Faraday Institution Fast Start
Multi-Scale Modelling

PI - Dr Gregory Offer
PM – Dr Jacqueline Edge
Imperial College London
The team
Multi-scale modelling (MSM)

• To develop improved models
  • Across length and time scales
  • From atoms to systems

• In collaboration with industry
  • To solve application relevant challenges

• Key scientific challenges
  • Bridging atomistic to continuum modelling approaches
  • Parameterisation and validation
  • Mathematical complexity & computational cost

• The first applications
  • Fast charging and cold temperature operation (i.e. lithium plating)
  • Coupling degradation mechanisms
Multi-scale modelling (MSM)

- 5 Research Expeditions
  - XP1 COLDSTART
    - Denis Kramer, Southampton
  - XP2 CELLDO
    - Monica Marinescu, Imperial
  - XP3 BATPACK
    - Billy Wu, Imperial
  - XP4 ROMCON
    - Dhammika Widanalage, WMG
  - XP5 LONGTERM
    - Charles Monroe, Oxford

- Understanding
  - Fast Charging
  - Degradation & Lifetime

- Industry Pull
  - Need for design Tools
  - Understanding
    - Fast Charging
    - Degradation & Lifetime

- AGM, JM, Nexeon, CoSeC, nVidia
- Williams, JLR, RR, Ford, Ricardo, JM, Arcola, Siemens, Potenza, CAT, Conti, BMW, BBOXX
- Shell

- Design Tools
  - Critical transition molecular and continuum models
  - Complexity reduction
  - Without loss of important fidelity

- CC1 Physics
  - CC2 Mathematical methods and solvers
  - CC3 Experimental parameterisation and validation
  - CC4 Visualisation and data management
  - CC5 Parameter Estimation

- Other FI projects
Multi-scale modelling (MSM)

- 5 Cross Cutting Activities
  - CCA1 PHYSMAT
    - Chris-Kriton Skylaris, Southampton
  - CCA2 MATHS
    - Giles Richardson, Southampton
  - CCA3 TEST
    - Emma Kendrick, WMG
  - CCA4 VISDAM
    - Harry Hoster, Lancaster
  - CCA5 PEACE
    - Dave Howey, Oxford
Innovate UK project links

All will provide rapid routes for exploitation into commercial applications

- Niche Vehicle Supply Chain
  - AGM, Lancaster & WMG (& Many Others)
  - Will benefit from MSM design tools (cell, pack and ROMs)

- EV-elocity V2G project
  - WMG, (& Many Others)
  - Will benefit from MSM models of degradation

- VALUABLE project
  - UCL
  - Will benefit second life/ end of life / recycling processes

- SUNRISE project
  - UCL
  - Will benefit from MSM modelling of silicon anode additives

- LiS:FAB project
  - UCL, Williams, (Cranfield, Ceetak, Oxis)
  - Will benefit from MSM PhD student modelling of LiS cells (@ Imperial)

- BATMAN
  - Imperial, CAT, (AVID)
  - Will benefit from MSM design tools (cell, pack and ROMs)

- BAFTA
  - Imperial, Aston Martin, Dukosi
  - Will benefit from MSM design tools (cell, pack and ROMs)

- WIZer
  - Imperial, Williams, (ZAPGO, PowerOasis, Codeplay)
  - Will benefit from MSM design tools (cell, pack and ROMs)

... There are quite a few more relevant 1 year feasibility studies
Recruitment

RA18 (XP1,XP5) Ben Morgan – Lucy Morgan - Empirical Potential Models
RA5 (XP1,XP5) Saiful Islam – Rana Islam - Coarse-Graining
RA6 (XP1,XP5) Sam Cooper - Rowena Brugge/Nina Meddings – COLDSTART validation
RA7 (XP1,XP5,CC1) Denis Kramer – Chao Peng - COLDSTART modelling
RA19 (XP2) Monica Marinescu – Simon O’Kane – CELPDO modelling
RA20 (XP2,XP5,CC3) Harry Hoster - Mike Mercer – Anode features in graphite data
RA16 (XP3) Billy Wu – Weilong Ai – Stress & strain in particles
RA12 (XP4) James Marco – Liuying Li – ROMCon modelling
RA4 (XP5) Charles Monroe – Maxim Zyskin - Property parameterisation of LiPF6/PC
RA11 (XP5, CC1) David Scanlon – Christopher Savory - Degradation modelling
RA23 (XP5) Aron Walsh - Hui Yang – Electrodes: charge and heat trapping at defects

