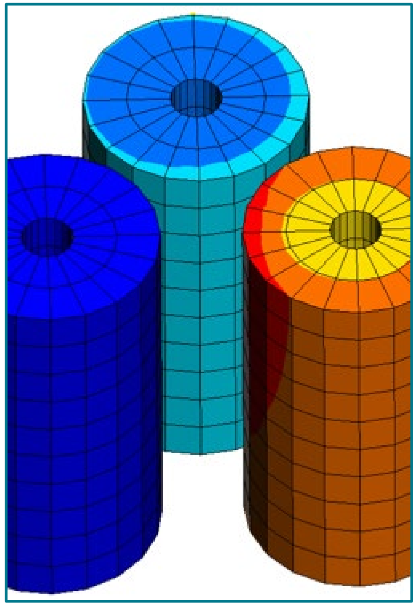

DYNAmore / ANSYS Information Day on Battery Simulation

Modular Multiphysics Simulation

of Li-Ion Batteries under Use and Abuse Load Cases

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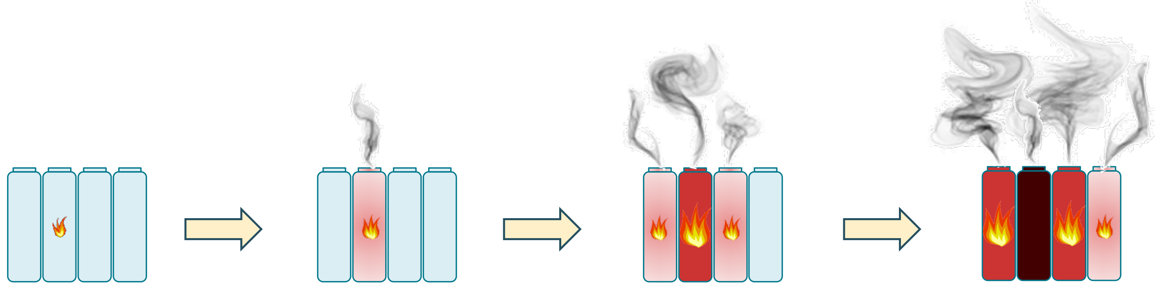
22 June 2022, Stuttgart, Germany

Overview

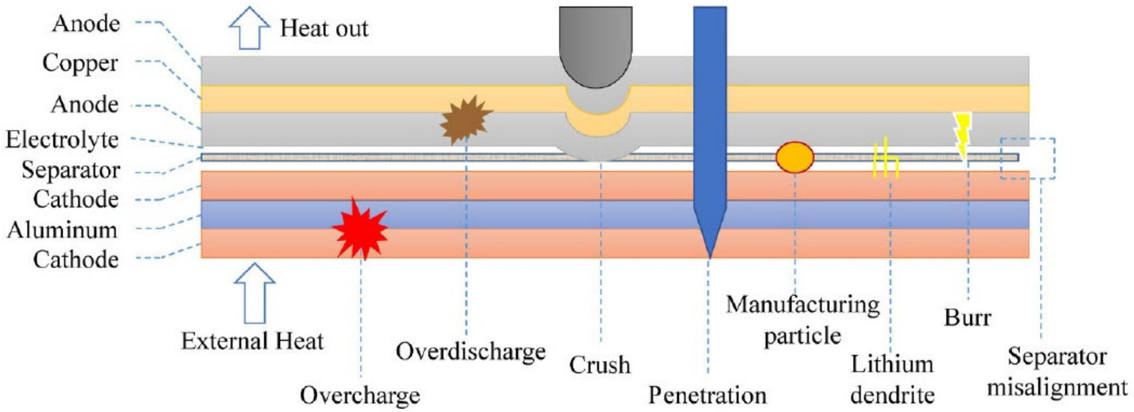
- Motivation
- Modular Single Cell Model
  - Thermal Module
  - Electro-Magnetics (EM) Module
  - Exothermic Reaction Module
- Modular Multi Cell Model
  - Thermal Contact Module
- Structural Module
  - Models on micro, meso and macro scales
  - Scale bridging strategies
- Bringing it all together
  - Time separation strategies
- Conclusion & Future Work

Motivation

- Greatest concern is the cascading cell failure in battery modules and packs
  - Goal is to understand
    - Mechanisms that trigger separator failure
    - If internal short circuit triggers a cell into a thermal runaway
    - How does thermal runaway of a cell propagate through the module/pack
    - How gas release causes structural damage or leaks in passenger cell



one cell in trouble → cell is shorted → exothermic reaction → neighbor cells triggered

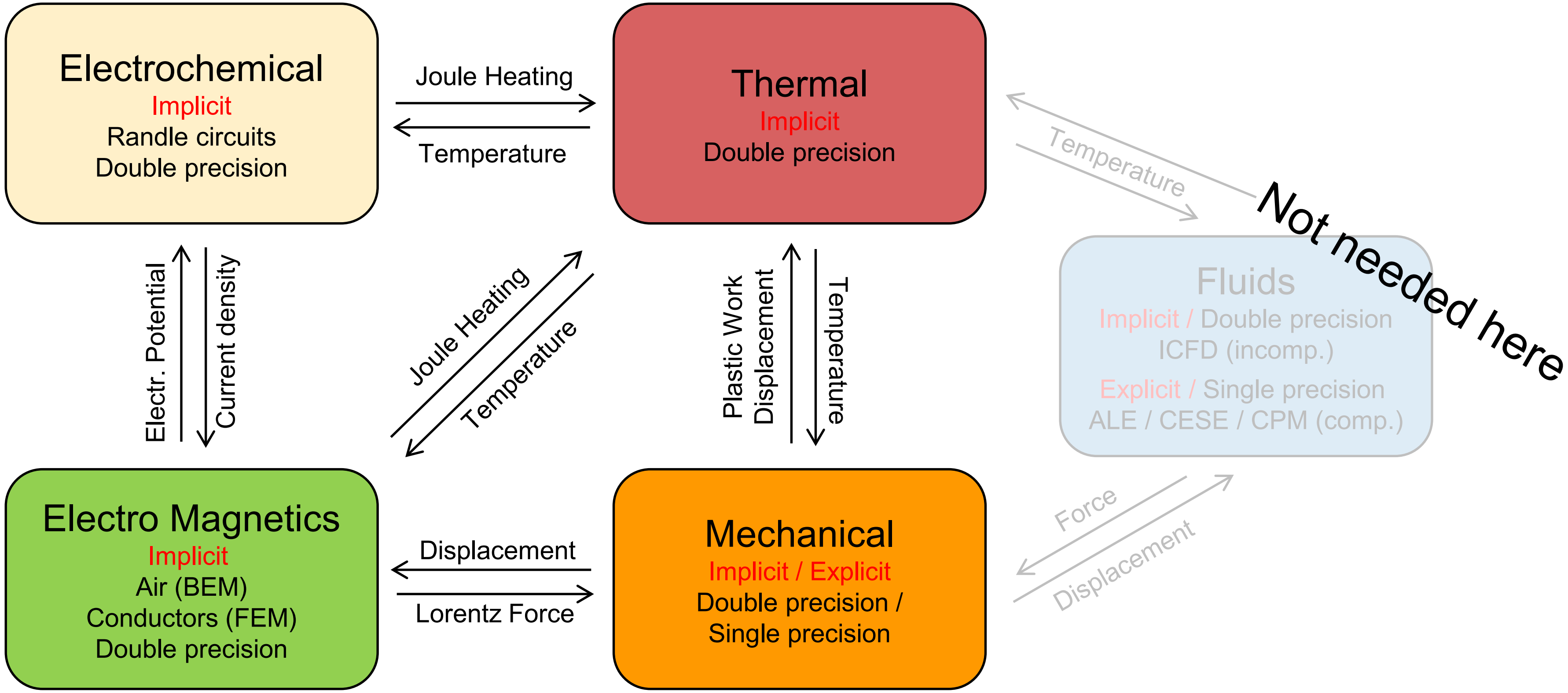


[Zhang, G., Wei, X., Tang, X., Zhu, J., Chen, S., & Dai, H. (2021)]

  - Build modular multi-physics model
    - Thermal module to characterize heat flow
    - Electro-magnetic (EM) module to characterize use and abuse
    - Structural module to capture deformation and separator failure

Coupled solvers in LS-DYNA

- Coupled solvers in LS-DYNA



Electrochemical
Implicit
Randle circuits
Double precision

Thermal
Implicit
Double precision

Electro Magnetics
Implicit
Air (BEM)
Conductors (FEM)
Double precision

Mechanical
Implicit / Explicit
Double precision /
Single precision

Fluids
Implicit / Double precision
ICFD (incomp.)
Explicit / Single precision
ALE / CESE / CPM (comp.)

Not needed here

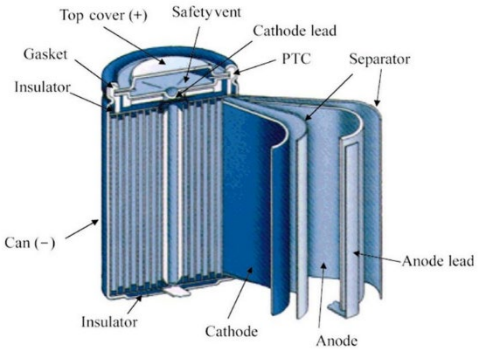
Modular Single Cell Model

Thermal Module

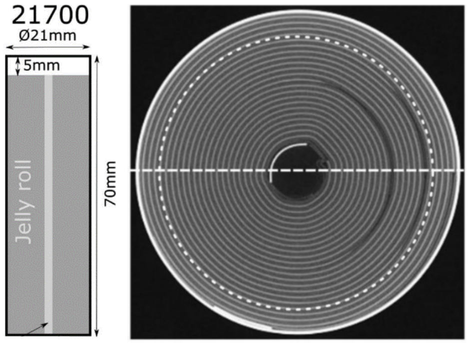
- Thermal material model
  - Orthotropic thermal conductivity of cell
    - In plane of the jelly roll layers (k1 & k2) is larger
    - Perpendicular (radial) to layers (k3) is smaller
  - Heat capacity C_p
  - Density ρ
  - Each cell needs own material due to different axis of symmetry

```
*MAT_THERMAL_ORTHOTROPIC
$#    tmid       tro     tgrlc    tgmult      aopt      tlat      hlat
      1002    2670.3                             4
$#      hc        k1        k2        k3
     928.0      25.8      25.8     0.998
$#      xp        yp        zp        a1        a2        a3
       0.0       0.0       0.0
$#      d1        d2        d3
       1.0       0.0       0.0
```

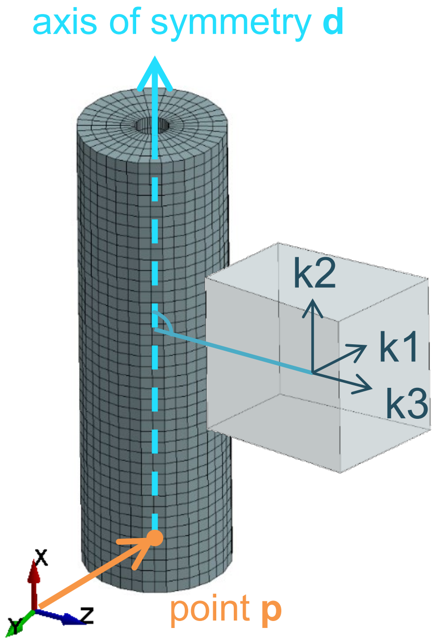
locally orthotropic
in cylindrical coordinate system
with material axis of symmetry



[Bankole et al. 2013]



[Quinn et al. 2018]

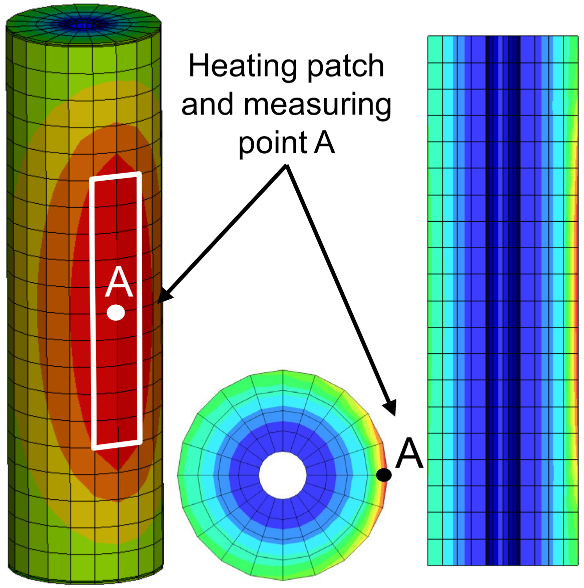


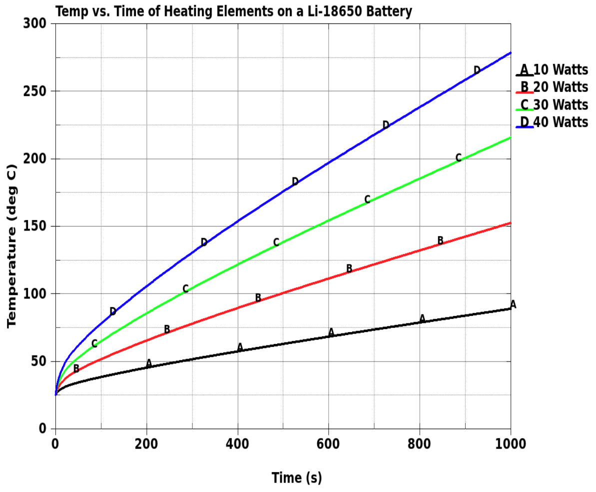
- Heat transfer boundary conditions
  - Flux boundary condition for heating patch
    - Application on segment set via **`*BOUNDARY_FLUX_SET`**

$$\dot{q} = \frac{P}{A} \quad \begin{cases} P = \text{power in Watt} \\ A = \text{segment set area in m}^2 \end{cases}$$

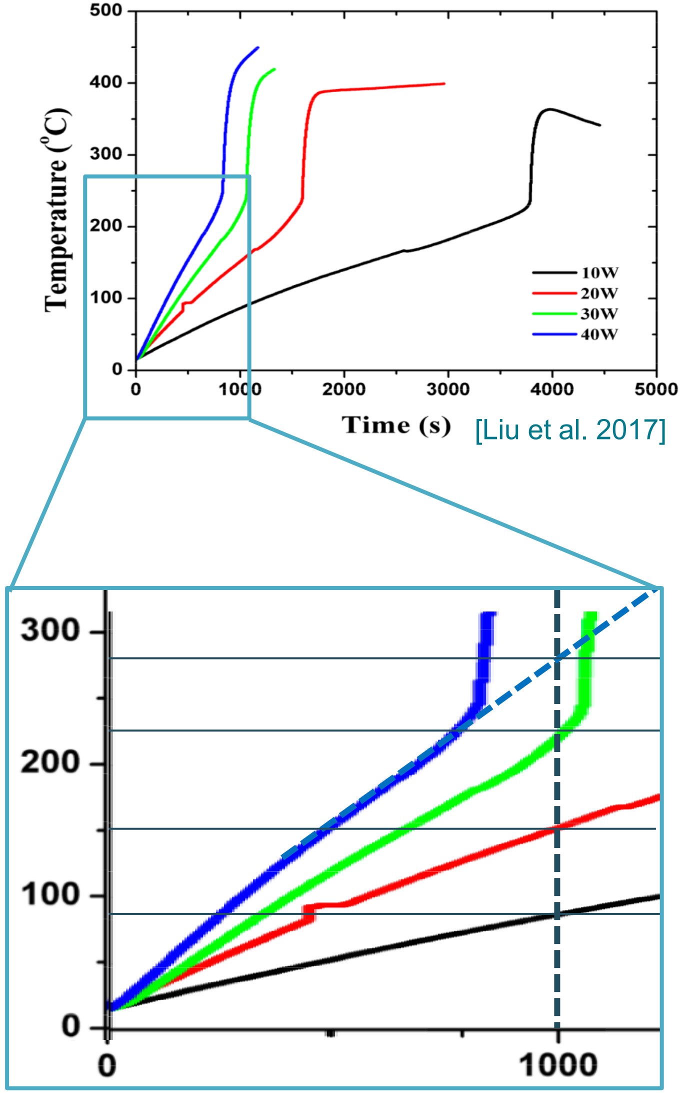
    - Surface temperature depends on heating power
    - Temperature at 1000 seconds

Power	Simulation	Experiment
10 W	89.0 ^{0}C	90.0 ^{0}C
20 W	152.0 ^{0}C	150.0 ^{0}C
30 W	216.0 ^{0}C	220.0 ^{0}C
40 W	278.0 ^{0}C	280.0 ^{0}C





simulation



[Liu et al. 2017]

experiment

Heat transfer boundary conditions

Convection model on segment set

```
*BOUNDARY_CONVECTION_SET
$#    ssid    pserod
     10021
$#   hlcid     hmult     tlcid     tmult       loc
    -10020       1.0     10022       1.0
```

h vs temp curve ID and h multiplier

T_∞ vs time curve ID and T_∞ multiplier

$$\dot{q} = hA(T - T_\infty)$$

- Typical heat transfer coefficients
  - ☐ Free convection: $3\ \frac{\mathrm{W}}{\mathrm{m}^2\mathrm{K}} < h < 9\ \frac{\mathrm{W}}{\mathrm{m}^2\mathrm{K}}$
  - ☐ Forced convection: $h \gg 10\ \frac{\mathrm{W}}{\mathrm{m}^2\mathrm{K}}$
  - ☐ Exact values need to be obtained by CFD simulations → Fluent

Surface radiation to open space (environment)

```
*BOUNDARY_RADIATION_SET
$#    ssid      TYPE
     10021         1
$#   flcid     fmult     tlcid     tmult       loc
    -10021       1.0     10022       1.0
```

f vs temp curve ID and f multiplier

T_∞ vs time curve ID and T_∞ multiplier

$$\dot{q} = \overbrace{\varepsilon\sigma F}^{f} A(T^4 - T_\infty^4)$$

Surface view factor (here 1.0)

Stefan Boltzmann constant

Emissivity (here 1.0)

- Typically, f equals the Stefan Boltzmann constant
- Temperature needs to be in Kelvin!
- Exact radiation model uses view factors (expensive)

- Heat transfer boundary conditions
  - Influence of convection vs. radiation

$$\dot{q}_{tot} = \underbrace{hA(T - T_\infty)}_{\dot{q}_{conv}} + \underbrace{fA(T^4 - T_\infty^4)}_{\dot{q}_{rad}}$$

