Li-Ion's roar: Unleashing the potential of battery simulation

GAMMA TECHNOLOGIES

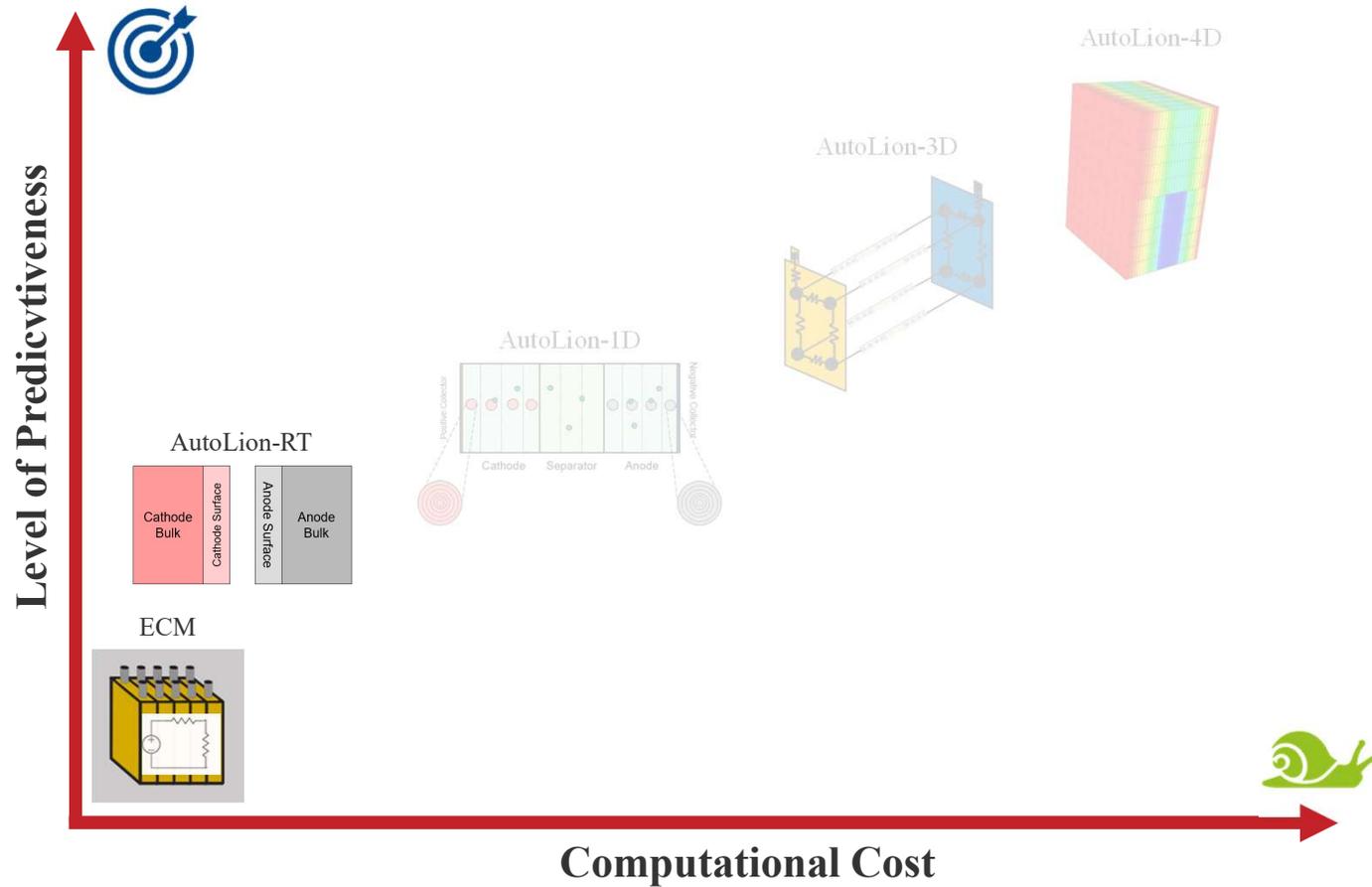Source: https://www.ast-reisen.de/tiere-afrikas/loewe/

GT

Development Cycle – various requirements

Vehicle Architecture Studies

Full Vehicle Validation & Control

DEVELOPMENT

VERIFICATION

Battery Architecture Studies

NMC

t

r

LMO

Battery Integration & Control (XiL)

Min Voltage

Feed-forward Calculation

Plant

V_{min} → $F(s)$ → P_{min} → ⊗ → $P_{corrected}$ → $G(s)$ → V_{actual}

$H(s)$

PI Controller

Detailed Battery Design & Analysis

GT

Flavors of Battery Modeling

Level of Predicvtiveness (vertical axis)

Computational Cost (horizontal axis)

AutoLion-4D

AutoLion-3D

AutoLion-1D

Positive Collector — Cathode — Separator — Anode — Negative Collector

AutoLion-RT

Cathode Bulk | Cathode Surface | Anode Surface | Anode Bulk

ECM

GT

Flavors of Battery Modeling

Level of Predicvtiveness (vertical axis)

Computational Cost (horizontal axis)

AutoLion-4D

AutoLion-3D

AutoLion-1D

AutoLion-RT

| Cathode Bulk | Cathode Surface | Anode Surface | Anode Bulk |

ECM

Bulk-Surface model
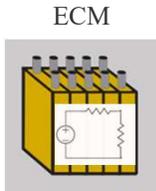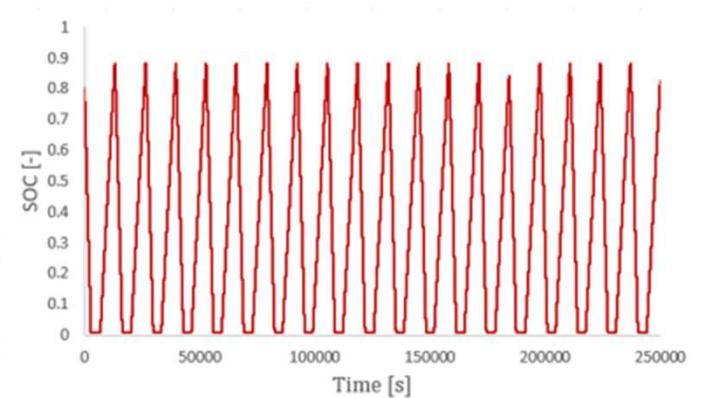

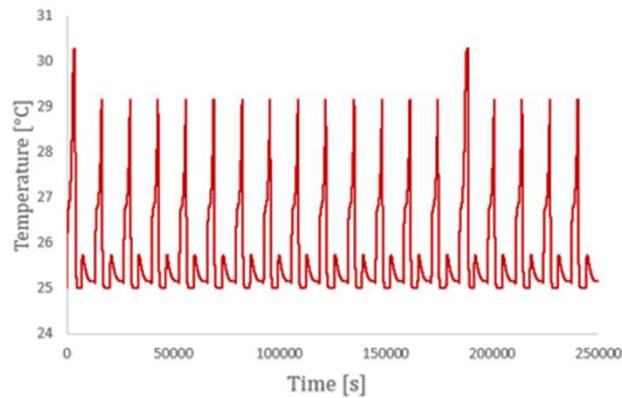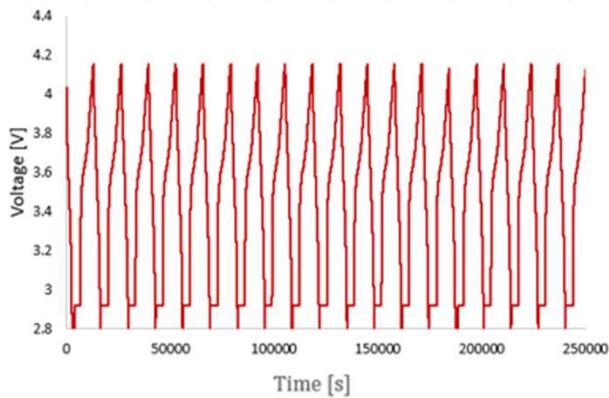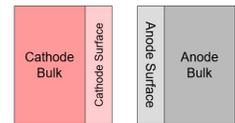- P2D model, a set of coupled partial differential equations (PDEs)
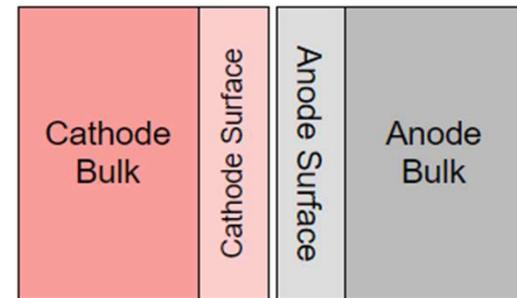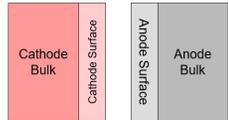
- Converting PDEs into ODE set
- Considering instantaneous diffusion between electrodes