RA22 (XP1,XP5,CC1) Chris-Kriton Skylaris – Marjan Famili - Linear Scaling DFT
RA17 (CC2) Giles Richardson – Ivan Korotkin - Continuum Models
RA8 (CC2) Colin Please – Robert Timms - Reduced order ‘Newman-type’ models
RA10 (CC2) Jon Chapman – Toby Kirk – Asymptotics; microfluidic channels
RA13 (XP2,CC3) Emma Kendrick – Changhui Chen – Experimental design & support
RA15 (CC3) Paul Shearing – Xuekun Lu - Microstructure characterisation & analysis
RA21 (CC4) Dénécs Csala – Violeta Gonzalez Perez – Visualisation & data management
RA3 (XP4,CC5) Dave Howey – Pedro Ascensio - Volume expansion model for Li-ion

PhDs:
• Rebecca Clements – XP1, CC1
• Antti Aitio - Developing Next Gen Li and beyond Li Battery Electrolytes through Synthesis, Electrochemical Characterisation and Modelling
• Malgorzata Wojtala – XP3
• Andrew Wang - Electrolyte experiments
• Robert Burrell - Cell models to quantify, predict & understand degradation
• Jordan Richards - Real-world automotive lifetime prediction via models informed by high-precision experiments
• Ethan Culverhouse – CC2
• Peter Kay - Fast-charging & recovery effects; reversibility of Li-plating

Missing:
RA1 (XP3) Greg Offer
RA2 (XP2,CC3) Greg Offer
RA9 (XP4,CC5) Dhammika Widanalage
RA14 (XP3) Dan Brett
**IP plan**

- “IP Guidelines” document in progress – to send out in July
- Risk: direct/indirect IP breach -> needs consistency & non-exclusivity
- Engagement through XP/CC’s, following RASIC
- Start off industry agreements Jul/Aug

### RASIC (responsible, approves, supports, is informed, is consulted)

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<thead>
<tr>
<th>Responsible</th>
<th>Institution leading relationship</th>
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<tr>
<td>Approves and Supports (directly involved in negotiations)</td>
<td>Institutions directly involved in XP/CCA -&gt; multi-party CA</td>
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<td>Informed at key milestones (i.e. initiation, first draft, final draft, completion)</td>
<td>All other institutions</td>
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<td>Consulted (i.e. need to be aware of all CAs)</td>
<td>PI and Project Manager (Greg &amp; Jacqueline)</td>
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*Faraday Institution Fast Start: Multi-scale Modelling*
Management plan

- Shared documents: RAG monitor; Researchfish (esp. publications) log; Reading list; Training log
- Shared Calendar: anyone can attend any meeting
- Virtual attendance possible at all meetings; brief minutes recorded
- Flipped meeting approach (averts Death by Powerpoint): pre-recorded, 3-minute videos by all RAs
- Weekly hotline with PM, Mondays 3-4 pm: dial-in to ask questions (optional)

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<th>Year 1</th>
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<td>2-day FI Annual conference</td>
<td>MSM meeting FI review</td>
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Collaborative working

MS Team created:

• Enables seamless sharing of Office files
• Secure, large file share
• Integrated conference calls
• Shared Calendar, integrates with Outlook
• Conversation threads for XP/CCs
• Extensive app library of MS & non-MS sharing tools
• OneNote repository for all members
• Task lists with notifications & scheduling
Software engineering

- Code & data: open source through Github, where possible
- Publish descriptions in appropriate journals (e.g. Journal of Open Source Software)
- Tools developed in partnership with software developers
- Evaluated against industry standards (COMSOL, Dymola, CD-Adapco, etc.)
- Might require hiring a software engineer to curate code
Expedition 1 (XP1): Low-Temperature Capabilities (COLDSTART)

Southampton: Denis Kramer, Chris-Kriton Skylaris, Giles Richardson, Marjan Famili (RA), Chao Peng (RA), Ivan Korotkin (RA), Rebecca Clements

Bath: Saiful Islam, Benjamin Morgan

Imperial: Sam Cooper, Nina Meddings (RA), WMG: Emma Kendrick
XP1: Low-Temperature Capabilities (COLDSTART)

• **Mission statement**
  • Which process is ultimately limiting (low temperature) intercalation rates and how can it be overcome?

• **Core objectives**
  1. Map DFT onto MC/KMC surface models incorporating temperature
  2. Model desolvation from electrolyte to solid and the double layer at the atomistic scale
  3. Validate against experiment
XP1: COLDSTART - Aim

Which process is ultimately limiting (low temperature) intercalation rates and how can it be overcome?

[Appl. Energy 164 (2016) 99]
XP1: COLDSTART - Intercalation

Map DFT energy landscape onto MC/KMC models to get the (sub)surface thermodynamics and dynamics as function of $T$.