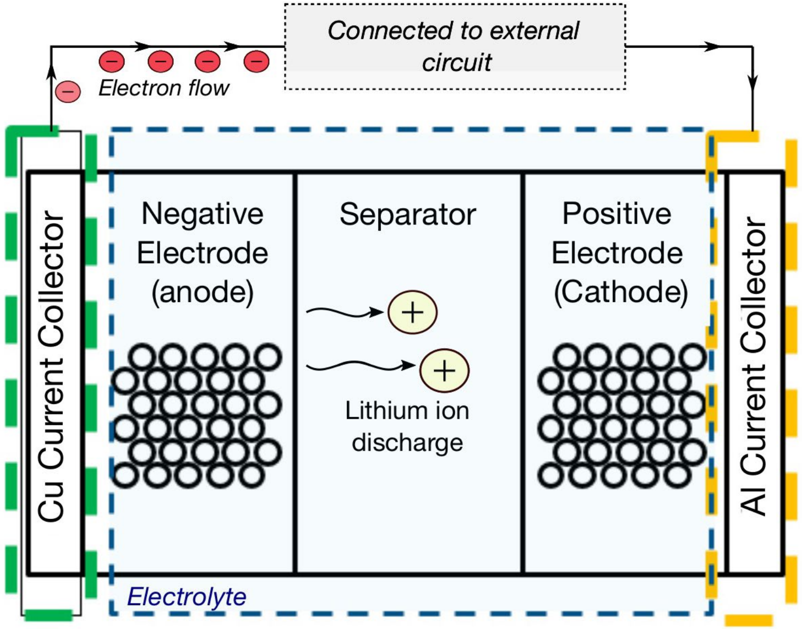
  - Examples for varying surface temperatures at constant ambient temperature
    - ☐ Assumptions: $A = 1\,m^2$; $h = 7.0\frac{\mathrm{W}}{\mathrm{m^2K}}$; $f = 5.67e^{-8}\frac{\mathrm{W}}{\mathrm{m^2K^4}}$; $T_\infty = 20^0$ C (293 K)

$T\ [^0C\ ]$	$T\ [K]$	T_∞ [K]	$\dot{q}_{conv}$ [W]	$\dot{q}_{rad}$ [W]	Dominance
50.0	323.0	293.0	210.0	199.0	Equal
100.0	373.0	293.0	560.0	680.0	Equal
150.0	423.0	293.0	910.0	1397.0	“Equal”
300.0	573.0	293.0	1960.0	5694.0	Radiation
400.0	673.0	293.0	2660.0	11214.0	Radiation
500.0	773.0	293.0	3360.0	19826.0	Radiation
600.0	873.0	293.0	4060.0	32516.0	Radiation

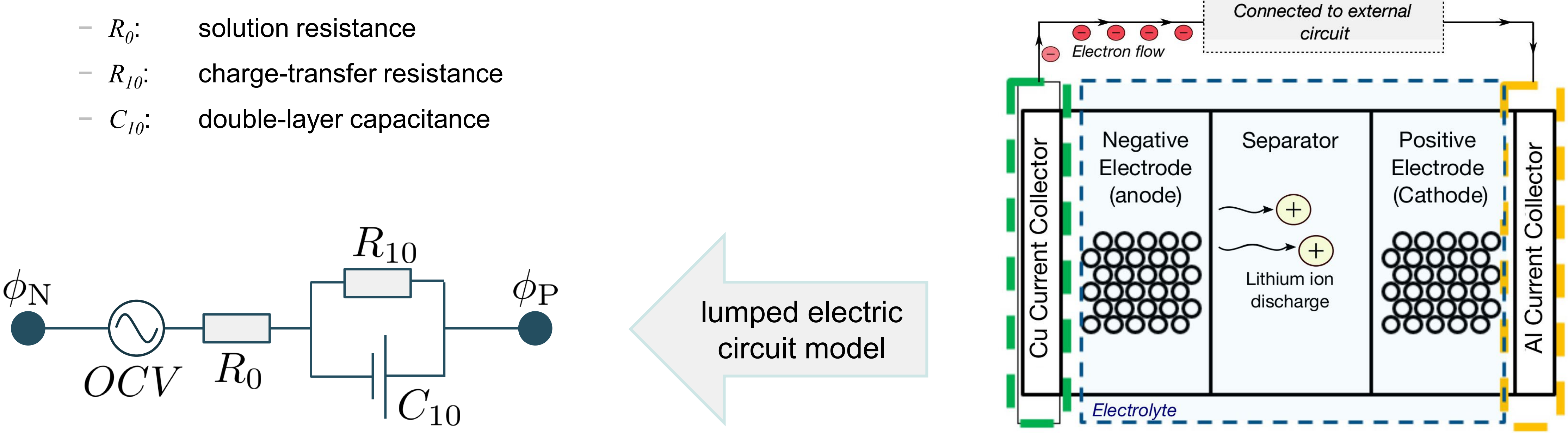
during the thermal runaway of a single cell surrounded by air, cooling is dominated by radiation

Electro-Magnetics (EM) Module

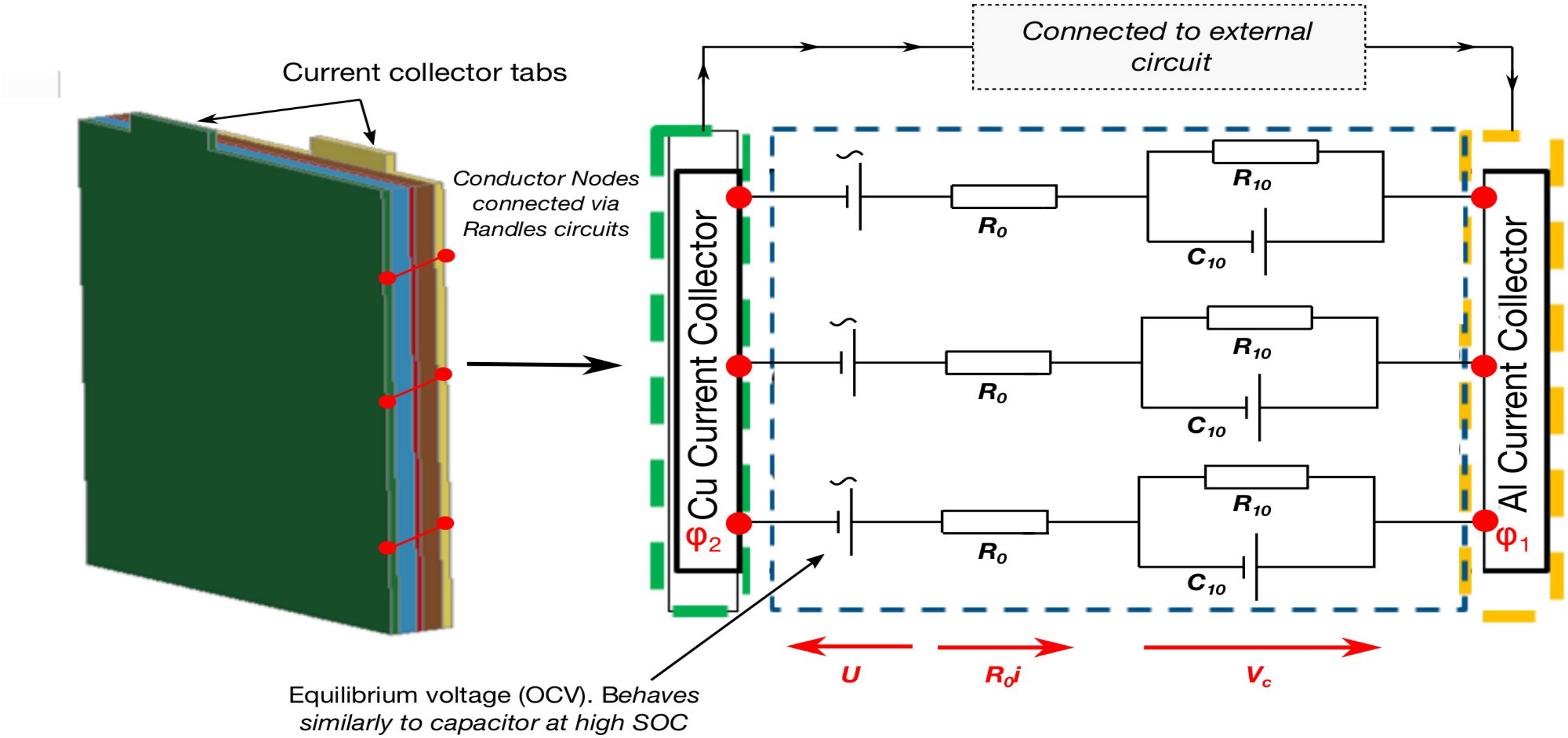
- Battery modeling requires the simplified resistive heating solver and not all Maxwell equations
- The unit cell is the basic electrochemical unit comprised of an
  - Anode, cathode, separator, electrolyte in between two current collectors (positive and negative)
    - Anode and cathode store the Lithium
    - Electrolyte carries positively charged Lithium ions
      - ☐ The separator is a selectively permeable membrane that can be passed only by Lithium ions
      - ☐ Ions move from cathode to anode during charging, vice versa during discharging
      - ☐ The movement of the lithium ions creates free electrons in the anode which creates a charge at the positive current collector through a device being powered to the negative current collector



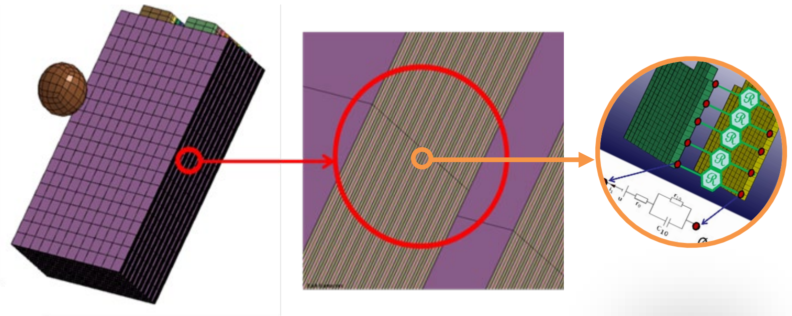
- Equivalent lumped electric circuit model
  - Computing the ion movement is possible but computationally intense
    - Solving the electrolyte in a porous chemically active anode & cathode is only useful in battery design
    - Idea: Define a set of equations that easily capture the gross behavior of the battery
      - Randles circuit is one of many approaches to this idea
        - $\phi_{\mathrm{N/P}}$ potential at anode & cathode
        - OCV: open circuit voltage as ideal voltage source
        - R_0: solution resistance
        - R_{10}: charge-transfer resistance
        - C_{10}: double-layer capacitance

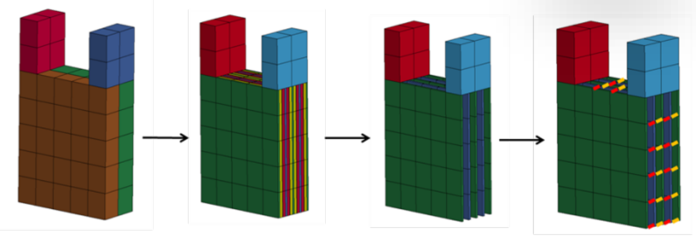


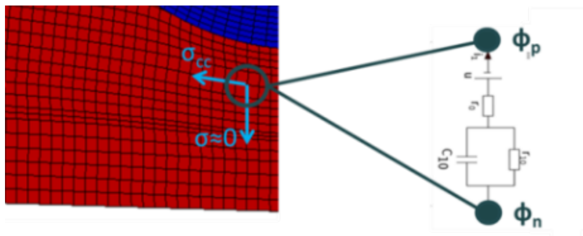
- The distributed Randles model
- Idea: Use several Randles circuits in parallel to account for 3d distribution in the battery
  - Circuits are placed between corresponding nodes on the two current collectors
  - Circuit elements depend on current direction and can be functions of state of charge (SOC) and temperature
  - This allows to capture localized discharge during internal short

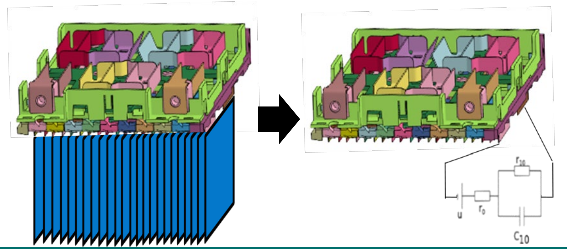


- Available Randle circuit models depending on scale & level of detail
  - Micro scale on cell level: Solid elements for each layer
    - All the layers of the jelly roll are meshed using solid elements
    - Same mesh used for mechanics, thermal and EM
    - Drawback: many elements with large aspect ratio & small mech. time step
  - Meso scale on cell/module level: `TSHELLS` with `*PART_COMPOSITE`
    - Mechanics part modeled using composite thick shells
    - EM and thermal use automatically generated solid mesh
    - Faster runs (mechanics solver has less elements with larger time step)
  - Macro scale for cell/module/pack level: Solid elements for everything
    - One (or a few) solid elements through thickness for mechanics, EM and thermal
    - 2 fields at each node (positive and negative current collectors)
    - Computationally cheap which allows for pack level simulations
  - Meshless model: module/pack level: External circuit only
    - One single equivalent circuit for the whole cell (lumped model)





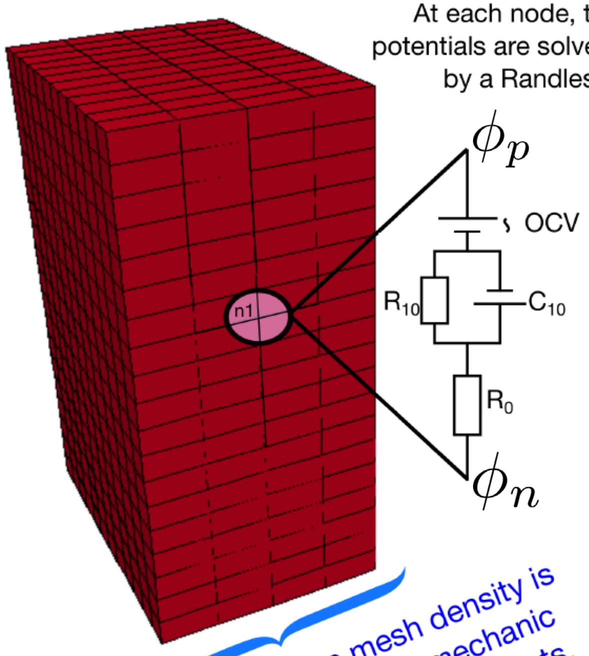




[L'Eplattenier & Çaldichoury 2019]

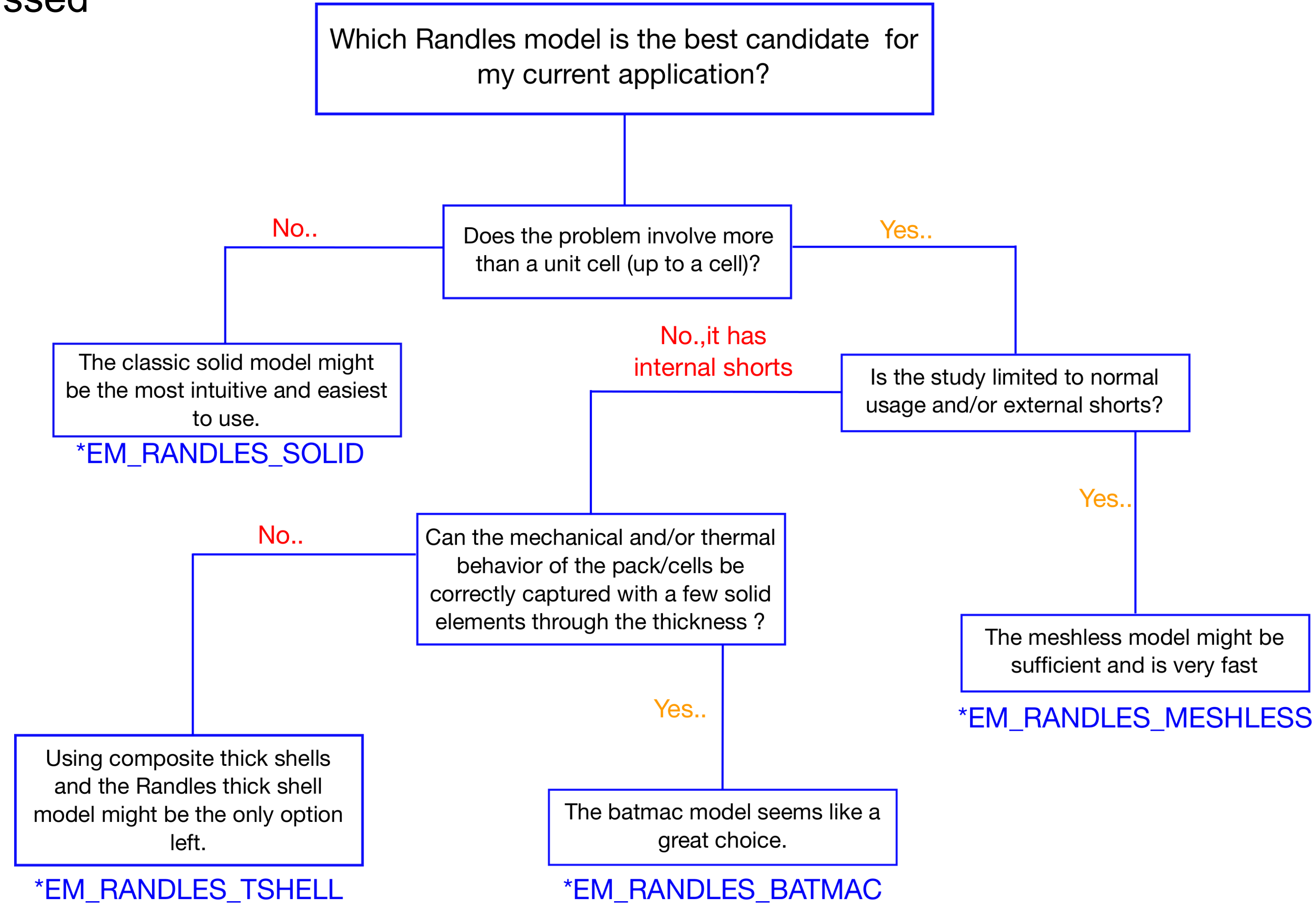
Decision Chart

- Here: BatMac model will be discussed



At each node, two scalar potentials are solved connected by a Randles circuit

Solid elements. The mesh density is determined by the solid mechanic and thermal solvers' requirements.



Which Randles model is the best candidate for my current application?

Does the problem involve more than a unit cell (up to a cell)?

No..

The classic solid model might be the most intuitive and easiest to use.

*EM_RANDLES_SOLID

Yes..

Is the study limited to normal usage and/or external shorts?

Yes..

The meshless model might be sufficient and is very fast

*EM_RANDLES_MESHLESS

No.,it has internal shorts

Can the mechanical and/or thermal behavior of the pack/cells be correctly captured with a few solid elements through the thickness ?

Yes..

The batmac model seems like a great choice.

*EM_RANDLES_BATMAC

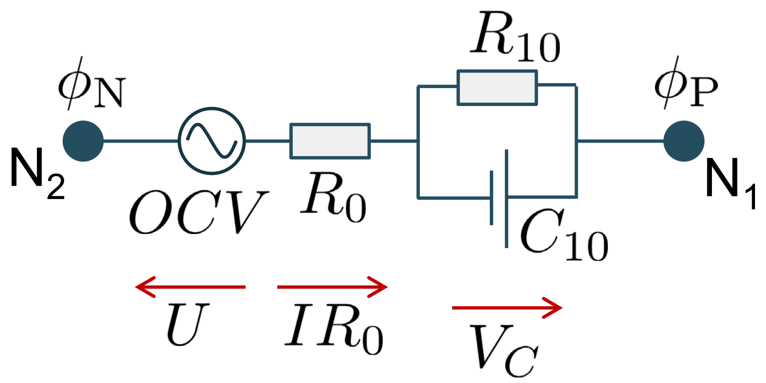
No..

