A Distributed Randles Circuit Model for Battery Abuse Simulations Using LS-DYNA®

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Introduction

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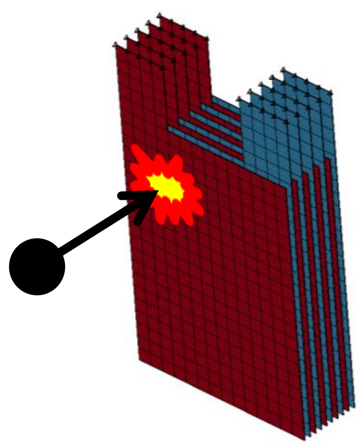
Car crash

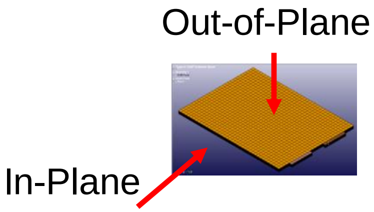
- Mechanical => Battery crush => local short circuits
- EM => large localized current densities => Joule heating
- Thermal => temperature increase => thermal runaway
  - CPM => fire, explosion



Case Study Development Assumptions

	Crash	Regulatory Crush	Overcharge/External Short/Thermal Ramp
Mechanics Time Scale	< 100 ms	> 10 s	> 10 s
EM/thermal Time Scale	ms to minutes		
Deformation Mode	Out-of-Plane or In-Plane Compression; Bending; Shear	Out-of-Plane Compression; In-Plane Compression	Internal Swelling; Separator Melting
Solver Assumption	Explicit to Implicit	Implicit	Implicit

- *3-D, transient finite element code needed to span these target applications*
- *Models that resolve mechanical properties of individual layers have higher potential robustness to multiple deformation modes*



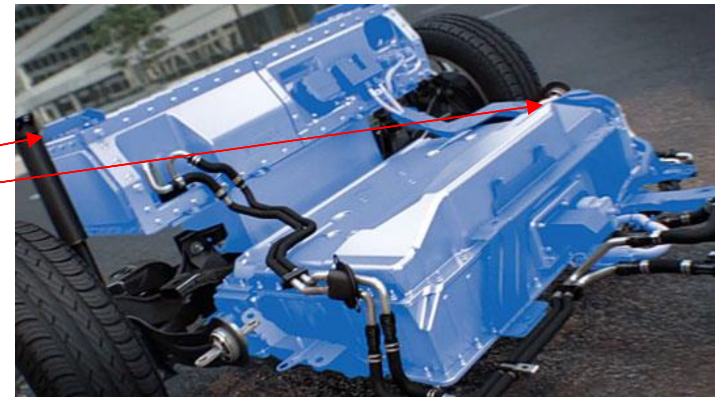
Outline

- Li-ion cell in an electric car
- The distributed Randles circuit model
- Validation on various electrical cycling experiments (“benign” use)
- Presentation of external short cases
- Presentation of internal short cases

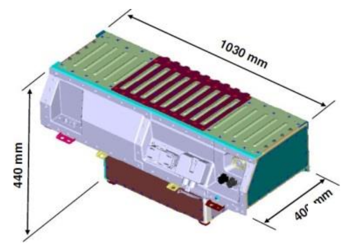
Li-ion cell

Vehicle

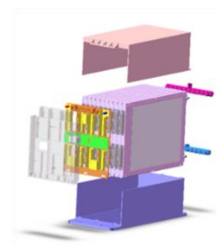
Dual-Packs



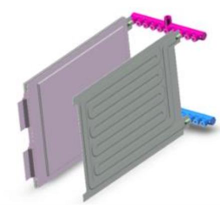
Pack



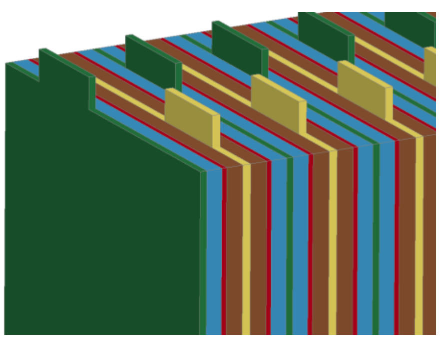
Module



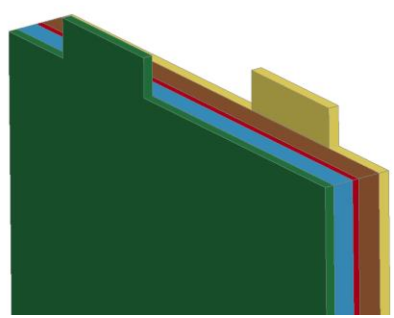
Cell

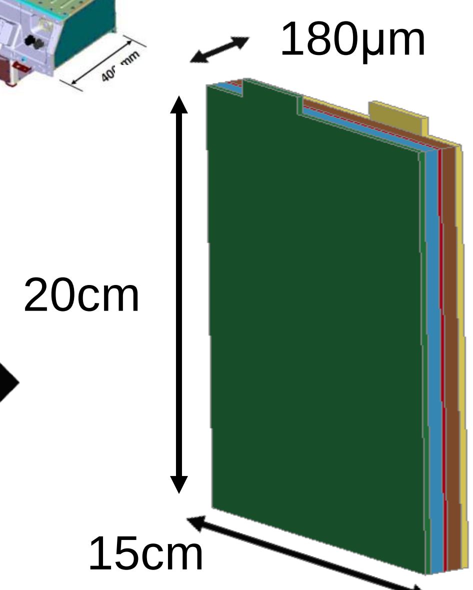


Cell (zoomed in z)



Unit cell (zoomed in z)





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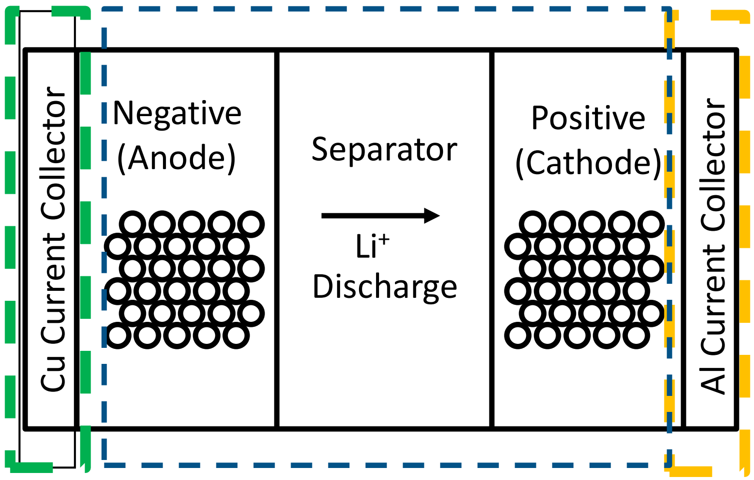
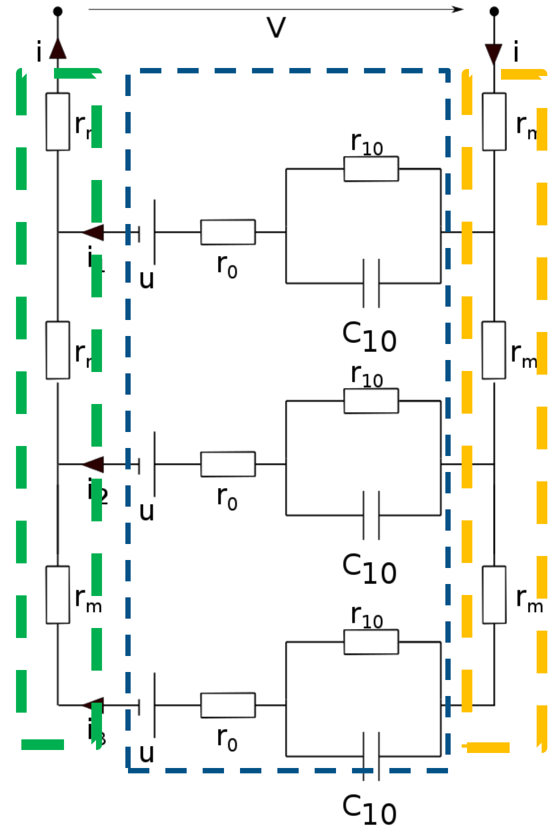
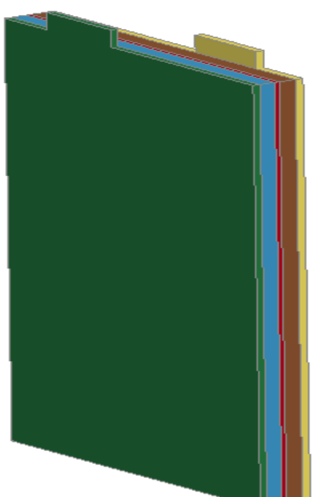
Distributed Equivalent Circuit (1st Order Randles)