[unpublished graphic]

[unpublished graphic]
XP1: COLDSTART - (De)solvation

- Model desolvation from electrolyte to solid at the atomistic scale using explicit/implicit solvent models (very challenging!)
- Model double layer and charge transfer w/ Onetep (DFT + tight binding)

XP1: COLDSTART - Validation

- Isotopic exchange on solid samples
  - Surface exchange in liquid electrolyte
  - Bulk diffusion in dense solid
- Tracking fraction of lithium-6
XP1: COLDSTART - Deliverables

Year 1
- Design Guides / Surface Treatments
- Graphite / Model Terminations

Year 2
- Large-scale atomistic + desolvation
- Graphite / Realistic Solvation
- Solvent Models from CC1/CC2

Year 3
- Large-scale atomistic + desolvation
- NMC / Realistic Solvation
- Correlated Oxides in ONETEP

Faraday Institution Fast Start: Multi-scale Modelling
XP1: COLDSTART - Staffing

• Core COLDSTART team
  • Chao Peng (Southampton/Kramer) Modelling - Start: 10 August
  • Nina Meddings (Imperial/Cooper) Validation – Start: October

• Cross-Cutting Activities support
  • Marjan Famili (Southampton/Skylaris) – Linear Scaling DFT
  • Ivan Korotkin (Southampton/Richardson) – Continuum Models

• Other partners
  • WMG – *In situ* experimental support
Expedition 2 (XP2): Tools for cell design and optimisation (CELLDO)

*Imperial:* Monica Marinescu, Gregory Offer, Simon O’Kane (PDRA), A.N. Other (PDRA)
*Lancaster:* Harry Hoster, Michael Mercer (PDRA), Robert Burrell (PhD)
XP2: Tools for cell design and optimisation (CELLDO)

• Mission statement
  • To develop accurate, fast and parameterisable cell models for cell design, to embed in pack simulations, & inform reduced order modelling

• Core objectives
  1. Couple electrochemistry and thermal effects, and allow inhomogeneity to reproduce observed cell behaviour
  2. Couple mechanical effects, including swelling and stress/strain at the particle level
  3. Target EOL design => Include degradation due to low temperature fast charging and cycling
  4. Include cell-cell interactions for pack simulations
Approach – parallel strands

Create model specification
- Minimum physics
- Inhomogeneity across cell
- Parameterisable
- Update-able with new degradation

Use existing tools
- Assess minimum required physics
- Introduce inhomogeneity via single cell results
- Solve bespoke problems
  - Balancing of cells for EOL Li plating effects

Gather experimental evidence
- Parameterisation & validation of
  - mechanisms & effects
  - proposed design solutions

Assess possible frameworks
- Assist OU with mathematically-reduced electrochemical models
- Compare to other solutions

=> BOL universal framework

Usage
T(t), I(t)
- BOL performance
- Cycle life

Cell design
- Tab size & location
- Layer thickness & number
- Electrode balancing
Thermal effects are stronger than electrical
Reduced order cell model

Thermal Management Strongly Influences Performance & Degradation

Simple electrical model, but complex thermal model can reproduce magnitude of effect

Next: upgrade the model to include degradation

Data-driven thermal models would predict the opposite result:
A tab cooled cell has higher average T => ages faster


Yan Zhao* et al. Paper in preparation (* final year PhD Faraday MSM associated)

Faraday Institution Fast Start: Multi-scale Modelling
Spatial effects in single cell mimicked in cell networks
Temperature and pressure controlled single-layer cells

High precision charge counting

HPC cycles

Coulombic efficiency

Faraday Institution Fast Start: Multi-scale Modelling
Deliverables and project links

**Deliverables**
- Year 1 - cell design tool for BOL with simple degradation
  - includes electrochemical-thermal coupling and inhomogeneity;
- Year 2 – cell design tool in universal framework for EOL for specific uses, e.g. fast charging
  - validated against bespoke cells by CC3
- Year 3 – cell design tool for EOL including all relevant degradation from CCs and XPs
  - In universal framework, include mechanical coupling, validate against long term degradation data

**Links within the project**
- Parameterisation and validation of design tools CC3
- Give cell models and obtain pack specs XP3
- Support reduced order model generation XP4
- Include relevant degradation CC2, CC4, XP5
- Test variable observability of designed tools CC6
Expedition 3 (XP3): Pack modelling (BATPACK)

*Imperial*: Billy Wu, Gregory Offer, Monica Marinescu, Weilong Ai (PDRA), A. Post-Doc (PDRA)

*UCL*: Dan Brett, A.N. Other (PDRA)
XP3: Tools for module/pack design and optimisation (BATPACK)

• **Mission statement**
  • To accelerate the development and improve the performance/lifetime of battery packs for current and future battery chemistries

