Faraday Institution Fast Start

Multi-Scale Modelling

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PL– Dr Jacqueline Edge
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The team

Imperial College London

UNIVERSITY OF BATH

UNIVERSITY OF OXFORD

UNIVERSITY OF Southampton

Lancaster University

UCL

UNIVERSITY OF BIRMINGHAM

WMG
THE UNIVERSITY OF WARWICK

The team


Saiful Islam (Bath)


Emma Kendrick (WMG)


Monica Marinescu (Imperial)


David Scanlon (UCL)


Dénes Csala (Lancaster)


Giles Richardson (Southampton)


Charles Monroe (Oxford)


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Denis Kramer (Southampton)


David Howey (Oxford)


Jon Chapman (Oxford)


Aron Walsh (Imperial)


James Marco (WMG)


Sam Cooper (Imperial)

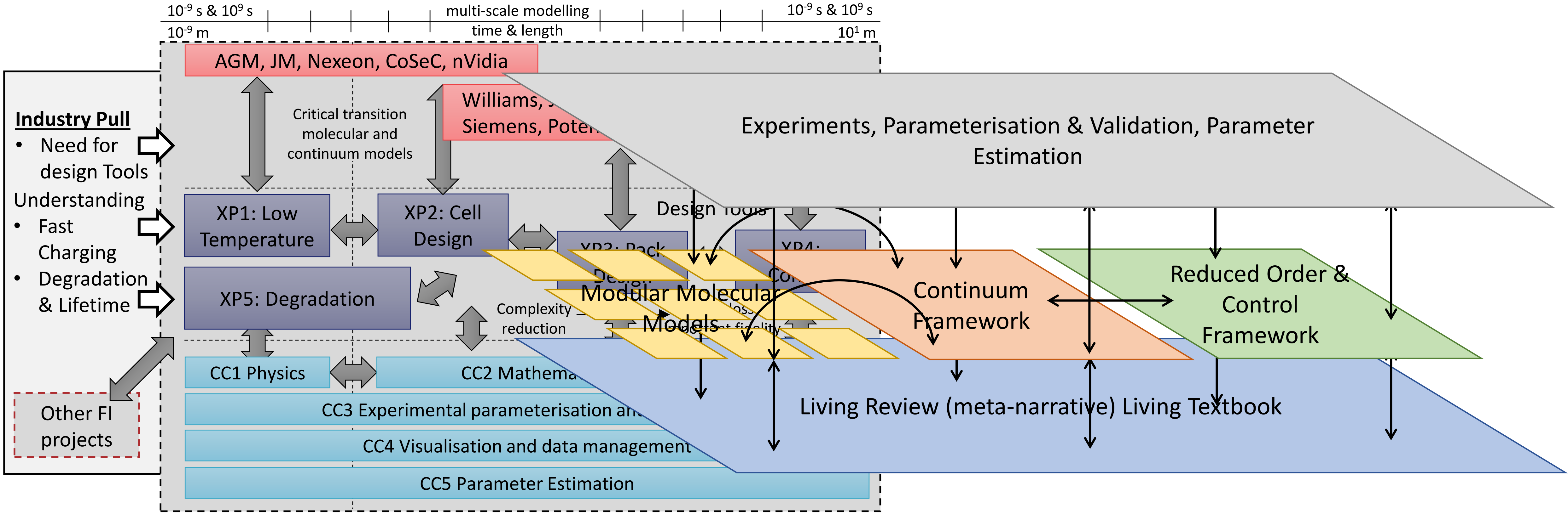

Paul Shearing (UCL)


Harry Hoster (Lancaster)


Chris-Kriton Skylaris (Southampton)


Colin Please (Oxford)

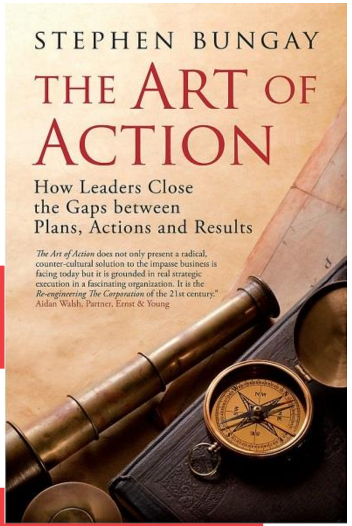
Project overview



The way the project is organised is changing as we understand what is needed in greater detail.

Strategy, operations & tactics (directed opportunism)

- Strategy is unitary and binding.
  - Created by academic investigators
  - Periodically reviewed (3 times/year)
  - Communicated to researchers to achieve alignment (Summer Visits and 121's)
- Operations is about execution and working out what to do at the time (objectives).
  - Researchers job, with periodic re-alignment against strategy with expedition leaders
  - Weekly/fortnightly meetings with supervisors to discuss technical details
- Tactics are standardised and binding procedures.
  - All contribute and benefit.



Strategy (Intent)

- Answering particular research questions
- Achieving certain goals & objectives

Execution (Operations)

- Exploiting advantage through independent thinking & obedience to strategy

Tactics

- Operating procedures to promulgate best practice, i.e. experimental test plans, training best practice coding, etc
- Standardisation of regular tasks to increase efficiency, i.e. common modelling framework and living review, etc

"What has not been made simple cannot be made clear and what is not clear will not get done."

