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Mechanical Modelling Approaches for Li-Ion Pouch Cells for Different Level of Detail

Table of contents

SafeLIB

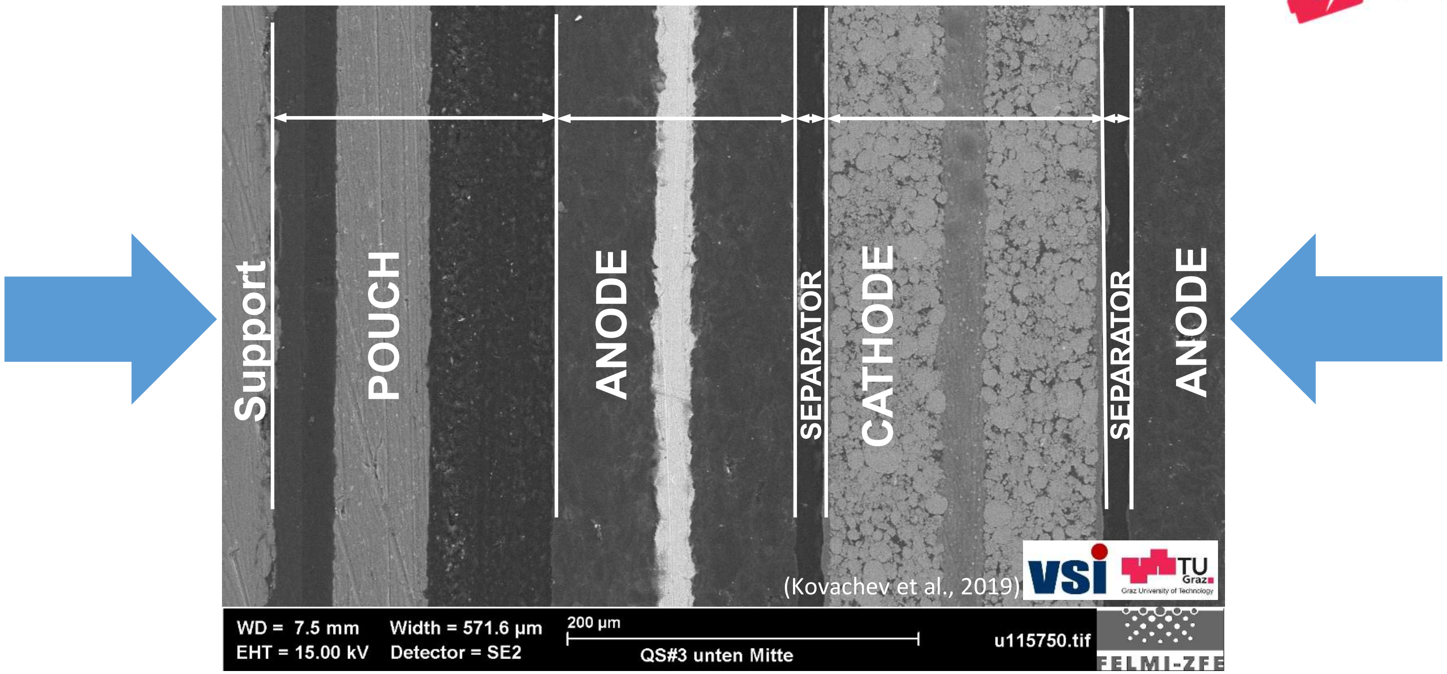
- Cell under study
- SAM vs. DLM
- Detailed Layer Model – DLM
- Simplified Applicable Model – SAM
- Vision of SafeLIB

SafeLIB

Cell under study

Cell under study

- NMC Pouch Cell
- Dimensions: 290x215x7.65mm
- Mass: 0.86kg
- Capacity: 41Ah
- **22 Anode layers**
- **21 Cathode layers**
- **42 Separator layers**

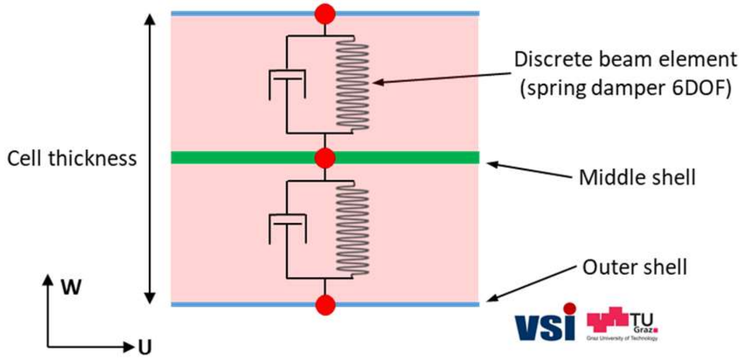


Mean thickness [µm]	
Anode	136
Cathode	165.2
Separator	19.5
Pouch	184.9

SAM vs. DLM

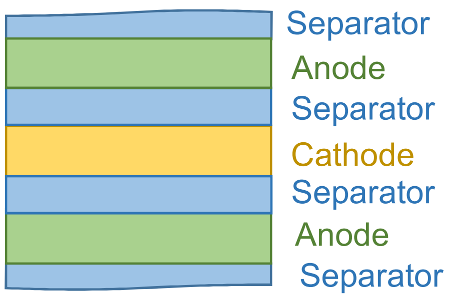
SAM

- **S**implified **A**pplicable **M**odel
- Macroscopic cell model
- Consisting mainly fast 1D and 2D elements (beam and shells)
- For full vehicle crash simulations
- Requirements for SAM
  - Representation of mech. Behavior
  - Simple handling and adaptability
  - Fast