- Current collectors transport electrons to/from tabs; modeled by resistive elements
- Jelly roll (anode – separator – cathode) transports Li+ ions; modeled with Randle circuit

r_0: Ohmic & kinetic

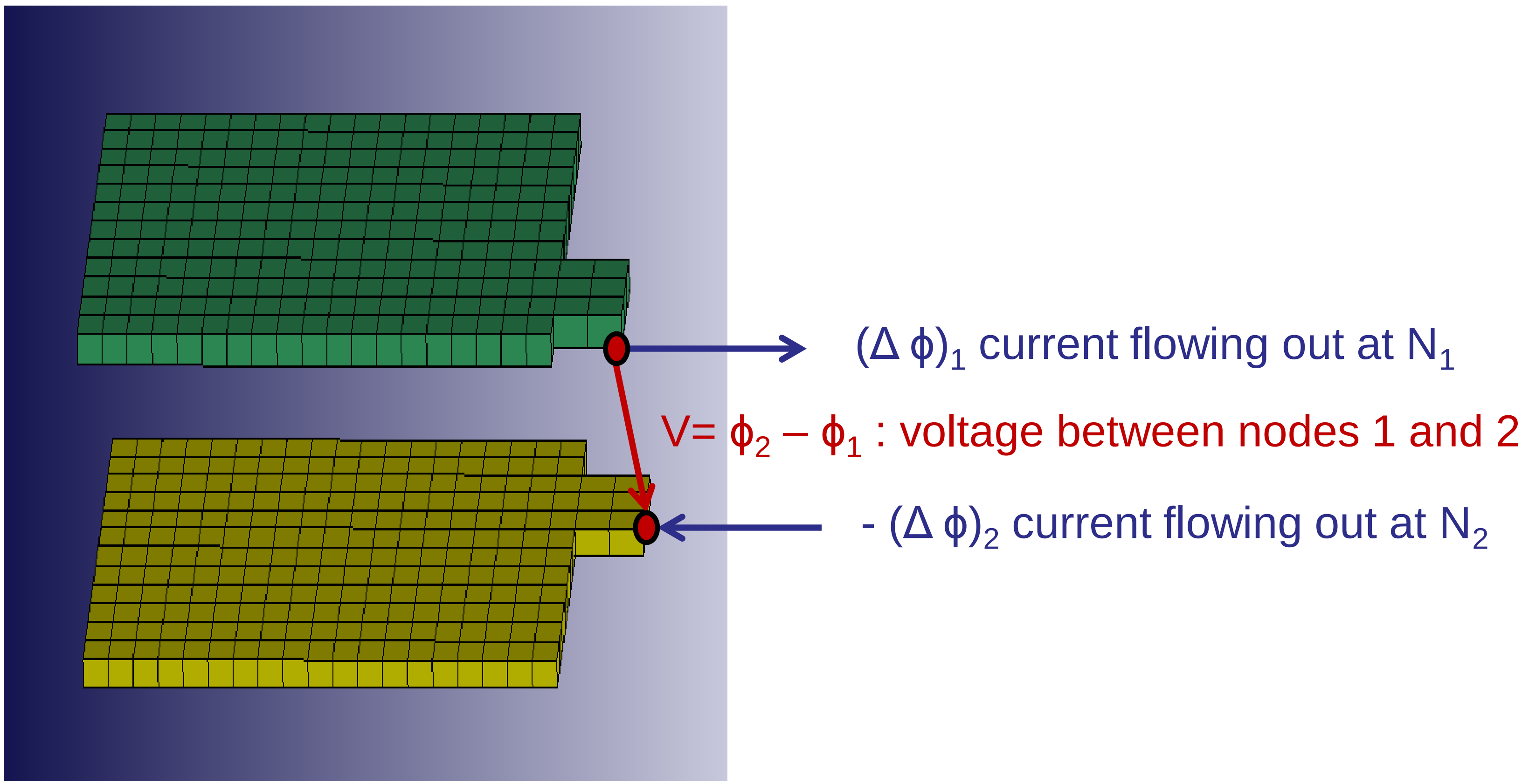
r_{10} & c_{10}: Diffusion

u: Equilibrium voltage (OCV)

r_m: Current collectors

Standard EM resistive solver

- ϕ : potential
- $E = -\,\mathrm{grad}(\phi)$: electric field
- $V = \phi_2 - \phi_1$: voltage
- $J = \sigma E$: current density (σ = electric conductivity)
- $\mathrm{div}(J) = 0 \Rightarrow \Delta\phi = 0$ + boundary conditions



Introduction of randles circuits in resistive solver

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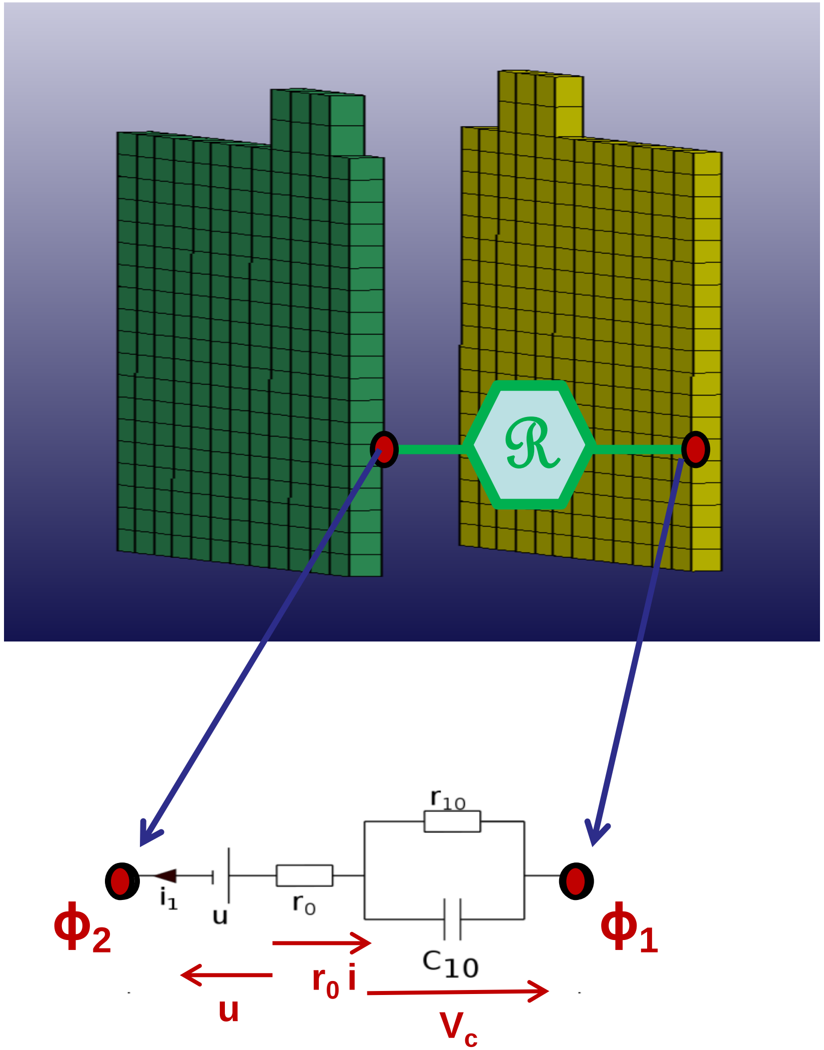


Randle circuit

Page 9

$\phi_2 - \phi_1 = u - r_0 * I - V_c$

$r_0 * i + \phi_2 - \phi_1 = u - V_c$

$i + (\phi_2 - \phi_1) / r_0 = (u - V_c) / r_0$

FEM solve:

$(S_0 + D) * \phi = b$

Where

- S_0 is the Laplacian operator (nds x nds)
- D has
  - $1/r_0$ at (N_1,N_1) and (N_2,N_2)
  - $-1/r_0$ at (N_1,N_2) and (N_2,N_1)
  - 0 elsewhere
- b has
  - $1/r_0(u-v_c)$ at N_1
  - $-1/r_0(u-v_c)$ at N_2
  - 0 elsewhere

Actualization of randle circuits:

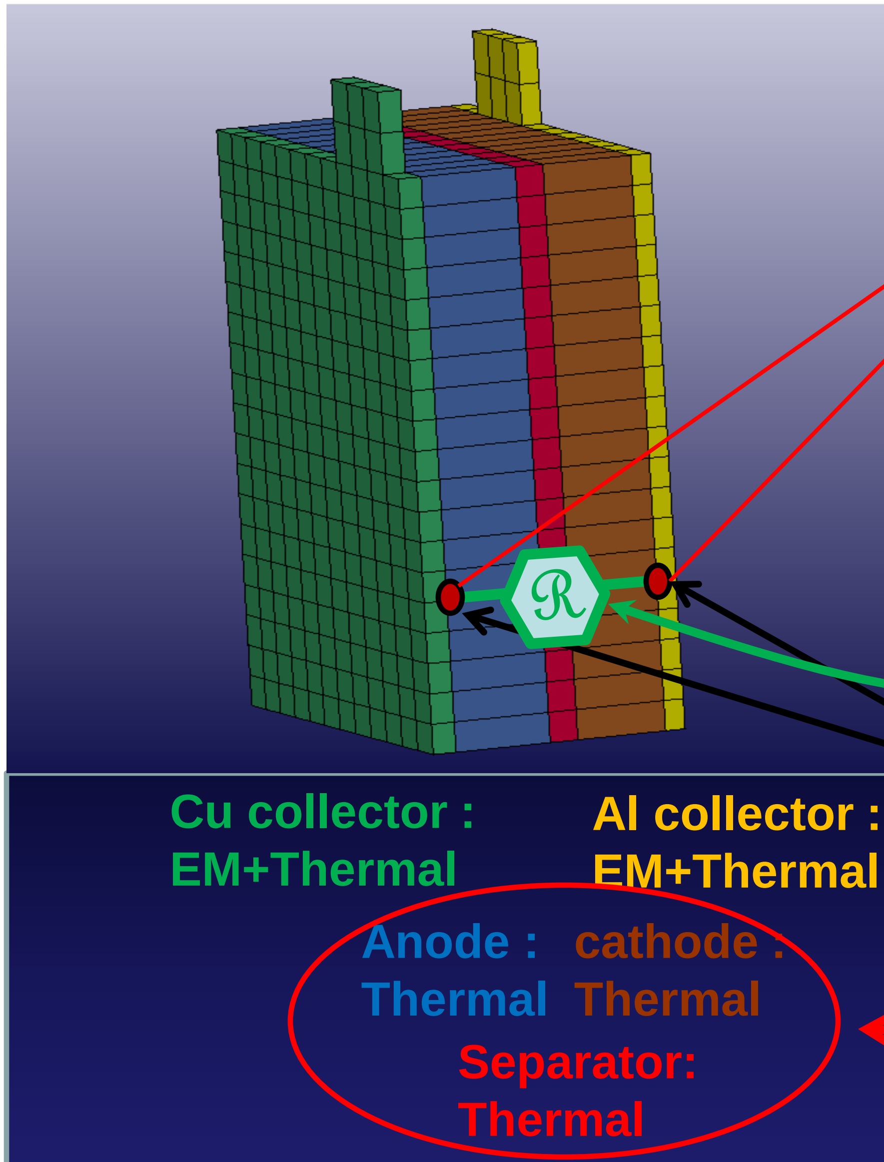
$i = (S_0 * \phi)(N_1)$

$V_c(t+dt) = V_c(t) + dt*(i/c_0 - V_c(t)/r_{10}/c_{10})$

$soc(t+dt) = soc(t) - dt*i*c_Q/Q$

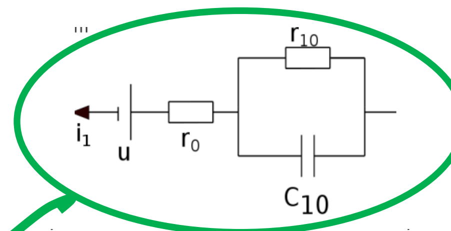
$u = u(soc)$

EM/thermal connection



T from thermal for r_0, r_{10}, c_{10} vs T

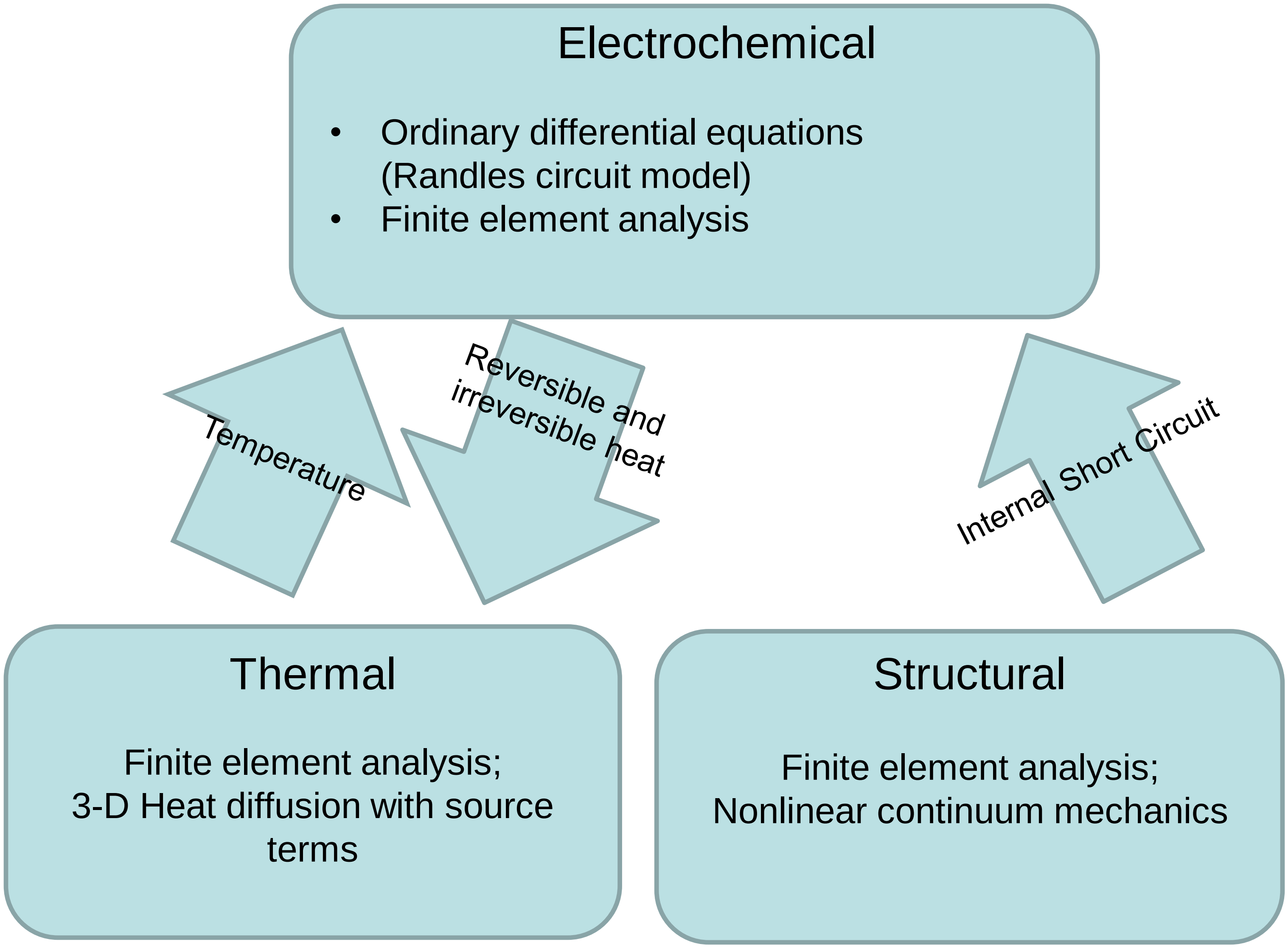
Randle circuit



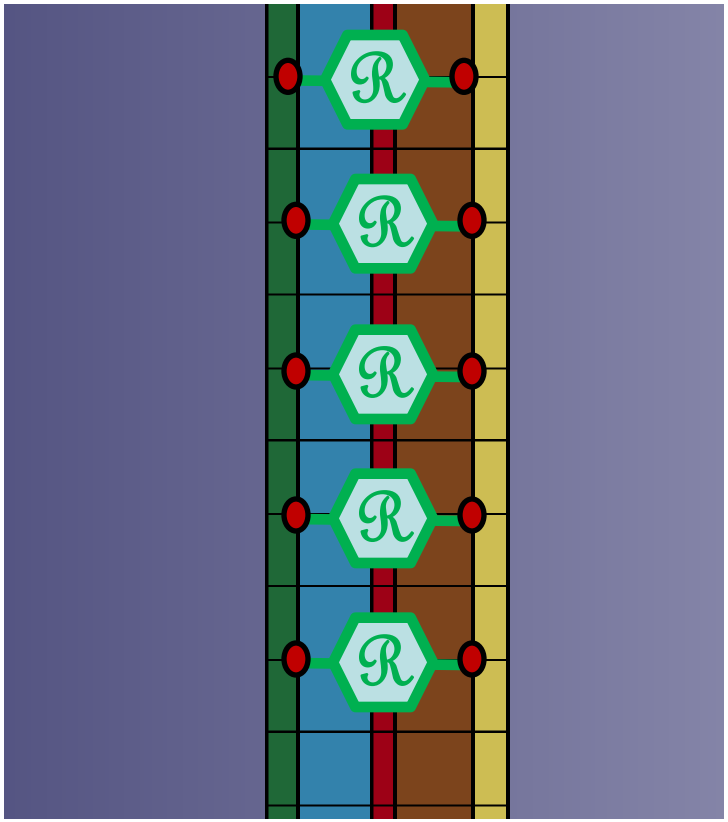
$r_0 * i^2$ added to thermal
ITdU/dT added to thermal

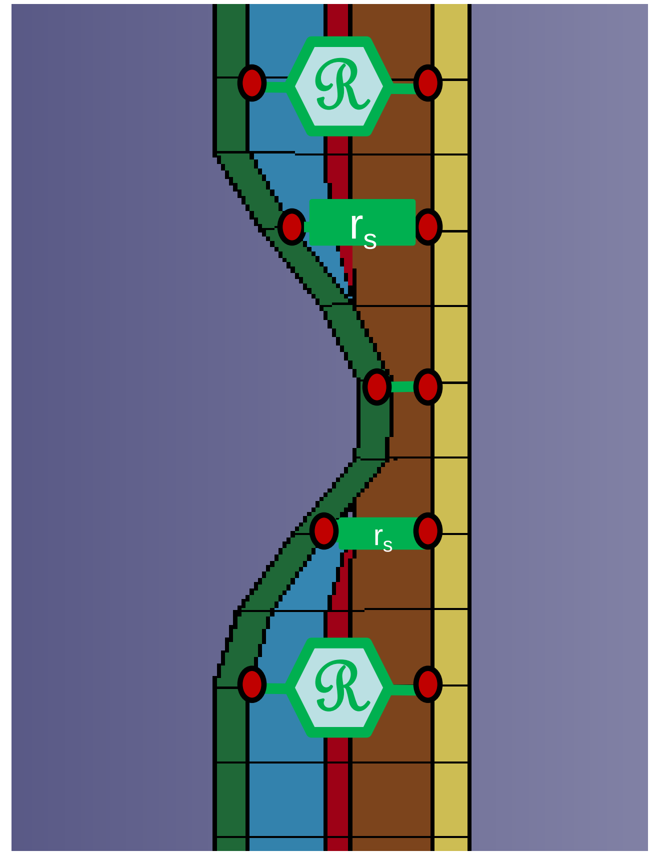
Allow correct material mass, heat capacity and thermal conductivity