Using composite thick shells and the Randles thick shell model might be the only option left.

*EM_RANDLES_TSHELL

Randle keyword for battery macro (BatMac) scale models

```
*EM_RANDLES_BATMAC
$#randleId randlType randlArea  ccp/psid
         1         1         2         2
$#       q        cq   socinit    soctou
      3.35  2.777e-2     100.0     -1000
$#   r0cha     r0dis    r10cha    r10dis    c10cha    c10dis
     -1001     -1002     -1101     -1102     -1501     -1502
$#    temp fromTherm r0ToTherm      dUdT     tempu
                   1         1                   1
$# useSocS   tauSocS     flcid
```

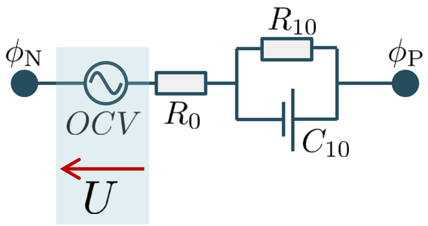


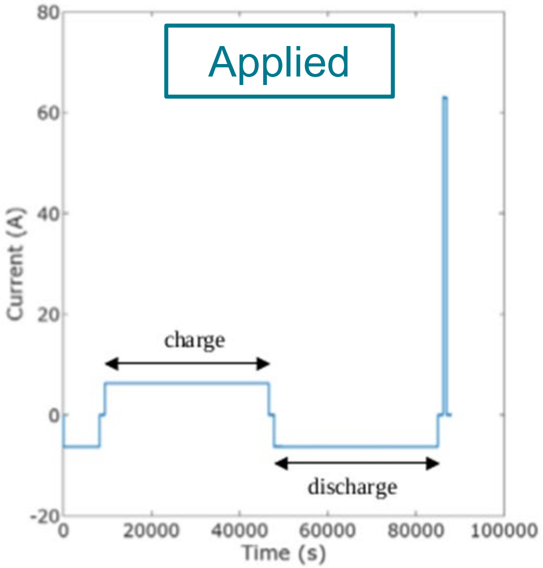
- Parameters can be obtained from a series of tests
  - First-order Randle cell – `randlType = 1`
  - Parameters defined for whole cell – `randlArea = 2`
  - Battery capacity in Ah – `q`
  - SOC conversion factor (1/36 in S.I. units) – `cq`
  - Open charge voltage (OCV) curve – `soctou`
  - Randle circuit parameters
    - ☐ `r0cha`, `r0dis`, `r10cha`, `r10dis`, `c10cha` & `c10dis`
    - ☐ Table ID for function of SOC and temperature

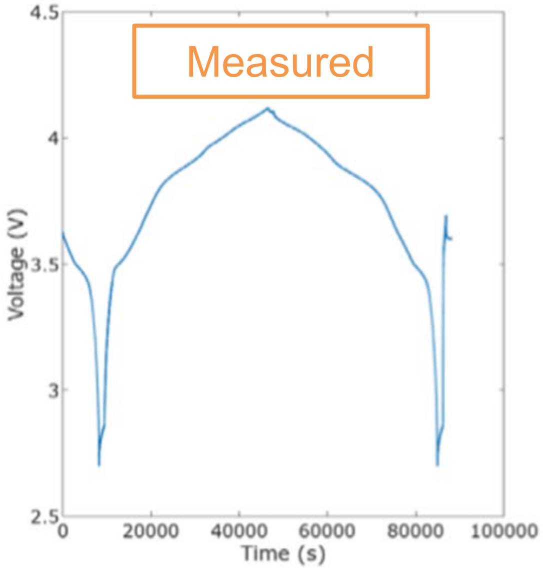
- Coupling to thermal solver
  - ☐ `fromTherm`, `r0ToTherm`, `tempu = 1` (Kelvin)
  - ☐ `dUdT` reversible heat as a function of SOC
- SOC shift to account for diffusion limitations at high-rate discharge
  - ☐ `useSocS`, `SocS` & `tauSocS` (not used here)

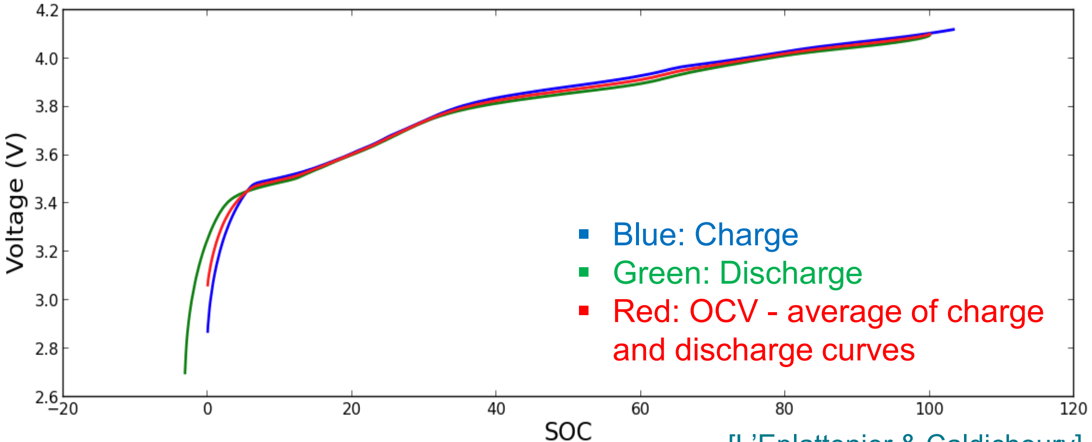
- Test #1: C/10 capacity charge and discharge test
  - Measurement of the open circuit voltage (OCV) curve
    - `soctou` defines the relationship between the voltage of the battery and its SOC (state of charge)
    - A low constant current is applied such that the charge and discharge time is equal to 10 hours
      - Charging time of battery = Battery Ah / Charging Current

```
*EM_RANDLES_BATMAC
$#randleId randlType randlArea      psid
         1         1         2         2
$#       q        cq   socinit    soctou
      3.35  2.777e-2     100.0     -1000
$#   r0cha     r0dis    r10cha    r10dis    c10cha    c10dis
     -1001     -1002     -1101     -1102     -1501     -1502
$#    temp fromTherm r0ToTherm      dUdT     tempu
                   1         1                   1
$# useSocS   tauSocS     flcid
```





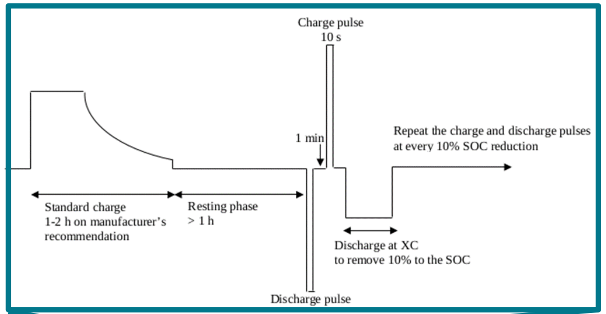


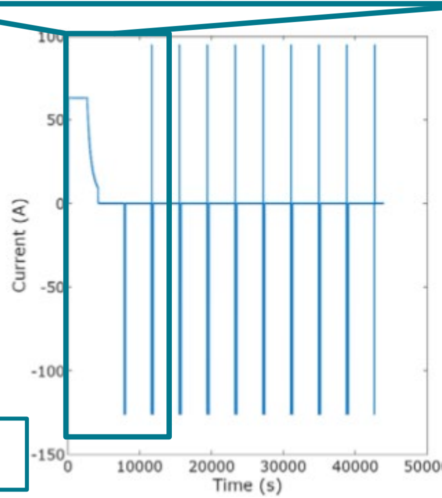


[L'Eplattenier & Çaldichoury]

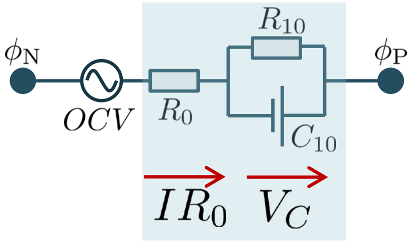
- Test #2: Hybrid pulse power characterization test (HPPC test)
  - Measure voltage curve during charge and discharge pulses with holding times
    - R_0 , R_{10} , C_{10} depend on SOC and temperature
      - ☐ R_0 captures the initial Ohmic voltage jump
      - ☐ R_{10} , C_{10} capture long term, relaxation behavior

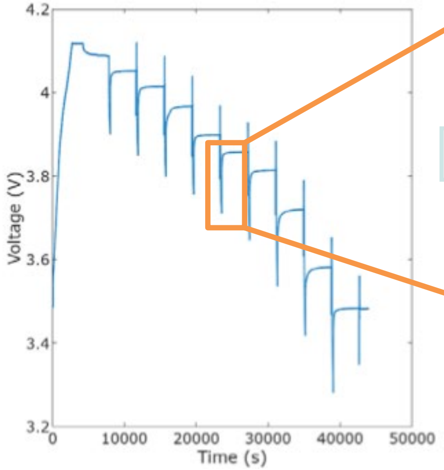
```
*EM_RANDLES_BATMAC
$#randleId randlType randlArea   ccp/psid
         1         1         2          2
$#       q        cq   socinit    soctou
      3.35 2.777e-2     100.0      -1000
$#    r0cha     r0dis    r10cha    r10dis    c10cha    c10dis
     -1001     -1002     -1101     -1102     -1501     -1502
$#    temp fromTherm r0ToTherm       dUdT     tempu
                   1         1                    1
$# useSocS   tauSocS     flcid
```



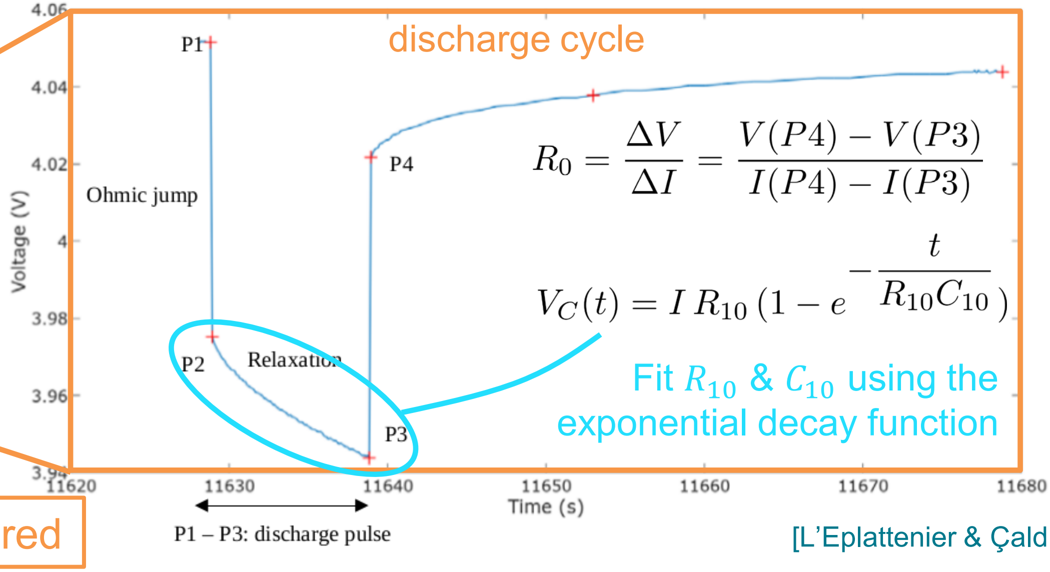


Applied





Measured



$$R_0 = \frac{\Delta V}{\Delta I} = \frac{V(P4) - V(P3)}{I(P4) - I(P3)}$$

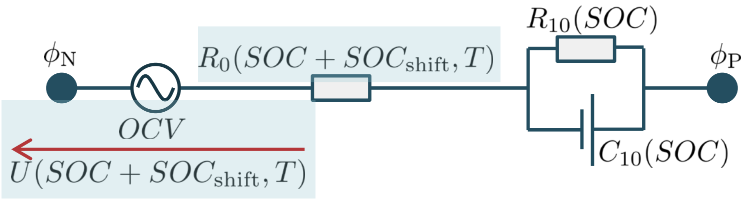
$$V_C(t) = I\,R_{10}\,(1 - e^{-\dfrac{t}{R_{10}C_{10}}})$$

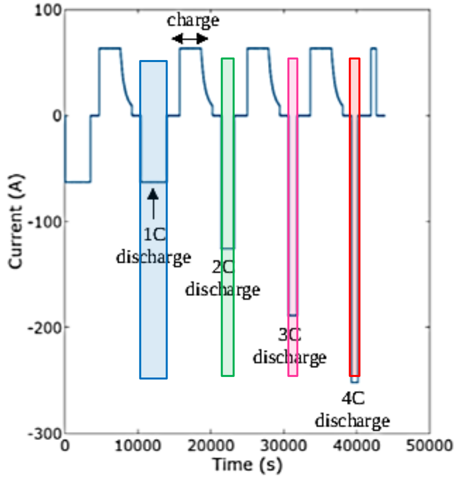
Fit R_{10} & C_{10} using the exponential decay function

[L'Eplattenier & Çaldichoury]

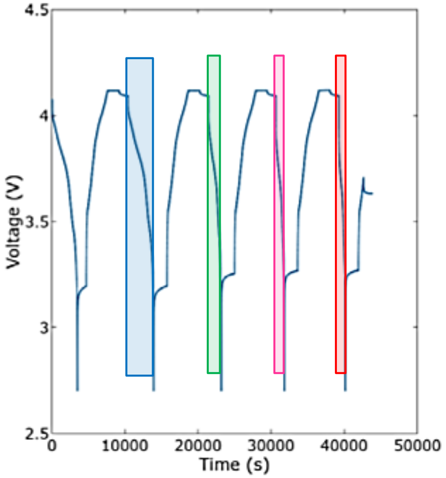
- Test #3: Multi-rate capacity discharge test
  - Characterize high-rate discharge scenarios
    - Needed to account for physical ion diffusion limitations
    - Identify state-of-charge shift
    - The cell is fully charged between each discharge

```
*EM_RANDLES_BATMAC
$#randleId randlType randlArea  ccp/psid
         1         1         2         2
$#       q        cq   socinit   soctou
      3.35 2.777e-2     100.0     -1000
$#   r0cha     r0dis    r10cha    r10dis    c10cha    c10dis
     -1001     -1002     -1101     -1102     -1501     -1502
$#    temp fromTherm r0ToTherm      dUdT     tempu
                   1         1                   1
$# useSocS   tauSocS     flcid
```

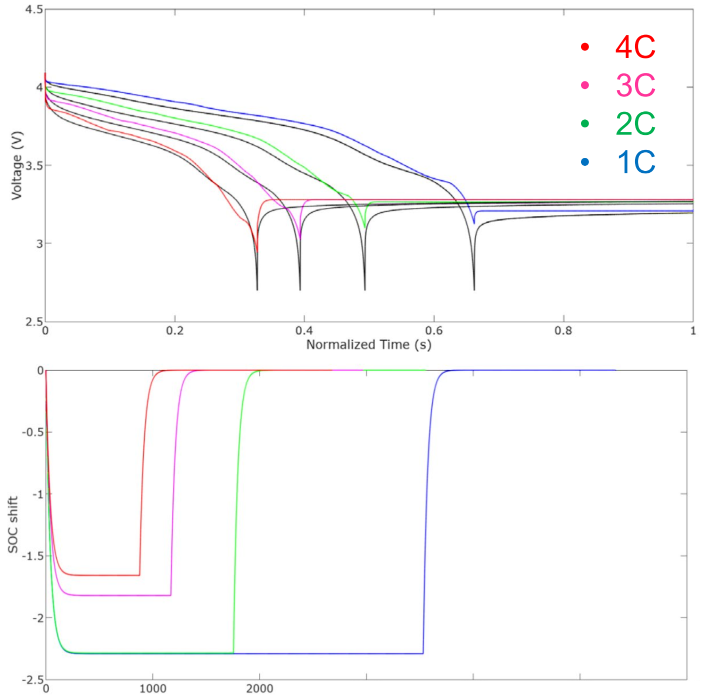


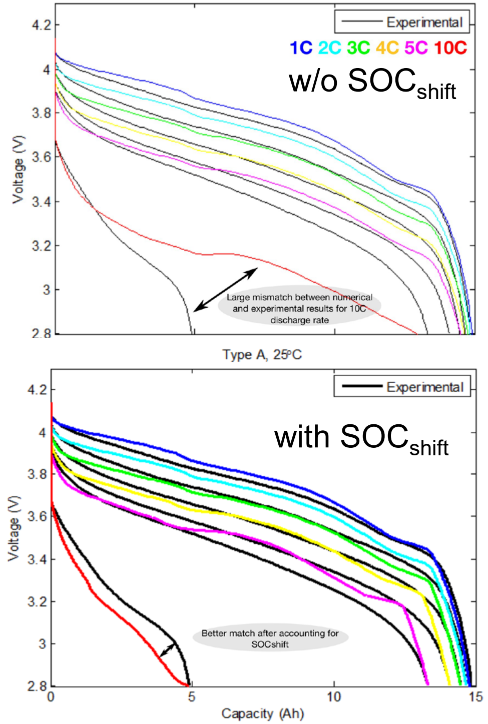


Applied



Measured





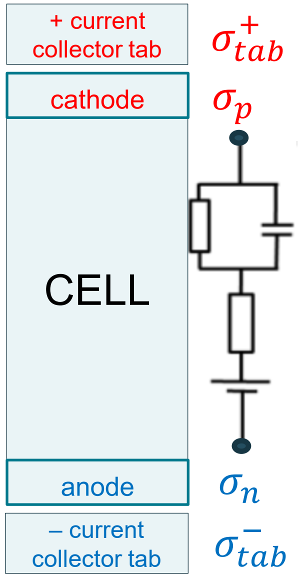
[L'Eplattenier & Çaldichoury]

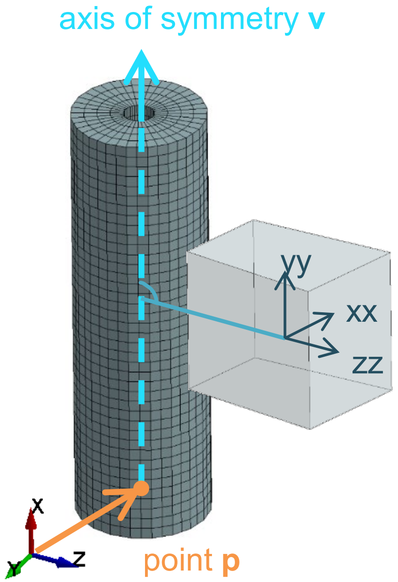
- Material cards for the BatMac model
  - Isotropic electrical conductivity of aluminum collector tabs σ_{tab}^{+} , σ_{tab}^{-}

```
*EM_MAT_001
$#     mid     mtype     sigma     eosid
      1002         2    36.9e6
```

  - Anisotropic electrical conductivity of anode and cathode σ_p , σ_n
    - Local orthotropy define like in the thermal material card