• **Core objectives**
  1. Develop a modelling framework which links pack level design decisions with electrochemical performance (thermal-mechanical)
  2. Understand and quantify the root cause of heterogeneous current distributions
  3. Develop diagnostic tools and figures of merit which would enable control algorithms which expand operating windows
  4. Explore novel pack architectures (hybrid cells/hybrid chemistries)
**XP3: BATPACK - Plan**

**Year 1**
- Thermally coupled pack model
- Understanding the impact of cell-to-cell variations
- Pack level diagnostics (ICA, DTV)
- Highly instrumented validation pack (pressure, voltage, current, temperature)
- Intelligent BMS

**Year 2**
- Develop figures of merit such as State-of-Balance (SOP) and State-of-available-power (SOAP)
- Derating techniques based on diagnostics
- Thermal-mechanical coupling
- Hybrid packs (HP-HE)

**Year 3**
- Mass parameterisation of cells in packs
- Li-S battery pack model
- Hybrid chemistry pack (Li-S/NMC)
- Application of pack design tools, diagnostics, integrated modelling and control for hybrid battery packs
XP3: BATPACK - Progress

- Starting to establish understanding of cell-to-cell variations
- First life and 2\textsuperscript{nd} life cells
- Tested to extra parameters for modelling
XP3: BATPACK - Progress

- Modelling the impact of cell-to-cell variations
- Placement of cells in packs impacts the accessible energy, especially at high C-rates

![Diagram of cell connections and voltage curves]

<table>
<thead>
<tr>
<th>Voltage (V)</th>
<th>Normalised Capacity (%)</th>
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<tbody>
<tr>
<td>0.1 C_cell voltage</td>
<td>3.0</td>
</tr>
<tr>
<td>0.1 C_pack voltage</td>
<td>3.2</td>
</tr>
<tr>
<td>1.5 C_cell voltage</td>
<td>3.4</td>
</tr>
<tr>
<td>1.5 C_pack voltage</td>
<td>3.6</td>
</tr>
</tbody>
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![Graph showing voltage and current over time for different conditions]

- Same cells
- Bad cell at 1
- Bad cell at 6

Faraday Institution Fast Start: Multi-scale Modelling
XP3: BATPACK - Progress

- Variation in the cell currents significant when aiming for high power densities
- Pack dQ/dV profiles give indications as to location of poorly performing cell
XP3: BATPACK - Exploitation and impact

- Workshop on battery pack modelling challenges and industry needs held with Delta Motorsport (02/03/2018) and McLaren (05/04/2018)
- Knowledge and model sharing with Delta Motorsport
- In discussions with Delta Motorsport to model AMPLIFII packs
- Follow on funding from Round 2 Innovate UK - £3M BAFTA project (Battery Advances For Transport Applications) with Aston Martin, Lagonda and Dukosi
- Modelling work feeding into Round 1 Innovate UK projects. IMPACT (IMproved bAttery Cooling Technologies) and ABLE (Advanced Battery Lifetime Extension)
- Working towards first pack modelling paper
Expedition 4 (XP4): Reduced Order Modelling & Control (ROMCon)

Warwick: Dhammika Widanalage, James Marco, Liuying Li (PDRA), A.N. Other (PDRA)

Oxford: Dave Howey, Pedro Ascencio (PDRA)
XP4: Reduced Order Modelling for Control (ROMCon)

- Mission statement
  - To produce reduced order models that can be embedded in commercial BMS systems that will solve real world problems

- Core objectives:
  1. To simplify and develop MSM electrochemical models with thermal and degradation phenomena for real time control applications
  2. To implement and benchmark ROM on real-time simulators
  3. Develop control strategies with ROMs for low temperature fast charging
XP4: ROMCon - Approach

- Full battery model consists of several sub-system dynamics, with input, states and outputs
- Will evaluate the dynamics (different time-scales) of the states to perform model reduction
- Will utilise techniques and analysis tools such as perturbation, asymptotic methods to perform model reduction
XP4: ROMCon – Approach, Short term

- Initial focus will be on:
  - Electrical, electrochemical and thermal dynamics at low temperature

- The simplified model will be
  - Validated
  - Implemented on a real-time platform
  - Used to evaluate charging control strategies
XP4: ROMCon – Approach, Long term

- Degradation dynamics coupled in second half
  - Degradation dynamics to include new learnings within project
- The simplified model will be
  - Further validated
  - Used for optimisation and control design of charging strategies and other BMS functions
Example of a reduced order model on a RT platform

Comparative study of the single particle model in real-time and pseudo two dimensional model in Comsol®

WMG, Chen Wang
Deliverables and partner engagement

• Deliverables
  • Four key deliverables of practical models for battery control that include thermal and degradation

