Python Battery Mathematical Modelling (PyBaMM)

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What is PyBaMM

- *Python Battery Mathematical Modelling* (PyBaMM) solves continuum models for batteries, using both numerical methods and asymptotic analysis.
- Designed as a Common Modelling Framework for the Multiscale Modelling Faraday project. Facilitates sharing and distribution of **model** and **numerical methodologies** .
- Not a general purpose solver (e.g. Comsol), focuses specifically on battery modelling.
- Use it for:
  1. Running a battery simulation using one of the pre-built models, either as a single simulation or within parameter estimation
  2. Inserting your own model, discretisation or solver. Compare with the pre-built pybamm components, or to share with other PyBaMM users.
  3. Develop within the PyBaMM framework, or use any of PyBaMM's components within your own code

Organisation

- developers:

Valentin Sulzer

Scott Marquis

Martin Robinson

Robert Timms

Ivan Korotkin

Jamie Foster

Organisation

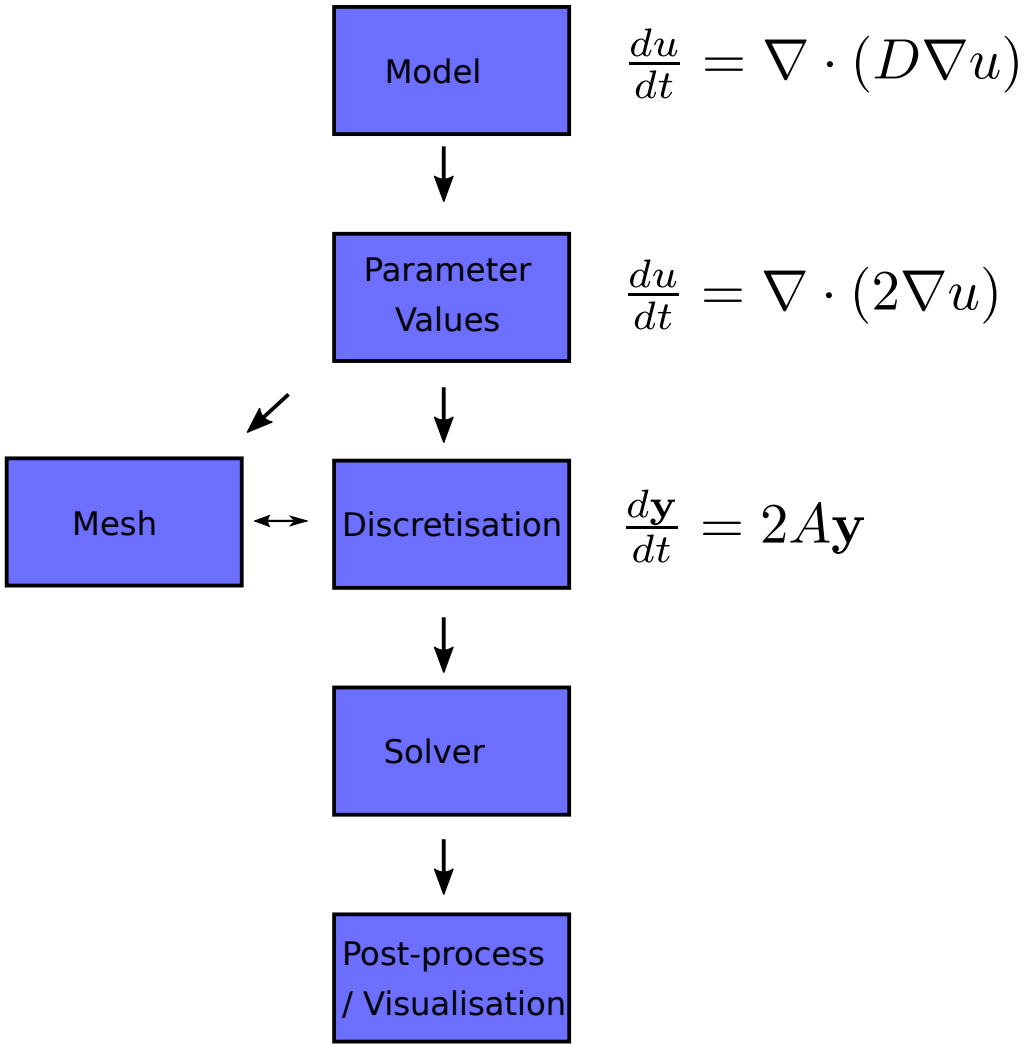
- developed as an open source (BSD licensed) Python library on GitHub:
  - `https://github.com/pybamm-team/PyBaMM`
- software engineering best practices:
  - Full suite of unit and integration tests
  - Automated testing on Linux, Mac and Windows using Python 3.5+
  - Generated API documentation and example notebooks/scripts demonstrating features
  - Project management, issue tracking and code review via GitHub

Current features

- Lithium-ion battery models:
  1. Single Particle Model (SPM)
  2. Single Particle Model with Electrolyte (SPMe)
  3. Doyle-Fuller-Newman (DFN)
- Lead-acid battery models:
  1. LOQS Model
  2. Composite Model
  3. Newman-Tiedemann Model
- Discretisations:
  1. 1D Finite Volumes (general purpose)
  2. 2 + 1D Finite Elements for current collector domain
  3. Control Volumes for electrode particle domains*
- Solvers:
  1. Scipy ODE solvers
  2. Scikits ODE & DAE solvers (SUNDIALS)
  3. Dae-Cpp DAE solver (Ivan Korotkin - Southampton)*