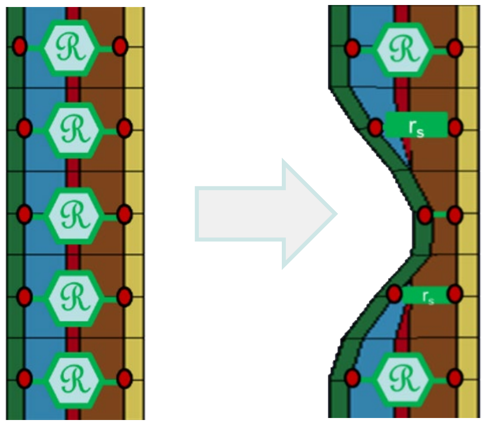
```
*EM_MAT_005
$#     mid     mtype    sigXXp    sigYYp    sigZZp
      1002         5     669.5     669.5       2.0
$#  sigXYp    sigXZp    sigYXp    sigYZp    sigZXp    sigZYp

$#                      sigXXn    sigYYn    sigZZn
                        1760.0    1760.0       2.0
$#  sigXYn    sigXZn    sigYXn    sigYZn    sigZXn    sigZYn

$#    aopt        xp        yp        zp        a1        a2        a3
         4       0.0       0.0       0.0
$#      v1        v2        v3        d1        d2        d3
       1.0       0.0       0.0
```



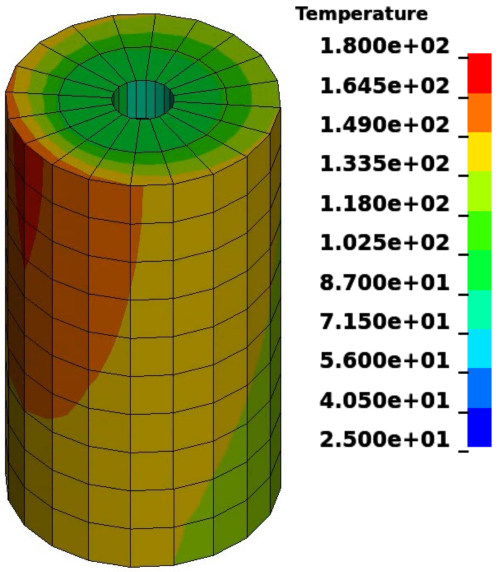


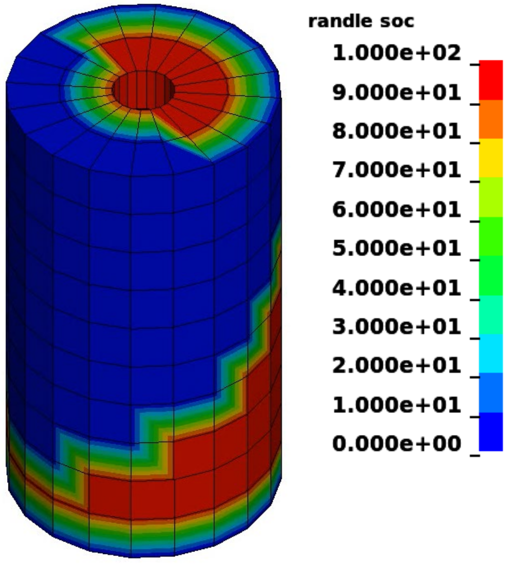
1 Positive pole
2 Positive Temperature Coefficient Device (PTC)
3 Gasket
4 Collector
5 Insulator
6 Cathode
7 Anode
8 Negative pole (cell can)
9 Separator
10 Current Interrupt Device (CID)
11 Exhaust gas hole

- Internal short circuit model during abuse
  - Short can be triggered based on combinations
    - Stress, strain, displacement, current, temperature, etc.
    - In case of an internal short, the respective Randle circuit is replaced by a resistance
    - Battery will then discharge through the shorted area which triggers resistive heating
      - ☐ SOC will go to zero after discharge
    - Here: Trigger temperature of the short is 180 ℃ (453 K)



```
*EM_RANDLES_SHORT
$#areaType    functId
         3        501
*DEFINE_FUNCTION
$#      fid                   heading
        501
float resistance_short_randle(float time,
                              float temp)  {
  if (temp >= 273.0 + 180.0)  {
    return 0.1;
  }else {
    return -0.1;
  }
}
```





Exothermic Reaction Models

- Decomposition reaction models are used to capture chemical reaction kinetics
- Approaches with analytical equations for the heat generation S
  - **`*LOAD_HEAT_EXOTHERMIC_REACTION`**
    - One-equation model (MacNeil et al. 2001)
      - Heat generation S by one exothermic reaction depending on temperature and constant input parameters

$$R(T,\alpha) = A_{\text{sei}} \times \alpha^{m_{\text{sei}}} \times (1-\alpha)^{n} \times (-\ln(1-\alpha))^{p} \times \exp\left(-\frac{E_{a,\text{sei}}}{R_u T}\right)$$

$$S = H_{\text{sei}} \times W_c \times R \quad \text{and} \quad \frac{d\alpha}{dt} = R$$

heat source

reaction kinetics

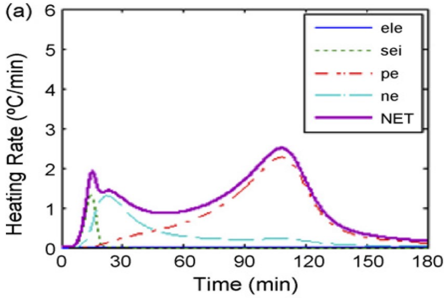
volume-specific carbon content

specific heat release

    - NREL's four equation model (Kim et al. 2007)
      - Separate heat generation from the decomposition reaction of the four components, i.e. solid electrolyte interface (sei), negative (ne) & positive (pe) electrode, electrolyte (ele)

$$S_{\text{abuse\_chem}} = S_{\text{sei}} + S_{\text{ne}} + S_{\text{pe}} + S_{\text{ele}}$$

Many parameters to determine!



$$R_{\text{sei}}(T,c_{\text{sei}}) = A_{\text{sei}} \times \exp\left(-\frac{E_{a,\text{sei}}}{R_u T}\right) \times c_{\text{sei}}^{m_{\text{sei}}}$$

$$S_{\text{sei}} = H_{\text{sei}} \times W_c \times R_{\text{sei}}$$

$$\frac{dc_{\text{sei}}}{dt} = -R_{\text{sei}}$$

$$R_{\text{pe}}(t,\alpha) = A_{\text{pe}} \times \alpha^{m_{\text{pe,p1}}} \times (1-\alpha)^{m_{\text{pe,p2}}} \times \exp\left(-\frac{E_{a,\text{pe}}}{R_u T}\right)$$

$$S_{\text{pe}} = H_{\text{pe}} \times W_p \times R_{\text{pe}}$$

$$\frac{d\alpha}{dt} = R_{\text{pe}}$$

$$R_{\text{ne}}(T,c_{\text{neg}},t_{\text{sei}}) = A_{\text{ne}} \times \exp\left(-\frac{t_{\text{sei}}}{t_{\text{sei,ref}}}\right) \times c_{\text{neg}}^{m_{\text{ne},n}} \times \exp\left(-\frac{E_{a,\text{ne}}}{R_u T}\right)$$

$$S_{\text{ne}} = H_{\text{ne}} \times W_{\text{cne}} \times R_{\text{ne}}$$

$$\frac{dc_{\text{neg}}}{dt} = -R_{\text{ne}}$$

$$\frac{dt_{\text{sei}}}{dt} = R_{\text{ne}}$$

$$R_e(T,c_e) = A_e \times \exp\left(-\frac{E_{a,e}}{R_u T}\right) \times c_e^{m_e}$$

$$S_{\text{ele}} = H_e \times W_e \times R_e$$

$$\frac{dc_e}{dt} = -R_e$$

[Kim et al. 2007]

- Engineering approach via curve definition for the exothermic energy release rate vs. temperature
  - Start with normalized energy release rate curve and scale with `&hexo` to fit sparse experimental data

```
*EM_RANDLES_EXOTHERMIC_REACTION
$#areaType    functId
         2        511
*DEFINE_FUNCTION
$#      fid                     heading
        511
float exothermic_reaction_randle(float time,
                                 float temp,
                                 float H_ex) {
  float t_burn = 273.0 + 247.0;
  float H_max  = 2.4;
  if (temp > t_burn && H_ex < H_max) {
    return &hexo*H_releaseVsT(temp-t_burn+offset);
  } else {
    return 0.0;
}}
*DEFINE_FUNCTION_TABULATED
$#      fid
        512
$# title
H_releaseVsT
$#        Temperature              H_release
                0.000                 0.0010
                7.198                 0.0057
                14.89                 0.0194
                  ...                    ...
```

definition of exothermic release rate

ignition temperature

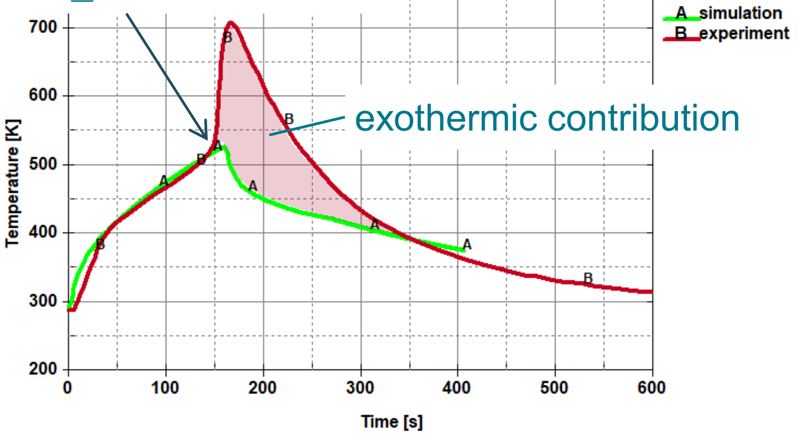
max. accumulated energy

burn only if ignition temp. `t_burn` is reached and not fully decomposed yet

activation offset

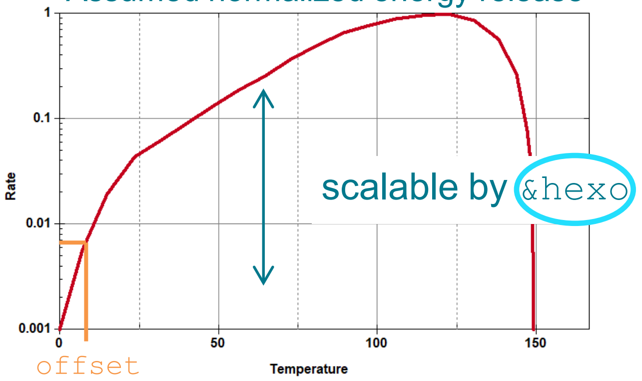
tune `T_burn, H_max, &hexo, offset` to match experimental results

`t_burn = 520.0`



exothermic contribution

Assumed normalized energy release

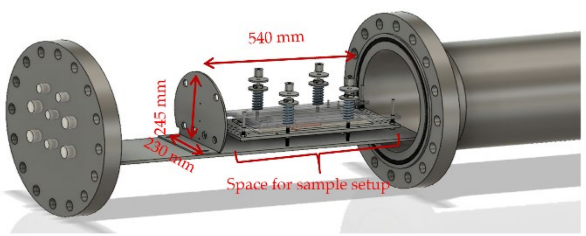


scalable by `&hexo`

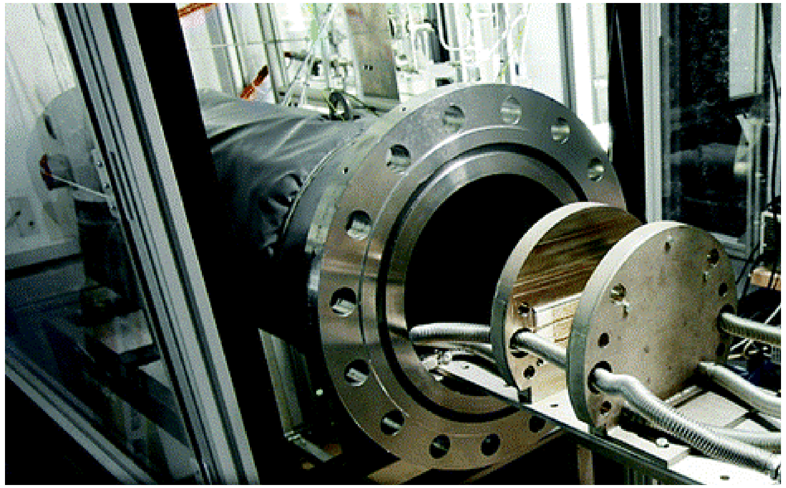
`offset`

Proof of Concept

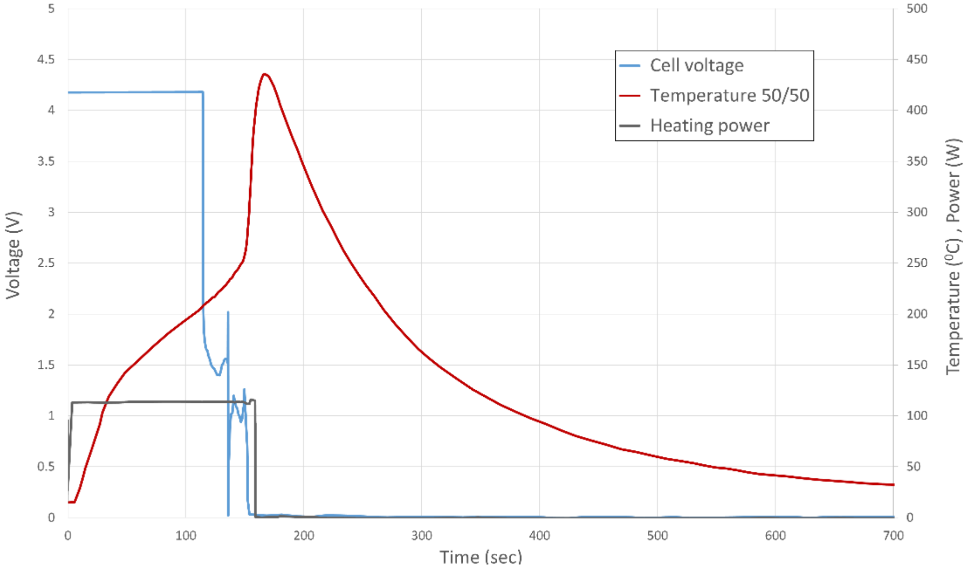
- Experimental setup
  - Heating wire is wrapped around the battery and
    - Heating power of 114 W is applied until onset of thermal runaway
  - Measurements
    - Temperature at 4 points on battery surface
      - ☐ Only point at the center of the battery is used for comparison
    - Voltage drop in battery after short



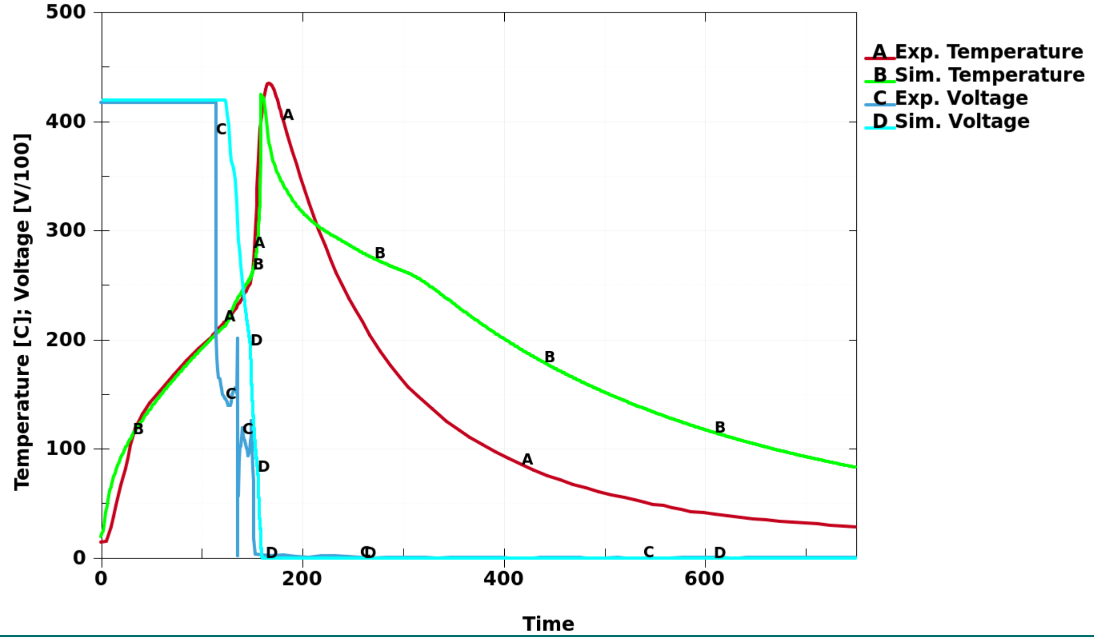
[Essl et al. 2018]

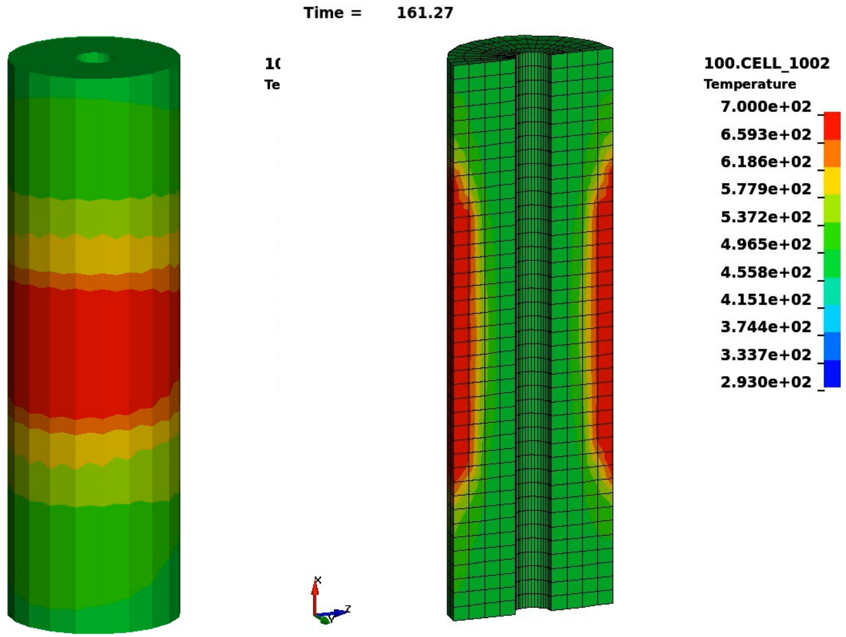


[Golubkov et al. 2018]



- Simulation results
  - Good agreement of the voltage drop
  - Good agreement of the temperature increase but room for improvement during cool down
    - Simulation results show temperature average of all surface nodes in the middle while experiment is at single point
    - Depends strongly on thermal boundary conditions where simplified convection models are always fuzzy without CFD
  - Batteries in a module/pack are usually connected by thermal paste such that there is no void space
    - Thermal propagation through contact plays probably bigger role than convection/radiation into free air