• Initial partner engagements to include:
  • Williams: BMS support for model
  • Claytex: Adapt battery libraries with ROM models
  • Delta Motor Sport: Interested in ROM models for pack development

• Close ties with other XP and CCAs
  • Knowledge on heat generation and electrochemical coupling XP2
  • Knowledge on newly understood transport and degradation mechanisms XP5
  • Data for parameterisation and validation CC3
  • New knowledge on physics and solvers CC2
  • Parameter identifiability/estimation CC5
Expedition 5 (XP5): Modelling Degradation (LONGTERM)

Bath: Saiful Islam, Ben Morgan
Lancaster: Harry Hoster
Imperial: Sam Cooper, Aron Walsh
Oxford: Jon Chapman, David Howey, Charles Monroe, Colin Please
Southampton: Giles Richardson, Denis Kramer, Chris-Kriton Skylaris
UCL: David Scanlon
XP5: Modelling Degradation (LONGTERM)

• Mission statements
  • To build and strengthen bridges between the atomistic/molecular and continuum modelling communities
  • To understand and model degradation mechanisms that are relevant for real world applications

• Core objectives:
  1. Produce computational frameworks including coupled phenomena that affect performance and degradation, e.g. thermal and mechanical effects
  2. Develop advanced continuum battery models to incorporate complementary multiphysical, microstructural, and atomistic data
  3. Use first-principles simulations to describe redox, thermal, and defect chemistry of key electrode materials
XP5: PDRAs identified, most are inducted

- **Bath (2 PDRAs):** Rana Islam, Lucy Morgan
- **Lancaster (1 PDRA):** Mike Mercer
- **Imperial (2 PDRAs):** Rowena Brugge, Hui Yang
- **Oxford (4 PDRAs):** Toby Kirk, Pedro Ascensio, Maxim Zyskin, Robert Timms
- **Southampton (3 PDRAs):** Ivan Korotkin, Chao Peng, Marjan Famili
- **UCL (1 PDRA):** Christopher Savory

In post
- In post within ± 3 weeks
- Due to start by fall
XP5: Research highlights

- (Chapman, Please) Formal methods to reduce order of ‘Newman-type’ physical models
- Derived in context of lead-acid batteries (BBOXX)
- (Monroe) microscopic property parameterisation of LiPF₆/PC

Simulated 5C discharges

- 0th order quasistatic
- Full porous-electrode theory
- Fast composite
- 1st order quasistatic

(Fig. credit: Mr V Sulzer)

- Fast composite solution matches full porous-electrode theory with dramatically reduced computation time
- First validation of the concentrated-solution transport theory (with solute-volume effects) for a Li electrolyte

(Figs. credit: Mr T Hou)
XP5: Research highlights

- (Hoster, Howey) Grand canonical ensemble Monte Carlo and mean-field approaches to OCV/entropy modelling here: influence of point defects on the signatures of phase transitions

\[ \text{Li in first sublattice} \]

\[ \text{Li in second sublattice} \]

→ *ab initio*-based Monte-Carlo simulations to create thermodynamically founded analytic expressions for OCV and entropy curves that suit fast modelling techniques

(Fig. credit: Dr M Mercer)
XP5: Collaborations and outreach

• External presentations

P Goyal and CW Monroe, “Mechanical basis of Nafion’s High-Frequency Inductive Impedance,” 233rd ECS Meeting, 5/2018, Seattle, WA, USA

CW Monroe, “Mechanical Consequences of Electrochemical Transport,” Helmholtz Institute Seminar, 6/2018, Ulm, Germany


M Mercer, D Howey, H Hoster, “Thermodynamic reduced order models to understand degradation in Li ion cells” 6th European Conference on Computational Mechanics (ECCM 6) & 7th European Conference on Computational Fluid Dynamics (ECFD 7) 6/2018, Glasgow, UK
Cross-cutting activity 1 (CC1): Fundamental Physics & Materials Science (PHYSMAT)

Southampton: Chris-Kriton Skylaris, Denis Kramer, Giles Richardson, Marjan Famili, Chao Peng, Ivan Korotkin, Rebecca Clements
Bath: Saiful Islam, Benjamin Morgan
Imperial: Aron Walsh, Sam Cooper
UCL: David Scanlon
WMG: Emma Kendrick
Oxford: Colin Please
Lancaster: Denes Csala
CC1: Fundamental Physics & Materials Science (PHYSMAT)

• Mission statement
  • To create simulation platforms to capture the necessary physics and materials science

• Core objectives
  1. Develop and deploy new simulation methods to the FI
  2. Simulate solvents at the high electrolyte concentration regime
  3. Accurately simulate charge dynamics in metal oxides
  4. Integrate with MD for extensive sampling of electrolyte degrees of freedom
Linear-scaling first-principles quantum mechanics for atomistic simulations

