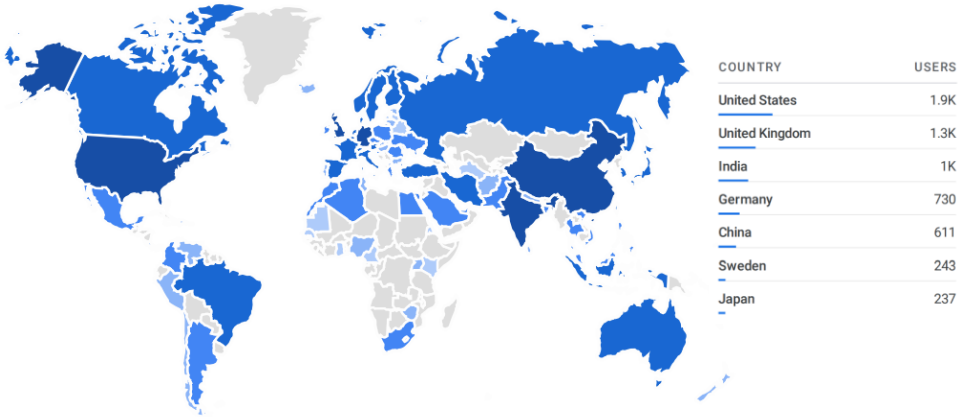
*PyBaMM's mission is to **accelerate battery modelling research***

*by providing an **open-source framework***

*for multi-institutional, interdisciplinary **collaboration**.*

Why PyBaMM?

- Provide fast, reliable battery simulations
- Facilitate development of new models
- Improve reproducibility of research
- Grow battery modelling community
- Increase impact and industry engagement



Try online

Install locally

Develop

*PyBaMM has fostered an active community with over **40 contributors** and **hundreds of users**. Our most recent training workshop attracted almost **400 participants**, **over 100** of which were from **industry**.*

What is PyBaMM?

PyBaMM is a framework for building and solving battery models

FAST

Models

- Standard lithium-ion models:
  - SPM, SPMe, DFN
- Plug and play multiphysics, including:
  - Thermal models
  - Degradation mechanisms
  - Mechanics

Experimental suite

- Easy interface to define custom protocols
- Any voltage, current or power control, e.g.:
  - GITT, PITT, CCCV, drive cycle
- Track degradation (e.g. capacity fade)

FLEXIBLE

Chemistries / Parameters

- NMC, LFP, $LiNiCoO_2$, LCO, NCA
- Graphite, graphite + SiO_x, Li metal
- $LiPF_6$
- Easy to add your own parameter sets