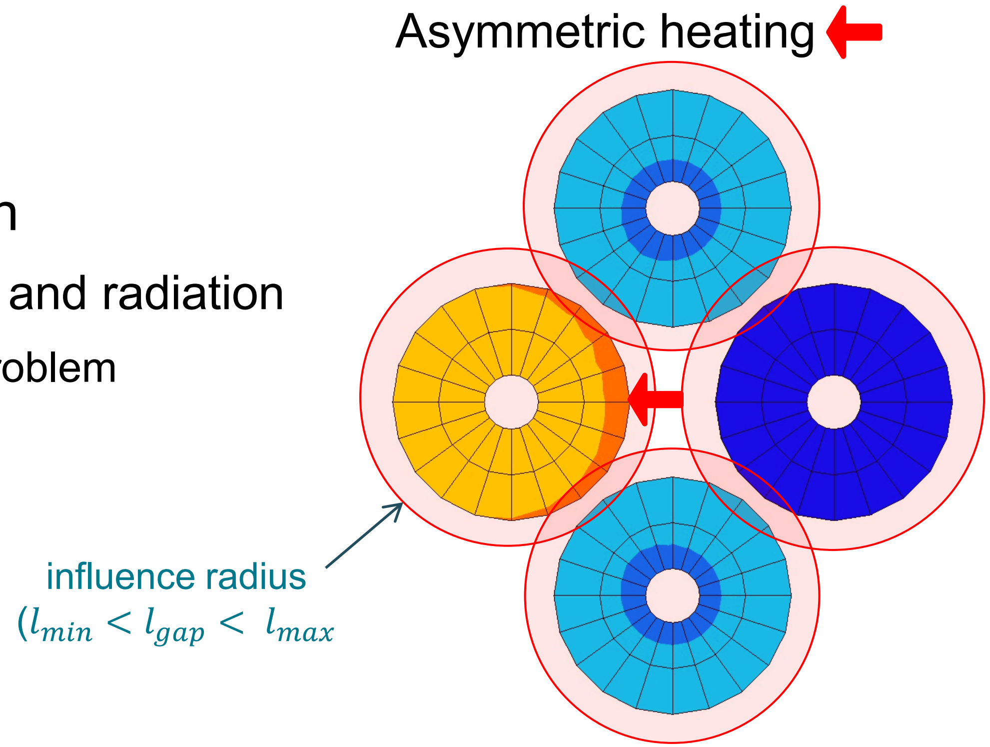




Modular Multi Cell Model

Thermal Contact Module

- Extension of the contact definition by the THERMAL option
  - Simple heat transfer model by contact, conduction through air and radiation
    - No view factor computation involved to solve boundary radiation problem
    - `K`: thermal conductivity of fluid between contact surfaces
    - `FRAD`: radiation factor between the contact surfaces
    - `H0`: heat transfer conductance for closed gaps
    - `LMIN / LMAX`: minimum / maximum gap size



Thermal Card 1.

THRM 1	1	2	3	4	5	6	7	8
Variable	K	FRAD	H0	LMIN	LMAX	FTOSLV	BC_FLG	ALGO
Type	F	F	F	F	F	F	I	I
Default	none	none	none	none	none	0.5	0	0

$$h_{\mathrm{cond}} = \frac{K}{l_{\mathrm{gap}}} \qquad f_{\mathrm{rad}} = \frac{\sigma}{\frac{1}{\varepsilon_1} + \frac{1}{\varepsilon_2} - 1}$$

σ = Stefan-Boltman constant

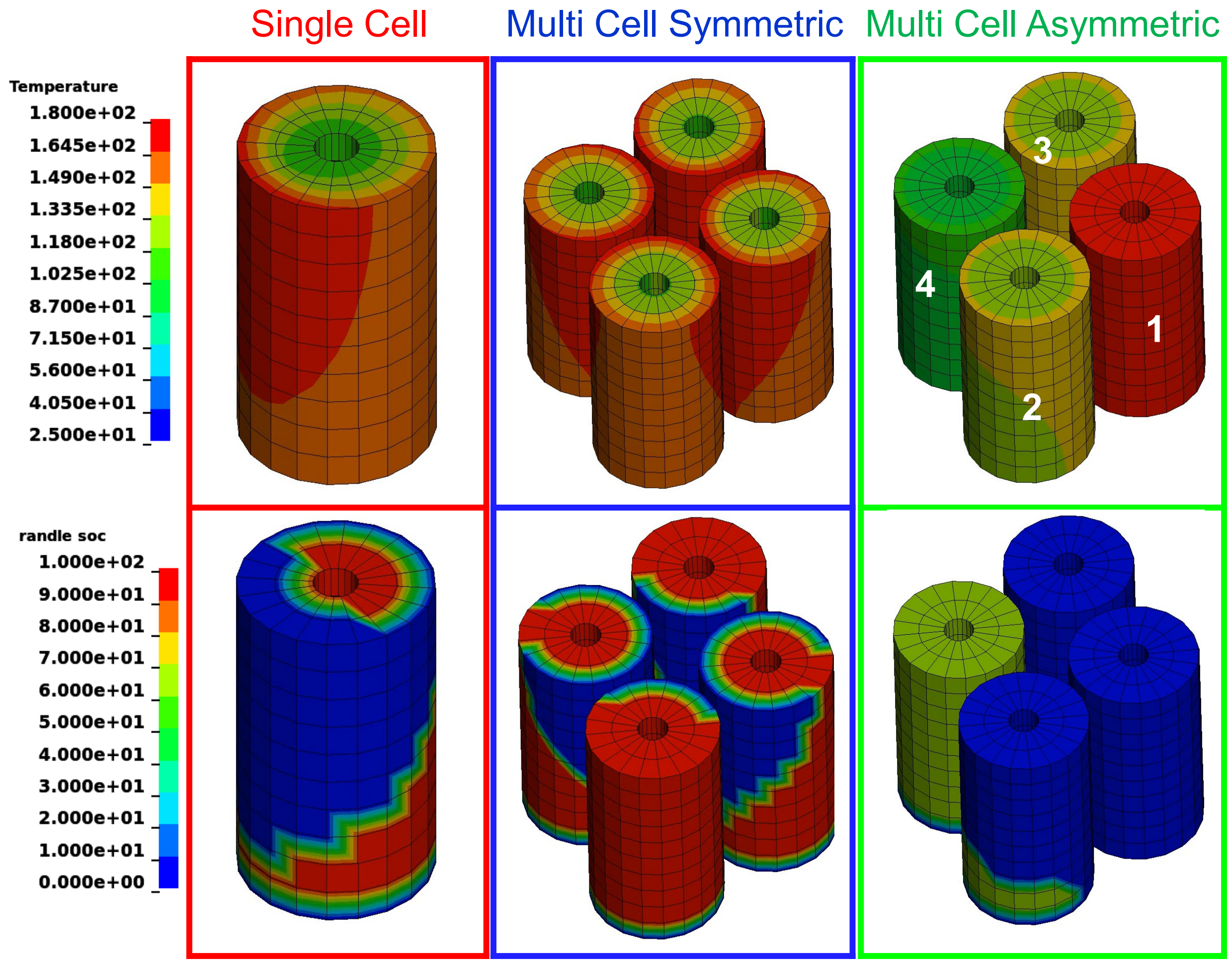
ε_1 = emissivity of master surface

ε_2 = emissivity of slave surface

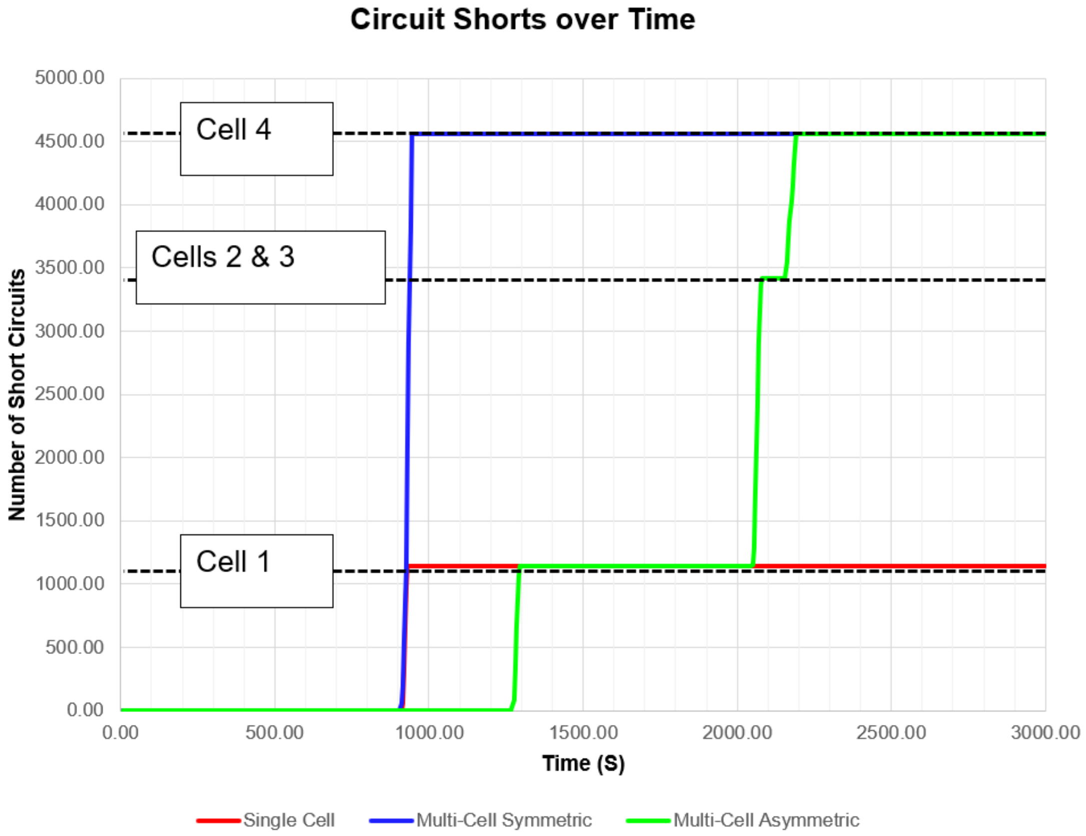
$$h = \begin{cases} h_0 & 0 \leq l_{\mathrm{gap}} \leq l_{\mathrm{min}} \\ h_{\mathrm{cond}} + h_{\mathrm{rad}} & l_{\mathrm{min}} < l_{\mathrm{gap}} \leq l_{\mathrm{max}} \\ 0 & l_{\mathrm{gap}} > l_{\mathrm{max}} \end{cases}$$

Proof of Concept

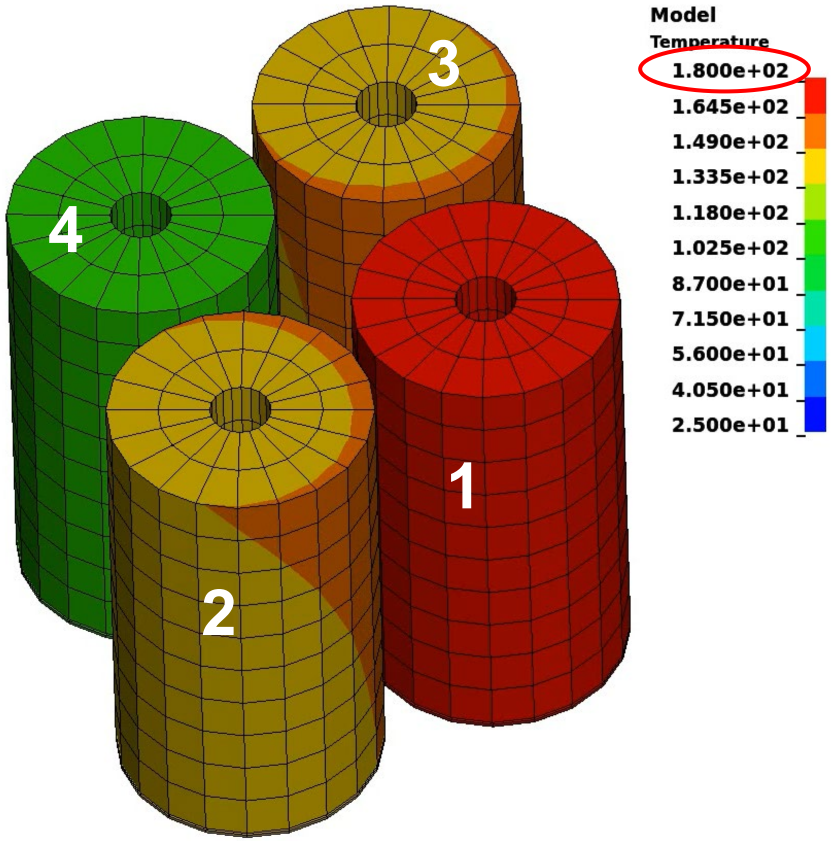
- Cascading cell failure with different heating patch application



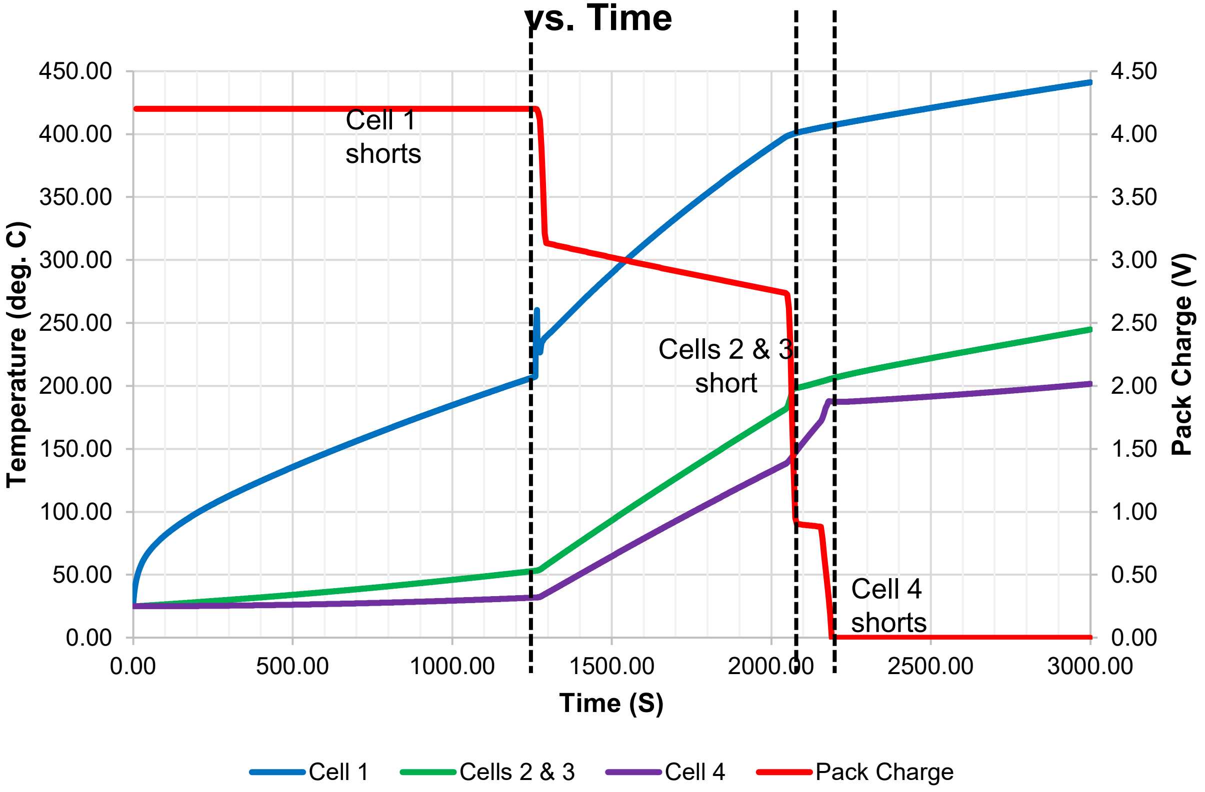
There is a circuit at each node, when the temperature reaches 180 deg. C



- Cascading cell failure with different heating patch application
  - Relationship Between Voltage Drop and Temperature Jump
    - Circuit shorts when temperature at the node reached 180 deg. C
      - ☐ Here: Thermal convection and radiation boundary not included; different exothermic energy release



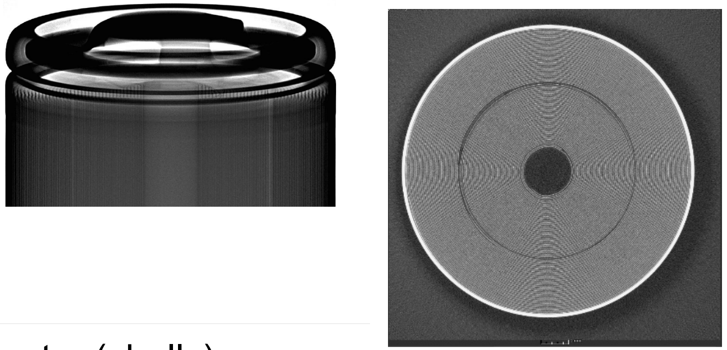
Cell Temperature vs. Time compared to Pack Voltage vs. Time



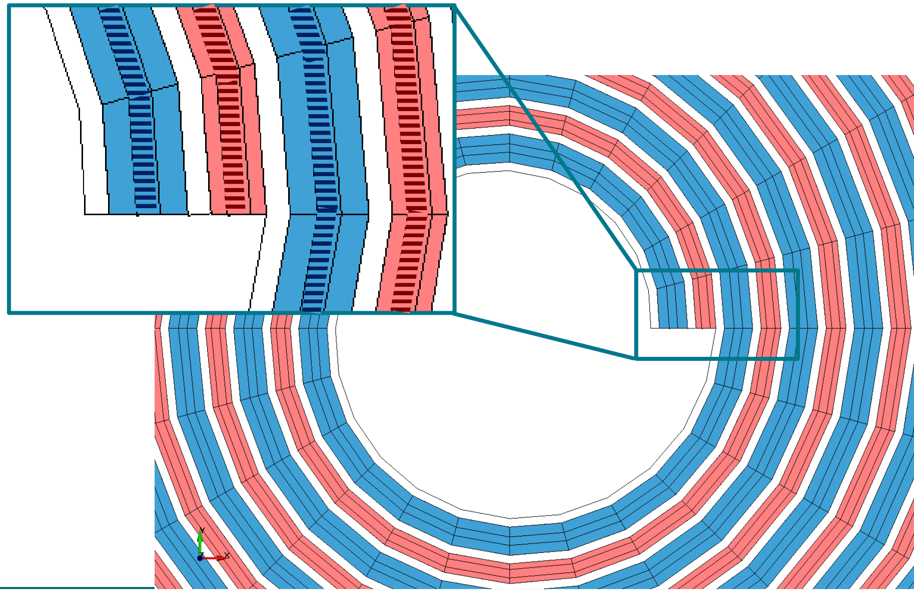
Structural Modul

Models on the microscale

- Idea: Model all components of the microstructure as they appear
  - Benefits
    - Each component can be modeled separately
      - Relatively simple material laws can be applied
      - Failure of each component can be included
    - Combination of shells, thick shells and solids possible
    - Structural effects from buckling laminate is automatically included
  - Drawbacks
    - Element count quickly explodes to unreasonable model sizes
      - Modul or pack simulations are close to impossible
    - If layers are allowed to slide, expensive contact modeling needed
    - Independent testing of the components needed (tedious)
    - Although layers are thin, some solids needed to capture compressibility