Hardware-in-the-Loop Simulations

ECM

AutoLion-RT

GT s-function → MathWorks → GT HiL Libraries → speedgoat
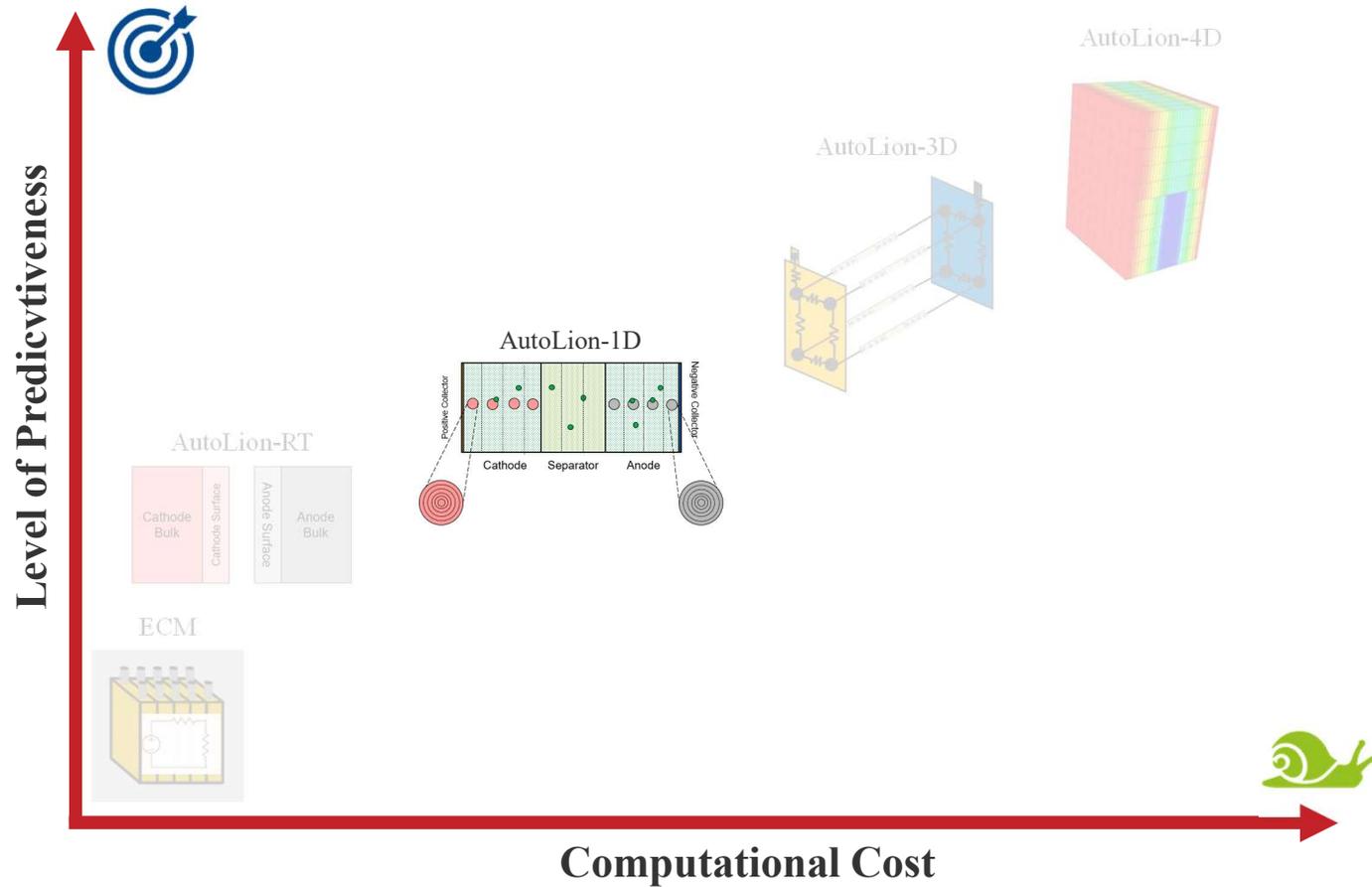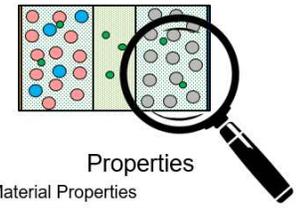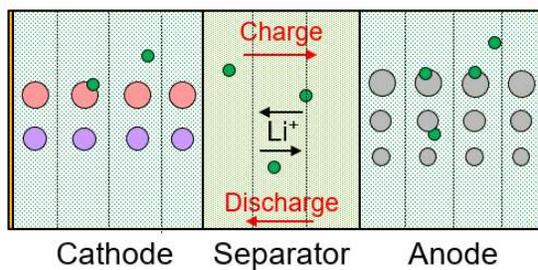real-time simulation and testing

Value Add:
Improved support for controls teams, who rely heavily on electrical-equivalent solutions today

GT

Flavors of Battery Modeling

Chart axes: Level of Predicvtiveness (vertical) vs. Computational Cost (horizontal)

Models labeled: ECM, AutoLion-RT, AutoLion-1D, AutoLion-3D, AutoLion-4D

AutoLion-1D labels: Positive Collector, Cathode, Separator, Anode, Negative Collector

