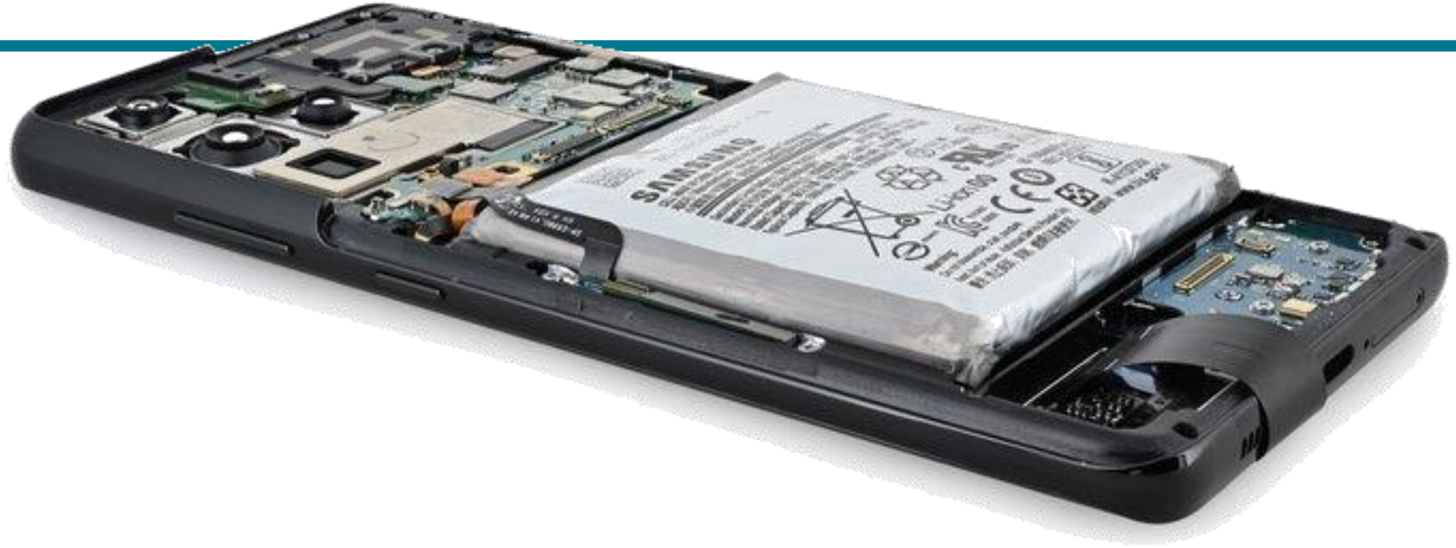
Information Day, Stuttgart, 22 June 2022

Overview on How Simulation Helps in Battery Development and Integration

Maik Schenke, DYNAmore GmbH



www.ifixit.com

Agenda

From physics to simulation models

- Introduction
- Inside battery
  - Physics
  - Cell geometry
  - Battery packs
  - Abuse
- Numerical simulations
- LS-DYNA
- Ansys product portfolio
- Summary

Introduction

First things first

Introduction

A personal story

"… Chestburster batteries are **not uncommon**."

"As startling as this swelling can be, it's **not a sure sign of danger**, … "

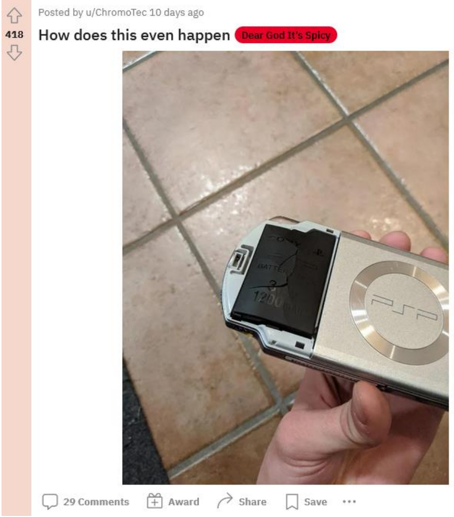
" … it's just that the battery **won't last for as long** as it used to."