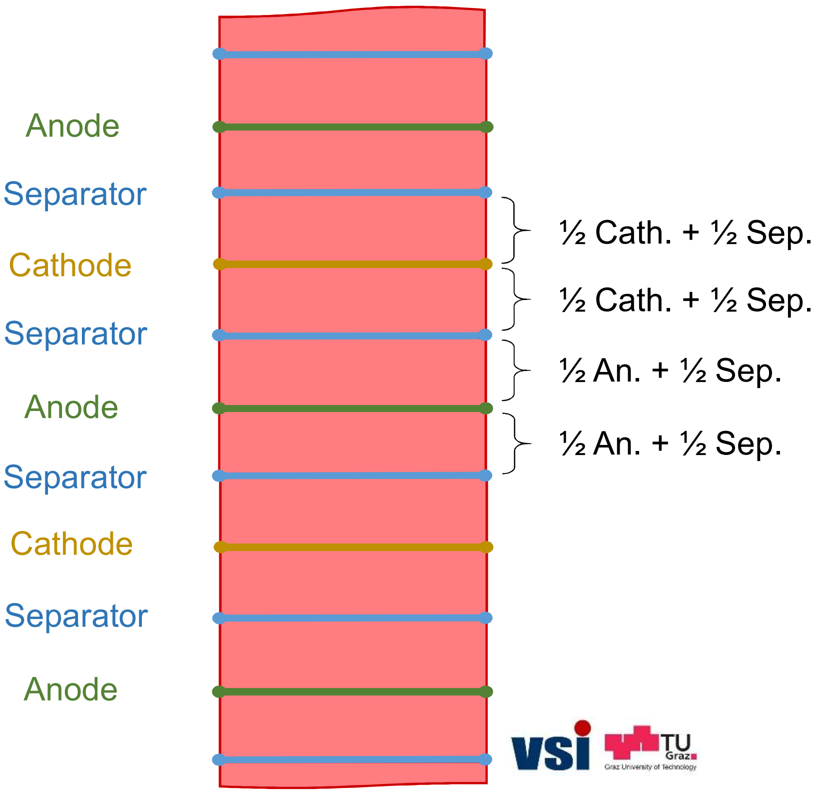
DLM

- **D**etailed **L**ayer **M**odel
- Layer-by-layer cell model
- Consisting 2D and 3D elements (shells and solids)
- Detailed model for cell simulations and profound analysis of mechanical behavior
- Requirements for DLM
  - High level of detail
  - Robust
  - Time efficient



Detailed Layer Model – DLM

Concept



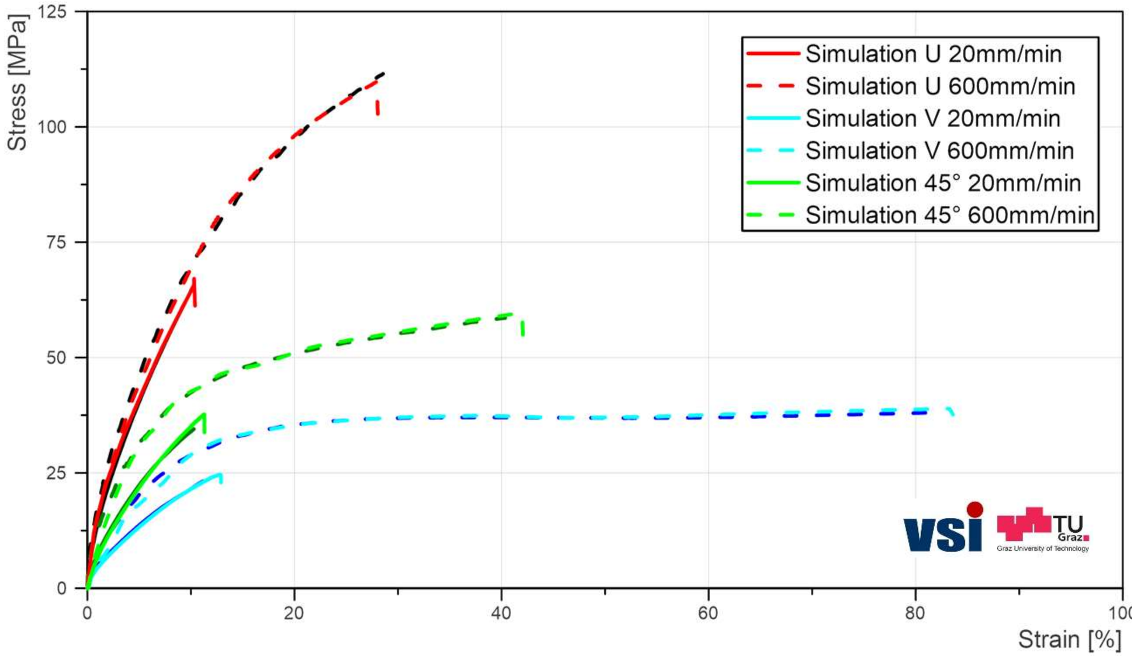
- **Key facts:**
  - Heterogeneous in-plane behaviour of components with shell elements
  - Homogenised out-of-plane behaviour with solid elements
  - No interlaminar penalty contacts
  - No subdivision into active material and current collector
  - Discrete element formulation for constant time step
  - Short circuit prediction due failure simulation of separator shells

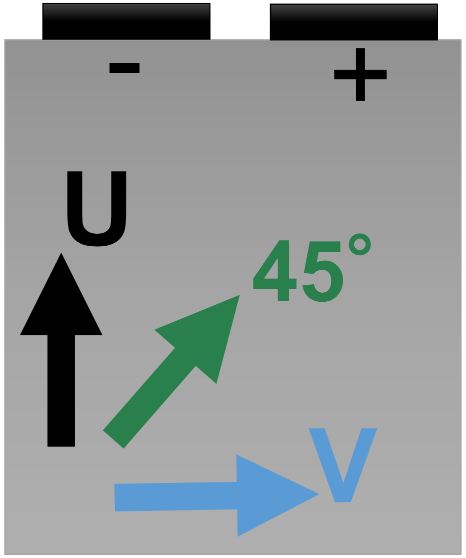
<u>Connection between Shell and Solid elements:</u>