AutoLion-RT labels: Cathode Bulk, Cathode Surface, Anode Surface, Anode Bulk
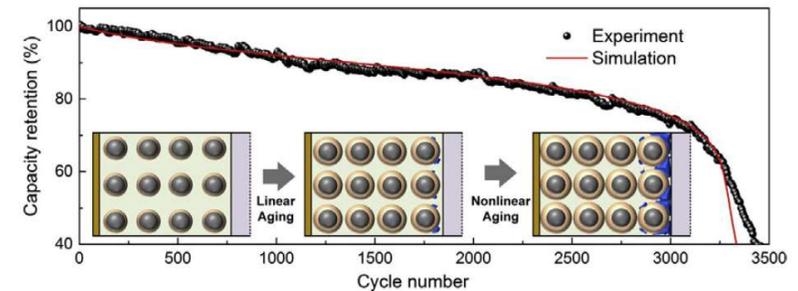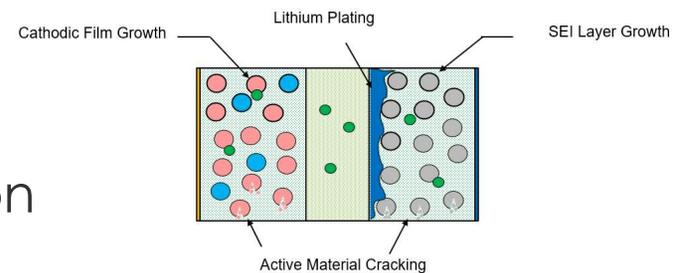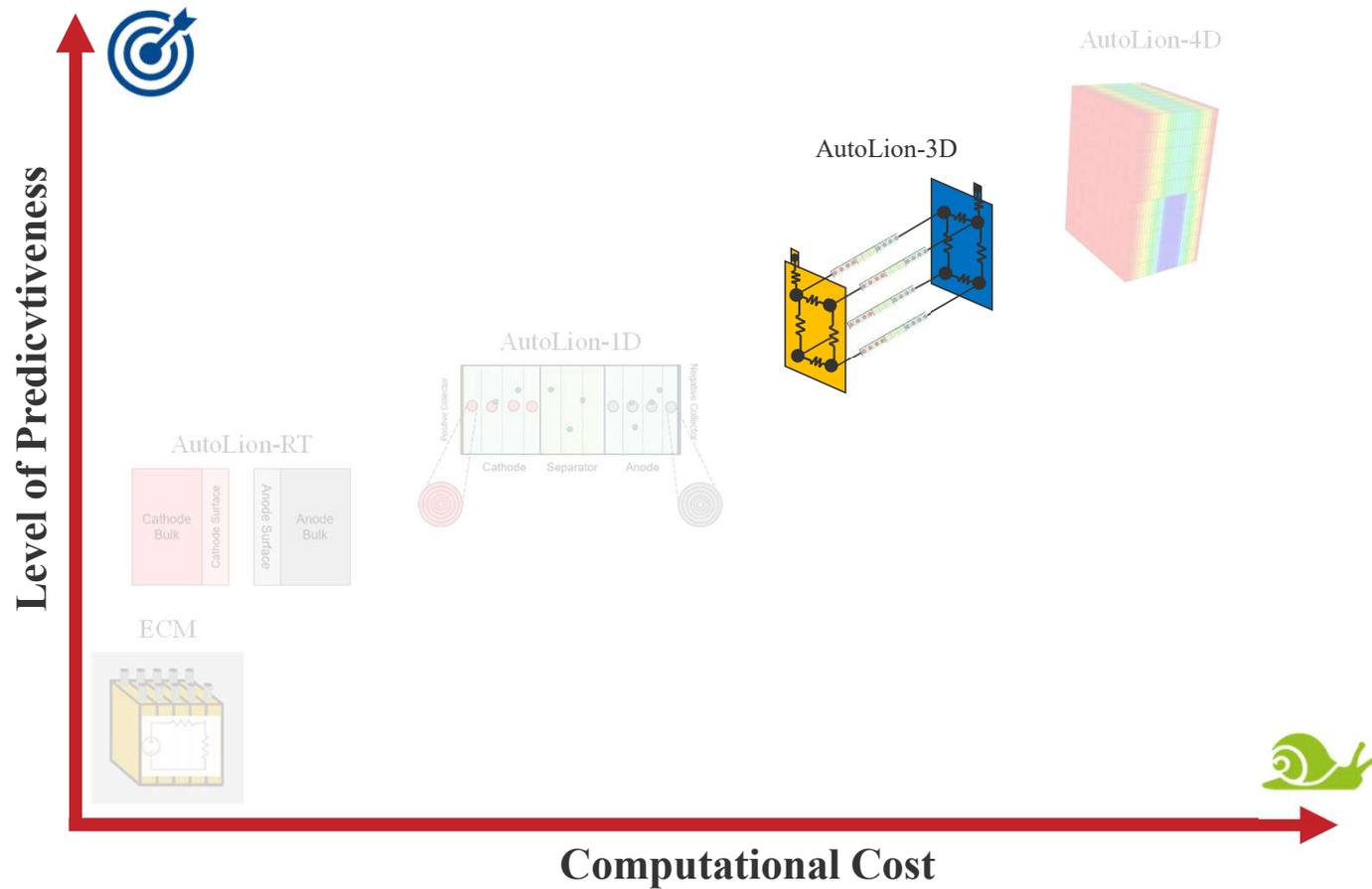
GT

Beyond P2D

- Material Properties Database

- Physics based models of degradation

- Integrated Multi-Domain Systems

- Thermal included - one thermal node

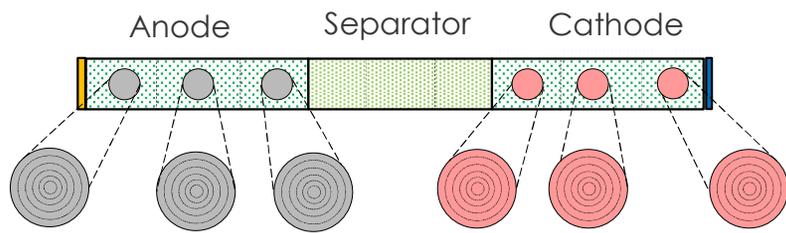- Blend electrodes & particle size distribution

Flavors of Battery Modeling

Level of Predicvtiveness (vertical axis)

Computational Cost (horizontal axis)

AutoLion-4D

AutoLion-3D

AutoLion-1D

Positive Collector · Cathode · Separator · Anode · Negative Collector

AutoLion-RT

Cathode Bulk · Cathode Surface · Anode Surface · Anode Bulk

ECM

GT

Introduction to GT-AutoLion-3D

GT AutoLion
Lithium-ion Battery Simulation

GT AutoLion3D
Lithium-ion Battery Simulation

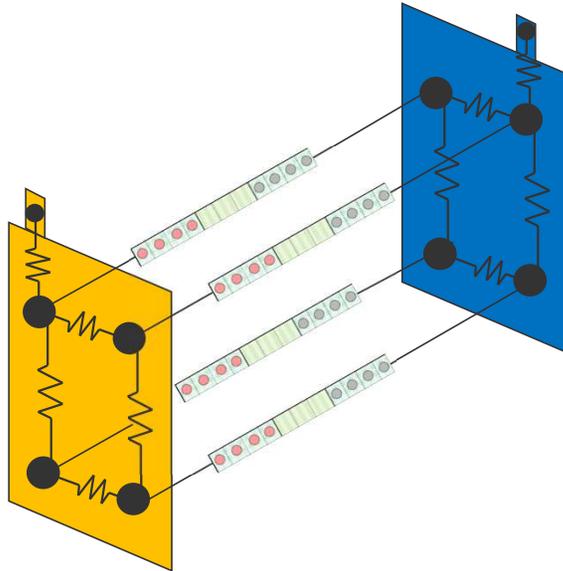Anode   Separator   Cathode

P2D electrochemical-thermal model

P3D electrochemical-thermal model

GT
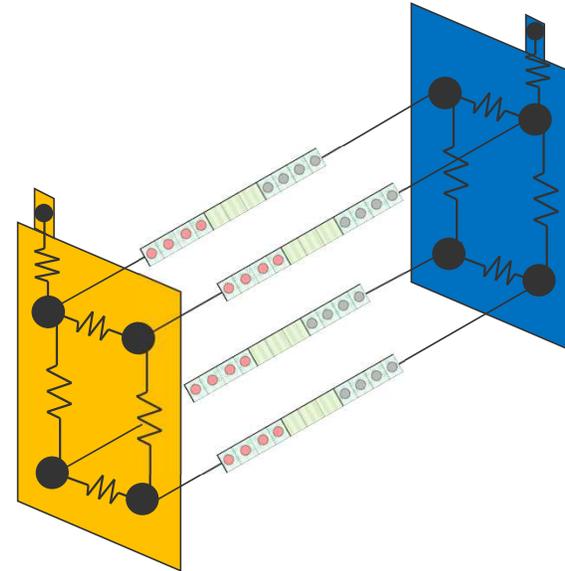
Introduction to GT-AutoLion-3D

P3D electrochemical-thermal model

**Electrical Solution:** Resistor network for current collectors

Electrochemical Solution: AutoLion-1Ds in parallel

- Same underlying solution (including aging models)