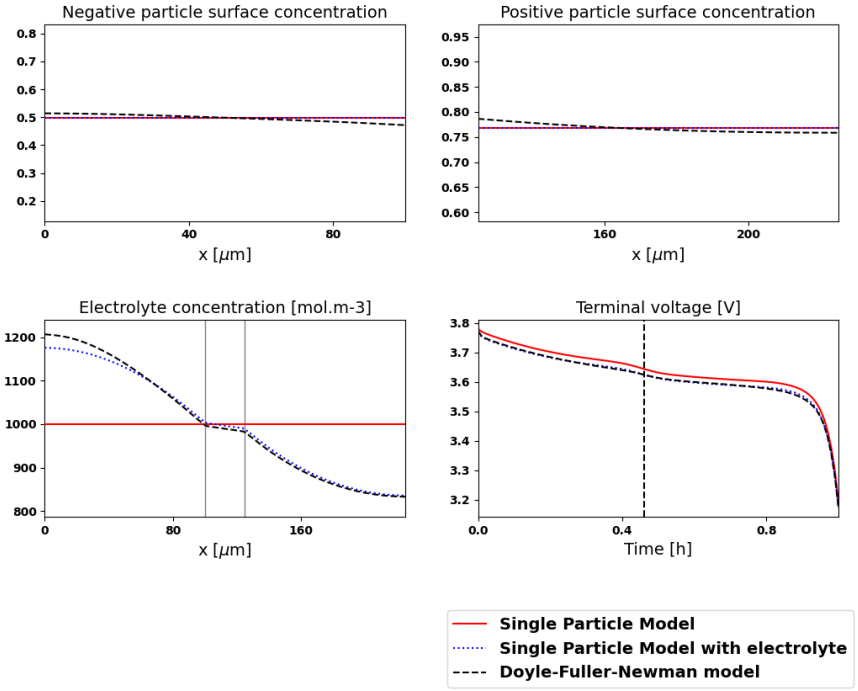
Functionality

- Choice of solvers and numerical methods
- Sensitivity analysis
- Seamless integration with Python workflows
- Interface with external software

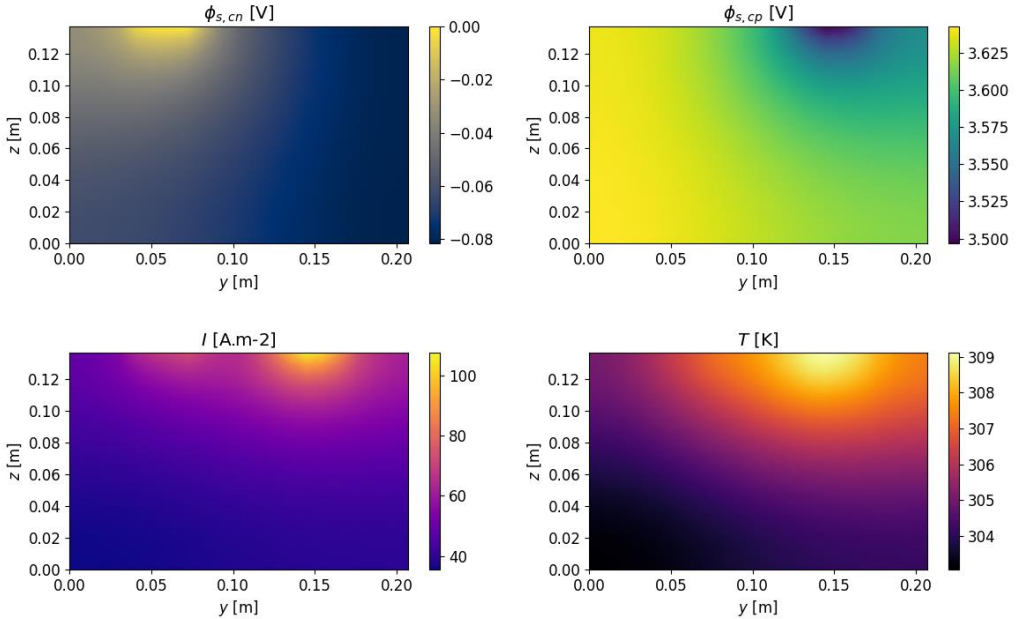
MODULAR

Fast, reliable simulations via a simple interface

```python
#
# Compare lithium-ion battery models
#
import pybamm

# load models
models = [
    pybamm.lithium_ion.SPM(),
    pybamm.lithium_ion.SPMe(),
    pybamm.lithium_ion.DFN(),
]

# create and run simulations
sims = []
for model in models:
    sim = pybamm.Simulation(model)
    sim.solve([0, 3600])
    sims.append(sim)

# plot
pybamm.dynamic_plot(sims)
```



Thermal models: pouch cells




```
options = {
    "current collector": "potential pair",
    "dimensionality": 2,
    "thermal": "x-lumped",
}
model = pybamm.lithium_ion.SPM(options)
sim = pybamm.Simulation(model)
sim.solve([0, 3600])
```

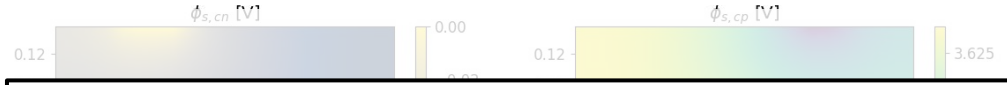
- Coupled electrochemical-thermal pouch cell models
- Full plug-play flexibility to include extra physics
- Enhanced computational speed through reduced-order models (e.g. SPMe)