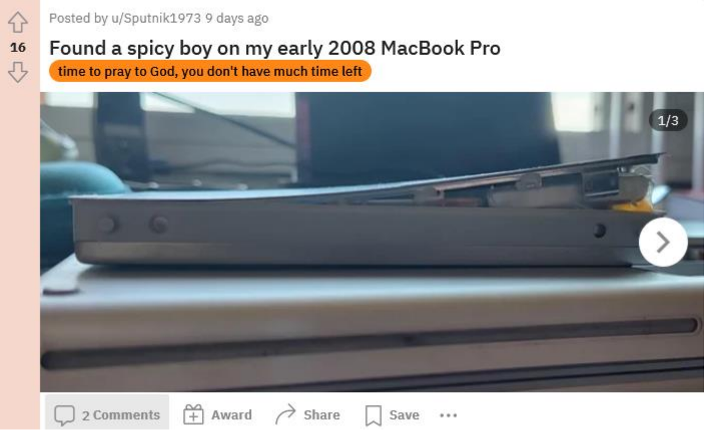
"… found a swollen battery … **stop using … the product it's inside. Don't charge it** again, either."

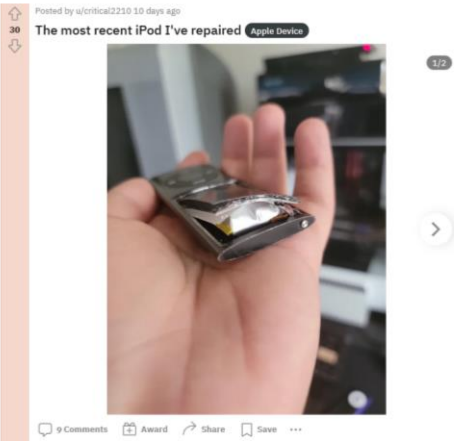
As the ions move during charging and discharging, the electrolyte begins to decompose and **produce gases as a byproduct**, thereby creating an excess pressure.