Thermal Solution: GT-SUITE's 3D finite element solution

- Anisotropic properties
- Ability to connect to other parts (i.e., case)
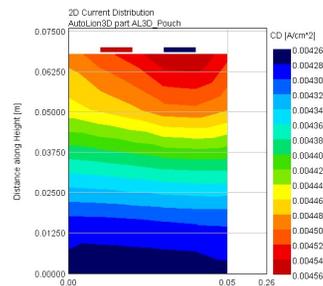- Ability to connect to flow domain
- GEM-3D support

Introduction to GT-AutoLion-3D

GT-AutoLion3D
Lithium-ion Battery Simulation
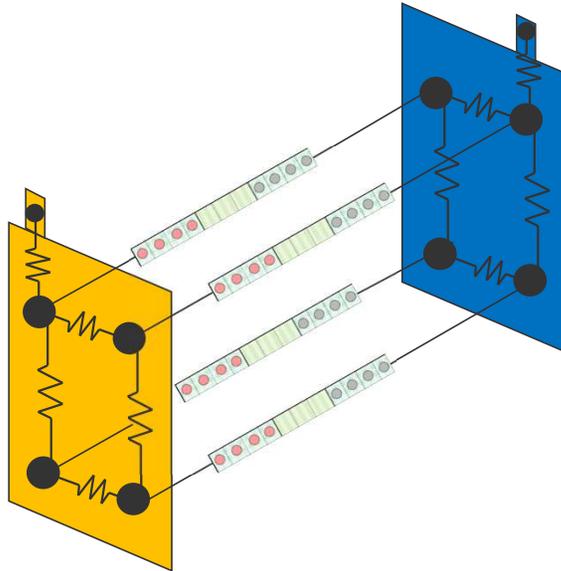
P3D electrochemical-thermal model

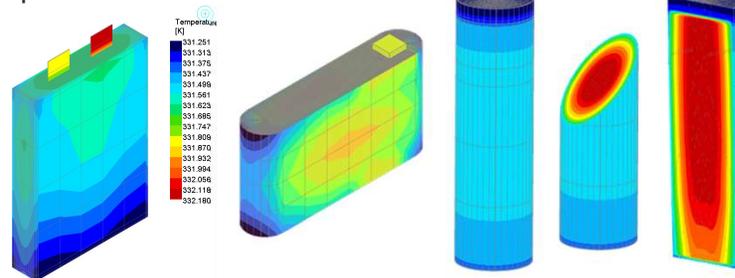## 2D/quasi-3D Electrochemical results:

- Current
- Voltage
- Heat Generation
- Aging
- State of Charge
- Stoichiometry

Current Distribution
(unrolled JR, cylindrical and prismatic)
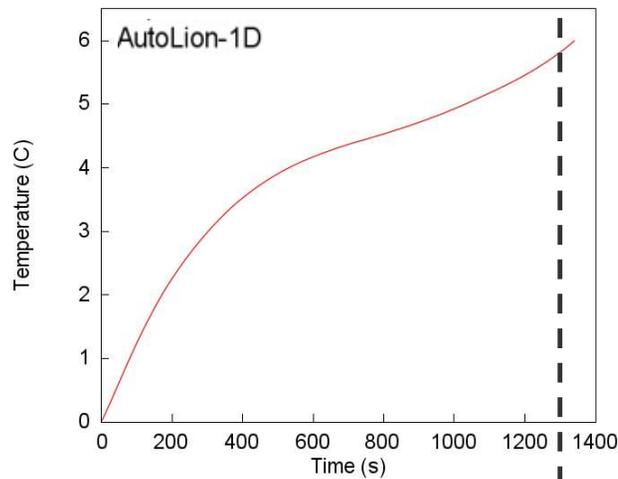
3D Thermal results:

- Temperature

GT-AutoLion-3D Use Cases

- **Detailed Cell Modeling**
  - Tab modeling, form factors

- **Inhomogeneities ask for discretization**
  - Extreme Operating Conditions (Load and Temperature)
  - Lithium Plating and Fast Charging Capability Analysis
  - Cell Cooling Design and Optimization

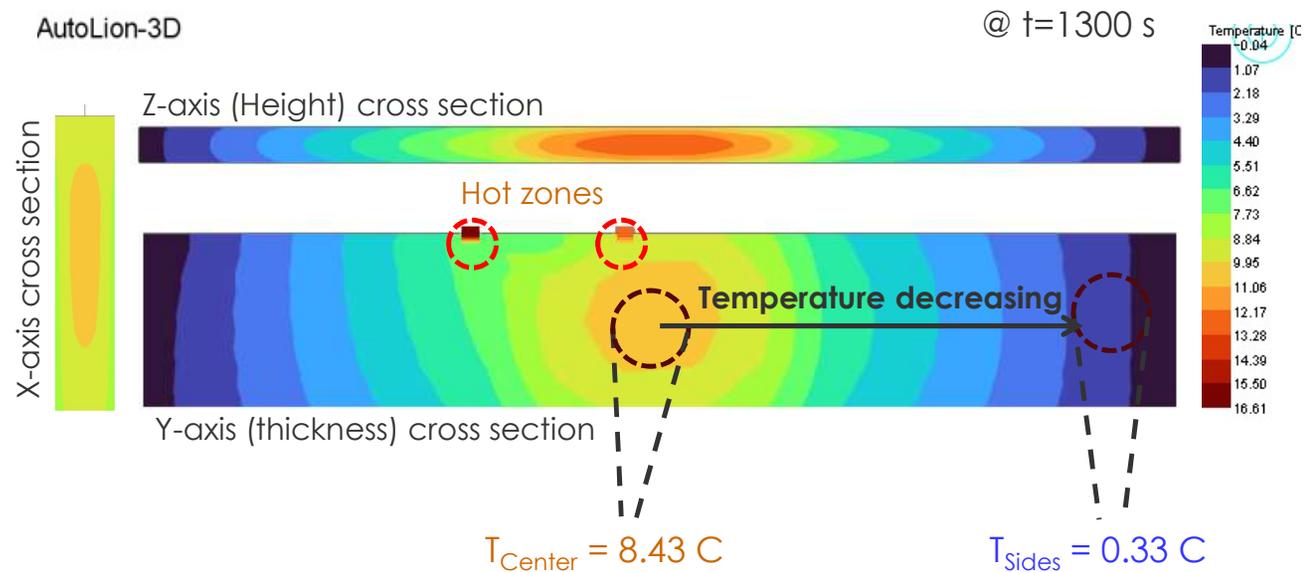- **Safety Events Analysis (Internal Short, Nail Penetration)**