The ONETEP linear-scaling DFT program

Conventional (cubic-scaling) DFT

Linear-scaling DFT (ONETEP)

Calculation time

Number of atoms

www.onetep.org


Picture taken from: A. A. Franco. RSC Advances. 3 (2013) 13027
CC1: PHYSMAT - Deliverables: Year 1

• New quantum and classical methods for simulation of solvent at the high electrolyte concentration regime

Scientific need - XP1

• Large-scale atomistic simulations of Li intercalation in graphite

• Methods to simulate charged solid/electrolyte interfaces

Background: development of electrolyte-free solvent model
CC1: PHYSMAT - Deliverables: Year 2

• New linear-scaling first-principles quantum methods for high accuracy calculations of metal oxides as well as force field-based approaches

Scientific need – XP5
• Accurately simulate charge dynamics in metal oxides
• Predictive simulation of defects, nano-structural modification and diffusion

Background: development of linear-scaling hybrid DFT exchange-correlation functionals

CC1: PHYSMAT - Deliverables: Year 3

- A linear-scaling DFT platform for electrochemistry
- Integrate with MD for extensive sampling of electrolyte degrees of freedom.
- Interface with visualisation and data management in CC4

Deliverables: 3-10 year horizon

- Mapping of atomistic outputs to coarser models from atoms to battery stacks
- Robust workflows for parameterisation of coarse grained and continuum models
- Providing parameterisation tools for continuum models of CC2
CC1: PHYSMAT - Pathways to impact

• Publications (new methods / applications with XPs), conferences, workshops
• Industrial collaboration with companies such as Dassault Systemes, Deregallera
• Release developments in the academic and the commercial (Dassault Systemes) versions of ONETEP
• Training users in the new methods within the annual ONETEP summer schools

Progress with hiring

• Postdoctoral Research Associate: Dr Marjan Famili will start on 2 July 2018
• PhD student: Rebecca Clements will start in October 2018 (within the NGCM CDT)
Cross-cutting activity 2 (CC2): Mathematical methods and solvers (MATHS)

Southampton: Giles Richardson, Ivan Korotkin (CCAP-PDRF), Ethan Culverhouse (PhD student)

Oxford: Jon Chapman, Colin Please, Robert Tims (PDRF) & Toby Kirk (PDRF)
CC2: MATHS - Aims

Aims

- Develop fast, flexible, robust and extensible code to solve core partial differential equation problems at heart of battery modelling.
- Use asymptotic techniques to systematically upscale detailed physical models to computationally simple engineering models.

Relationship to XPs

Underpins all expeditionary projects
Foster et al., J. Power Sources 350, p.140 (2017)
Causes of binder damage in porous battery electrodes and strategies to prevent it.

- Lateral binder delamination observed on particles and current collector after manufacture before cycling.
- Delamination becomes worse after repeated cycling.
- Explained by viscoelastic model of for binder around growing/shrinking electrode particles.
- Initial lateral delamination a consequence of binder swelling.
- Cycling produces delamination in vertical plane.
CC2: MATHS - Deliverables, Year 1

• Robust computational code to solve 1+1-dimensional porous electrode theory (PET) models.
  • Incorporate Non-Fickian transport models in electrode particles
  • Accurately conserve lithium (control volumes) over many cycles
  • Deal with sharp reaction fronts

• Develop accessible well-documented front end to code (e.g. GUI)

Deliverables, Year 2

• Multiscale reduction of PET models
  • Chemistry specific reductions (e.g. derivation of single particle models)
  • Operation regime specific reductions (e.g. derivation of equivalent circuit models)
  • Validate reduced models against full PET numerics
  • Derive equivalent circuit model parameters from cell microstructure

• Computational code to solve 3+1 & 3+2-dimensional PET models.
  • Address non-spatially uniform currents in pouch cells
  • Non-spherical electrode particles.
CC2: Deliverables: Year 2-3

• Incorporate mechanical and thermal effects into PET code.
  • Non-local heating
  • Stress build up in electrode particles and binder into PET code
  • Study binder delamination and electrode particle cracking

• Develop continuum models for lithium transport in electrode materials
  • Adopt multiscale approach based on DFT to determine appropriate transport models of Li in different materials (e.g. Cahn-Hilliard & nonlinear diffusion models).

Longer term

• Implement models for Li transport across electrolyte/SEI-layer/electrode region.
• Use tomography data with averaging techniques to calculate PET model parameters from cell microstructure
• Develop models for SEI formation and effects on cell performance
Faraday Institution Fast Start: Multi-scale Modelling
Cross-cutting activity 3 (CC3): Experimental parameterisation & validation (TEST)

**WMG:** Emma Kendrick, Dhammika Widanalage

**Imperial:** Gregory Offer, Billy Wu, Sam Cooper

**UCL:** Dan Brett, Paul Shearing

**Lancaster:** Harry Hoster

**Oxford:** Charles Monroe, David Howey
CC3: Experimental parameterisation & validation (TEST)

• Mission statement
  • Support the modelling through parameterisation and validation.