Scope, goals & objectives

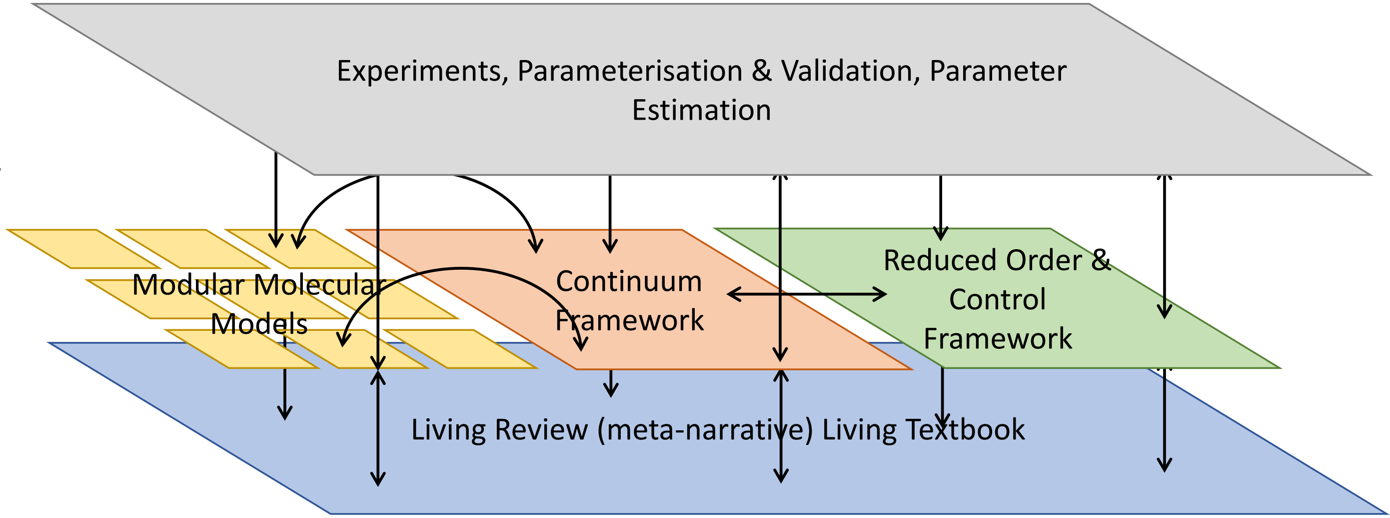
- Scope & Goals (Strategy) are the same
  - Ab initio modelling
    - Understand degradation mechanisms
    - Calculate parameters for continuum models
    - Explore material properties -> industry
  - Continuum models
    - Create common framework
    - Add coupled degradation mechanisms, lithium plating for fast charging first
    - Cell and pack design studies -> industry
    - Lifetime prediction studies -> industry
  - Control models
    - Create reduced order models
    - Implement in real-time controllers -> industry

- Objectives (Operations) adapt and change as required
  - Continuum modelling part of XP5 to work with XP2 working with CC2*, and focus on common framework, and then add science
  - Ab initio modelling part of XP5 to focus on the interface with continuum modelling to be led by Ben

* Still kept discrete as role is to keep an eye on long term vision

The importance of cross-cutting activities

- Living review emerges as critical tool
  - Documents science and justification of the research
  - Glues all parts of the project together and anchors it into external literature
  - Visualises research and makes it easily accessible to outside the project
- Experimentation spans all scales
  - Experiments must validate outputs at every length scale
  - Experiments alongside ab initio modelling critical for parameterisation
  - Leveraging multiple links with Degradation Fast Start



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Project Management

Led by: Jacqueline Edge

- Every 10 weeks, each XP and CCA reports on progress/highlights of previous period and plans for next
- Collaboration through MS Teams: shared files; chatting; video conferencing
- Monthly newsletter: project highlights; events/news/opportunities alerts
- Website in progress: batterymodel.co.uk
- Quarterly project meetings
- Fortnightly updates with TFI -> reports
- Flexibility is key
- Identified four cross-cutting subprojects:
  - Common Modelling Framework
  - Living Review
  - Coordinated experimental plan
  - Big Data Management
- Identified areas for collaboration between Fast Starts:
  - Workshops planned to map out links

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Common Modelling Framework

Led by: Monica Marinescu and Jacqueline Edge

- Publishable code
- Common platform:
  - Github
  - Python
- Design core continuum models & solvers: SPM, P2D, etc.
- Ongoing modifications through pair/peer programming: code review
- Series of collaborative sessions

- First Software Engineering workshop held in Oxford 29 Oct – 2 Nov:
  - Version control
  - Collaborative coding
  - Builds
  - Test-driven programming
  - Documentation
  - Agile methodology

-> Skills for producing robust, reproducible code to industry standard

-> Good progress on simple models

Coordinated Experimental Plan

Led by: Emma Kendrick & Changhui Chen

- Single layer pouch cells ordered from AGM Batteries – expected November 2018
  - Thermal gradients removed as an error
  - Standardisation easier
  - Electrolyte batches reserved
  - All undergo same formation before delivery
  - Same tabbing geometry
  - Characterisation of electrodes
  - Pressure and temperature impacts

-> Papers produced can be coordinated

- Experimental design for model validation:
  - Parameterisation set
  - Characterisation set
  - Measurement techniques: degree of accuracy, define standard condition suites
    - Environmental conditions
    - Charge-discharge conditions
  - Drive cycle definitions
  - Sample numbers
- First research questions:
  - Effects of tabbing
  - Effects of formation

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Big Data Management & HPC


Led by: Harry Hoster & David Scanlon

Data management

- To be set up alongside living review

- UCL Supercomputer cluster, *Michael*, launched on Wed 31st October.
- Access plan to be managed by David Scanlon.
- Further need for HPC for certain RAs.