**NODE_MERGE_SET*

Shell Elements – In-Plane Behaviour

- Tensile tests are basis of the in-plane behaviour of all components
- Two to three different sample orientations → Evaluation of anisotropy
- Two test velocities (20mm/min and 600mm/min) → Evaluation of strain rate influence
- **Only the separator samples showed a relevant influence of direction and strain rate**





Anode, Cathode and Pouch:

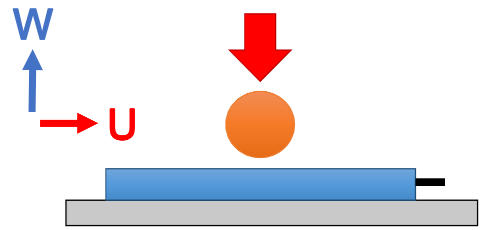
**MAT_PIECEWISE_LINEAR_PLASTICITY*
**MAT_ADD_EROSION*

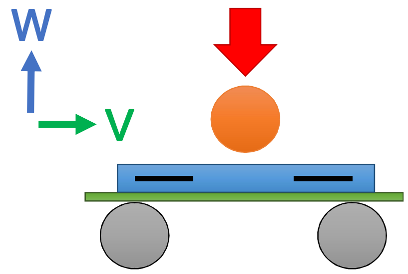
Separator:

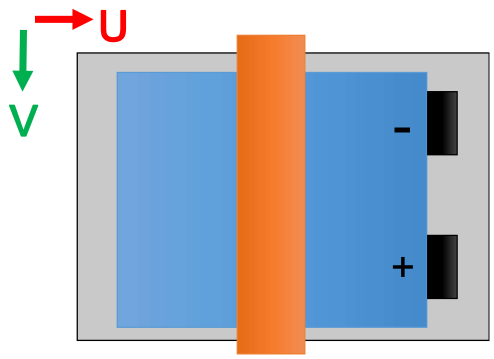
**MAT_EXTENDED_3-PARAMETER_BARLAT*
**MAT_ADD_GENERALIZED_DAMAGE*

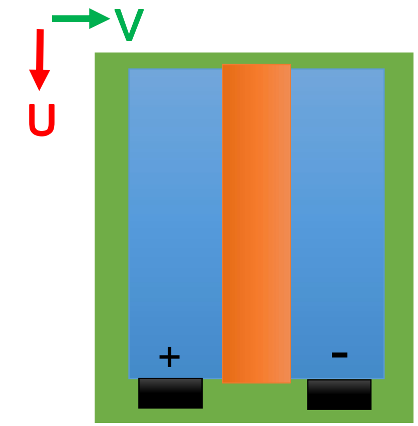
Solid Elements – Out-of-Plane Behaviour

- Transversal behaviour
- Shear behaviour (component and interlaminar)
- In-plane behaviour already due shell elements → Decoupled material
- Calibration due Cell tests
  - Indentation test for transversal behaviour
  - 3-Point Bending test for shear behaviour







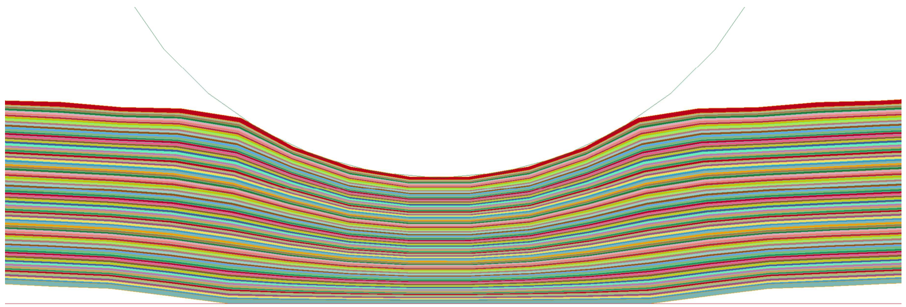


<u>Solid Elements:</u>

**MAT_MODIFIED_HONEYCOMB*
with
**SECTION_SOLID ELFORM 9*

<u>Representing the electrolyte:</u>

**AIRBAG_LINEAR_FLUID*



Due *SECTION_SOLID ELFORM 9 the time step size is constant: 1.33E-5ms

Results

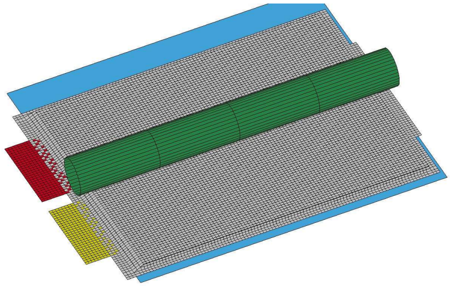
Cylindrical indentation test – long side

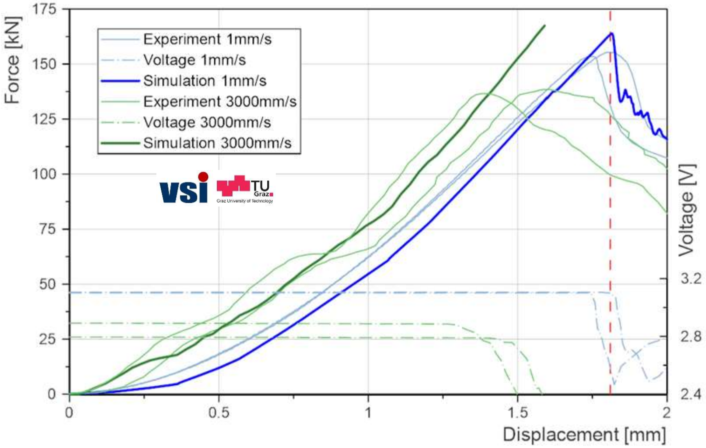
Impactor diameter: 30mm

Impactor orientation: long side

Velocities: 1mm/s (quasi-static)