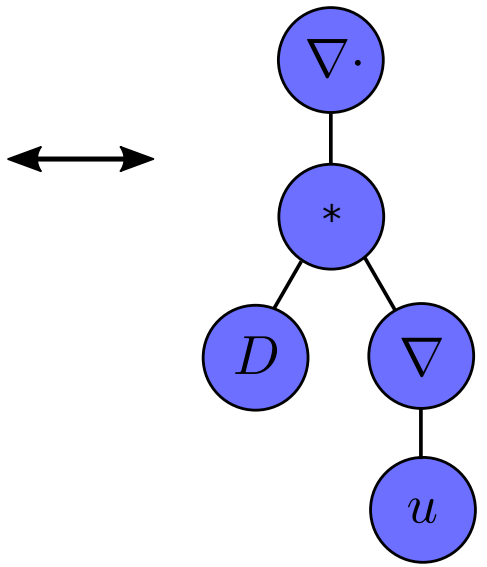
PyBaMM Pipeline

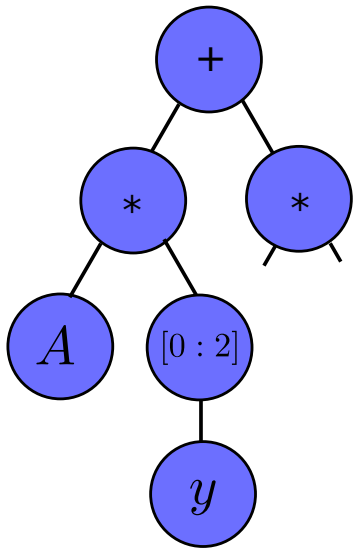
- PyBaMM's design separates the different stages solving a model, can develop or customise each stage separately
- Construction of a pipeline is a python script, reuse the stages as you see fit (e.g. comparing different models, re-solving with different parameters, custom plotting, ...)



PyBaMM's Expression Tree

- Communication between the stages is done via *expression trees* representing equations
- Different stages operate on these. E.g. Parameter Values walks though tree replacing symbolic parameters with scalars.
- Pybamm can take *derivatives* of expression trees (i.e. for Jacobians)

$\nabla \cdot (D \nabla u)$ 

$Ay[0:2] + By[2:4]$ 

Use Case 1 - Adding your own model

1. Create a Python class representing your model[1]
2. Define `rhs`, `algebraic`, `boundary_conditions`, `initial_conditions`, `variables` as **expression trees**
3. An expression tree is built from building blocks such as `pybamm.Variable` or `pybamm.Parameter`, and normal Python operators such as `+`. e.g., the expression

$$\nabla \cdot D(c)\nabla c + ac$$

written as:

```
c = pybamm.Variable('c')
a = pybamm.Parameter('a')
D = lambda x: pybamm.FunctionParameter('D', x)

expr = pybamm.div( D(c) * pybamm.grad(c) ) + a * c
```

[1] see repository documentation for more details

Use Case 1a - Add/Customise your own submodel

- **Note:** In-built models in PyBaMM consist of sub-models (e.g. electrolyte diffusion or interface kinetics). Often simpler to replace/add a new sub-model rather than write a new model from scratch

Use Case 2 - Using your own parameters

- Each model has a set of default parameters that you can use, for example:

```
model = pybamm.lithium_ion.SPM()
param = model.default_parameter_values
```

- You can change individual parameters in a python script:

```
param['Typical current [A]'] = 1.4
```

- ... or, the default parameter sets are defined as `csv` files in dimensional units, so can supply your own to specify an entire parameter set.

Use Case 3 - Plotting additional variables

- Each model has a list of variables that are calculated from the solution variables. These can be dimensional versions of solution variables or other useful quantities for comparing different battery models.

```
voltage = pybamm.ProcessedVariable(
            model.variables['Terminal voltage [V]'],
            solution.t, solution.y, mesh=mesh)


t = np.linspace(0,1,250)
plt.plot(t, voltage(t))
```

- Users can defined *custom variables* using expression trees. These are discretised along with the other equations in the model (can therefore contain derivatives)

Other potential use cases

1. **Custom discretisation**: discretisation is set on a per-domain basis (electrolyte, positive electrode particle, etc.). Can supply your own discretisation for one or more domains. Can be as general purpose or as model-specific as you require.
2. **Parameter estimation**: Those parameters that do not affect the discretisation can be altered and a new solutions obtained just be re-running the solver (i.e. no need to re-generate and discretise your model)
3. **Others..?**: We are keen to hear your ideas! PyBaMM is in a formative stage so keen to receive and incorporate feedback into the library.

Live demo time!!

Summary

- PyBaMM is a library for describing and solving continuum battery models
- Exposes a decoupled pipeline design for solving a model, so that users can customise with new models, discretisations, parameterisations, solvers etc.
- We welcome new developers at this beta testing stage, and are keen to get your feedback, bug reports and suggestions!
- Holding a 2-day PyBaMM workshop on the 31st July in Oxford, spaces available.
- Get the code, browse the documentation, or get in contact at: `https://github.com/pybamm-team/PyBaMM`