Timms, R., Marquis, S. G., Sulzer, V., Please, C. P., & Chapman, S. J. (2021). Asymptotic Reduction of a Lithium-Ion Pouch Cell Model. *SIAM Journal on Applied Mathematics*, *81*(3), 765–788. https://doi.org/10.1137/20M1336898

Marquis, S. G., Timms, R., Sulzer, V., Please, C. P., & Chapman, S. J. (2020). A Suite of Reduced-Order Models of a Single-Layer Lithium-Ion Pouch Cell. *Journal of The Electrochemical Society*, *167*(14), 140513. https://doi.org/10.1149/1945-7111/abbce4

For more information contact Dr Robert Timms (University of Oxford)

Thermal models: pouch cells




```
options = {
    "current collector": "potential pair",
```

```
pybamm.print_citations()
```


[1] Joel A. E. Andersson, Joris Gillis, Greg Horn, James B. Rawlings, and Moritz Diehl. CasADi – A software framework for nonlinear optimization and optimal control. Mathematical Programming Computation, 11(1):1–36, 2019. doi:10.1007/s12532-018-0139-4.

[2] Marc Doyle, Thomas F. Fuller, and John Newman. Modeling of galvanostatic charge and discharge of the lithium/polymer/insertion cell. Journal of the Electrochemical society, 140(6):1526–1533, 1993. doi:10.1149/1.2221597.

[3] Charles R. Harris, K. Jarrod Millman, Stéfan J. van der Walt, Ralf Gommers, Pauli Virtanen, David Cournapeau, Eric Wieser, Julian Taylor, Sebastian Berg, Nathaniel J. Smith, and others. Array programming with NumPy. Nature, 585(7825):357–362, 2020. doi:10.1038/s41586-020-2649-2.

[4] Scott G. Marquis, Valentin Sulzer, Robert Timms, Colin P. Please, and S. Jon Chapman. An asymptotic derivation of a single particle model with electrolyte. Journal of The Electrochemical Society, 166(15):A3693–A3706, 2019. doi:10.1149/2.0341915jes.

[5] Valentin Sulzer, Scott G. Marquis, Robert Timms, Martin Robinson, and S. Jon Chapman. Python Battery Mathematical Modelling (PyBaMM). Journal of Open Research Software, 9(1):14, 2021. doi:10.5334/jors.309.

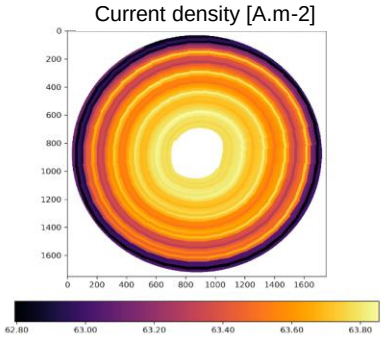
[6] Robert Timms, Scott G Marquis, Valentin Sulzer, Colin P. Please, and S Jonathan Chapman. Asymptotic Reduction of a Lithium-ion Pouch Cell Model. SIAM Journal on Applied Mathematics, 81(3):765–788, 2021. doi:10.1137/20M1336898.

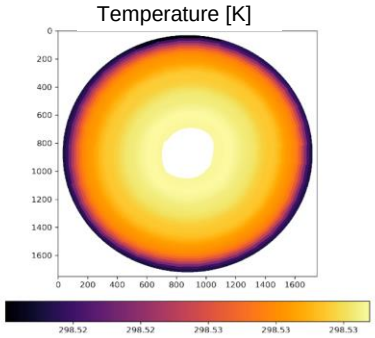
Marquis, S. G., Timms, R., Sulzer, V., Please, C. P., & Chapman, S. J. (2020). A Suite of Reduced-Order Models of a Single-Layer Lithium-Ion Pouch Cell. *Journal of The Electrochemical Society*, *167*(14), 140513. https://doi.org/10.1149/1945-7111/abbce4