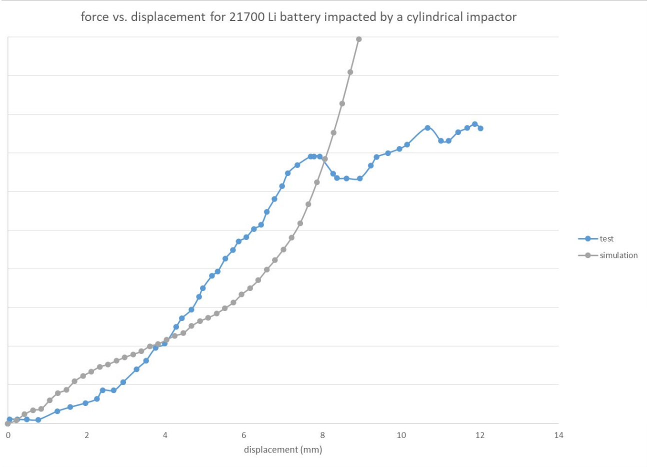
☐ Separator (shells)
🟦 Negative electrode (solids)
🟥 Positive electrode (solids)
▤ Neg. current collector (constrained shell in solid)
▤ Pos. current collector (constrained shell in solid)

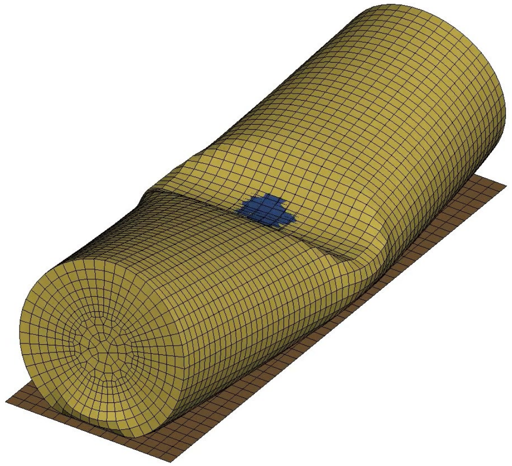


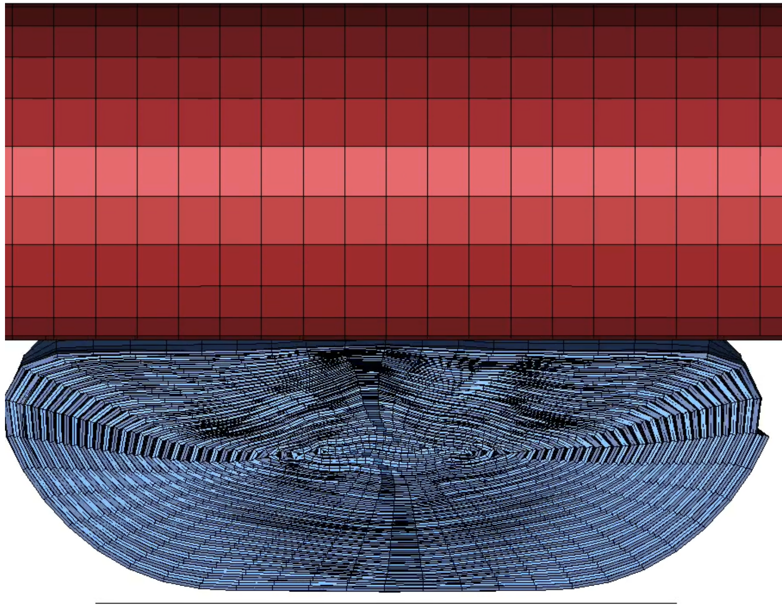
Models on the microscale

- Simulation results for cylindrical impactor test
  - Model size roughly 0.5 mio. elements
    - Elements must be small enough to be able to slide without locking
  - Here: All materials are `*MAT_PIECEWISE_LINEAR_PLASTICITY`
    - Currently still based on literature values.
  - Goal: Testing and calibration with failure models
    - Isotropic anode and cathode
      - ☐ `*MAT_PIECEWISE_LINEAR_PLASTICITY`
      - ☐ `*MAT_ADD_EROSION`
    - Anisotropic separator
      - ☐ `*MAT_EXTENDED_3-PARAMETER_BARLAT`
      - ☐ `*MAT_ADD_GENERALIZED_DAMAGE (anisotropic failure behavior)`

Failure separator → short-circuit

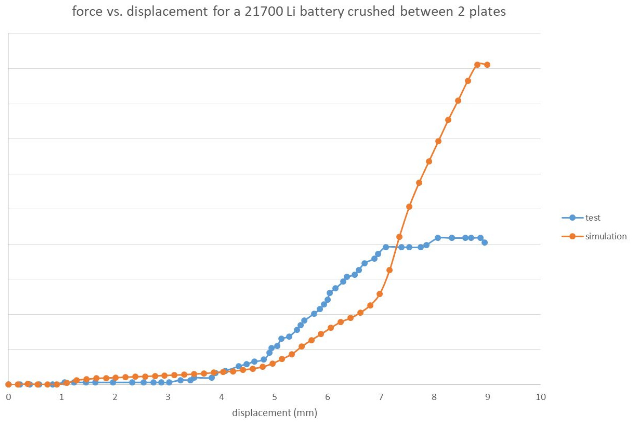


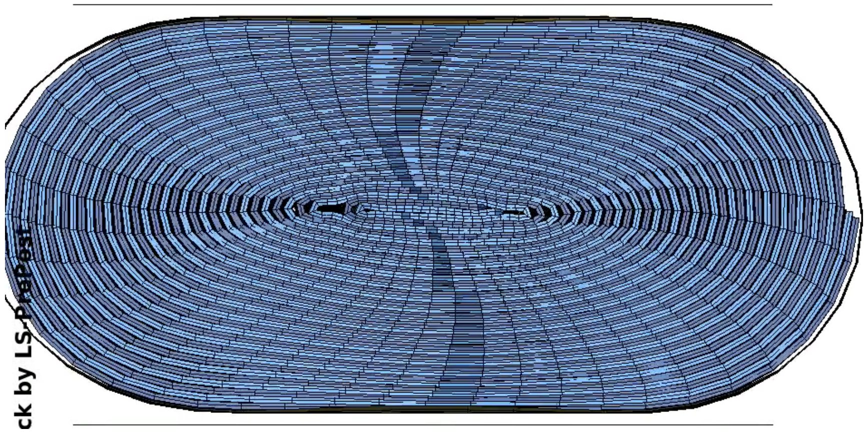




Models on the microscale

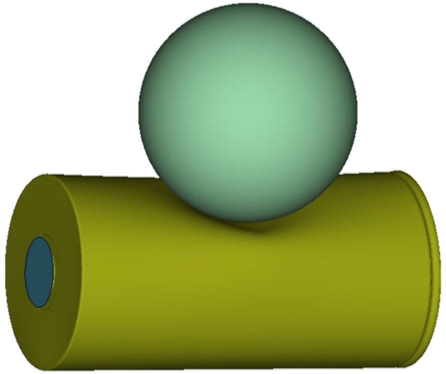
- Simulation results for plate impactor test
  - Model size roughly 1 mio. elements
    - Elements must be small enough to be able to slide without locking
  - Here: All materials are `*MAT_PIECEWISE_LINEAR_PLASTICITY`
    - Currently still based on literature values.
  - Goal: Testing and calibration with failure models
    - Isotropic anode and cathode
      - ☐ `*MAT_PIECEWISE_LINEAR_PLASTICITY`
      - ☐ `*MAT_ADD_EROSION`
    - Anisotropic separator
      - ☐ `*MAT_EXTENDED_3-PARAMETER_BARLAT`
      - ☐ `*MAT_ADD_GENERALIZED_DAMAGE (anisotropic failure behavior)`
  - Also: Investigate influence of electrolyte
    - `*AIRBAG_LINEAR_FLUID` or `*MAT_ADD_PORE_FLUID`

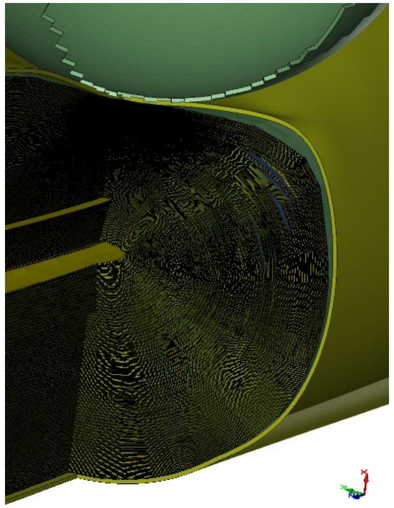


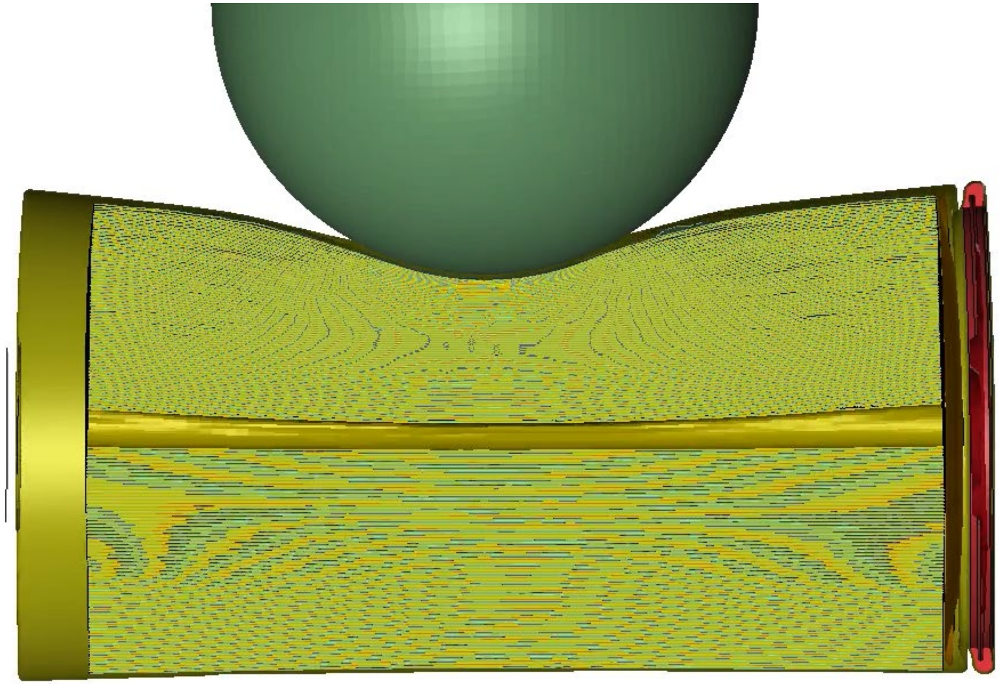


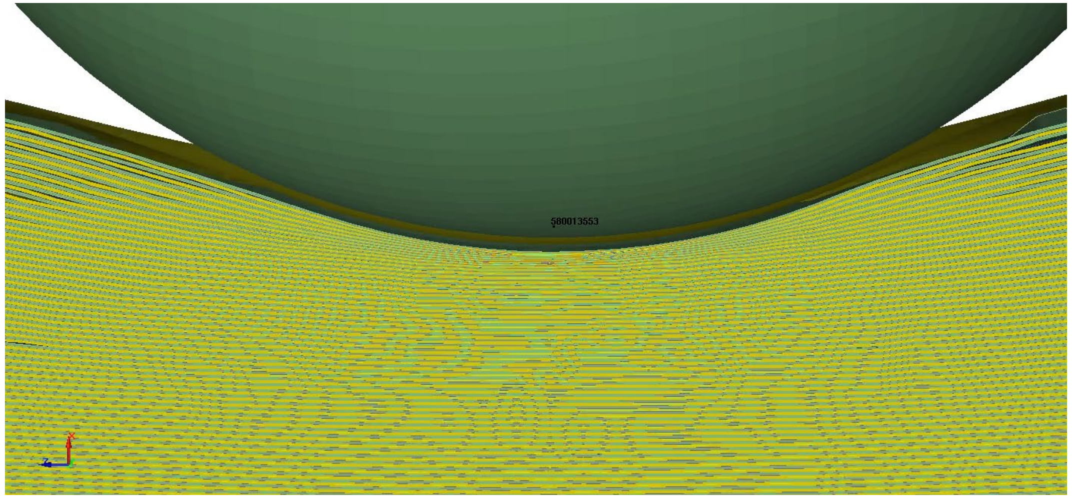
Models on the microscale

- Models can still get refined
  - Model size at around 6 mio. elements
  - Mostly thick shells with more sophisticated material models



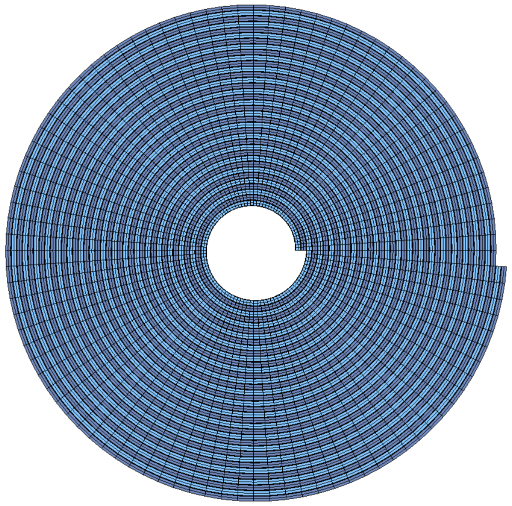




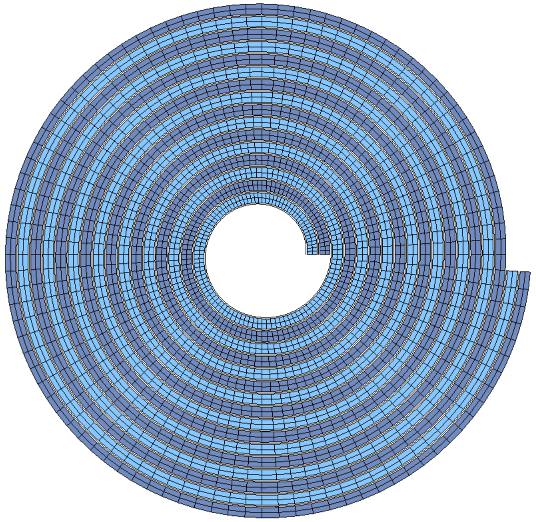


Models on the mesoscale

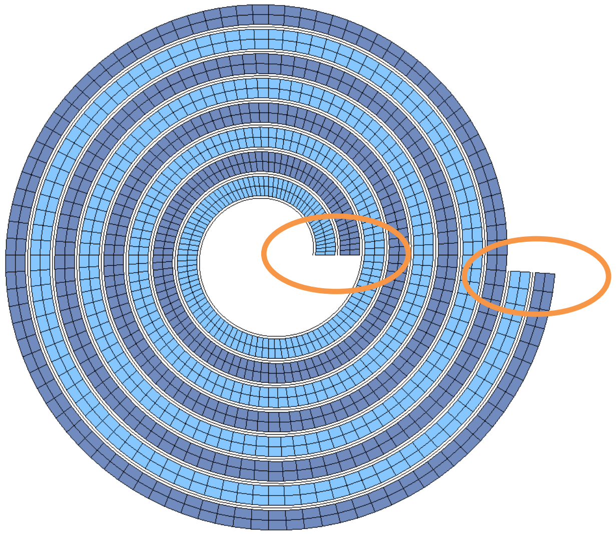
- Idea: Resolve some of the microstructure but keep element count lower
  - Homogenization of several patterns of layers into one pattern
    - PART_COMPOSITE could be used to represents layers in one homogenized layer
    - How coarse can it get without loosing the structural effect or introducing big gaps?



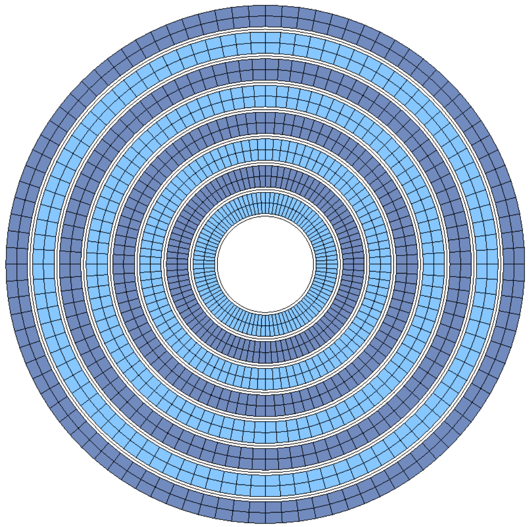
original



coarse 1



coarse 2a

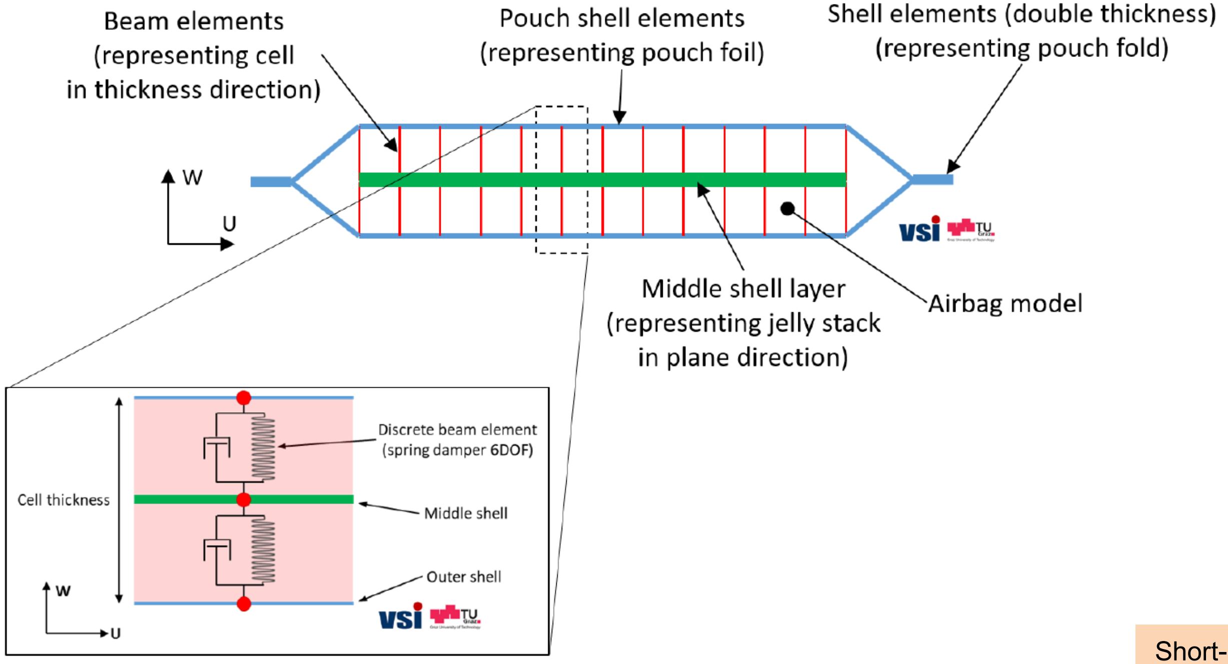


coarse 2b

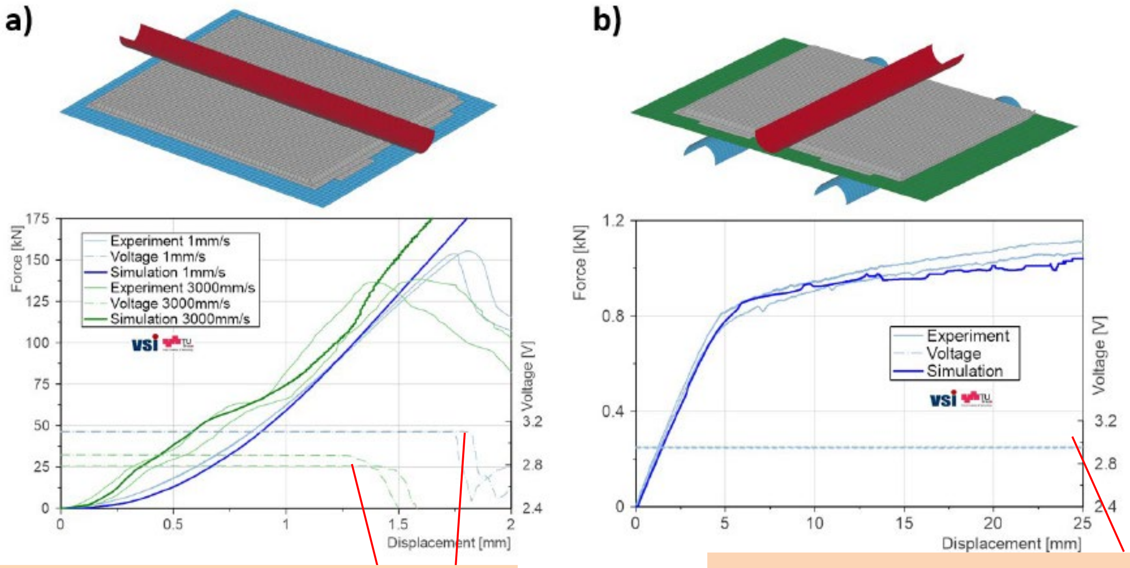
    - Note: Thicker layers introduce higher bending stiffness to the homogenized layer
      - In case of shell elements, this can be compensated by squeezing the z-coordinate of the integration points