3000mm/s (dynamic)





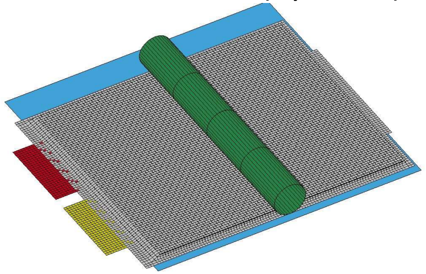
Cylindrical indentation test – short side

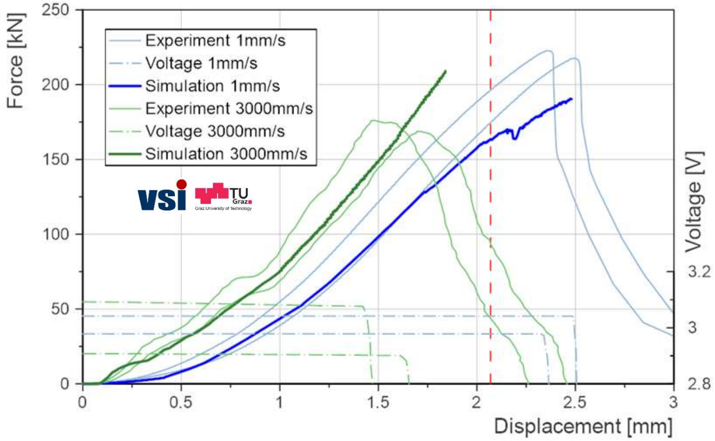
Impactor diameter: 30mm

Impactor orientation: short side

Velocities: 1mm/s (quasi-static)

3000mm/s (dynamic)





Short Circuit Criterion

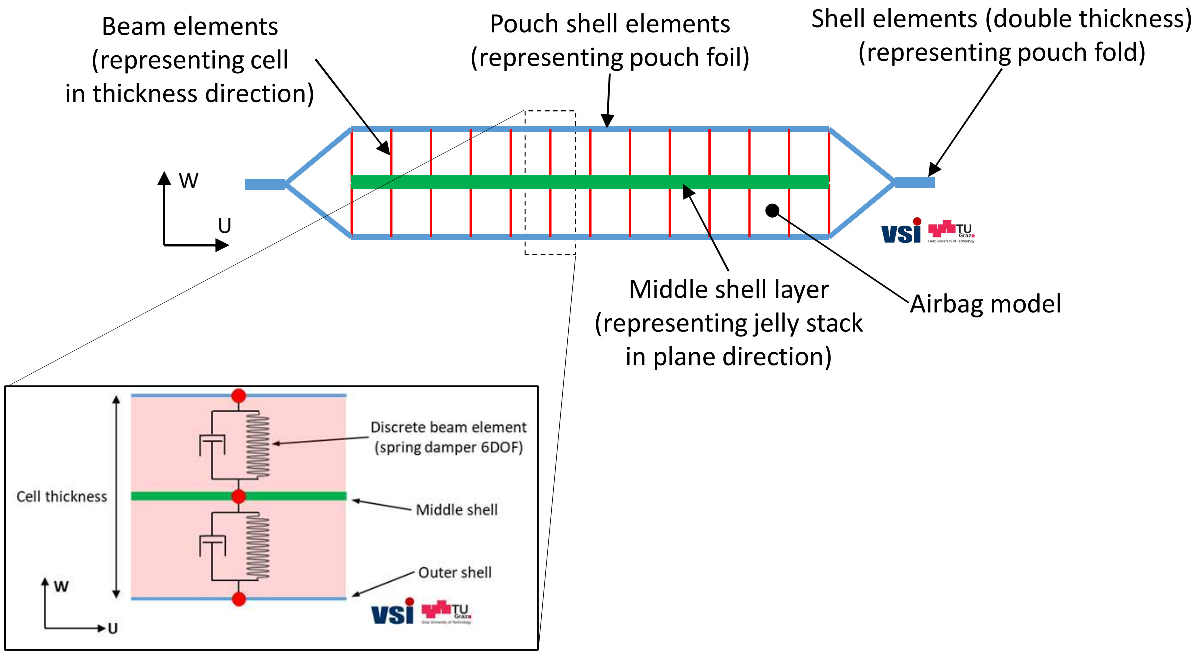
- Physic-based criterion
- Simulation of the failure of the separator shells (**MAT_ADD_GENERALIZED_DAMAGE*)
- The erosion of the first separator elements determines the simulated short circuit