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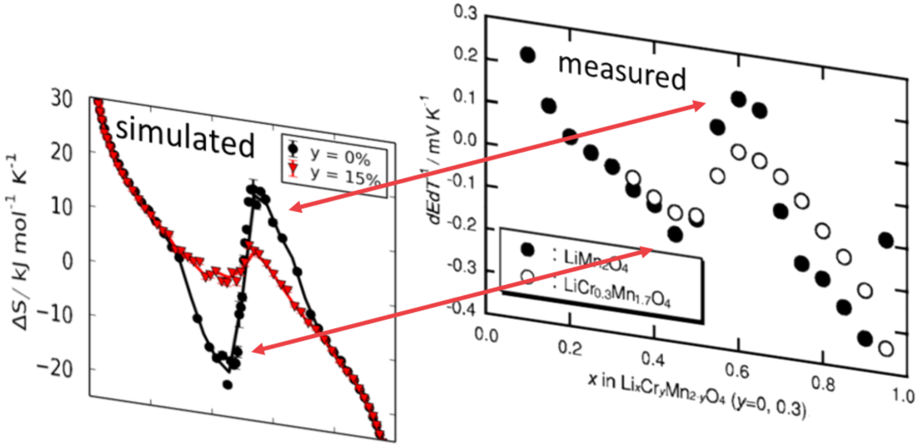
Living Review

Led by: Dénes Csala
Violeta Gonzalez-Perez, Jacqueline Edge

Connect researchers at **different** modelling **scales**, while maintaining full **attribution** and facilitating **collaborative publications**

"Computational notebooks are essentially laboratory notebooks for scientific computing. (…) a document that allows researchers to supplement their code and data with analysis, hypotheses and conjecture. (…) For data scientists, that format can drive exploration. "

[J. M. Perkel (2018 October 31) *Nature*]



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Living Review



Led by: Dénes Csala
Violeta Gonzalez-Perez, Jacqueline Edge

AUTHOREA Beta

Multiscale Modelling

Researcher Consortium at Imperial College London

figures have code attached

Jupyter

re-run the code in the cloud with new parameters for new outputs

plotly

plots are interactive for quick exploration

Dash by plotly

others run new scenarios without writing code

LATEX

edit paper collaboratively in Word, LATEX or HTML

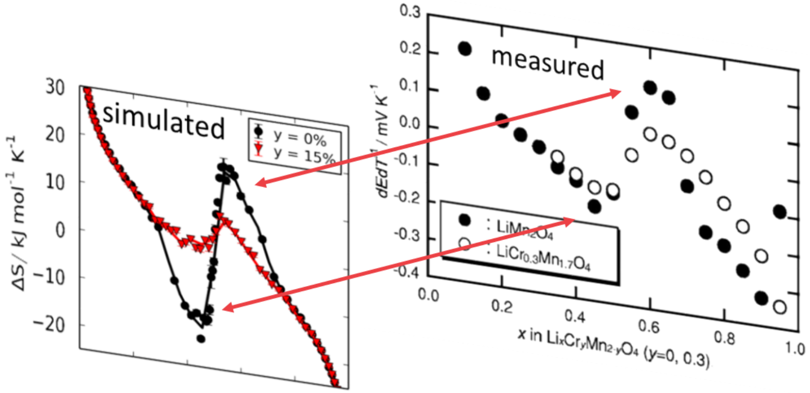
standardized coding

code in version control

GitHub

paper becomes a code repository of *.*tex* files

Connect researchers at **different** modelling **scales,** while maintaining full **attribution** and facilitating **collaborative publications**



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Living Review

- [The Faraday Institution Multi-Scale Modelling Living review demo article]
- [GitHub repository behind the paper]
- [Jupyter notebook with interactive plots]
- [Plotly Dash tutorial repository]

Scientific Progress: Overview

Publications & Outputs

Papers published:

- *Electrochimica Acta* **- 1**
- *Nature Catalysis* – **1**
- *Batteries & Supercaps* - **1**
- *Physical Chemistry Chemical Physics* **- 1**
- *Applied Energy* - **2**
- *J. Electrochem. Soc.* - **1**
- *Nature Materials* - **1**

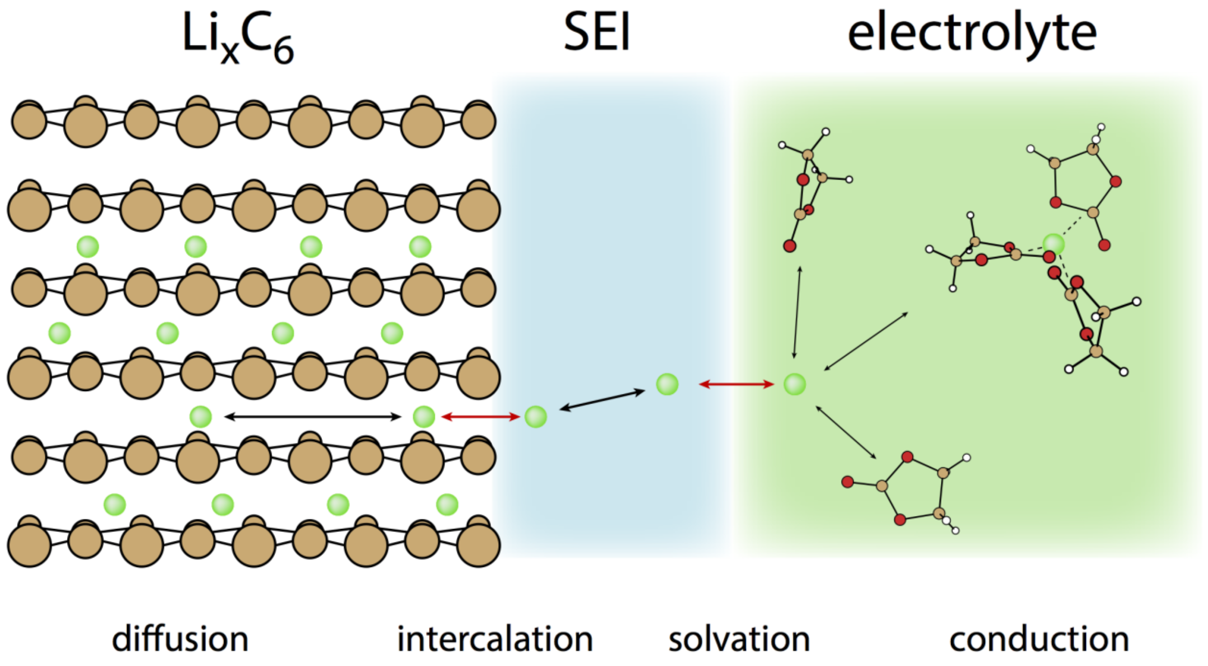
- Antonopoulos, B.K. *et al.* ”Solid electrolyte interphase: Can faster formation at lower potentials yield better performance?” *Electrochimica Acta* **269** pp. 331-339 (2018)
- Hoster, H.E. "Catalysing surface film formation." *Nature Catalysis* **1** (4), pp. 236 (2018)
- Antonopoulos, B.K. *et al*. "Formation of the Solid Electrolyte Interphase at Constant Potentials: a Model Study on Highly Oriented Pyrolytic Graphite." *Batteries & Supercaps* (2018)
- Schlueter, S. *et al*. "Quantifying structure dependent responses in Li-ion cells with excess Li spinel cathodes: matching voltage and entropy profiles through mean field models." *Physical Chemistry Chemical Physics* **20**, pp. 21417-21429 (2018)
- Liu, X. “The effect of cell-to-cell variations and thermal gradients on the performance and degradation of lithium-ion battery packs.” *Applied Energy* (2018)
- Zhao, Y. *et al.* “Modelling the effects of thermal gradients induced by tab and surface cooling on lithium ion cell performance.” *J. Electrochem. Soc.* (2018)
- Li Y. *et al.* “Fluid-enhanced surface diffusion controls intraparticle phase transformations.” (2018)
- Walsh, A. et al. “Oxidation states and iconicity.” *Nature Materials* (2018)
- Ai, W. “On uneven currents and the effect of thermal gradients on battery pack performance.” *Applied Energy* (2018)