• Core objectives
  1. Provide models with experimentally derived parameters.
  2. Perform analysis on materials, electrodes and cells with known compositional, physical and mechanical properties.
  3. To determine chemical, electrochemical and thermal properties through characterisation of components and cells.
  4. Evaluate throughout life time, at different temperatures, SOC and lifetime.
CC3: TEST - Activity 1, Cell Materials Selection

Power vs Energy design – effect of coat weights (1 - 2 - 3 mAh/cm²)

Existing Chemistry and Technology
- NMC622 (BASF) vs Graphite (Hitachi)
- Known and established mixing and coating protocols
- Stability in air for assembly
- Consistent cell manufacturing
- Establish experimental techniques and parameters
- Structural / thermal and electrochemical evaluations

Future Chemistry and Technologies
- NMC811 vs Graphite / Silicon
- New mixing and coating methodologies need established for consistency of cell production
- Air sensitive materials – different handling protocols
- Typically used in cylindrical not pouch. Need to establish pouch formats with this technology for testing.
CC3: TEST - Activity 2, Parameterisation Testing

**Chemical / Structural**
- Young’s Modulus
- Chemical composition
- Physical dimensions
- Tortuosity
- Packing / densities

**Thermal**
- Heat transport
- In plane / through plane
- Heat Generation
- Heat distribution
- $dT/dV$

**Electrochemical**
- Electronic / ionic transport
- OCV curves
- Diffusion / Transfer numbers
- Activation Energy
- $dQ/dV$
CC3: NMC electrode microstructure characterisation

Three phase gray scale
Three phase segmentation
AM particles
Particle orientation
Pore size distribution
Reaction sites

Xuekun Lu, Antonio Bertei, Paul Shearing: Work in Progress towards Paper
The Effect of Microstructural Heterogeneity on the Electrochemical Performance of Li-ion Battery
CC3: NMC electrode microstructure characterisation

Xuekun Lu, Antonio Bertei, Paul Shearing: Work in Progress towards Paper
The Effect of Microstructural Heterogeneity on the Electrochemical Performance of Li-ion Battery
CC3: TEST - Activity 3, Testing (drive cycle protocols)

- Testing protocols
- Cycling drive cycles (non standard)
- To be determined
- Drive cycle data from BMW / JLR / Charging stations etc.

- Testing protocols
- Require input from partners to what is required
CC3: TEST - Deliverables and partner engagement

• Deliverables
  • To support all XPs with experimental parameter and validation.
  • Statistically Robust Data
  • Bespoke Cells for Parameterisation

• Initial partner engagement:
  • AGM batteries will provide reproducible cells for testing at cost, and access to facilities and training
  • Charging data for charge protocols
  • JLR / BMW – drive cycles for testing
  • Dukosi, support and protocols for testing and validation

• Close ties in Year 1
  • XP1 – cold testing and parameterisation, electrolytes
  • XP2 – experimental parameters for cell models
  • XP3 – instrumented packs for validating pack models
  • XP4 – Data for parameterisation and validation
Cross-cutting activity 4 (CC4): Visualisation and Data Management (VISDAM)

**Lancaster:** Harry Hoster, Denes Csala

**Imperial:** Gregory Offer
CC4: Visualisation and Data Management (VISDAM)

• Mission statements
  • To create the data and model management and visualisation tools to maximise the impact of the research of the whole project

• Core objectives:
  1. Can improve data sharing and communication tools, bridge scale gaps and improve experimental validations of battery modelling?
  2. How can connections between existing publications become more visible - and how can that inform the future research agenda?
CC4 aims:

1. break up silos
2. bridge gaps
3. to achieve truly integrated Multi-Scale Modelling

make model & experiment results available and understandable to wider research community

provide value to industry

data exchange

Visualisation and Data Management

VISDAM

data exploratorium
data kiosk
Living review paper

- Connect communities: model ↔ experiment
- Standardize procedures and metadata
- Collaboratively flag challenges
- Comment/vote on priorities
- Express interest in further development of ideas
- Track attribution of credit and provenance of data
- Share human resources and equipment

Activity for next ‘Third’: to write specification for this and identify the most suitable platform.
CC4: VISDAM - Deliverables Year 1