EM/thermal/mechanical connections



Contact for Internal Short Models

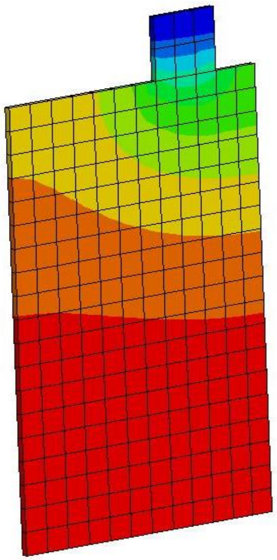




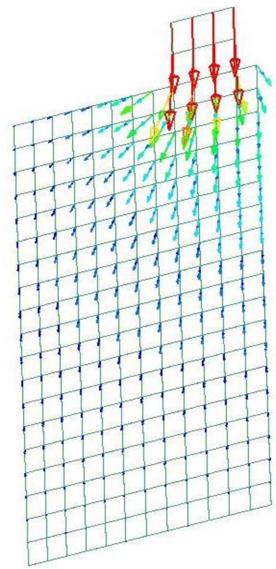
Replace randle circuit by resistance r_s
R_s * i ^{2} added to thermal

Experiment + simulation (voltage, current, temperature) should give good models

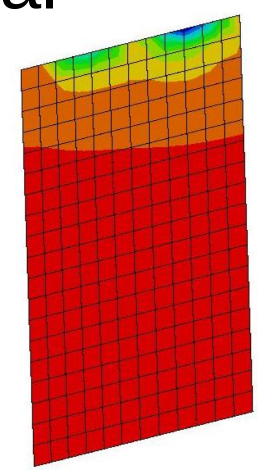
Randle circuits in LS-PREPOST



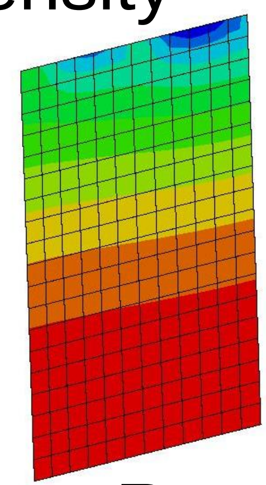
Scalar potential



Current density



Randle r0

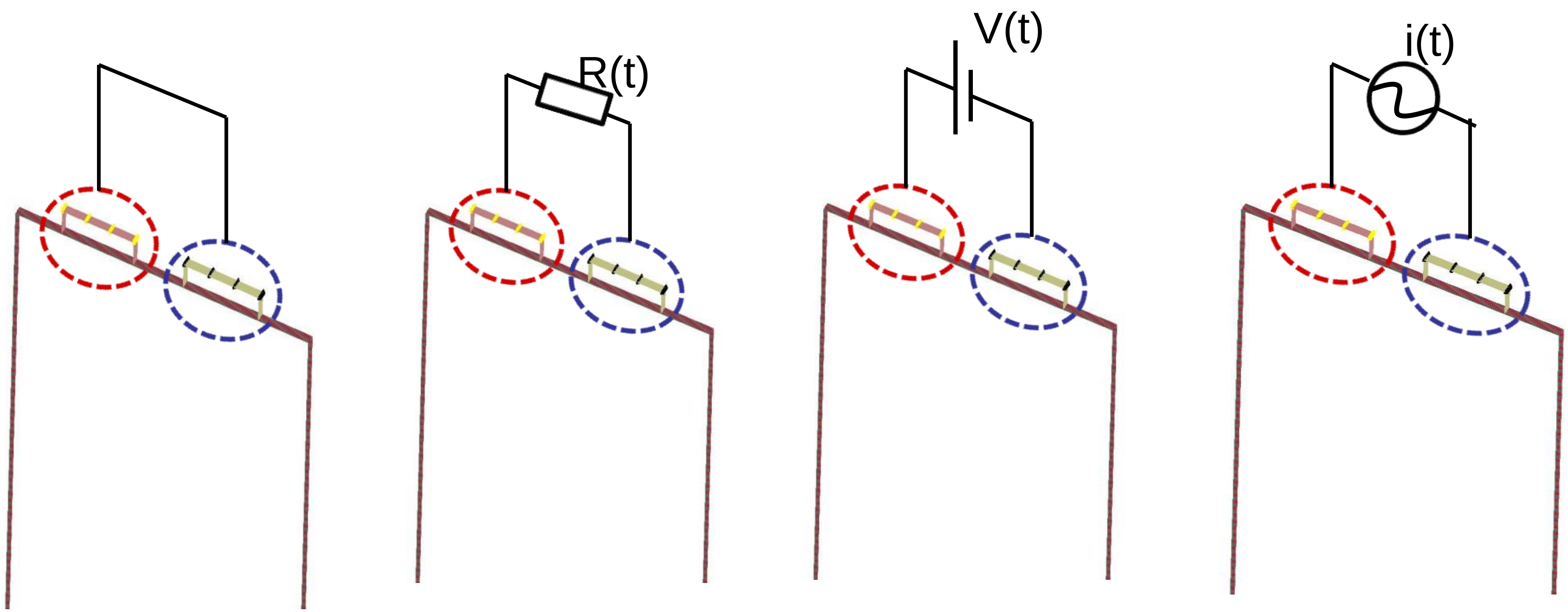


Randle SOC

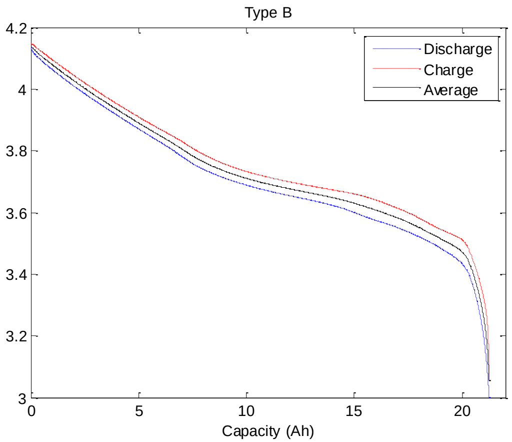
Connection to external circuits

Isopotentials can be defined and connected:

- The connectors do not need to be meshed.
- Enables alignment of cell simulations with experimental conditions (low rate cycling, HPPC, continuous discharge, …).

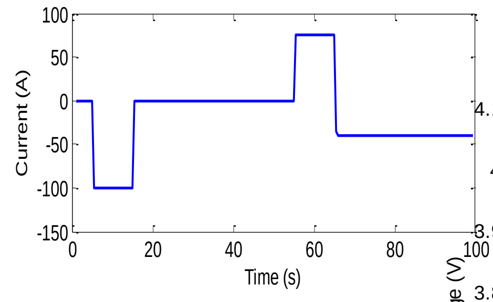


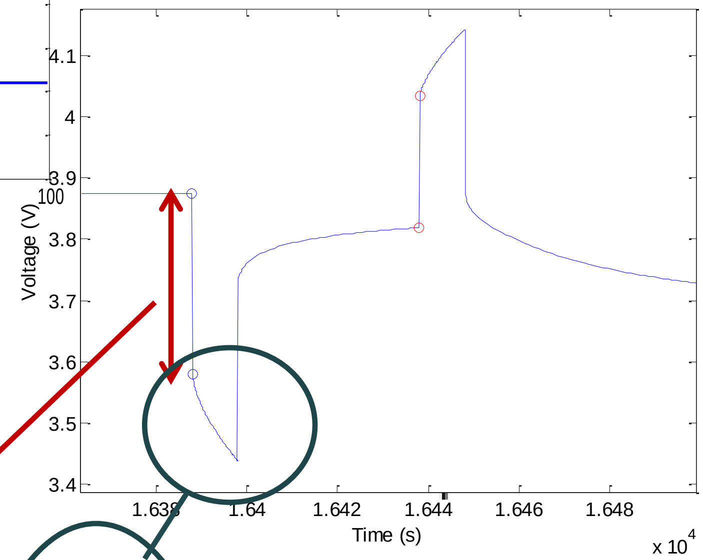
Evaluation of the circuit parameters

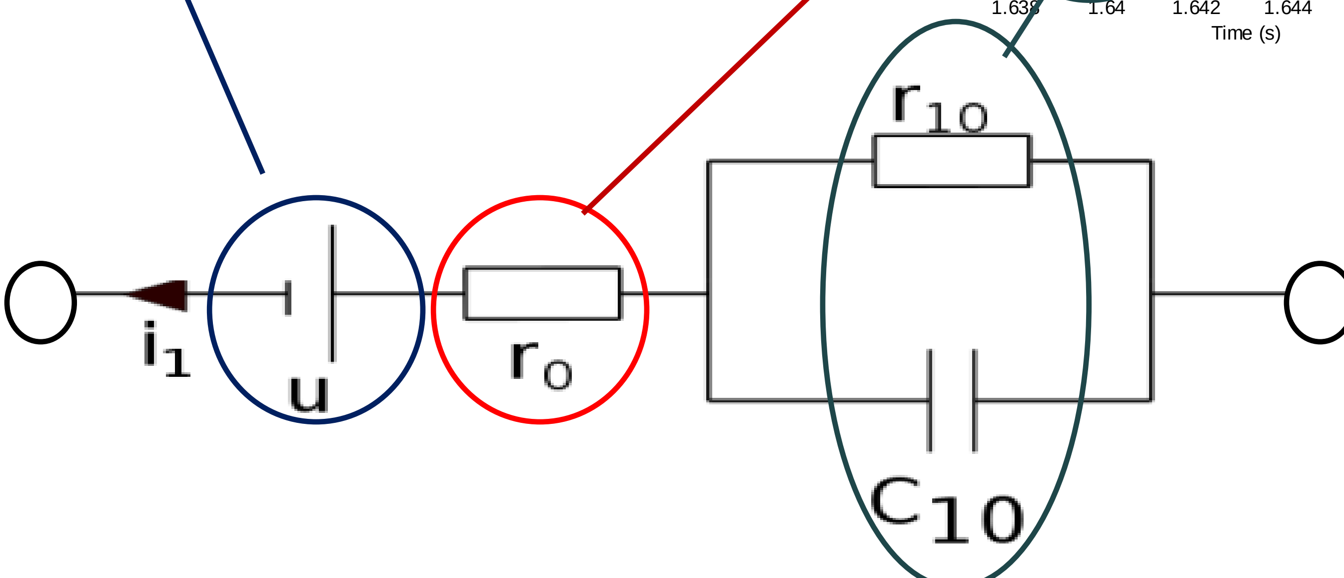


C/10
capacity tests

HPPC tests







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Benchmarking with experimental results