- **Cell Swelling**

2D Lithium Plating Potential, Charging at 1C,

0.1 sec

GT
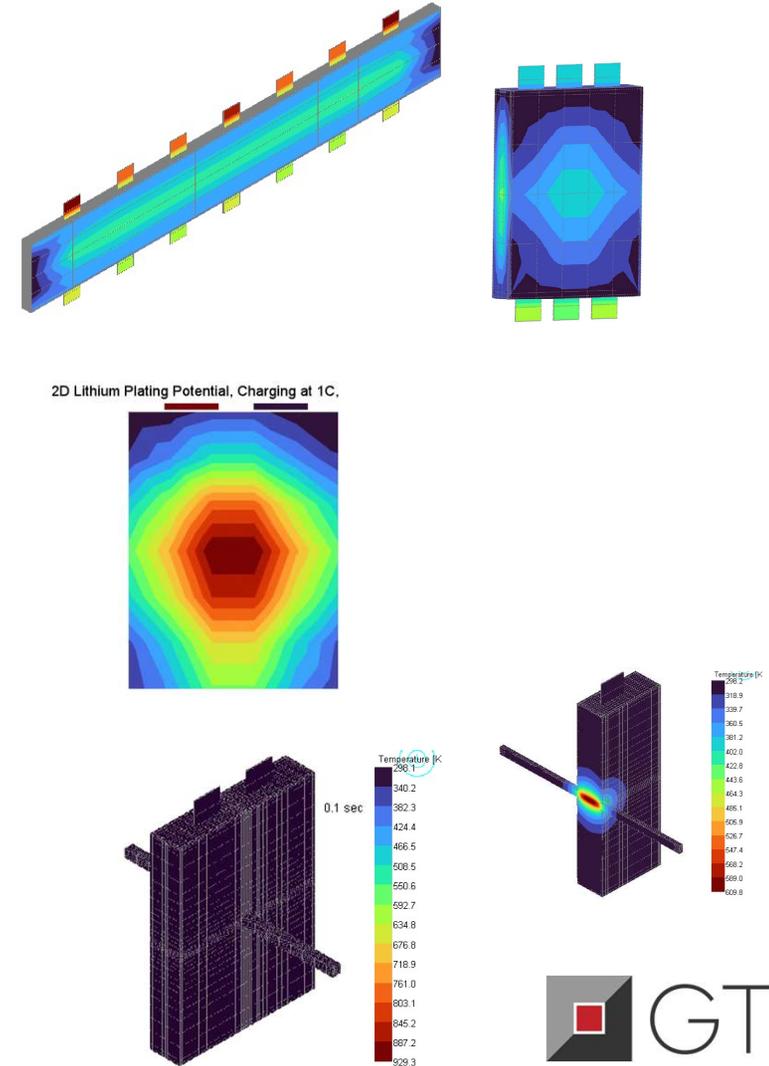
Model Results: Thermal Behavior

Constant current discharge process at the temperature of 0 ˚C – 1C rate

AutoLion-1D

T = 5.81 C @ t=1300 s

Single value across the cell!

AutoLion-3D

@ t=1300 s

Z-axis (Height) cross section

X-axis cross section

Hot zones

Temperature decreasing

Y-axis (thickness) cross section
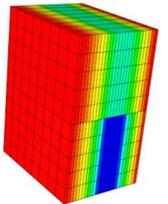
T_{Center} = 8.43 C

T_{Sides} = 0.33 C

Temperature distribution across the cell!

Flavors of Battery Modeling

Level of Predicvtiveness (vertical axis)

Computational Cost (horizontal axis)
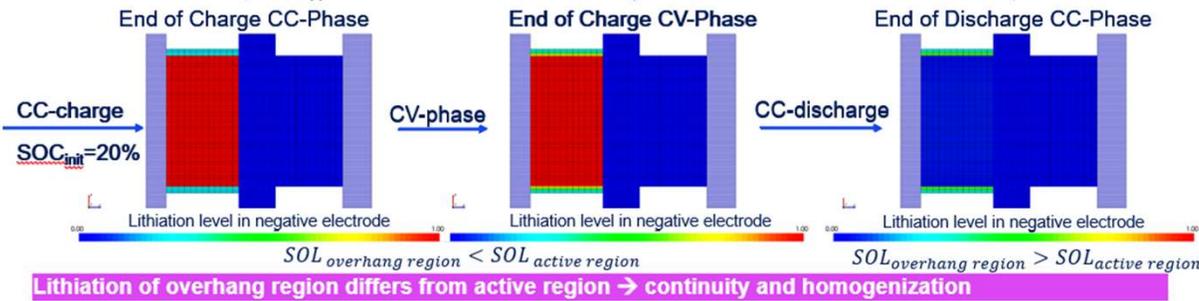
ECM

AutoLion-RT

AutoLion-1D

AutoLion-3D
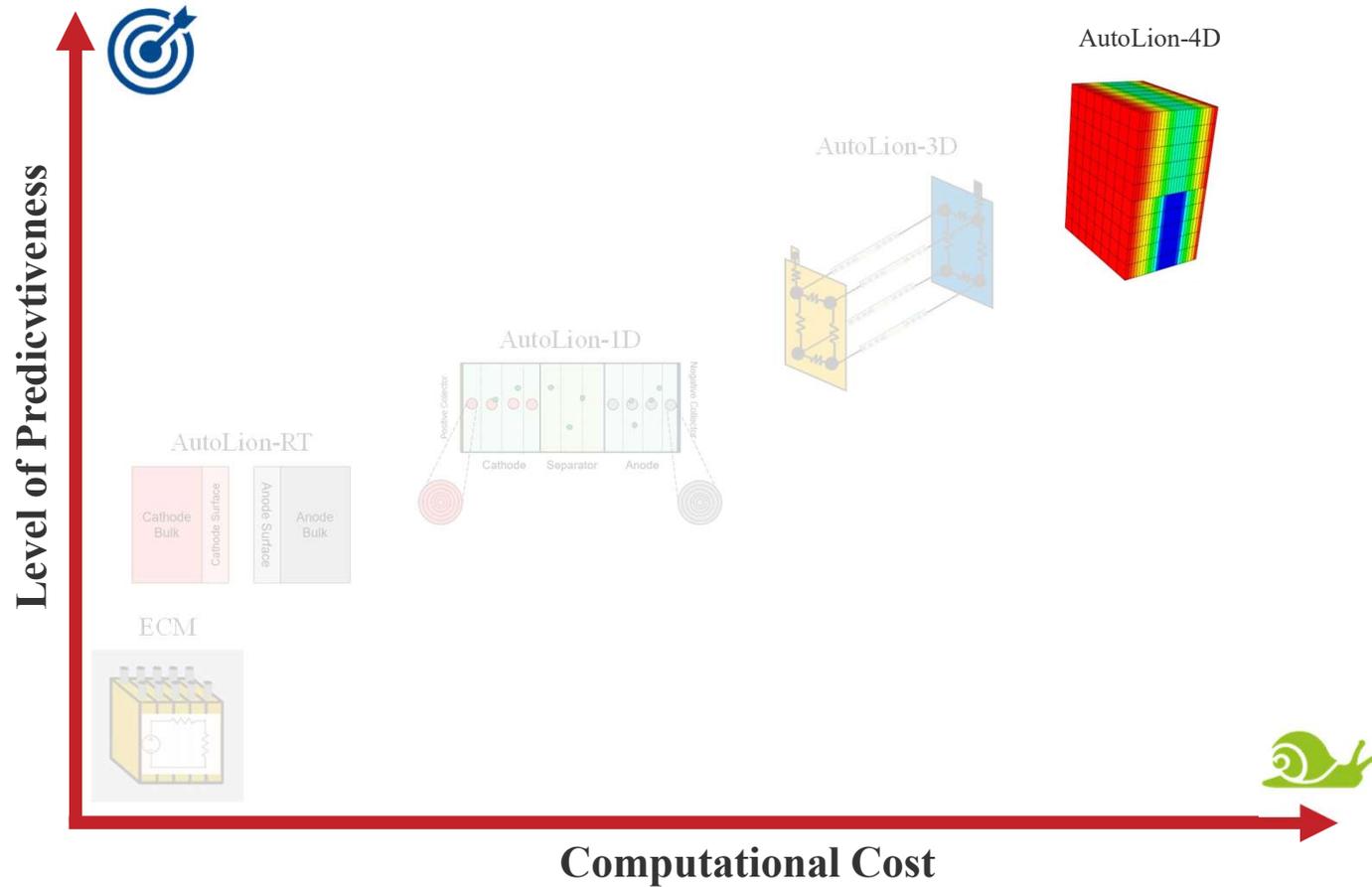
AutoLion-4D

Anode Overhang

AutoLion-4D

Simulation Results

GT

Δ=0.005 Ah (2.2%)