SafeLIB

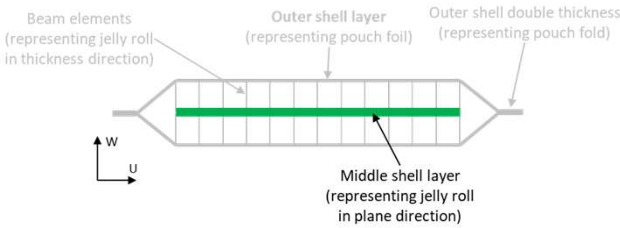
Simplified Applicable Model – SAM

Design of SAM Approach

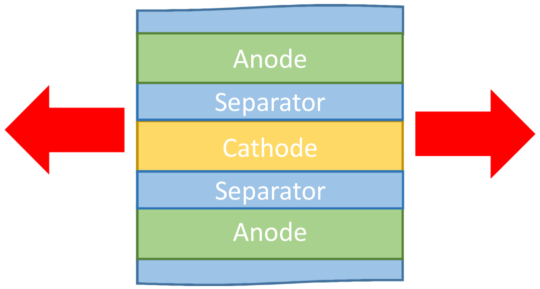
- **Combination of simple and fast 1D and 2D Elements:**
- One main shell layer in the middle (stiffness of jelly stack in U and V direction)
- Beam elements in thickness direction (stiffness of jelly stack in W direction)
- Outer shell elements represent pouch foil
- Additional solid elements for dynamic behaviour

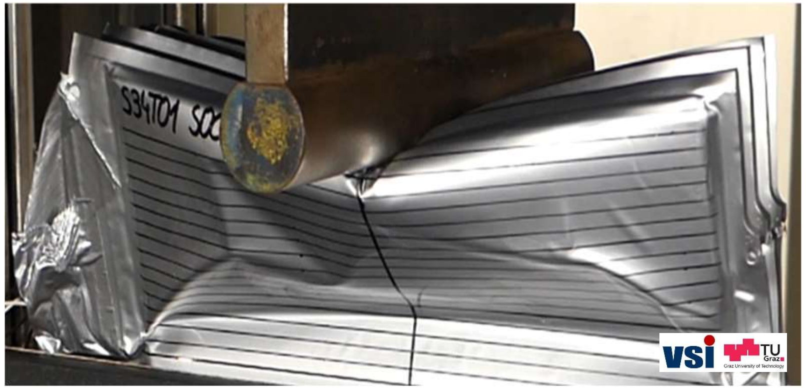


Jelly Stack – Middle Layer



- Middle Shell Layer represents the whole jelly stack
  - Anodes
  - Cathodes
  - Separators
- Tension behaviour due jelly tensile test (fictive)
- Compression behaviour due lateral indentation test
- Behaviour of the separator has minor influence
- **Jelly stack can be assumed to be isotropic**

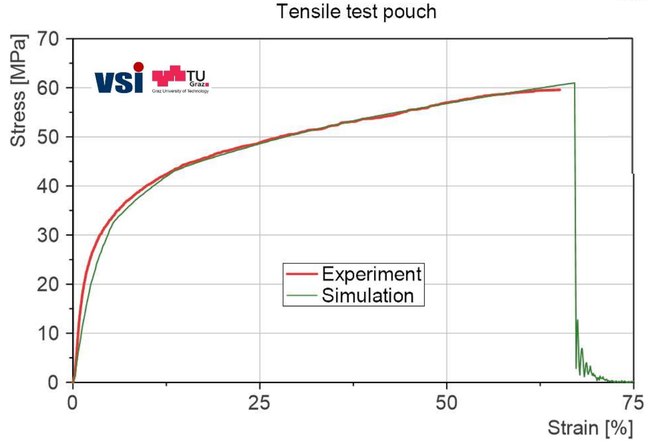


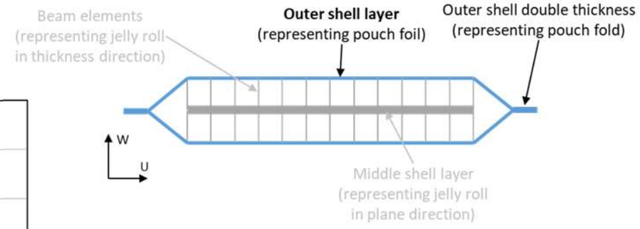


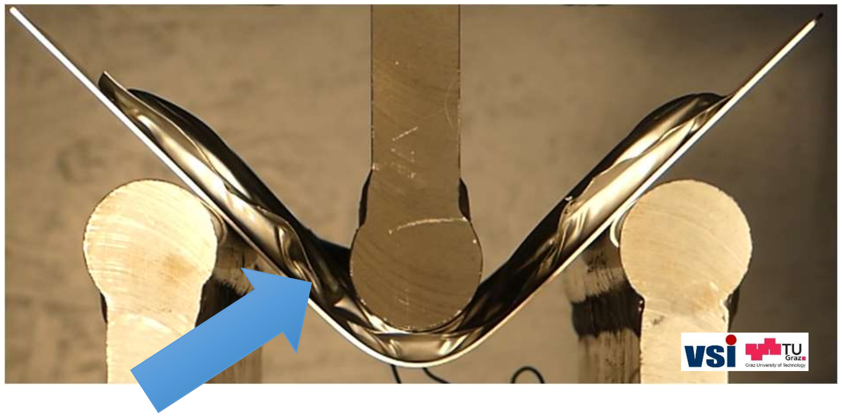
Material:
**MAT_PLASTICITY_COMPRESSION_TENSION*

Pouch Foil

- Major influence on the bending behaviour
- Characterisation due tensile test of pouch samples
- Isotropic behaviour
- Adaption of compression behaviour for buckling (bending)
- Representation of electrolyte due airbag model
  - mass properties
  - Incompressibility of fluid (bulk-modulus)







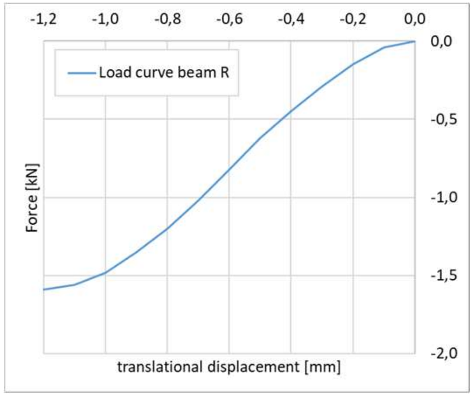
Material:
MAT_PLASTICITY_COMPRESSION_TENSION