Towards an atomistic understanding of intercalation across charged interfaces

Rationally mitigating rate limitations requires understanding of interface processes involved in (de)intercalation

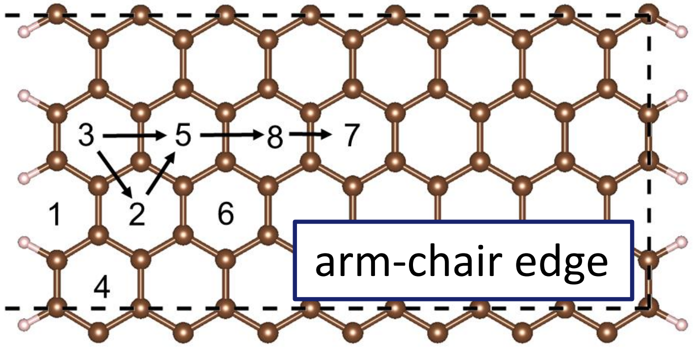
Last quarter:

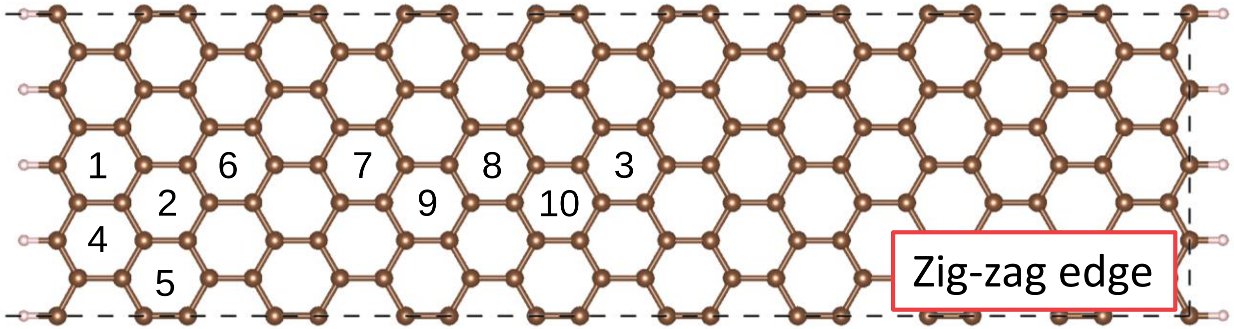
- *Work on sub-surface intercalation energetics*
- *Implementation of implicit electrolyte model*



Sub-surface energetics of Li in graphite

Chao Peng, James Womack, Chris-Kriton Skylaris, Denis Kramer





Results:

- Site energies of Li **substantially** different from bulk graphite
- Depends on edge type and termination

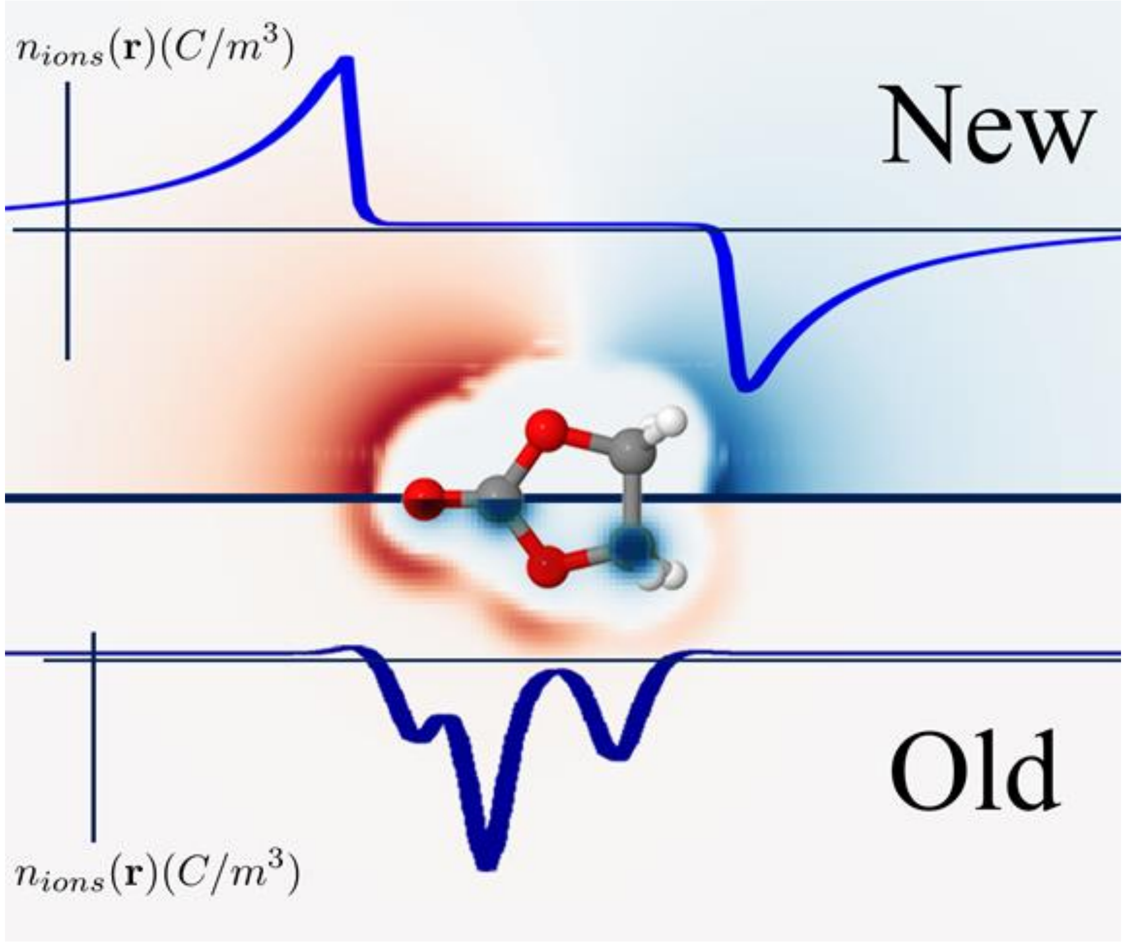
Importance:

- Sub-surface Li can “clog” interfaces during intercalation
- Opportunity to improve rates by
    - destabilizing Li via surface treatments and doping
    - synthesis routes favoring arm-chair edges over zig-zag edges

Implicit solvent model for charged interfaces

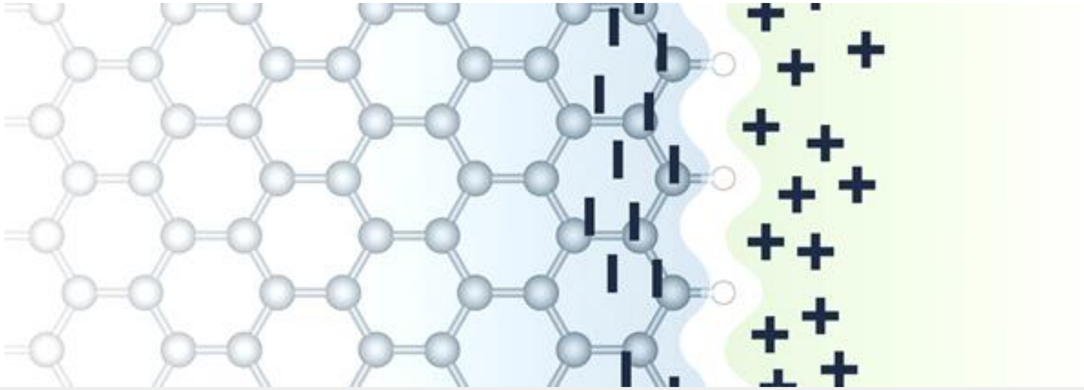
Marjan Famili, James Womack, Denis Kramer, Chris-Kriton Skylaris

Example: Electrolyte distribution around a molecule of ethylene carbonate (red: +ve ions, blue: –ve ions)



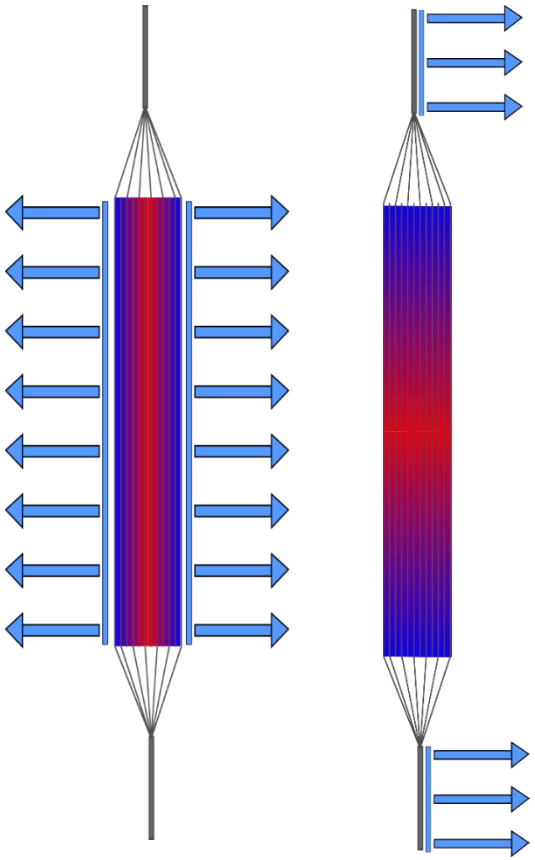
Result:
- New, physically correct linearised implicit electrolyte model implemented and tested on small molecules

Importance:
- Allows large-scale DFT calculations of charged interfaces (i.e., under constant potential rather than charge neutrality)

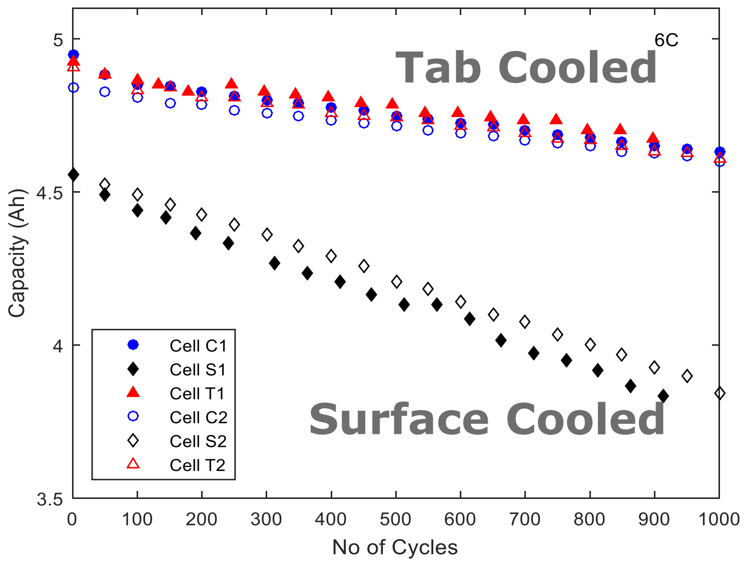


Continuum Modelling: Problem

- Previous work[2] has shown effect of thermal gradients highly important
- Affects useable capacity & lifetime
- Question: How to model this effect and enable industry to accurately predict lifetime for different thermal management systems