End of Charge CC-Phase

End of Charge CV-Phase

End of Discharge CC-Phase

CC-charge
SOC_{init}=20%

CV-phase

CC-discharge

Lithiation level in negative electrode

Lithiation level in negative electrode

Lithiation level in negative electrode

$SOL_{overhang\ region} < SOL_{active\ region}$

$SOL_{overhang\ region} > SOL_{active\ region}$

Lithiation of overhang region differs from active region → continuity and homogenization

for illustration: scaling factor 1000 applied for axial dimension

IAV

True 3D Diffusion "Edge Effects" with AL-4D

Anode

Separator

Cathode

Li⁺ Diffusion

GT

User-Defined Reactions

Flavors of Battery Modeling

Different Flavours of Battery Modeling

ECM

Vehicle Architecture Studies

Full Vehicle Validation & Control

ECM

AutoLion-RT

DEVELOPMENT

VERIFICATION

Battery Architecture Studies

AutoLion-1D

Positive Collector   Cathode   Separator   Anode   Negative Collector

Battery Integration & Control (XiL)

AutoLion-RT

Cathode Bulk | Cathode Surface | Anode Surface | Anode Bulk

ECM

Detailed Battery Design & Analysis

AutoLion-3D

AutoLion-4D

Cathode Bulk | Cathode Surface | Anode Surface | Anode Bulk

GT

Integrated Multi-Domain Modelling

GAMMA TECHNOLOGIES

AutoLion-1D Real-world Aging
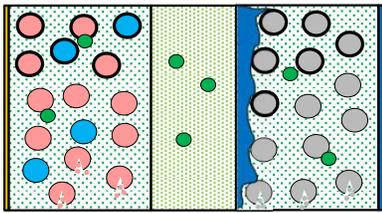
Physics-based aging models

+

Full System Model

More meaningful aging predictions (Miles, Years of operation)

+
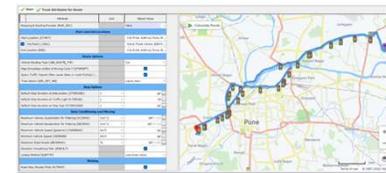
Commuting / Usage Patterns
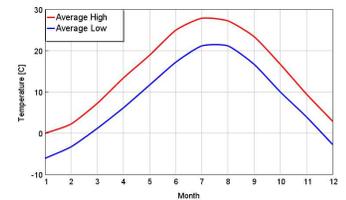
**Weather Patterns**

Charging Patterns

Vehicle/Powertrain Model

- Electrical Load on cell calculated based on vehicle „operating point"

- Low Voltage circuit with consumers

- Electrical domain allowing for modeling of

  - BMS, cell balancing over module

  - Circuit Protection

Full System Model

GT
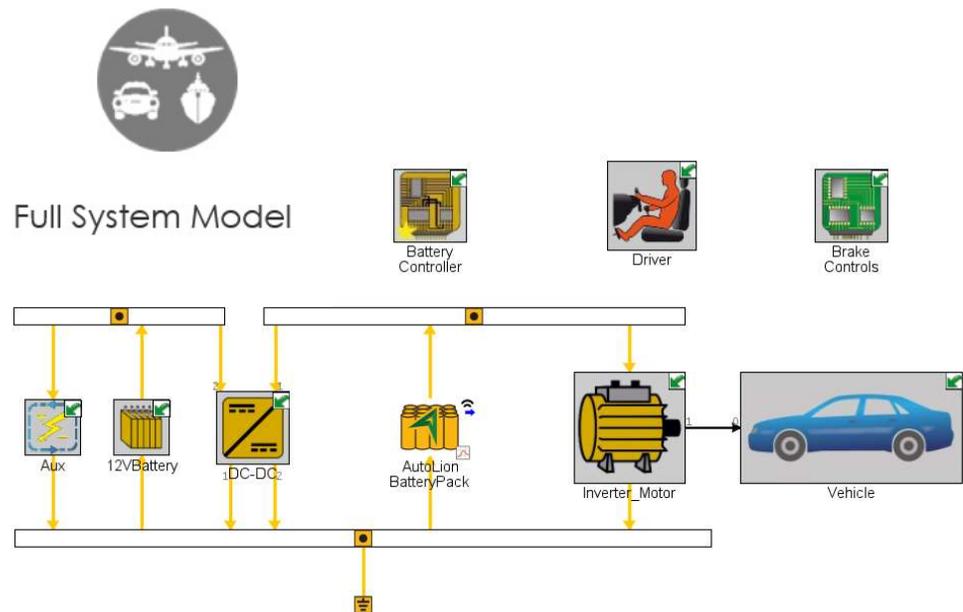
Model Setup for a Single Cell

- A compound was created with the following architecture

- GT-AutoLion cell & 3D thermal finite element cell exchange heat rate and temperature through control objects

- Gases ejected from TR pass through a pressure release valve through the ambient where combustion occurs

- Heat generated from the combustion of gases is also fed back to the battery pack

Compound Template
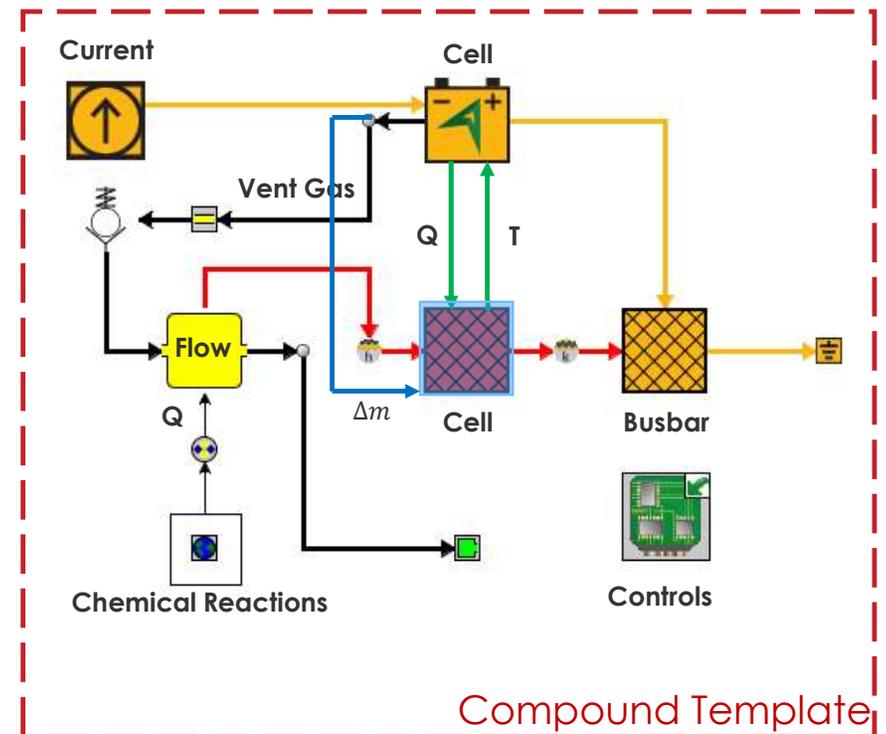
Mechanical Connectivity

In addition to cell performance (Voltage, Heat Generation), GT-AutoLion can predict stress & strain on a cell