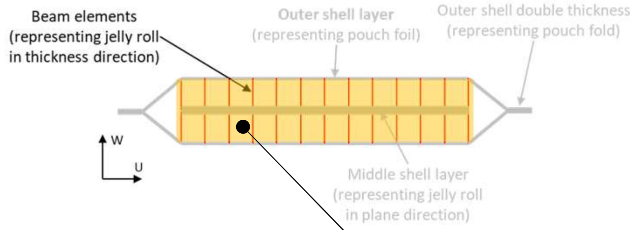
Electrolyte:
AIRBAG_LINEAR_FLUID

Beam Elements and Additional Solid Elements

- Representing the transversal behaviour
- Beam elements for quasi-static
  - Constant Load curve for in-plane (S/T in beam coordinates) and rotation
  - Non-linear load curve for thickness direction (R in beam coordinates)
- Additional solid elements for dynamic
- Calibration due cylindrical indentation test

Compressive beam load curve in R:





Overlapping solids with MAT_MODIFIED_HONEYCOMB

<u>Quasi-static behaviour:</u>

**GENERAL_NONLINEAR_6DOF_DISCRETE_BEAM*

<u>Dynamic behaviour:</u>

**MAT_MODIFIED_HONEYCOMB*

Results

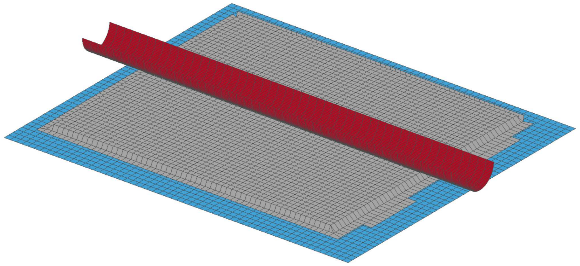
Cylindrical indentation test – long side

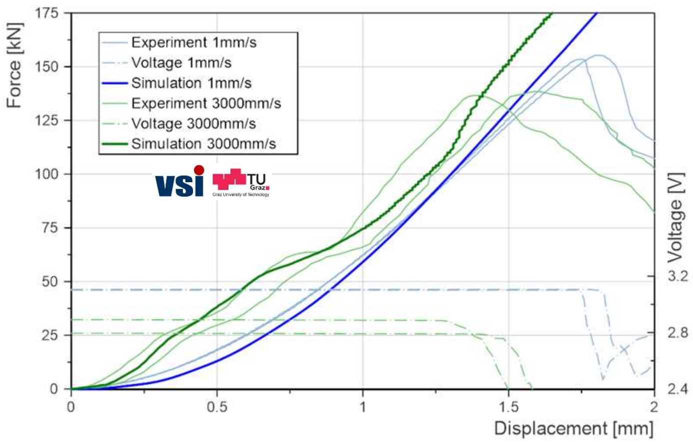
Impactor diameter: 30mm

Impactor orientation: long side

Velocities: 1mm/s (quasi-static)

3000mm/s (dynamic)



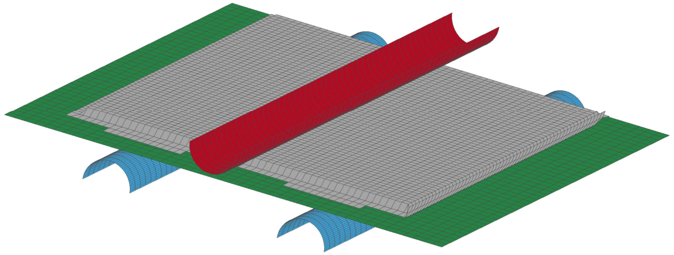


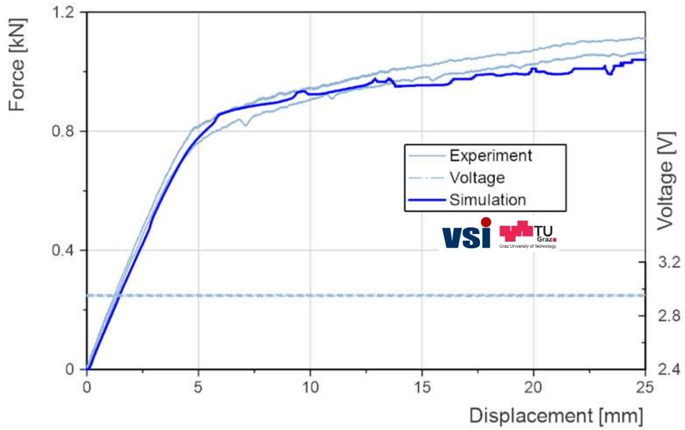
3-Point bending test

Impactor diameter: 30mm

Impactor orientation: long side

Velocities: 1mm/s (quasi-static)





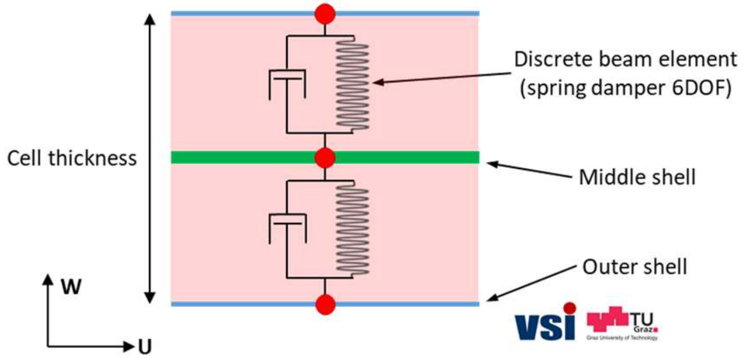
Short Circuit Criterion

- Calibrated criterion
- Evaluation of Beam-Forces
- $C_{SC} = a \cdot U + b \cdot V + c \cdot W \geq 1$
- U, V and W are the Forces
- a, b and c are the calibrated Parameters