- 1000 cycles
  - 6C discharge and 2C charge
- Tab cooling is better
  - Useable and lifetime capacity



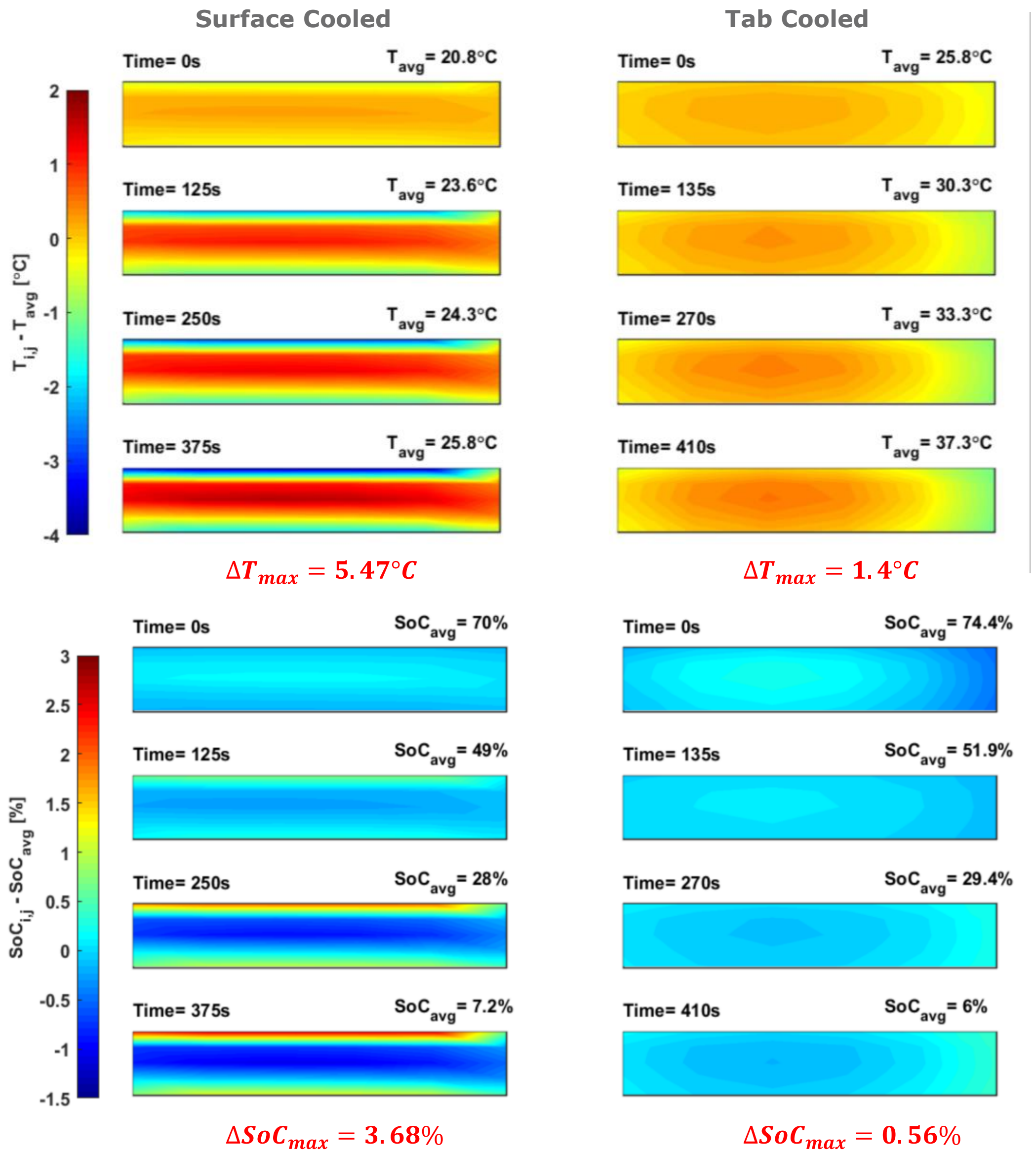
[1] Zhao et al. J. Electrochem. Soc., 2018, Vol 165, A3169–A3178

[2] Hunt et al. J. Electrochem. Soc., 2016, Vol 163, A1846-A1852

Continuum: Results

Effect can be modelled[1], but:

- Sophisticated thermal model is more important than electrochemistry (simple ECN)
- Non-core components & boundaries critical for thermal model (i.e. tab weld points)
- Parameterisation of thermal model is important, including reversible heat generation
- Validated across wide range of operating conditions