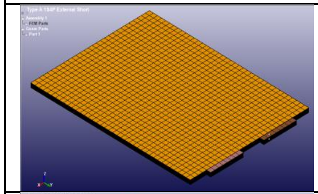
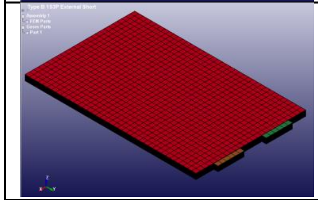
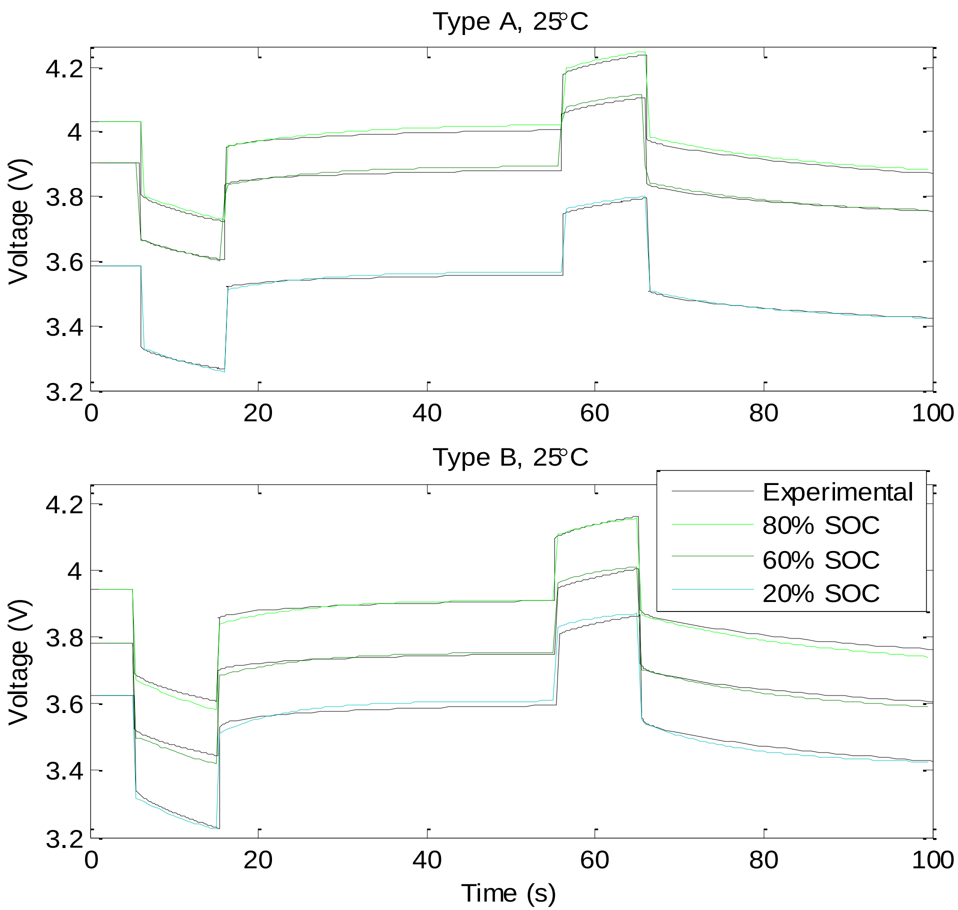
Image	Type	Cathode Chemistry	Dimensions	Number of Elements
	A	NMC/LMO	195 mm x 145 mm	151k
	B	NMC	195 mm x 125 mm	153k

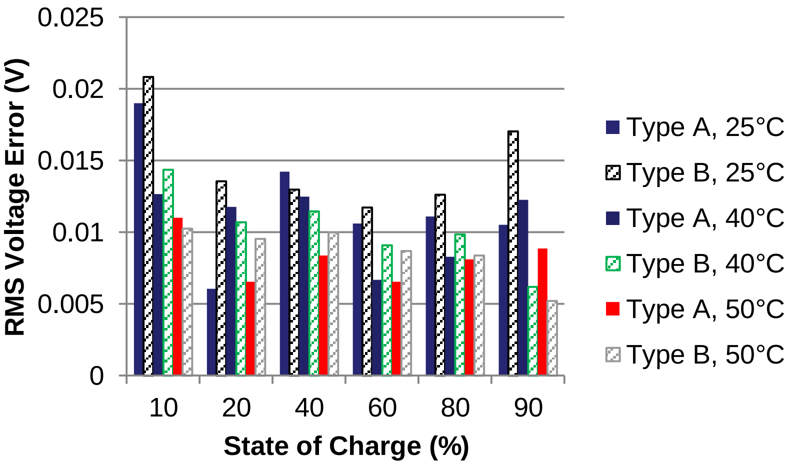
Table 1: Cell characteristics for experimental benchmarking study.

- 2 types of cells
- Various electrical cycling experiments
  - Quick tests : transient response
  - Longer tests: coupling between thermal and electrochemical

HPPC validation



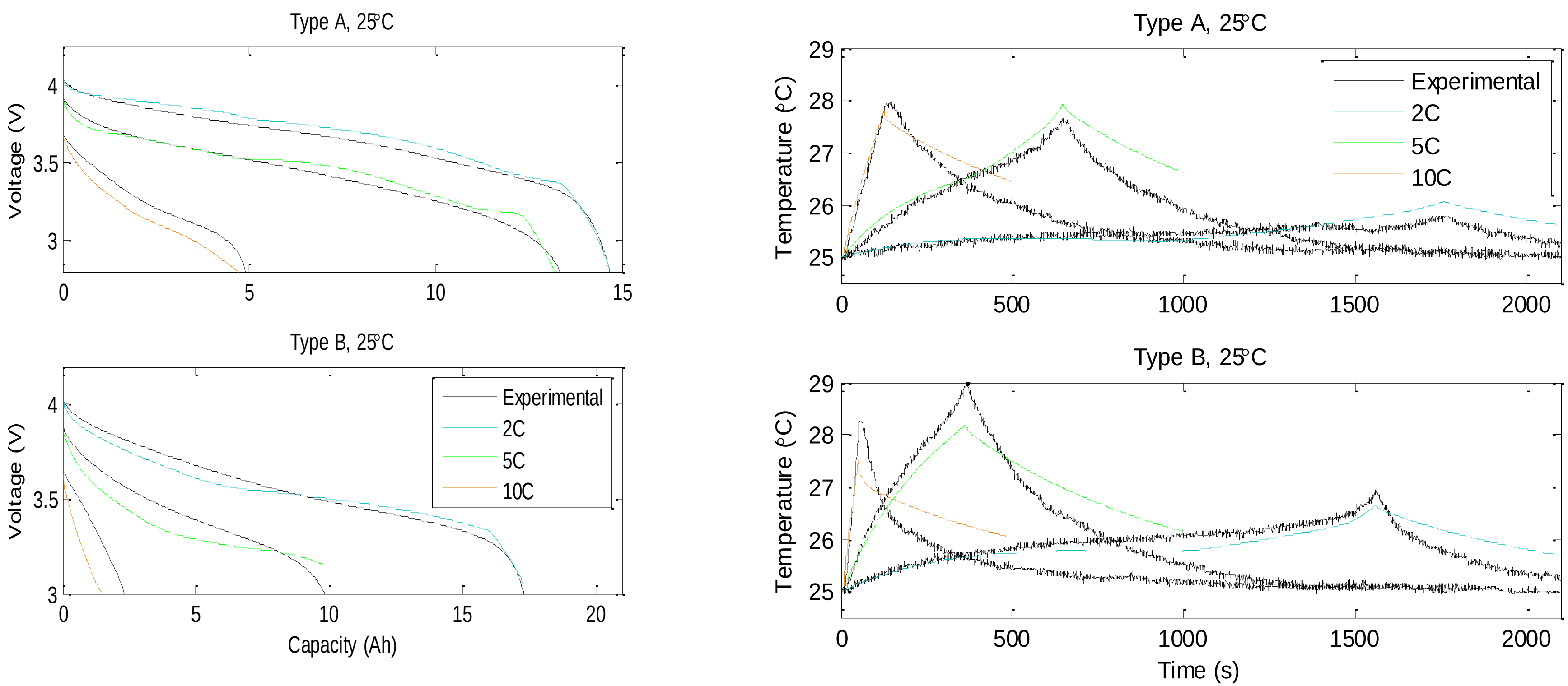
HPPC tests at different current magnitude (different SOC)