Highlights

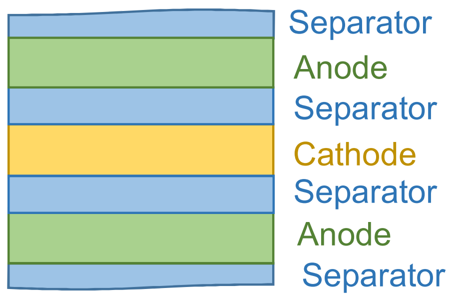
Simplified Applicable Model – SAM

- Macroscopic cell model
- Consisting mainly fast 1D and 2D elements (beam and shells)
- For full vehicle crash simulations
- Number of nodes: 15 007
- Number of elements: 17 800
- Initial time step: 7.63E-4 ms
- Simulation time (HPC cluster 20 cores):
  - Quasi-static loading → 2 h
  - Dynamic loading → 42 sec.



Detailed Layer Model – DLM

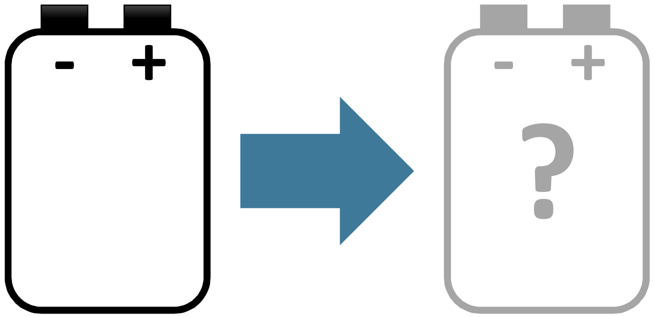
- Layer-by-layer cell model
- No penalty contacts
- Detailed model for cell simulations and profound analysis of mechanical behavior
- Number of nodes: 2 191 089
- Number of elements: 1 325 192
- Initial time step: 1.33E-5 ms
- Simulation time (HPC cluster 64 cores):
  - Quasi-static loading → 48 h
  - Dynamic loading → 10 h