Zhao et al. J. Electrochem. Soc., 2018, Vol 165, A3169–A3178

Hunt et al. J. Electrochem. Soc., 2016, Vol 163, A1846-A1852

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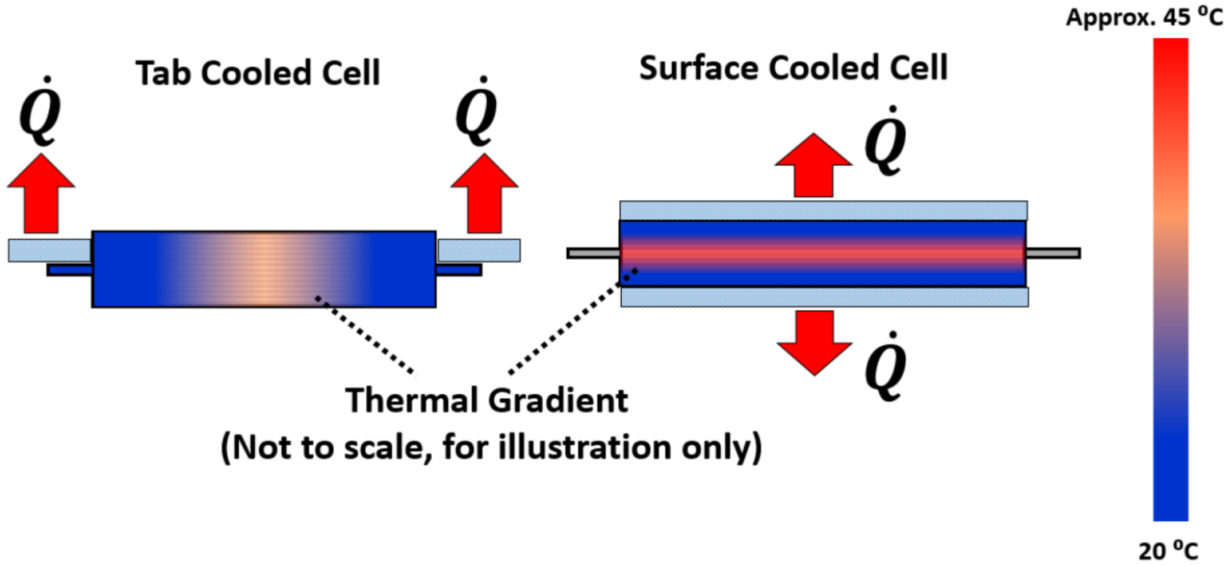
Continuum Modelling: Impact

Conclusions

- Surface cooling more effective at removing heat, even for relatively big tabs at both sides
- This is because of thermal resistance bottleneck between current collectors and tabs
- Surface cooling induces large thermal gradients, of many degrees, even across a thickness of just 10-12mm

Future work

- Explore the opportunities of redesigning cells to open up bottleneck
- Adding degradation to enable the effect on lifetime to be predicted



https://www.youtube.com/watch?v=_jd8REVB-c8

Zhao et al. J. Electrochem. Soc., 2018, Vol 165, A3169–A3178

Hunt et al. J. Electrochem. Soc., 2016, Vol 163, A1846-A1852

Workflow for control-oriented models (XP4 / CC5)

1 Define the modelling objective

e.g. estimate hotspots,
e.g. estimate anode potential,
etc..

2 Full order model based on fundamental physics (PDEs)

e.g. Moyels et at. *Asymptotic Reduction of a porous electrode model for Lithium-ion batteries*, 2018

3 Simplified approximate model (PDEs)

Parameter estimation and adaption (offline or online)

e.g. Bizeray. A. et al. *Identifiability and Parameter Estimation of the Single Particle Lithium-Ion Battery Model*, IEEE Trans. Control Systems Technology, 48, 2018.

4 Discretised + numerically solved model (ODEs)

e.g. Kandler A. Smith et al. *Model Order Reduction of 1D Diffusion Systems Via Residue Grouping* , Journal of Dynamic Systems, Measurement, and Control, 130, 2008.

5 Reduced order model (ODEs)

6 Real-time estimation and control

Challenges for control-oriented models

How can we simplify complex battery models but keep the physics we most care about?

↳ *Asymptotic analysis* (Moyels et at. 2018)

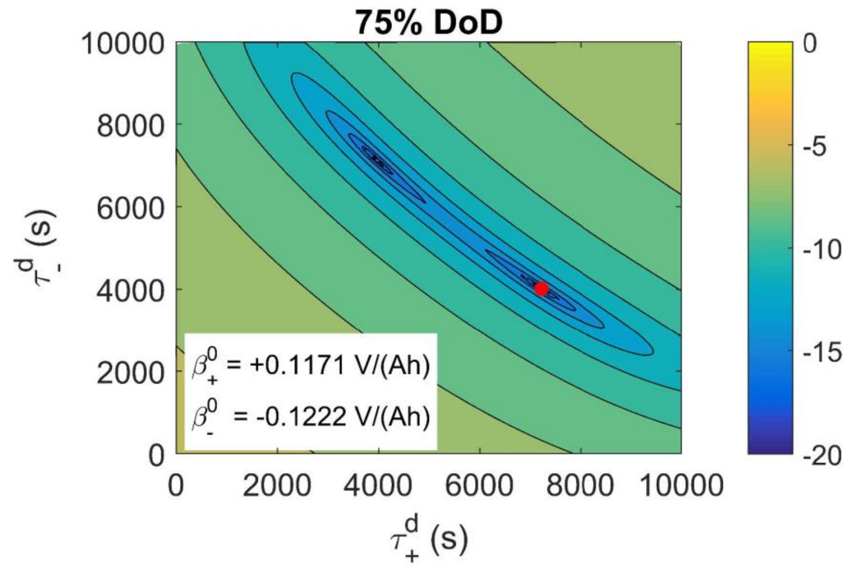
How can we make our models more computationally efficient?

↳ *Model order reduction* (K. A. Smith et al., 2008)

How do we fit model parameters from cell measurements, and check they are valid?