Simulation/experiment voltage error for different SOC for each cell

Multi-rate capacity test validation

Experiments on longer time scale => the temperature effects are more important



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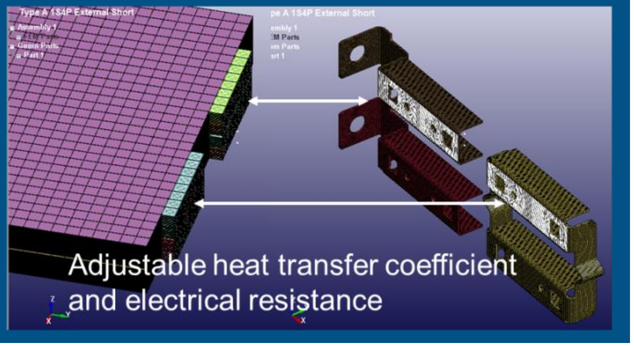
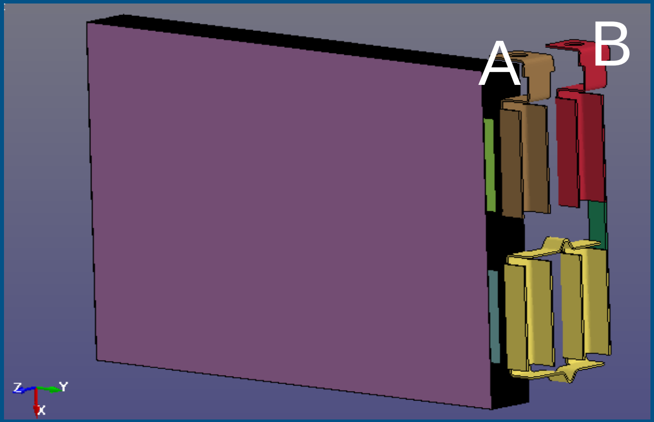
External Short Model Setup

Cell to Bus Thermal & Electrical Connections

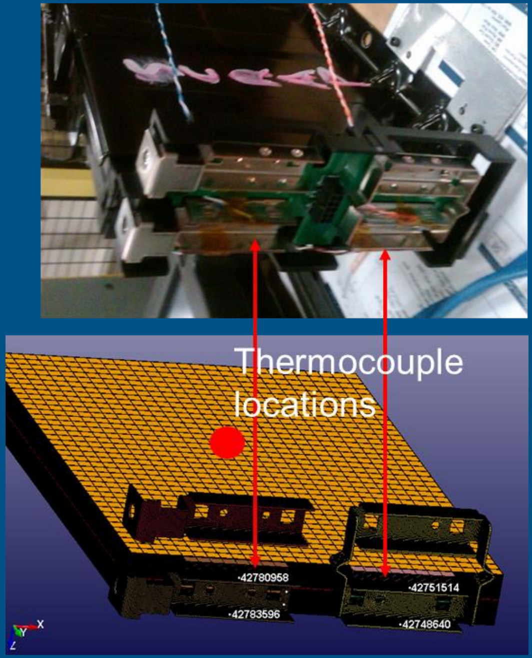


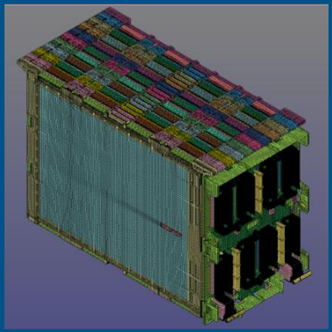
Cells and Bus Bar



Short circuit resistance applied between A and B creates current pathway

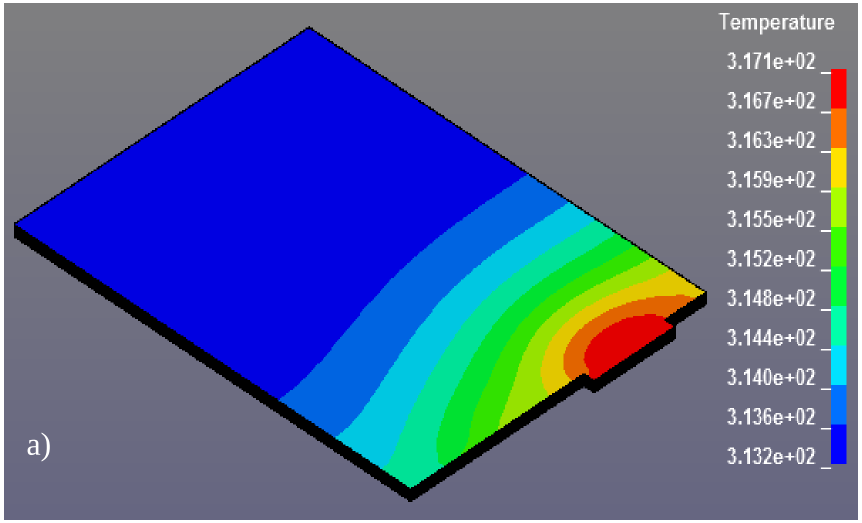
Sensors

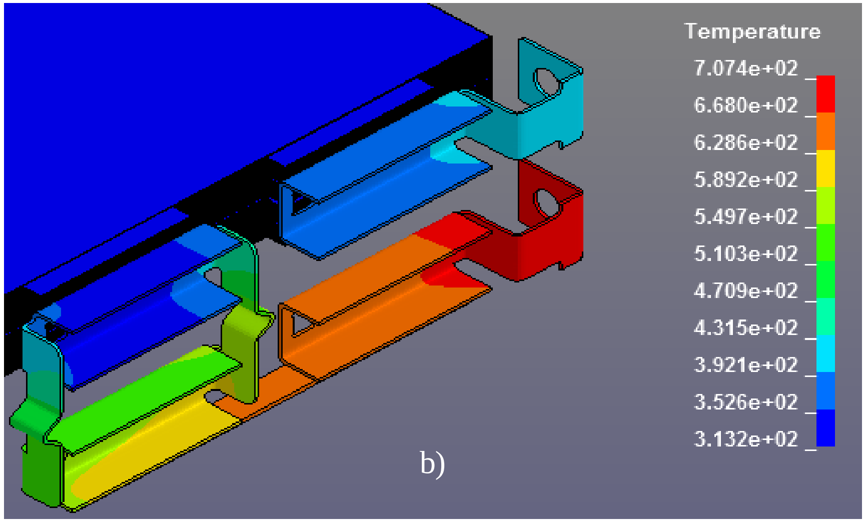




Inactive Components

External Short
Thermal Fringe Plot

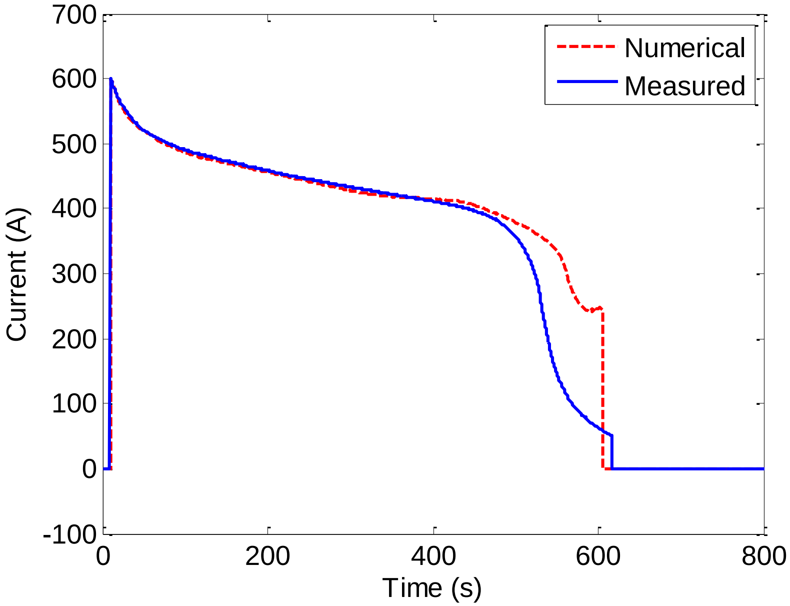




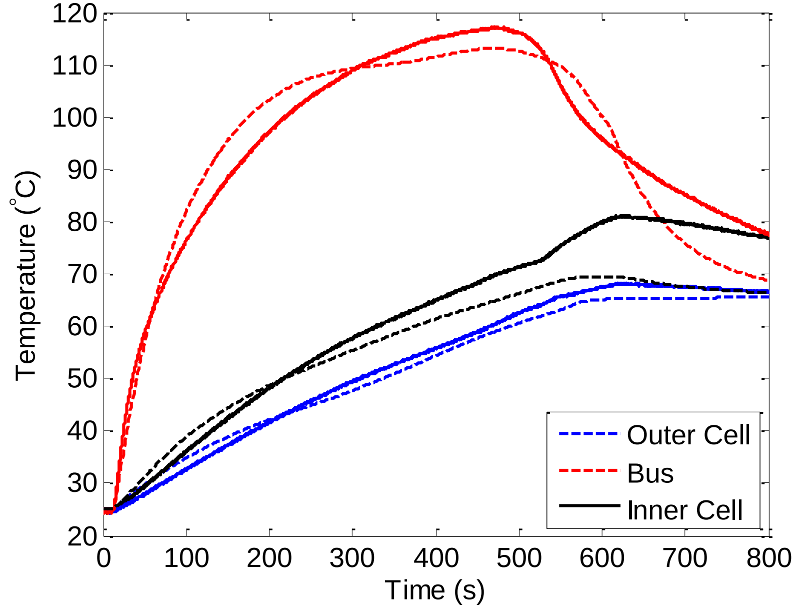
- Average short resistance is 6.5 mOhm, equivalent to ~2 mm^2 steel connection across terminals
- Heat propagates from bus to cells; higher bus temperatures observed where cells are not connected.