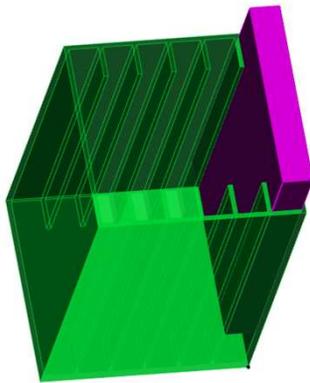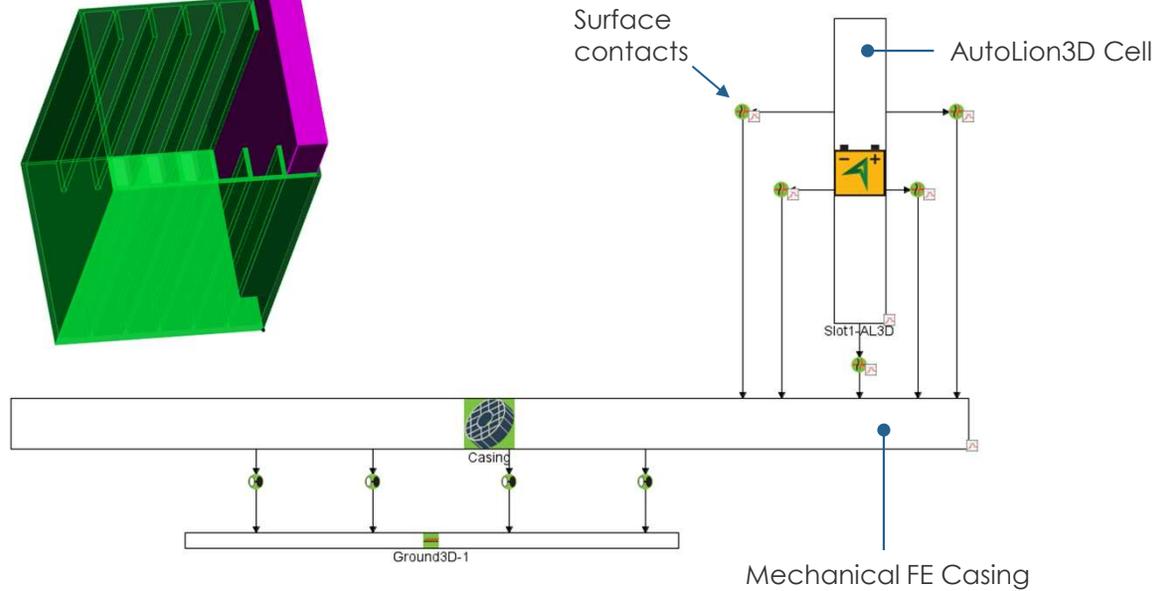Interaction with Aging

Swelling

ΔPorosity

Stress

Cathode   Separator   Anode
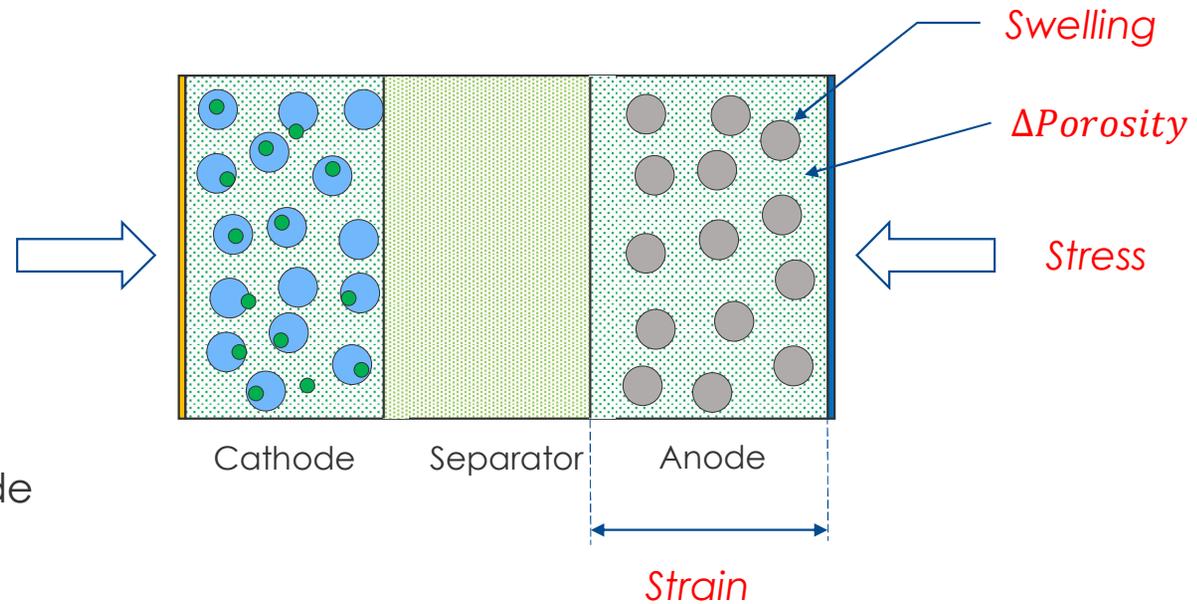
Strain

🔵 Active material in cathode

⚫ Active material in anode

🟢 Lithium-ion (Li$^+$)

GT

Mechanical Connectivity

Example Cell in Module Casing Slot
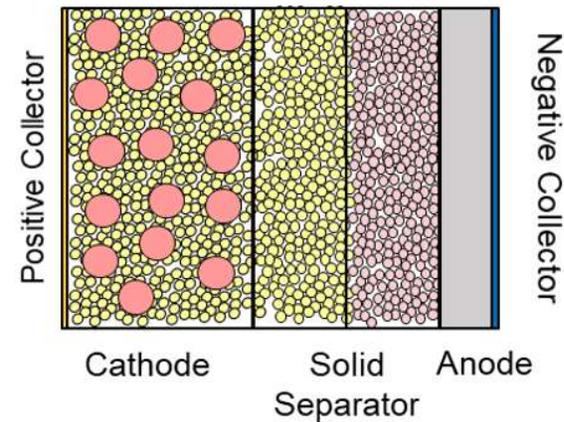
Electrochemical-Mechanical Model