Models on the mesoscale

- Extreme case of only one layer in a thin pouch cell
  - Shell elements + discrete beams + airbag model (~1.800 elements)
  - Good representation of the deformation
  - Difficult to predict separator failure



No separator to predict short-circuit



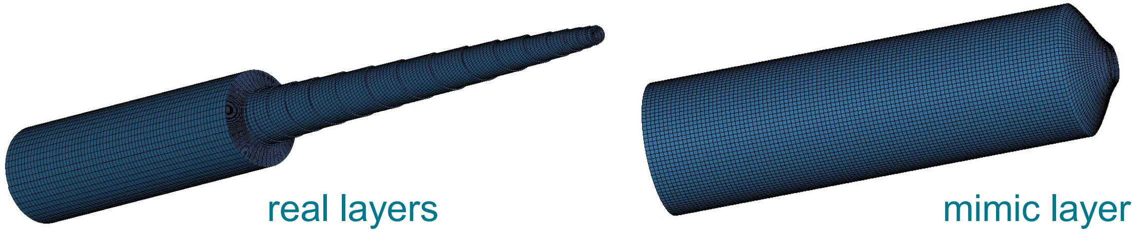
Short-circuit at displacements around **1.3-1.7mm**

25mm displacements **no short-circuit**

[Schmid et al. Uni Graz 202

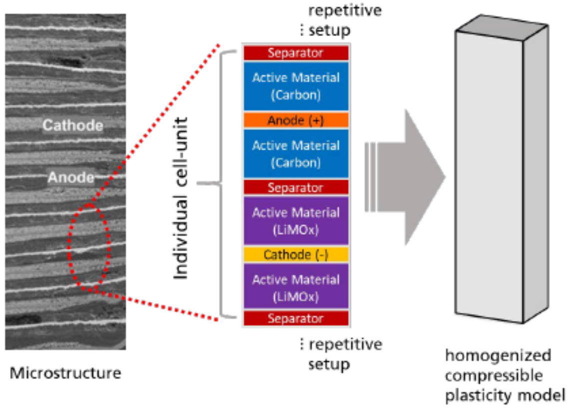
Macro scale models

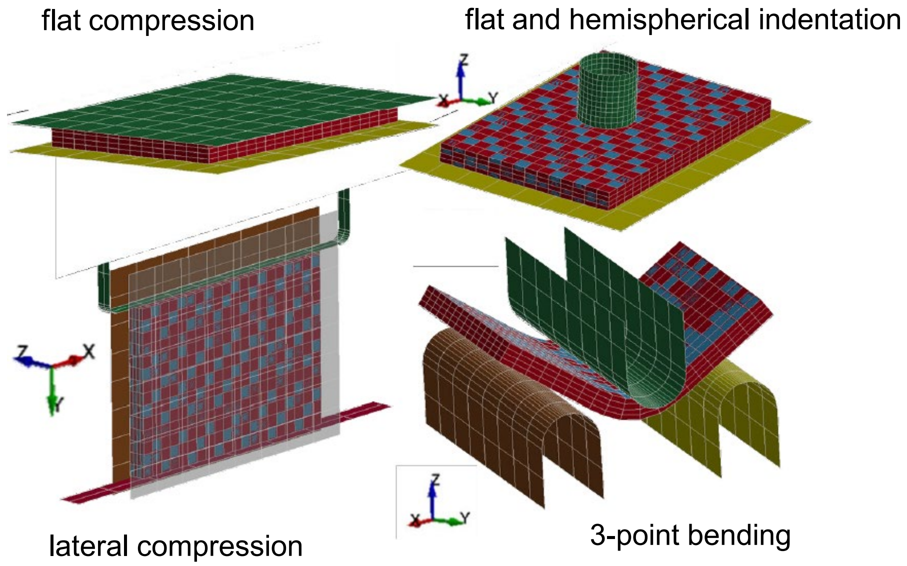
- Idea: Homogenization over all layers to be able to use much coarser solid elements
  - Typically, all structural effects are ruled out from the model
  - Material models need to include these through the back door
  - Example: `*MAT_MODIFIED_HONEYCOMB`
    - Anisotropic material that allows to decouple normal from shear stresses
    - Three yield surfaces are available
      - ☐ The first yield surface defines the nonlinear elastoplastic material behavior separately for normal and shear stresses
      - ☐ The second yield surface considers the effects of off-axis loading (transversely isotropic)
        - Because of the definition of the second yield surface, the material can collapse in a shear mode due to low shear resistance
        - There was no obvious way of increasing the shear resistance without changing the behavior in purely uniaxial compression
      - ☐ The third yield surface allows to prescribe the shear and hydrostatic resistance without affecting the uniaxial behavior
    - Summary
      - ☐ Rather complicated to calibrate
      - ☐ Allows to mimic to some degree the sliding of the layers on a solid mesh without internal contact



Macro scale models

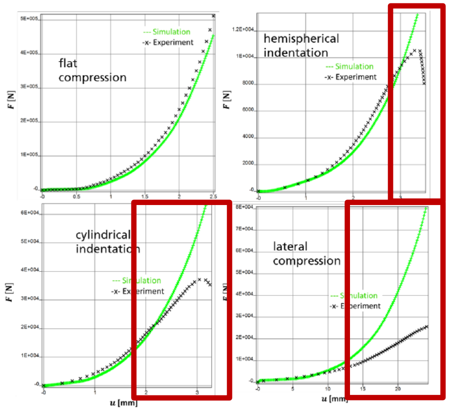
- Examples of homogenized models
  - With coupled and decoupled material cards



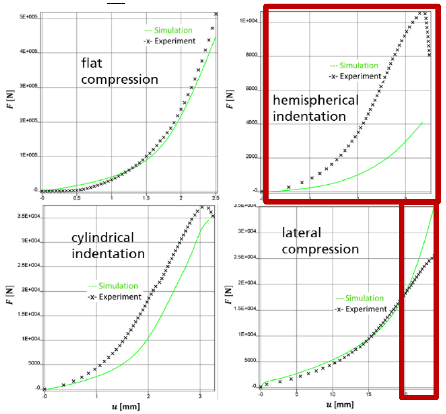


[Trondl at al. / Fraunhofer 2021]

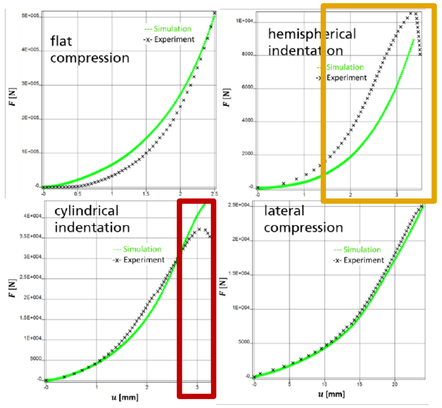
`*MAT_CRUSHABLE_FOAM`



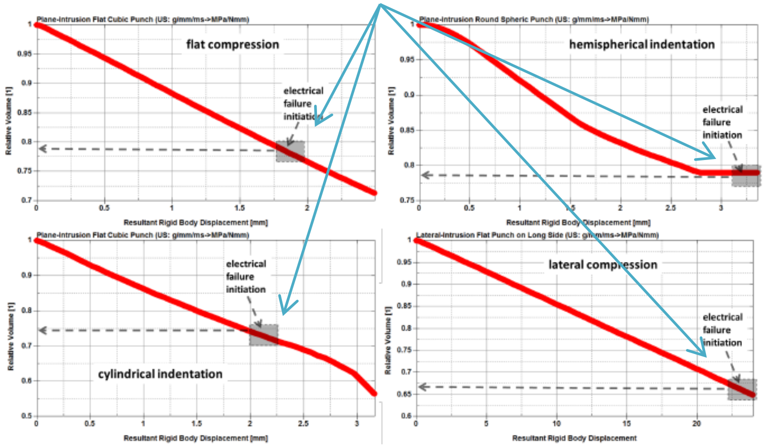
`*MAT_CSCM`



`*MAT_MODIFIED_HONEYCOMB`

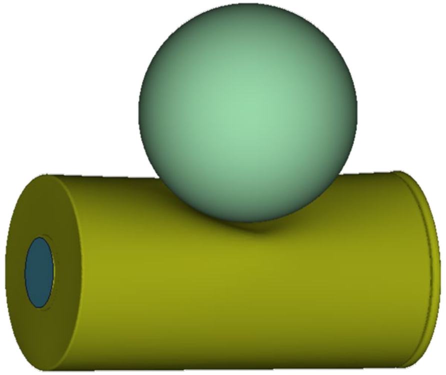


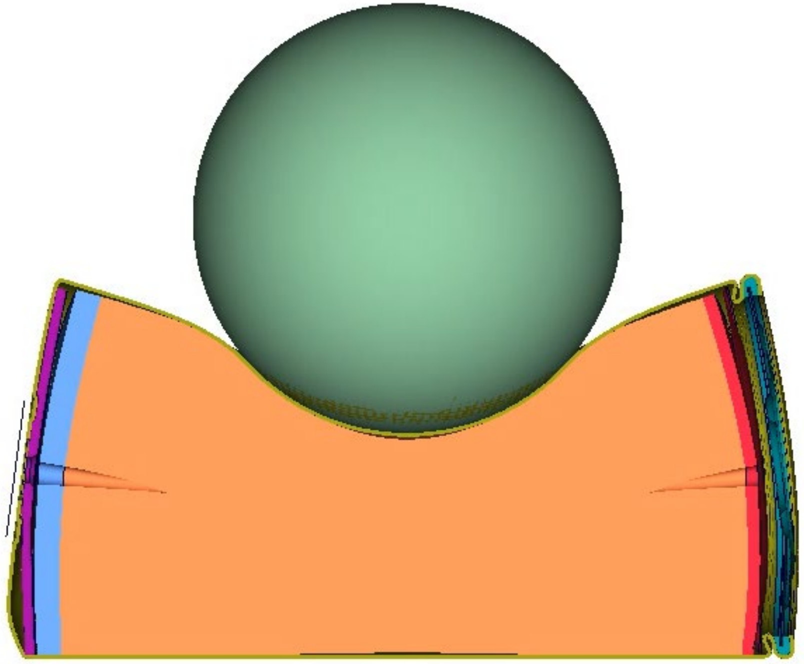
Short circuit areas from experiments
→ relative volume vs. intrusion

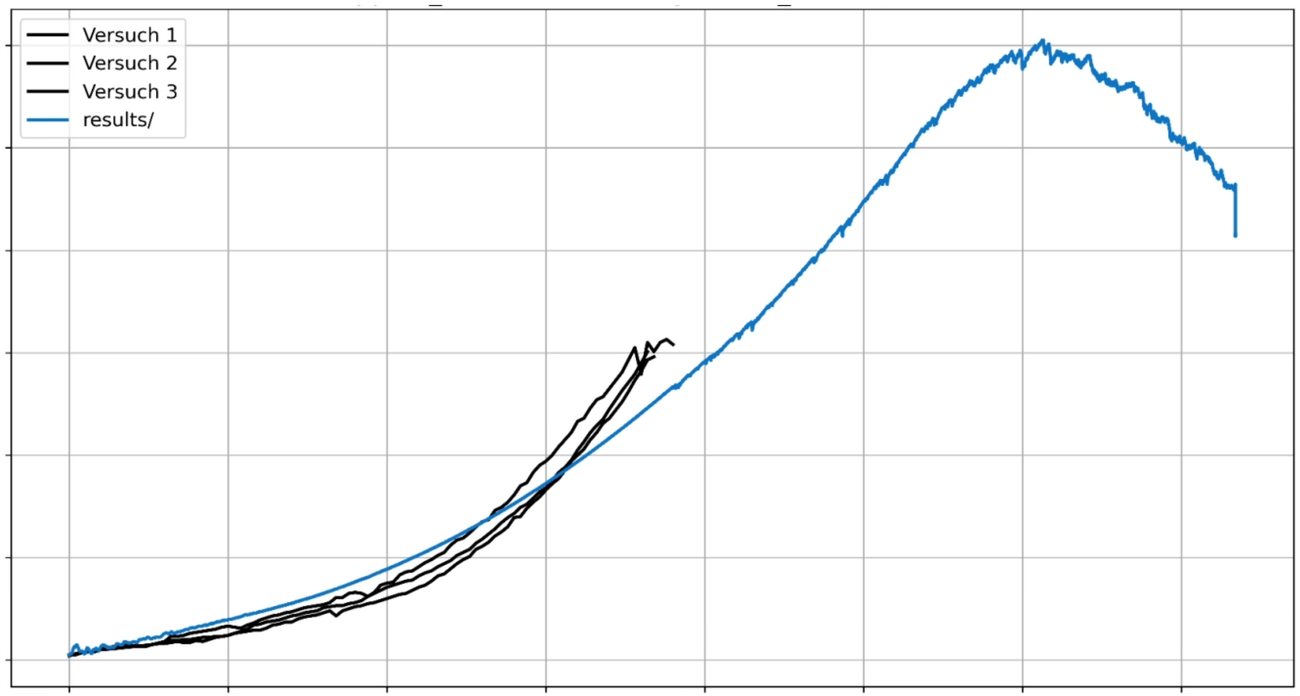


Macro scale models

- Decoupled models seem to be most promising
  - Here: `*MAT_MODIFIED_HONEYCOMB`

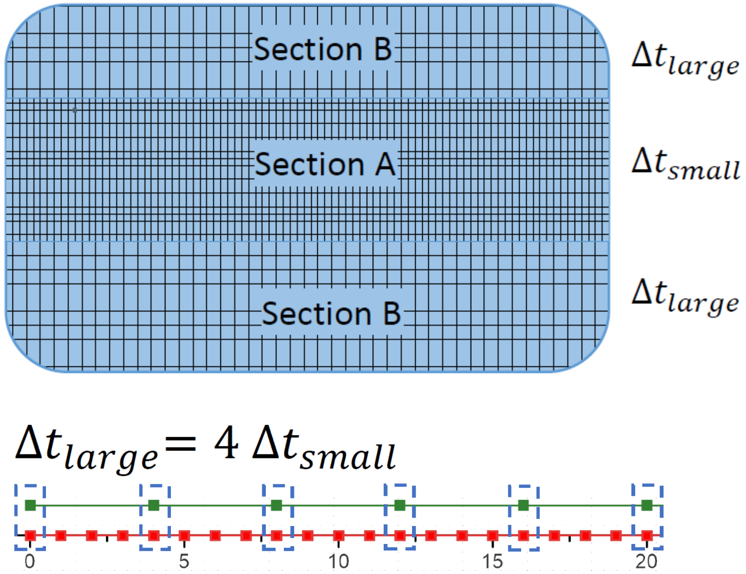






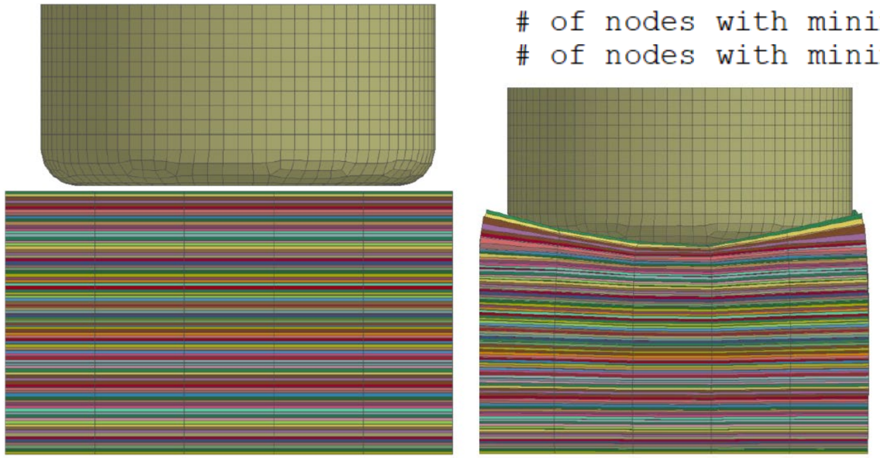
Scale bridging strategies in time

- Sub-cycling to reduce simulation time in explicit simulations
  - Areas with small timestep are computed in 2n sub cycles
  - Synchronize with other areas every large time step



$$\Delta t_{large} = 4\ \Delta t_{small}$$

```
minimum time step size          =    0.9639E-05
maximum time step size          =    0.7711E-04
external time step size         =    0.9639E-05
# of nodes with minimum time step size x 1 =     14068
# of nodes with minimum time step size x 2 =         0
# of nodes with minimum time step size x 4 =       864
# of nodes with minimum time step size x 8 =       756
# of nodes with minimum time step size x 16=         0
# of nodes with minimum time step size x 32=         0
# of nodes with minimum time step size x 64=         0
```