External Short Circuit Validation

Model Predicted Current versus Experiment



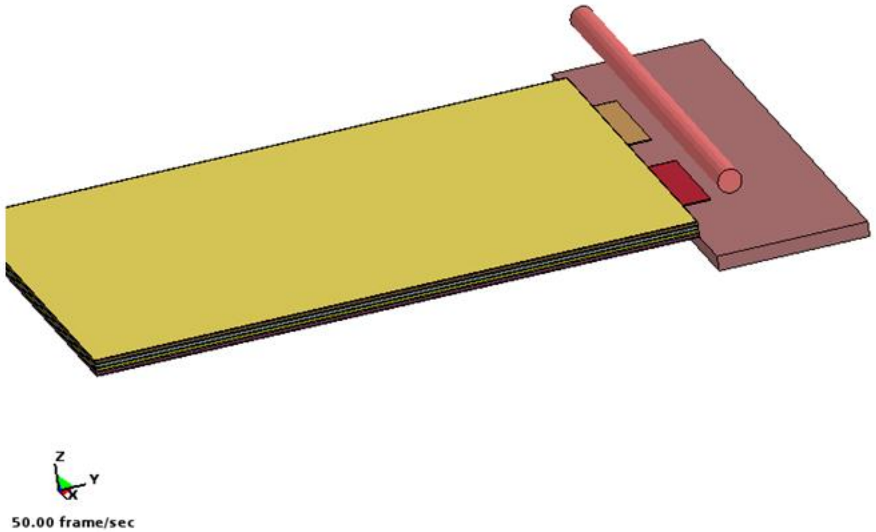
Model Predicted (Dashed) Temperatures versus Experiment (Solid)

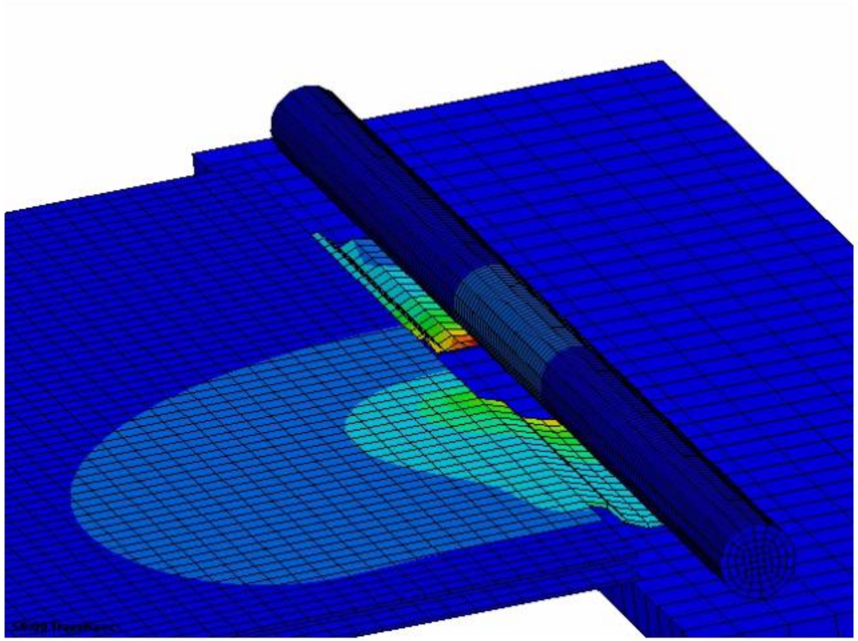


- Good agreement between numerical and measured data for electrical variables
- Thermal predictions demonstrate agreement of 5-10 °C between numerical and experimental data (excluding >550 s for inner cell)

External short example 2

Conducting cylinder falling on the tabs of a cell creates an external short





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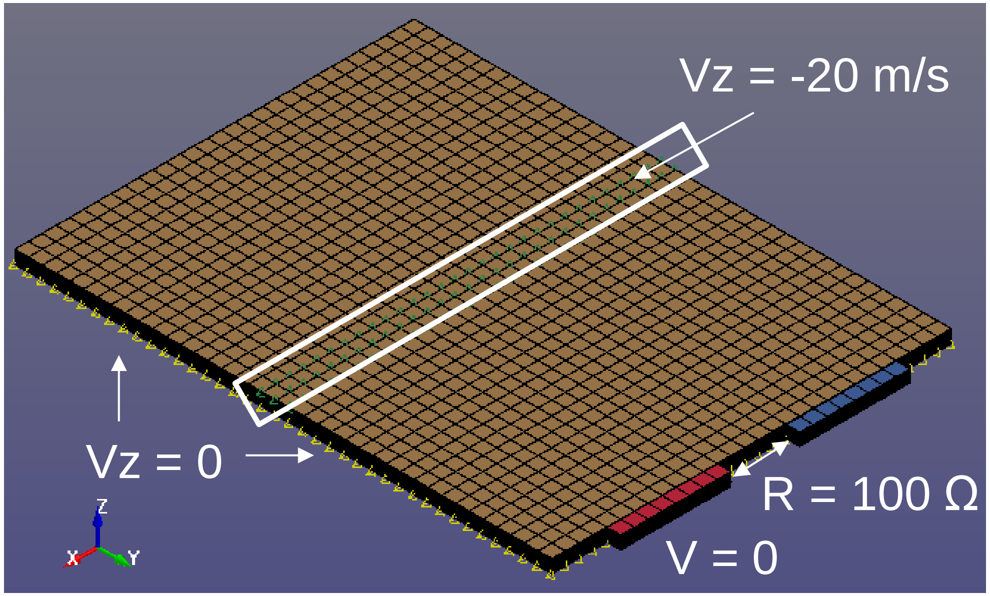
Internal short case 3
Cell Crush Case Study

Boundary Conditions



Mech + Electrical + Thermal
tf = 50 μs
dt = 0.2 μs

"Freeze" mechanics

Electrical + Thermal
tf = 50 s
dt = 1 s

- Thermal boundary conditions same as previous simulations
- Failure criteria is unit cell compressive strain threshold
- Randles circuits replaced by direct short once failure criteria is exceeded

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Internal short case 3
Cell Crush: Thermal results

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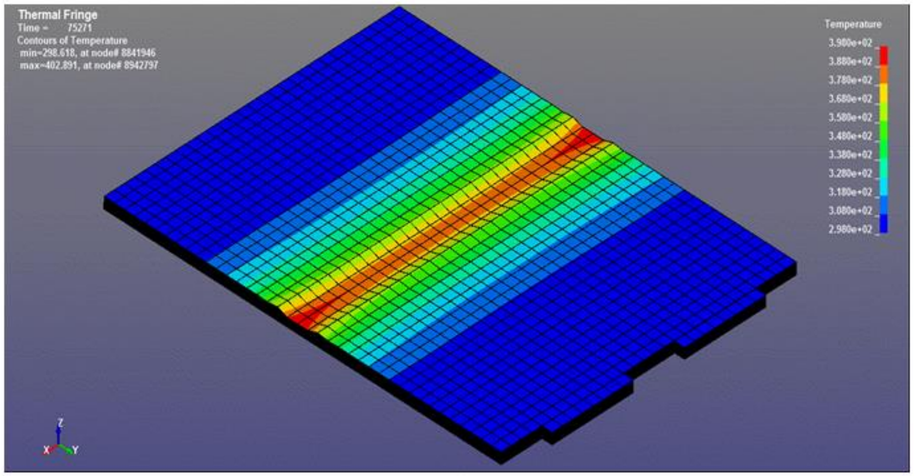
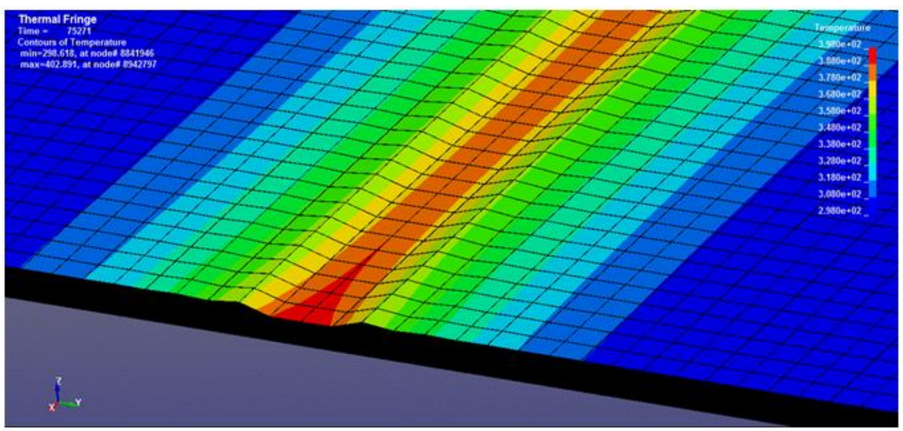
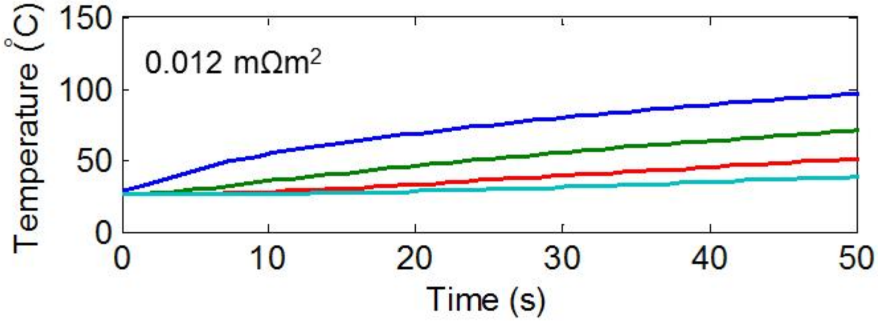
Thermal Fringe Plot