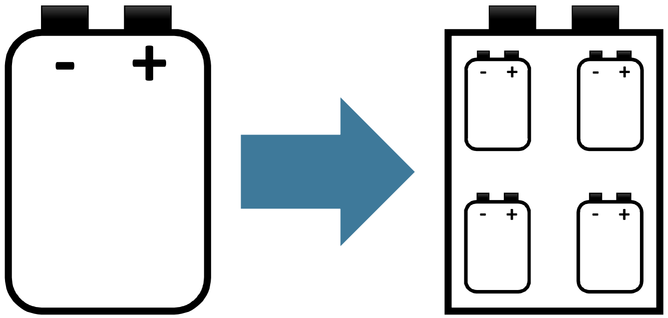
Vision of SafeLIB

Vision of SafeLIB – Transferability

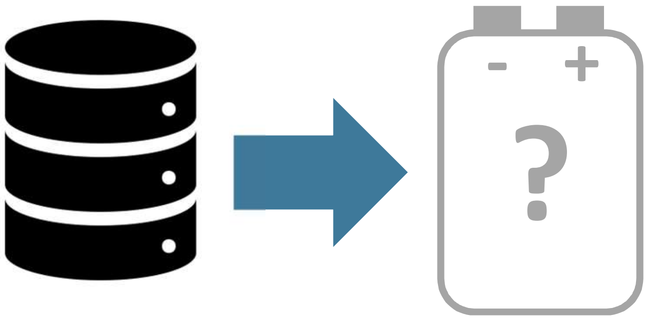
Cell 2 Cell



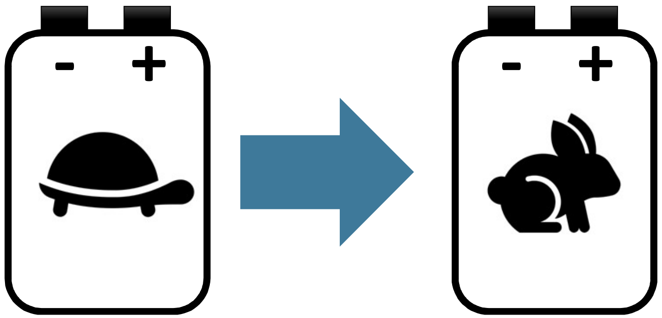
Cell 2 Module



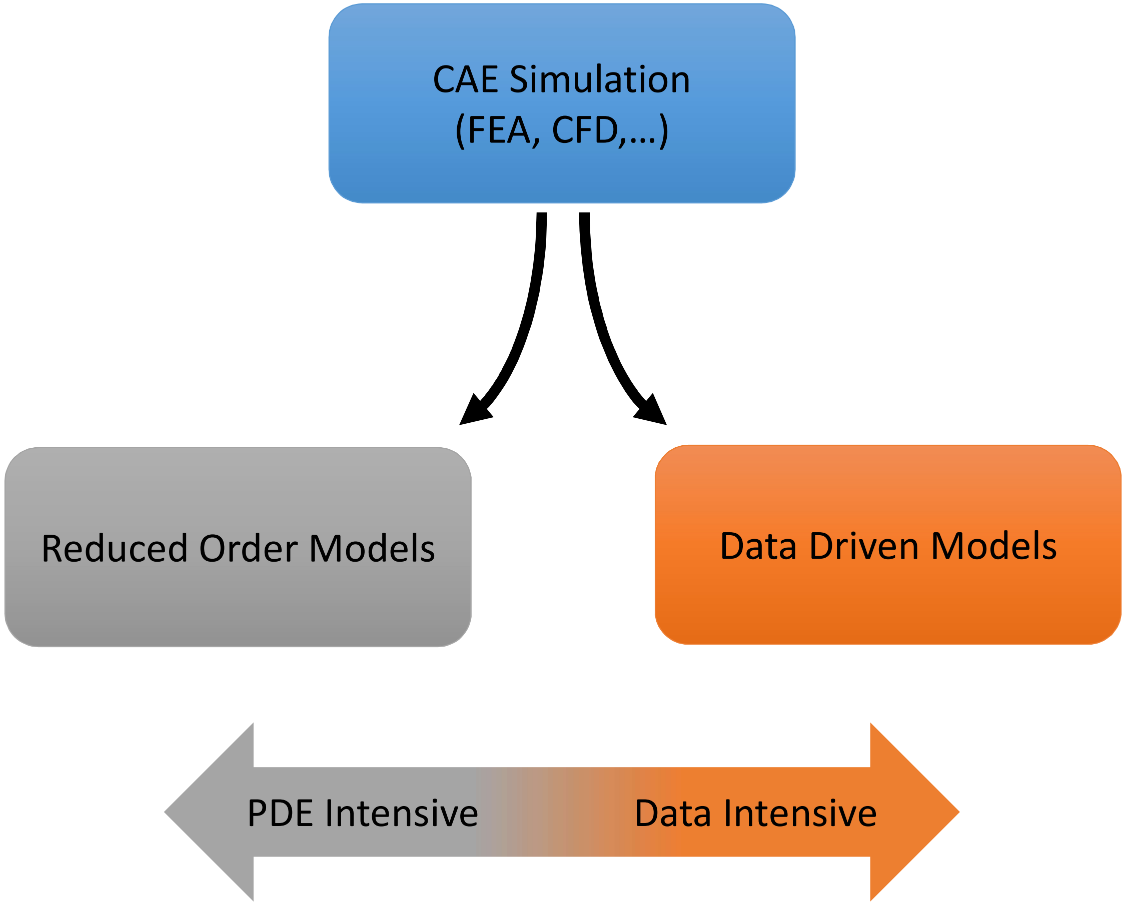
Data 2 Cell



Cell 2 reduced Cell



Upcoming Methods as Great Hope….



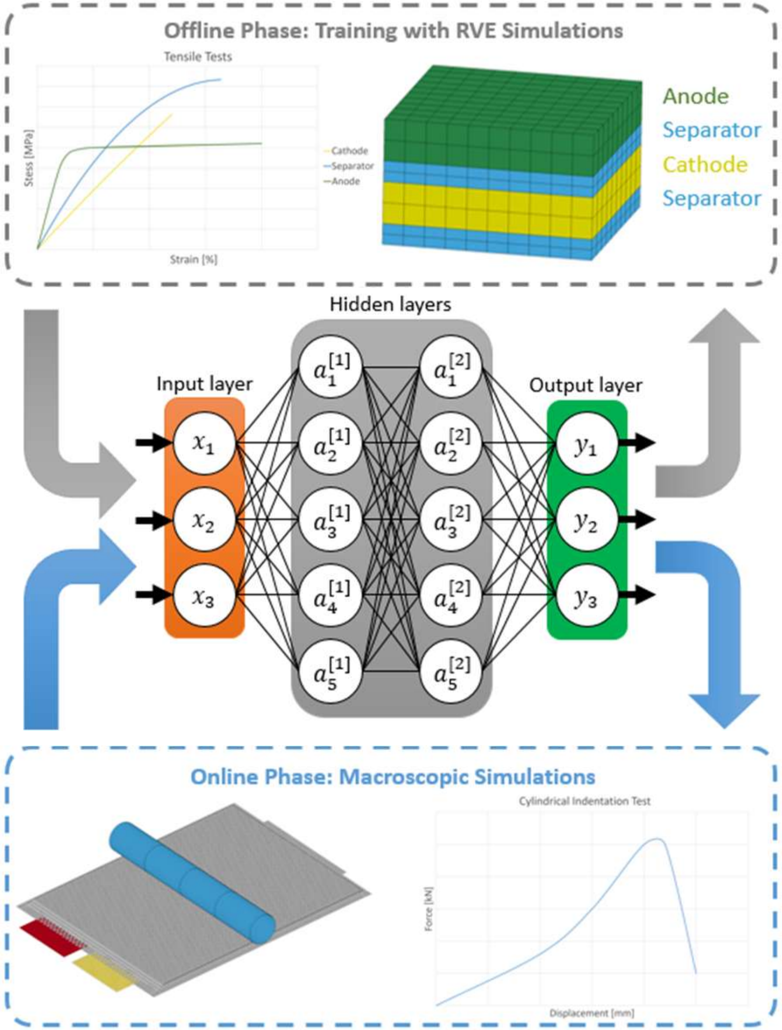
- Upcoming methods, such as **Model Order Reduction** or **Data Driven Modelling**
- The combination of both would also be promising
- **Aim: Generation of a detailed and yet time-efficient model of a Li-Ion cell**

Data Driven Modelling – Artificial Neural Network

1. **Offline Phase:**
   - Modeling of the microstructure
   - Testing against a huge among of load cases
   - Collecting the essential data of interest

2. **Training Phase:**
   - Data preparation
   - Definition of architecture
   - Training of neural network

3. **Online Phase:**
   - Using the trained ANN to bring the behavior from RVE-level to cell-level
   - Including all the essential data of interest



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JKU
LIT Law Lab

Funding

SafeLIB

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