- VISDAM will adopt an “Agile Management” approach
- Pilot in the first 12 months, focus on one well-known chemistry end-to-end
- **Interact** with all modelling scales to deliver non-trivial knowledge from the simulation and experimental data outputs
- Design and deliver the **data exchange** and a basic interactive tool (kiosk) for industry partners (first trial user **BMW**)
- Coordinate with **high precision coulometry experiments** in XP2 and XP5

CC4: Deliverables year 2+

- Integrated data acquisition and management for efficient modelling-experiment validation loops
- Include more chemistries and modelling aspects
- Refine the exploratorium and kiosk interfaces and implement extrapolation and forecasting tools necessary to scale up limited experimental data to real-world applications
- Virtual/augmented reality and other advanced visualisations for better understanding of multi-dimensional processes and problems.
CC4: VISDAM - Pathways to impact

- Delivery of collaboration and showcase tools
- Development of data standards and hosting in data safe haven
- Publications on new data collection and sharing methods and joint publications with the XPs
- Presentations in conferences and workshops
- Curation of code repository with version control
- Training of users in the new methods within the annual data workshops
- Potential service extension to other FI projects

Progress with hiring

- **PDRA**: Dr Violeta Gonzalez-Perez – will start in October 2018
  supported by XP2 researchers for pilot delivery:
  - PDRA: Dr Michael Mercer – started March 2018
  - PhD student: Robert Burrell – started June 2018 (in partnership with BMW)
Cross-cutting activity 5 (CC5): Parameter estimation and model analysis

*Oxford*: David Howey, Pedro Ascencio (PDRA)

*WMG*: Dhammika Widanalage
CC5: Parameter estimation and model analysis (PEACE)

• Mission statements
  • Provide tools to support model selection, analysis and parametrisation.

• Core objectives:
  • Develop new approaches to structural identifiability and parameter sensitivity analysis of battery models
  • Develop new techniques and implement established techniques from other fields applied to battery model parameter estimation
  • Produce a toolbox of analysis and estimation techniques for use by the project consortium
CC5 – Parameter estimation and model analysis

- **Aim:** Model selection, analysis and parametrisation.

- **Why?** Battery models contain many parameters. Best fits of outputs do not mean the model structure or states are ‘correct’.

- **Example:** Fast charging → estimate anode potential → requires accurate estimation of internal overpotentials. Depends on parameters e.g. $i_0, \kappa, D$ etc.

Log of voltage error cost functions (colour) vs. normalised diffusivity in positive (x-) and negative (y-axis) electrodes, at various DoD. [Arxiv pre-print 1702.02471](https://arxiv.org/abs/1702.02471)
CC5 – Achievements this quarter

• Oxford appointed Dr Pedro Ascencio – background in control engineering, including adaptive observers (Imperial), and modelling silicon anodes (WMG).

• Hosted 2-day visit to Oxford by Dr Scott Moura (Berkeley), 4-5/6/18, including talk on “Identification and Control of PDE Battery Electrochemistry Models”.

• Gave invited talks and conference presentations:
  • “Parameterisation of the Single Particle Model for Lithium-ion Cells”, D. Howey, Warwick Battery Workshop 7-8/6/18.
  • “A Volume Expansion Model for Li-ion Batteries and its Numerical Solution”, P. Ascencio, Warwick Battery Workshop 7-8/6/18.
  • “Parameterisation of the Single Particle Model for Lithium-ion Cells”, D. Howey, ECCOMAS ECCM-ECFD, 11-15/6/2018, Glasgow.
CC5 – Plans next quarter, and engagement

• CC5 Year 1 aim is to understand parameter sensitivities in an already established model (e.g. SPM/P2D). Working towards this, we are:
  • extending Oxford’s previous work on parameterising the single particle model to include electrolyte parameterisation (the so-called “SPM-e”)
  • considering how to estimate functions rather than constants (e.g. charge transfer resistance as a function of SOC)
  • exploring non-linear EIS as a parameterisation approach (new equipment from Ivium capable of measuring NLEIS arrives week 1 July)

• Interactions
  • XP2, 3, 5: apply our techniques to the new models being developed
  • CC3: be involved in the design of experiments
  • Industry: Continental, Siemens, BBOXX → explore their available datasets
MSM: Plans for next quarter (Jun-Aug)

• PI/PM to visit each institution & meet with each RA personally
  • Discuss progress, training and CPD
• Plan for PhD cohort starting in October (FI, DTA, Industry, Ad hoc Etc)
  • Also, how to integrate FI-MSM associated PhD students
• Industry collaboration agreement negotiations kick-off
• Living Review document: understanding the state-of-the-art
• Project Coordinator (Nicholas Dean) started 2\textsuperscript{nd} July
  • First job to formalise our communication strategy (websites, videos, conferences, etc) to help establish the FI as the international point of contact for electrochemical energy storage in the UK
Thank You

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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