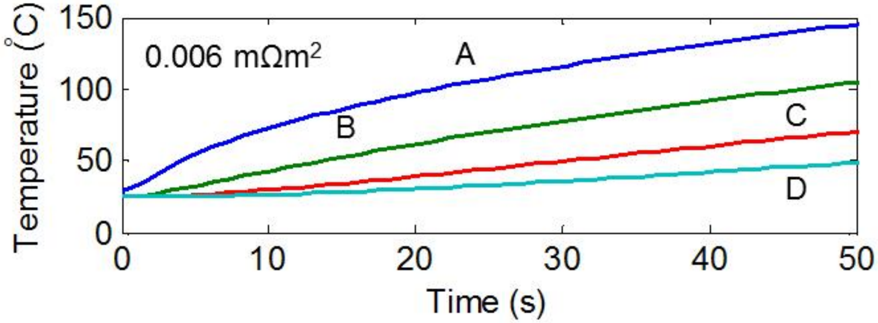


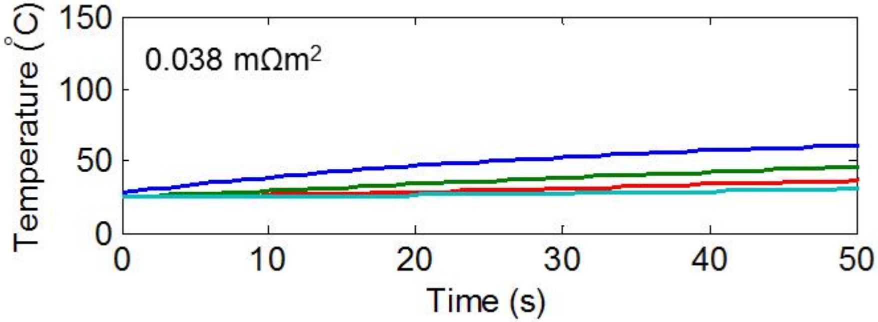
Thermal Fringe Plot Zoomed



Temperature of Cell Surface versus Time







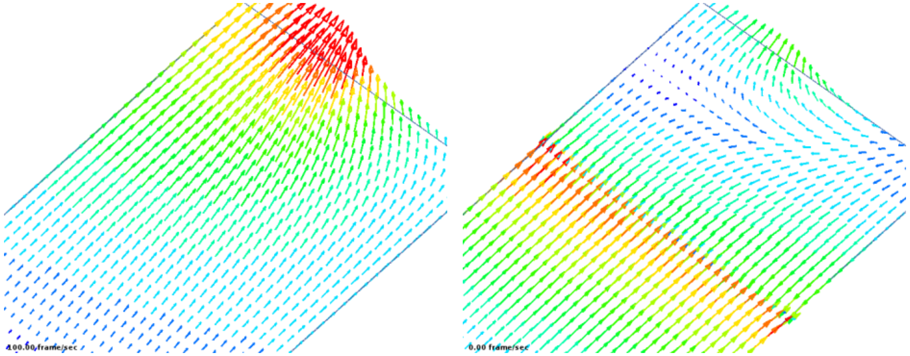
A: center of crush; B: 10 mm from center
C: 20 mm from center; D: 30 mm from center

Internal short case 3
Short Circuit Characteristics

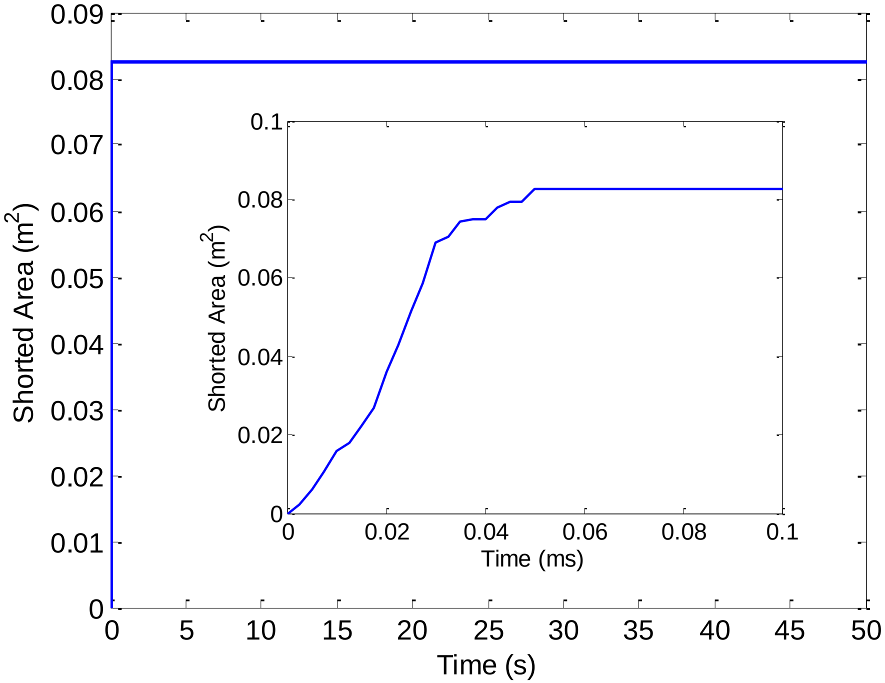
Current Density Vector Plots

Before Internal Short

After Internal Short



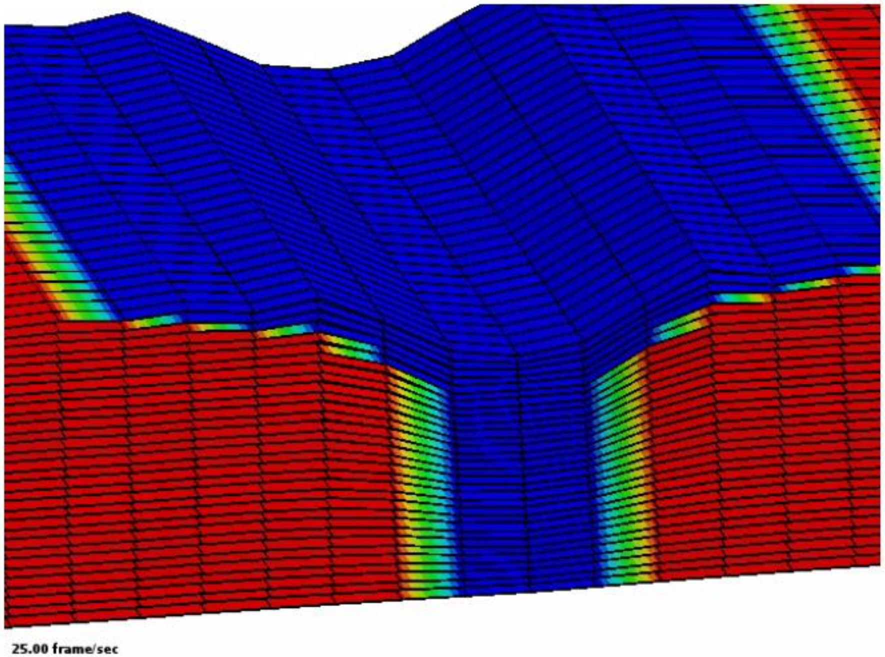
Shorted Area versus Time



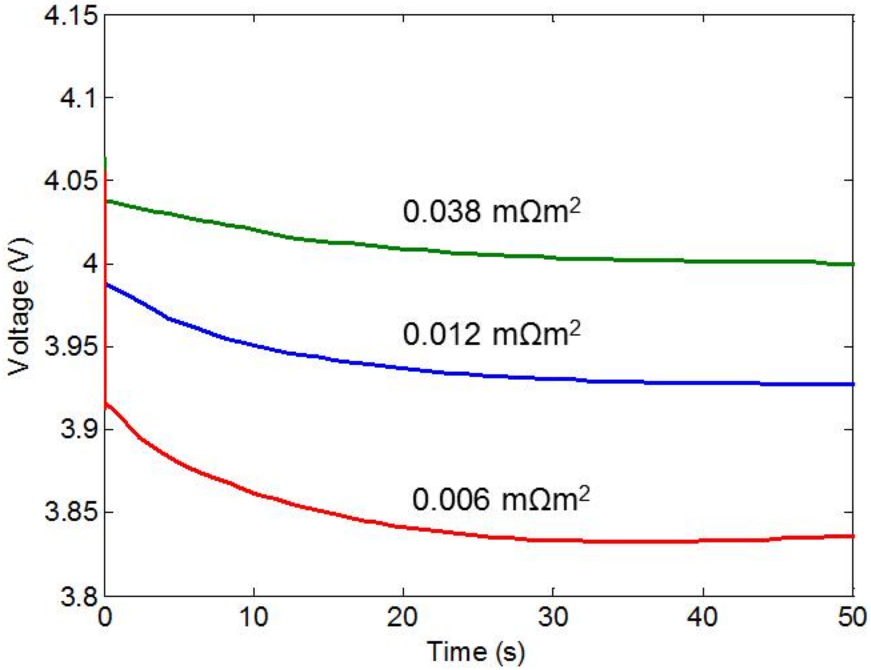
Shorted area increases upon application of external load, then stabilizes
Resistivity combines with shorted area to compute corresponding current response

Internal short case 3
Cell Crush: Electrical results

SOC Fringe Plot



Terminal Voltage versus Time



Charge depletion occurs locally, then proceeds globally, with corresponding heat generation
Voltage drop increases with decreasing short resistivity

Summary

- A three-dimensional finite element model has been developed for battery abuse case studies
- The model is parameterized using benign experiments on cells and cell components
- The model is available on solid and thick shells as a beta version
- Validation activities are underway

Future Work

- Add a “Battery packaging” in LS-PREPOST to easily create the models
- Extend the model to composite thick shells
- Develop higher-fidelity failure models and examine more complex loading conditions
- Improve models for short resistance, based on comparisons with experiments
- Replace empirical inputs with an increasingly analytical approach