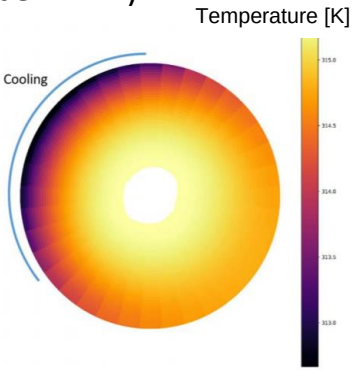
For more information contact Dr Robert Timms (University of Oxford)

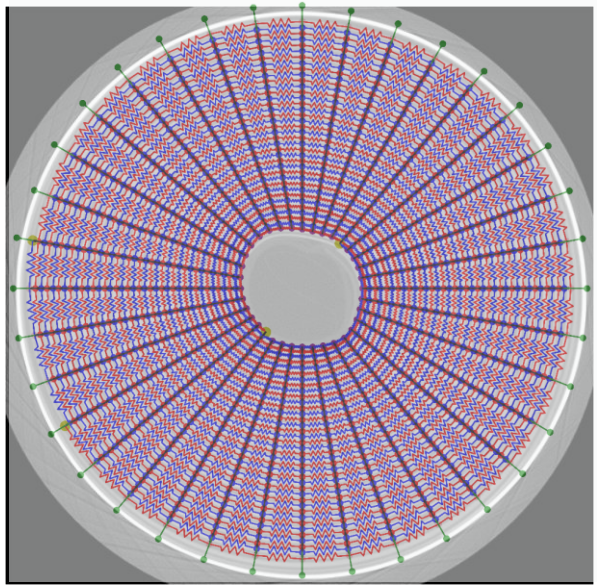
Thermal models: cylindrical cells

- Internal temperature differences lead to non-uniformities in current flow, state of charge, particle stress and levels of degradation. A 2D heat-transfer problem for spirally rolled cylindrical batteries shows effect of varying # tabs and cooled surface area.
  - particle scale electrochemical modelling (PyBaMM)
  - cell level electrical and thermal modelling (OpenPNM)









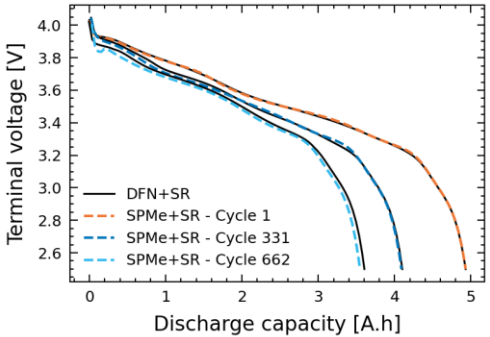
Tranter, T. G., Timms, R., Heenan, T. M. M., Marquis, S. G., Sulzer, V., Jnawali, A., … Brett, D. J. L. (2020). Probing Heterogeneity in Li-Ion Batteries with Coupled Multiscale Models of Electrochemistry and Thermal Transport using Tomographic Domains. *Journal of The Electrochemical Society*, *167*(11), 110538. https://doi.org/10.1149/1945-7111/aba44b

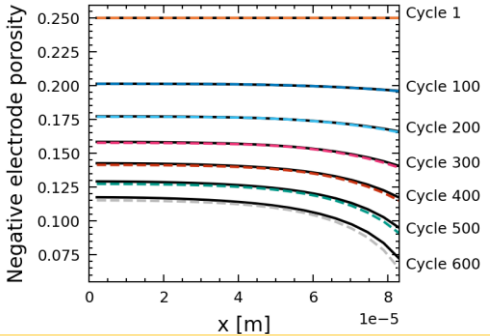
For more information contact Dr Thomas Tranter (UCL Electrochemical Innovation Lab)

Degradation models: SEI growth and lithium plating

- Multiple SEI growth and lithium plating models available.
  - SEI:
    - reaction limited
    - solvent-diffusion limited
    - electron-migration limited
    - interstitial-diffusion limited
  - Lithium plating:
    - irreversible
    - reversible

- Can be coupled with various electrochemical and thermal models, and further effects can also be included (such as porosity change).