Cell Swelling during charge

Surface contacts

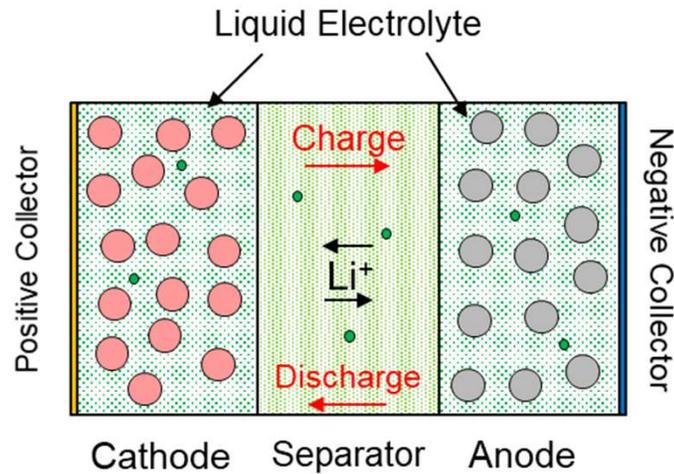AutoLion3D Cell

Slot1-AL3D

Casing

Ground3D-1

Mechanical FE Casing
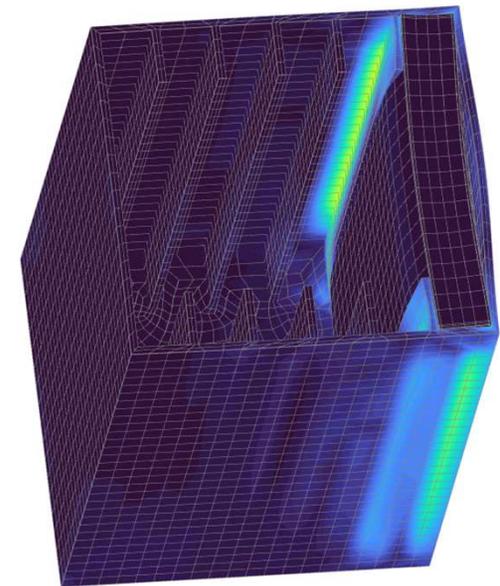
Stress/Strain on Casing
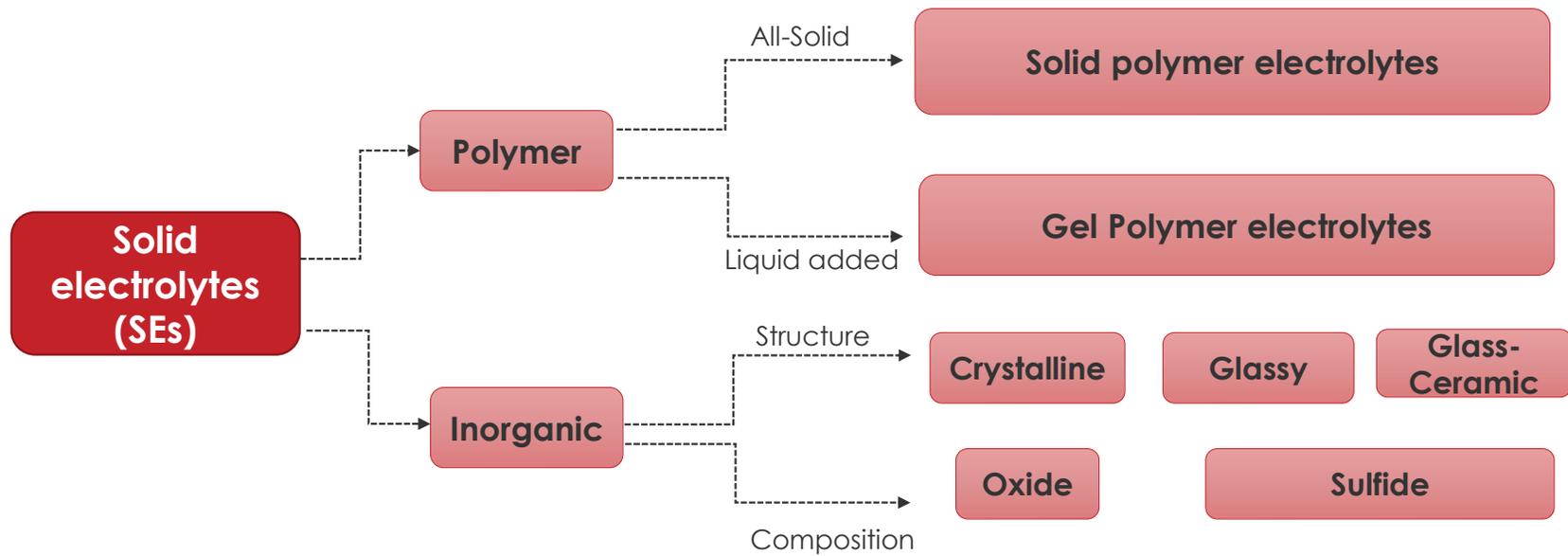-> Impact on Cell Performance
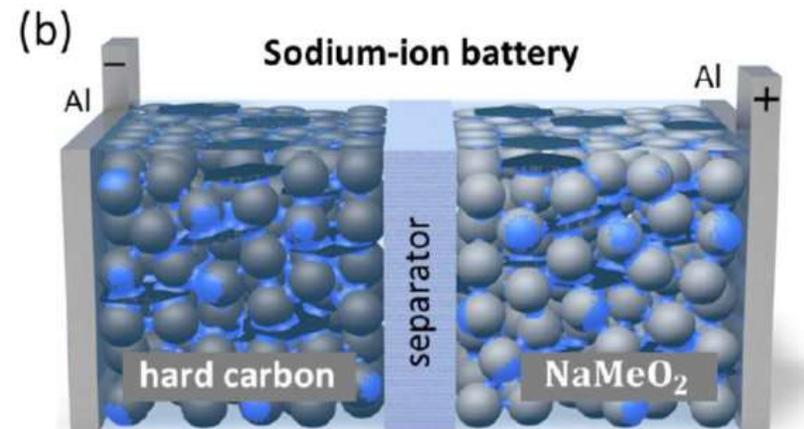
GT

Solid-State Batteries

- **SSB related features includes**:
  - Defining different electrolytes for anolyte, solid separator, and catholyte
  - Modelling capability of reaction surface area
  - Einstein's relationship for ionic diffusivity
  - Defining multiple layer of solid separators in contact with Li metal anode
  - Multiple solid electrolytes support

Types of solid electrolytes

```
Solid electrolytes (SEs)
├── Polymer
│   ├── All-Solid ──> Solid polymer electrolytes
│   └── Liquid added ──> Gel Polymer electrolytes
└── Inorganic
    ├── Structure ──> Crystalline | Glassy | Glass-Ceramic
    └── Composition ──> Oxide | Sulfide
```
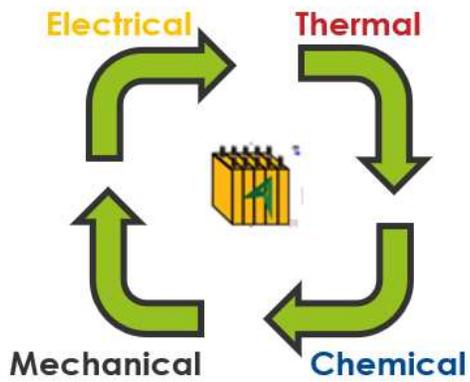
GT

Sodium-Ion Batteries

Sodium-Ion Batteries
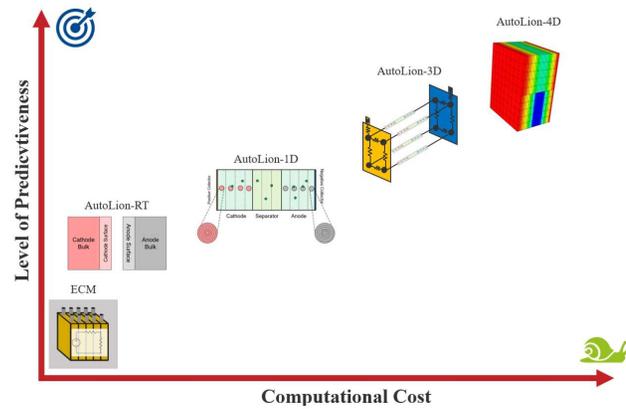
- Material Properties Database
  - Anode materials: Hard Carbon
  - Cathode material: $Na_3V_2(PO_4)_2F$ (NVPF)
  - Electrolyte: $NaPF_6$ in $EC_{0.5}:PC_{0.5}$ (w/w)

- Physics based models of degradation
- Blend electrodes & particle size distribution
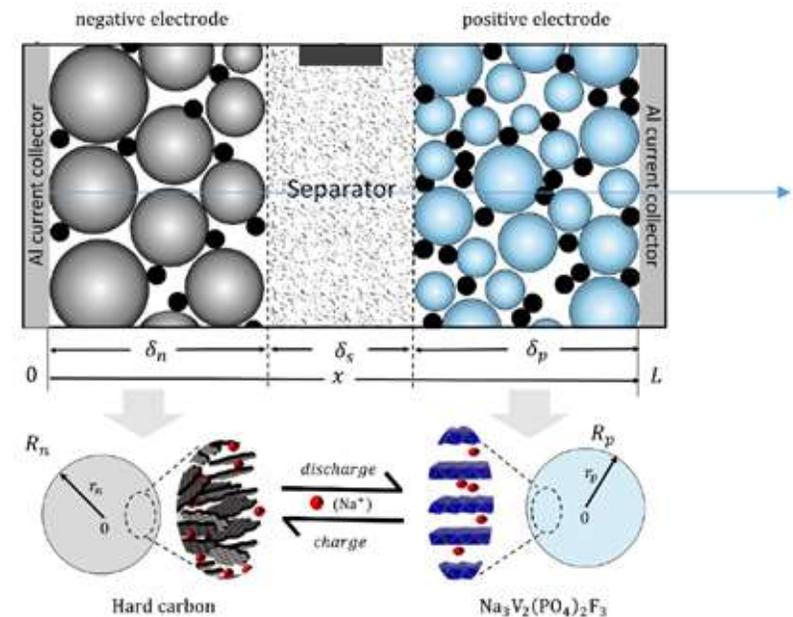
Conclusion

Perspectives - Connectivity

Different Flavors - Flexibility

Ready for the future

Thanks for listening…hungry?

Source: https://www.ast-reisen.de/tiere-afrikas/loewe/

GT