↳ *Identifiabilty analysis* (Bizeray. A. et al. 2018)

Example: Parameter fits may have multiple minima



Voltage error between model and experiment as a function of electrolyte diffusion timescale parameters (Bizeray. A. et al. 2018)

Example results

Moyels, et at. 2018 showed that

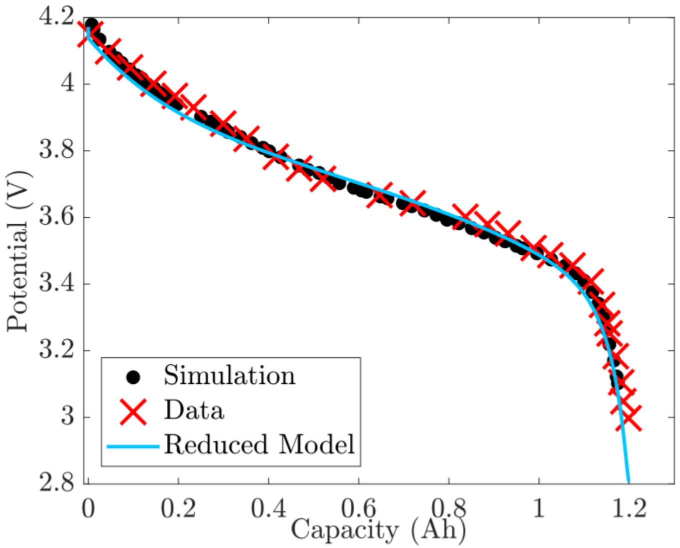
Electrochemical models can be systematically reduced to equivalent circuit models

K. A. Smith, et al., 2008

Model order reduction can give accurate results (depends on objective). E.g. 3rd order model was 1.2% within full order model.

From Bizeray, Howey, et al. 2018

Battery models are over parametrised and should be grouped for identification purposes



Moyels et at. 2018

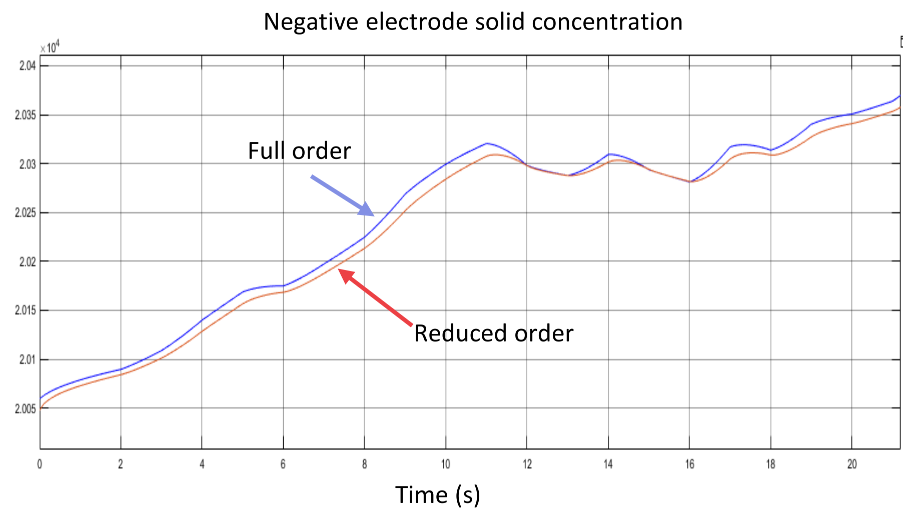
Impact of this work

Following on from these papers:

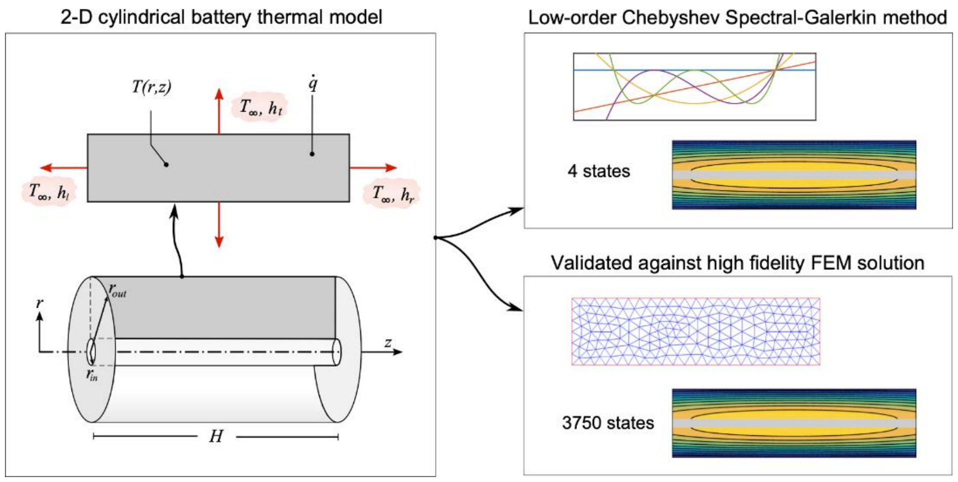
We have a good starting point to analyse coupled thermal-electrochemical models

We can develop the control algorithms for a BMS

We have a framework to study parameter validity for the coupled models that we will develop



Example of simulation of ROM vs. full order



Example of accurate hotspot modelling with ROM

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Next steps

- Other Fast starts:
  - **Degradation**: meetings held; workshop planned
  - **ReLib**: JE met with Prodip Das in Newcastle; workshop for Y2 planned
  - **SOLBAT**: 3 postdocs attended Software Engineering workshop; modelling coordination will be necessary in Y3; could do a workshop on experimental coordination
- Cross-cutting themes for workshops identified:
  - Design for Safety
  - Design for recycling
  - Experimental coordination
- Battery Modelling Conference, Oxford, March 2019

Next steps

Justify

- Researchers identify gaps or needs for research, define a hypothesis to be tested
- Discuss with supervisor, ensure it is aligned with objectives of expedition & strategy of project
- Justify and reference in living review (i.e. like introduction to a paper, hence can be used for this)

Conduct

- Researchers are free to use whatever modelling platform to explore the science
- Researchers can work in private, without having to disclose their best ideas until they are ready to publish, however, upon submission they must reintegrate with the core.

Record

- In addition to a paper, the result must be fully described in the living review, adding to the story
- The methodology must be fully described and reproducible, experimental test plans & data deposited in shared repository, well commented codes & documentation deposited in Github (all length scales), core equations implemented & tested in the common modelling framework (continuum length scale)