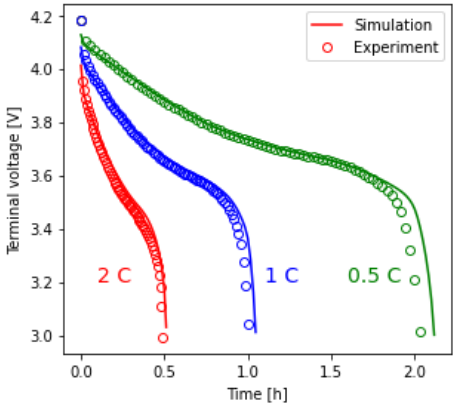


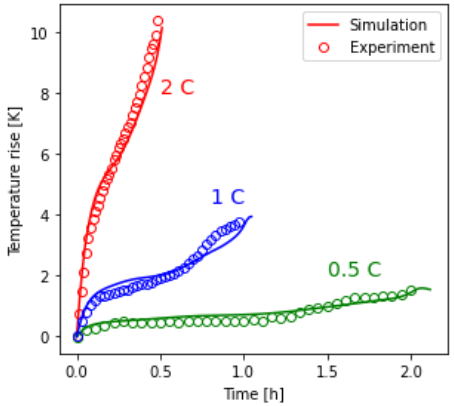


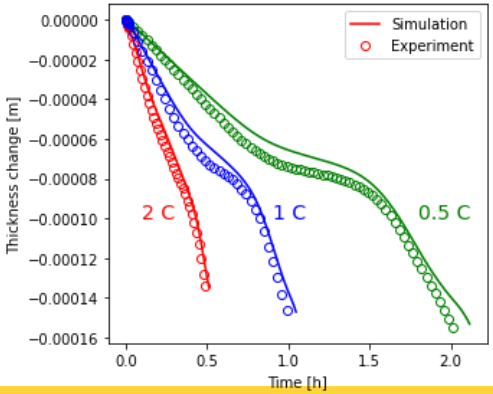
Brosa Planella, F., Widanage, W. D. (2022). Systematic derivation of a Single Particle Model with electrolyte and a side reaction (SPMe+SR) for degradation of lithium-ion batteries. *In preparation.*

For more information contact Dr Ferran Brosa Planella (University of Warwick)

Degradation models: mechanical effects







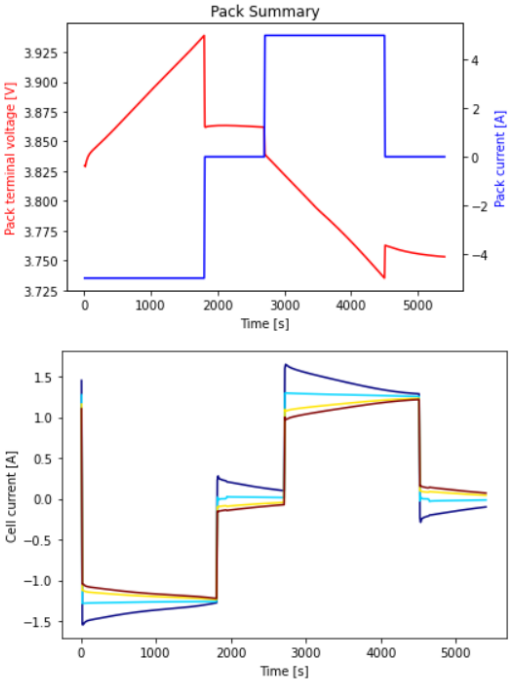
- Stress response in electrode particles investigated through a DFN model.
- Mechanically coupled diffusion physics
- Voltage, temperature and thickness change for a lithium cobalt oxide-graphite pouch cell agrees well with experimental results