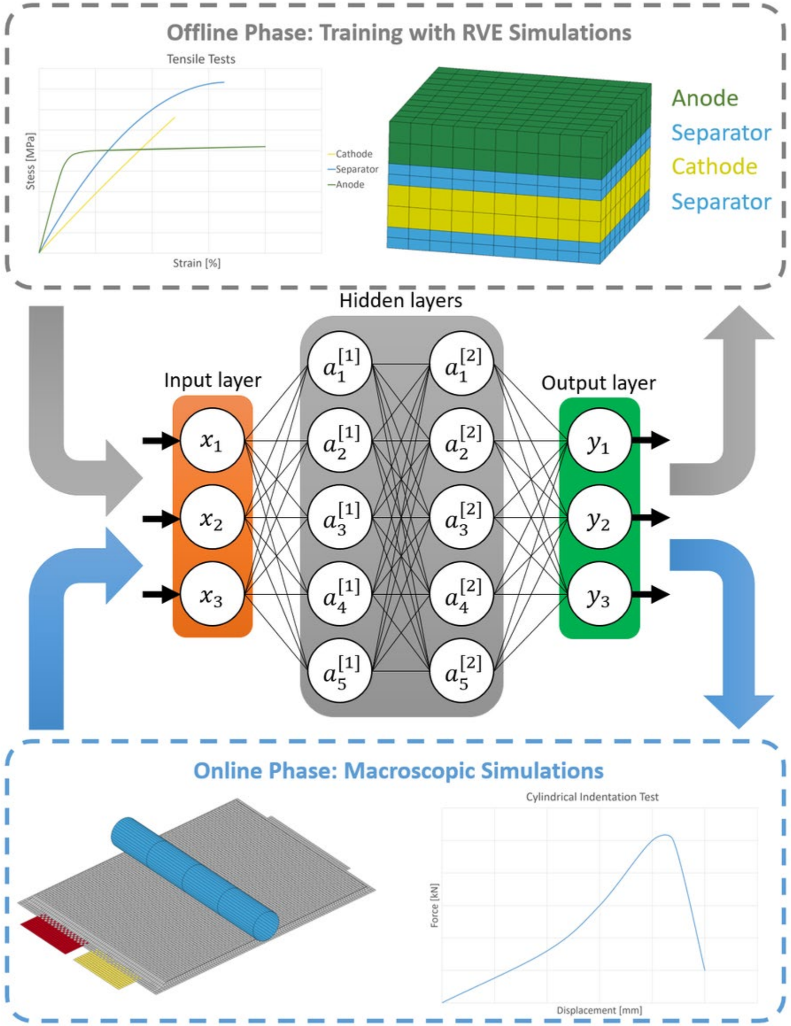


Simulation time [s] (%)	Local smp_d_R13.0
FULL	697 (100%)
SUBCYCLE_16_1	290 (42%)

[Schmid et al. / SafeLIB / Uni Graz]

Scale bridging strategies in space

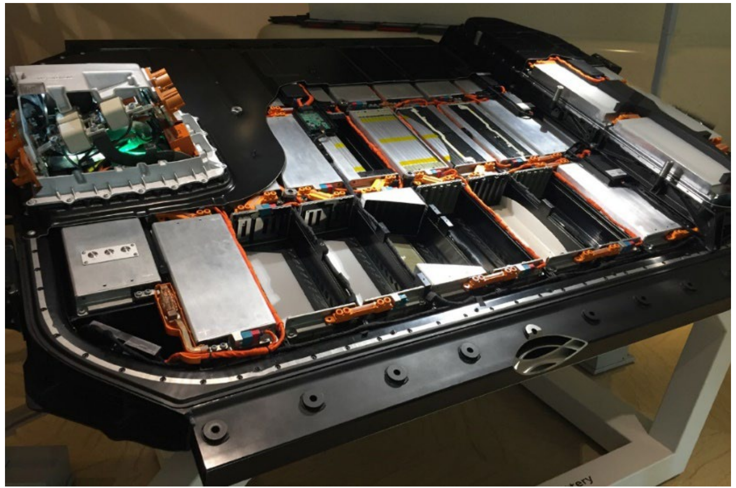
- Data-driven multi-scale modeling
  - Machine learning approach
    - Training of the neural network
      - Perform micro-scale analysis on Representative Volume Element (RVE)
      - Homogenization of stress data
    - Apply trained neural network
      - Use it as material model on a coarse mesh
      - Will output stress based on an applied strain
    - Available in LS-DYNA R13 SMP/MPP
      - `*RVE_ANALYSIS_FEM` for RVE analysis
      - `*DATABASE_RVE` for homogenized output

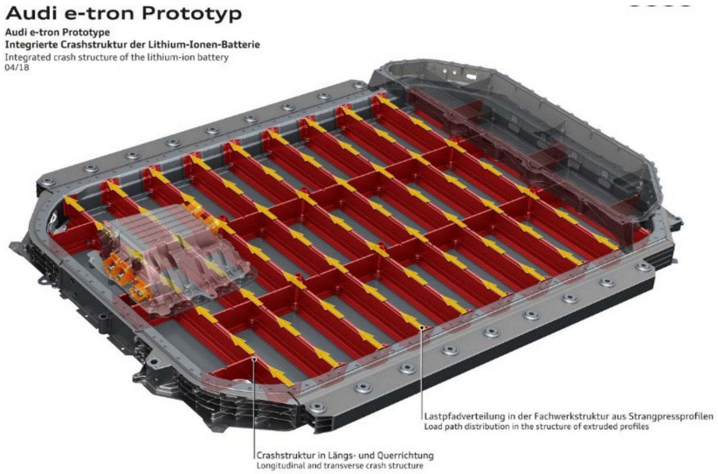


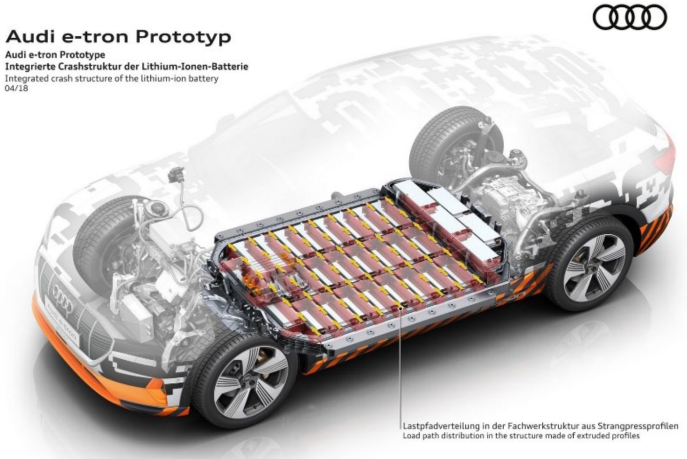
[Schmid et al. / SafeLIB / Uni Graz]

Other challenges around the battery pack

- Deformation chain before the battery needs to be correctly modeled
- Old challenges come back in a different context
  - Extruded aluminum
  - Fiber-reinforces plastics
  - Adhesives, thermal paste
  - Welds
  - Connection to BIW







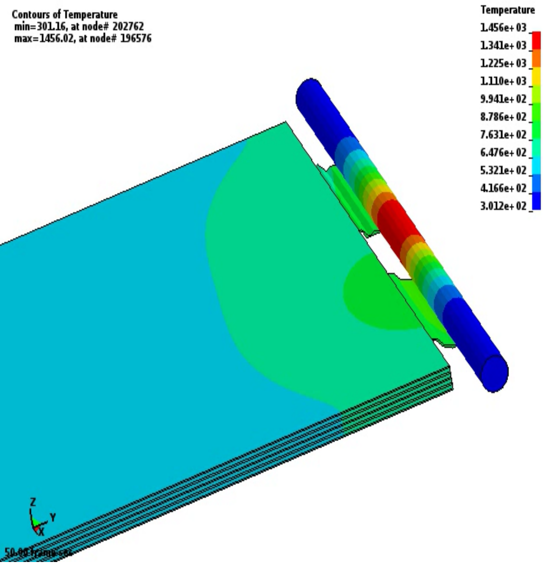
[Courtesy Audi AG]

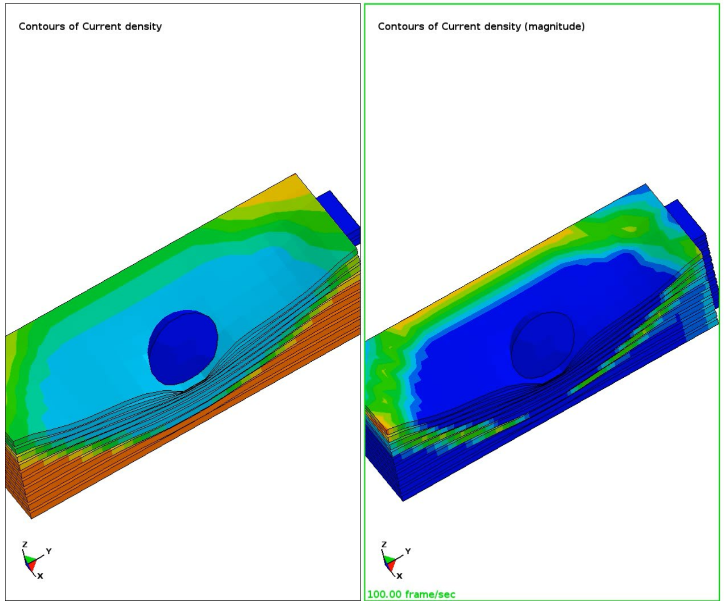
Bringing it all together

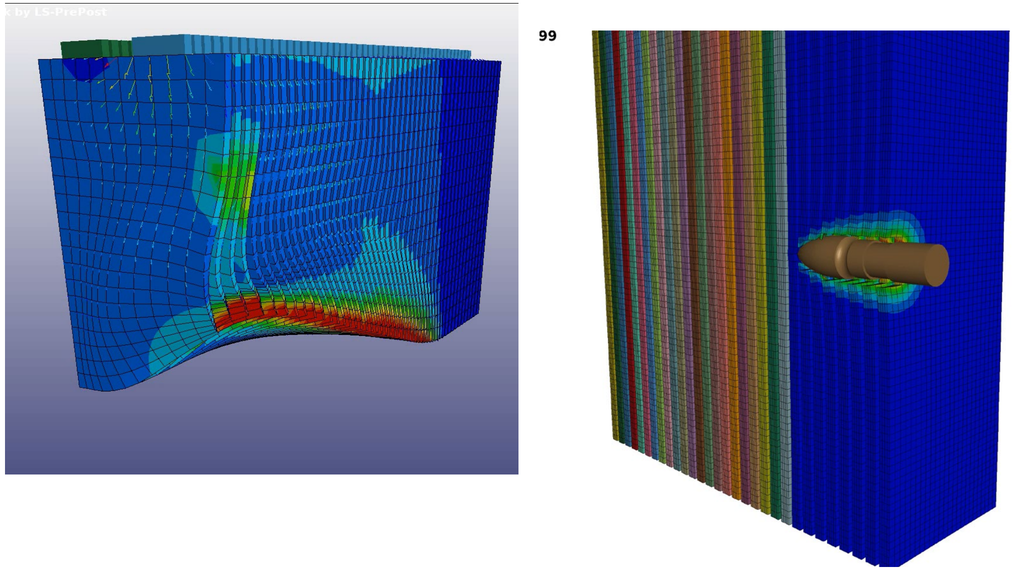
Misc. Examples

Download examples from
www.dynaexamples.com

- Fully coupled simulations
  - External short: Solid
    - Conducting rod shorting the tabs of a cell (temperature)
  - Internal short: Tshell
    - Sphere impacting a 10-cells module (current density)
  - Internal short: batmac
    - Wall and object impact
    - (Current density + temperature)



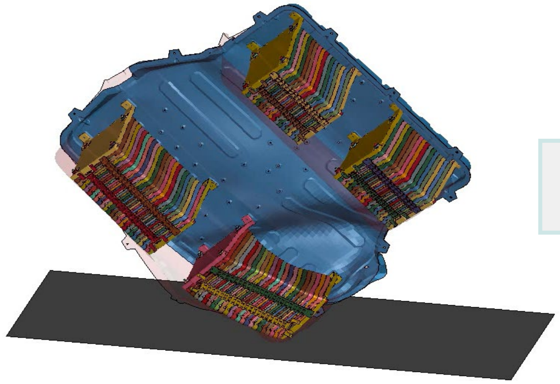




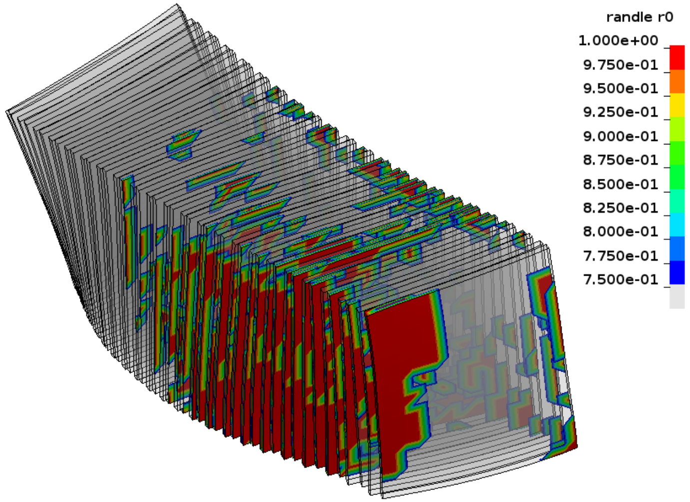
[L'Eplattenier & Çaldichoury 2019]

Time separation strategies

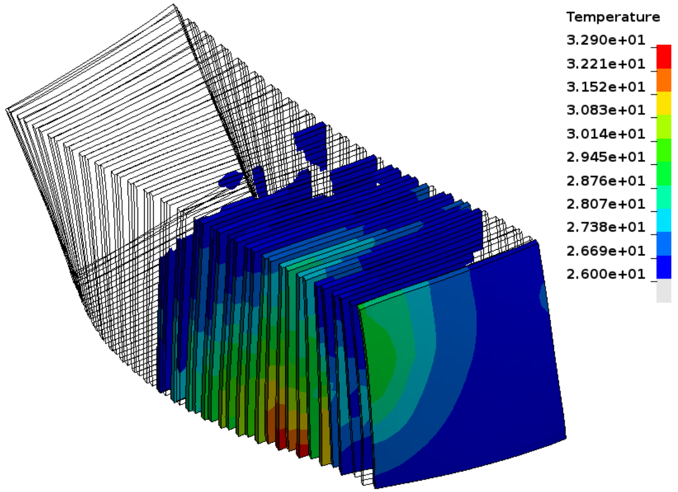
- Two-step approach
  - Crash or impact events usually last less than 100 ms
  - From short circuit due to separator failure to thermal runaway can be hours
  - Idea: decouple structural simulation from EM-thermo coupled simulation
    1. Do structural only simulation to predict deformation and internal short due to separator failure
    2. Do EM-thermal simulation to predict how battery discharges and if it remains stable
  - Example of a drop test



freeze



local internal shorts



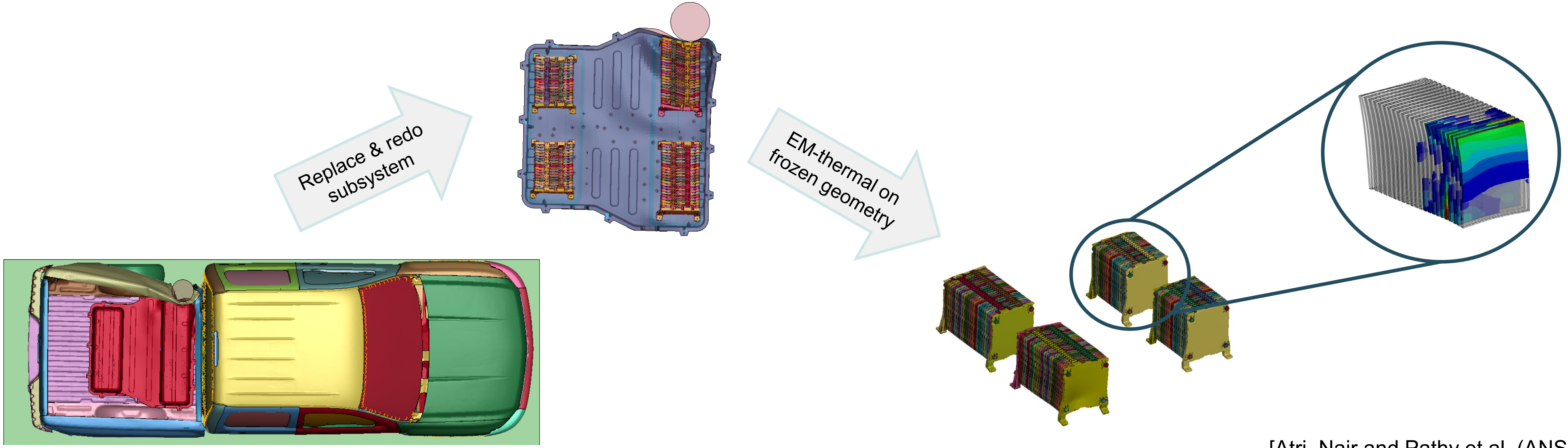
Temperature rise due to resistive heating

Time separation strategies

- Extended two-step approach

  1. Perform full vehicle crash with macro scale battery models
  2. Replace most critical cell with micro model and redo simulation on sub system
  3. Apply short circuit at location of separator failure and do EM-thermal simulation on frozen geometry

  → Requires matching battery models on micro and macro scale



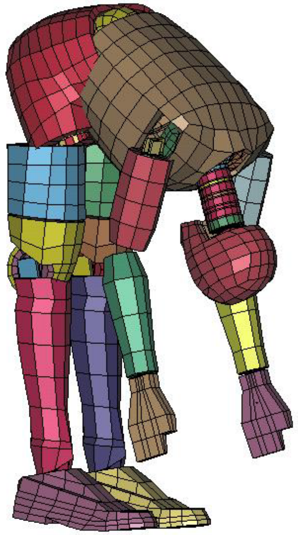
[Atri, Nair and Pathy et al. (ANSYS)]

Conclusion & Future Work

- Successful coupling of the structural and thermal solver with the EM solver
  - Capability to capture the main chain of events
    - Heating triggers internal short, discharge at the shorted area increases temperature, which triggers thermal runaway
  - Heat transfer via contact to neighboring cells included to assess cascading failure in battery packs
  - Different structural models available to predict deformation and on the micro scale even separator failure
  - Coupling to structural solver is possible to capture thermal runaway triggered by shorts due to deformation
- Open questions
  - Thermal boundary conditions
    - Influence of hot vent gases on neighboring cells for the stability of the pack? → CFD simulations needed (e.g., Fluent)
  - Exothermic energy release
    - Is the simple engineering approach enough to capture the complex chemical decomposition?
    - Does it need an extension of the exothermal module to include dependencies on temperature rates and SOC?
  - Mechanical deformation models
    - Best way to predict separator failure in structural simulations

Thank you
for your attention!

Questions: nils.karajan@dynamore.com



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