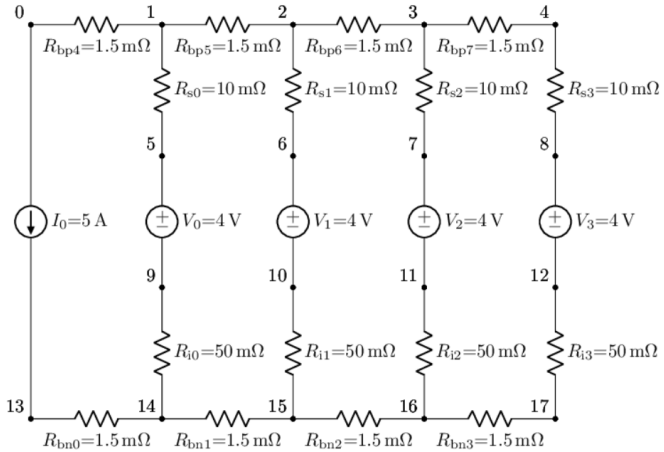
Ai, W., Kraft, L., Sturm, J., Jossen, A., & Wu, B. (2020). Electrochemical Thermal-Mechanical Modelling of Stress Inhomogeneity in Lithium-Ion Pouch Cells. *Journal of The Electrochemical Society*, *167*(1), 013512. https://doi.org/10.1149/2.0122001jes

For more information, contact Dr Weilong Ai (Southeast University) or Dr Billy Wu (Imperial College London)

Pack modelling: liionpack

- New open-source package in the PyBaMM ecosystem.
- Simulate pack configurations using PyBaMM models.
- Completely written in Python.
- Specify pack design or load a circuit netlist.



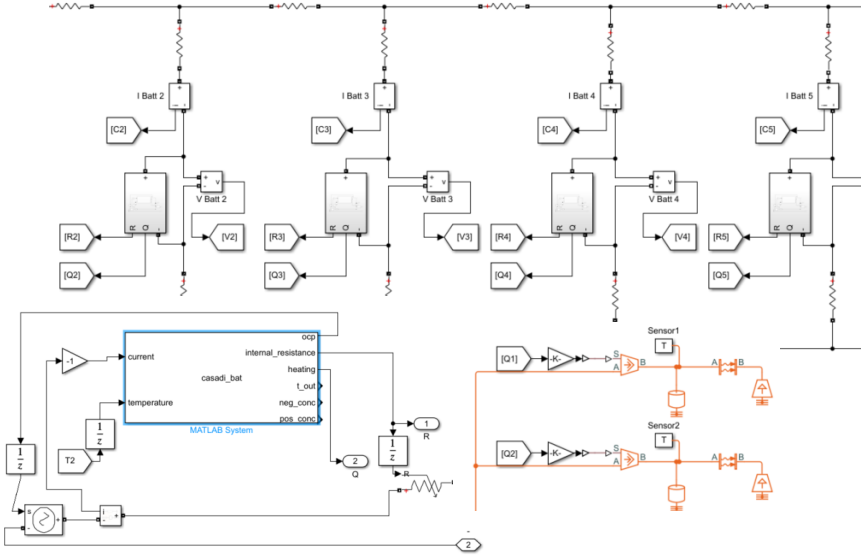


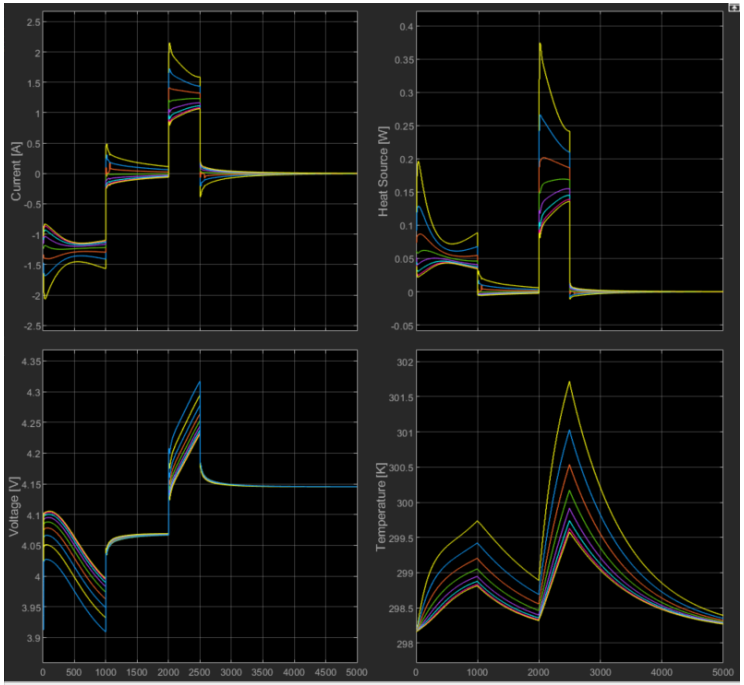
Tranter, T. G., Timms, R., Sulzer, V., Brosa Planella, F., Wiggins, G. M., Karra, S. V., … Brett, D. J. L. (2022). liionpack : A Python package for simulating packs of batteries with PyBaMM. *Journal of Open Source Software*, *7*(40), 4051. https://doi.org/10.21105/joss.04051

For more information visit https://github.com/pybamm-team/liionpack

Interface with Simulink

Initial work to demonstrate the extensibility and interoperability of PyBaMM





- "White box" PyBaMM model in MATLAB system
- Pack level electrical/thermal problem solved in Simulink
- Input currents and temperatures
- Output heat and voltage sources and internal resistance calculated with physics-based models

Accessing support

PyBaMM doesn't do something you think it should?

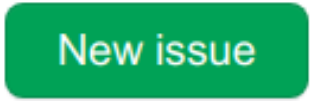
Not sure how to use existing features or implement your own model?

Interested in commercial or academic collaboration?

Please get in touch!

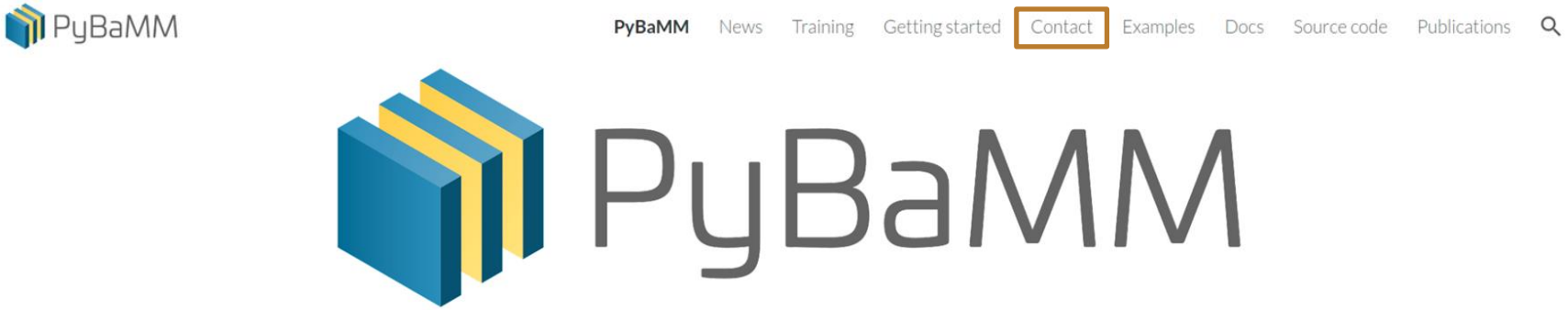
Get in touch on Slack or email
Use the #technical-questions channel, send a direct message, or send us an email

Create an issue or discussion
Head over to GitHub and post an issue or start a discussion



Implementation Sessions
One-on-one or group session to workshop your ideas, discuss implementation details and help with any issues

Further information – pybamm.org



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