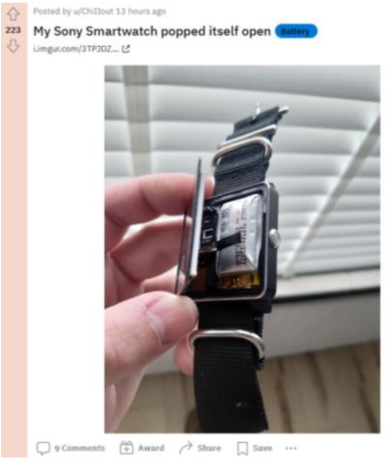
Introduction

A not so personal story





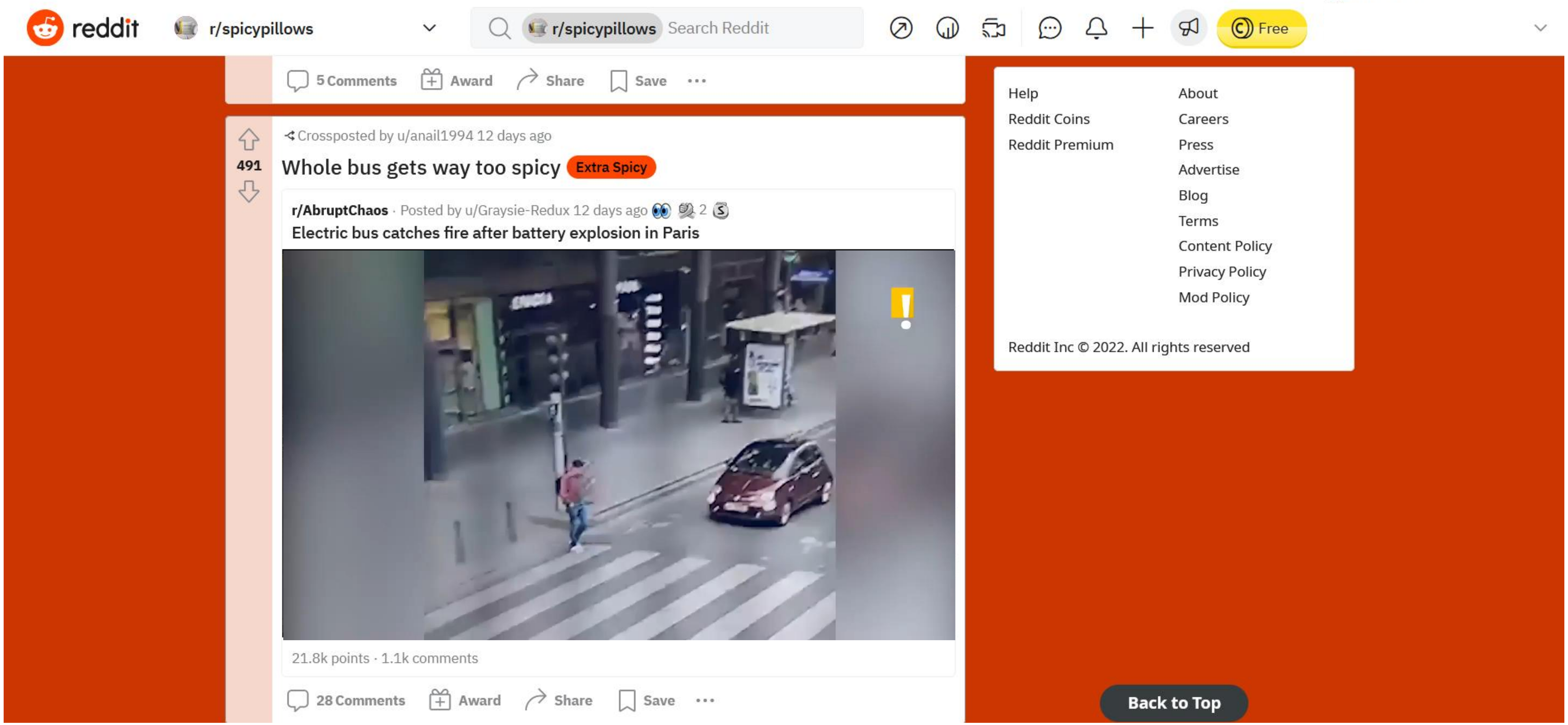




www.reddit.com/r/spicypillows/

Introduction

More serious spicy pillow



Introduction

US bans all Samsung Galaxy Note 7s from flights

The Federal Aviation Administration ban comes just after a second recall of the phone.

Ben Fox Rubin
Oct. 14, 2016 1:12 p.m. PT
2 min read

The Note 7 was pulled from production after multiple reports of phones catching fire.
Juan Garzón/CNET

The Samsung Galaxy Note 7 is no longer flight ready.

A group of US regulators on Friday banned of the device from all flights to, from or within the country, describing the phone as a "forbidden hazardous material" under federal regulations.

The ban, which goes into effect on Saturday at noon Eastern Time, is a significant expansion of a previous restriction on Note 7s. Beforehand, people were allowed to bring the phones onto planes but were told to power them down and to not use, charge or stow them in checked baggage.

- Nearly **100 dangerous battery incidents** reported in US
- **Recall of 2.5 million devices** before production was eventually ceased
- **Errors in both design and manufacturing** by two different manufactures
  - **Too tight space** to safely accommodate the batteries' electrodes (Samsung SDI)
  - ~~Insufficient~~ **Missing insulation material** and sharp protrusions (Amperex Technology)

Danger of an internal short!

Introduction

Rechargeable batteries everywhere

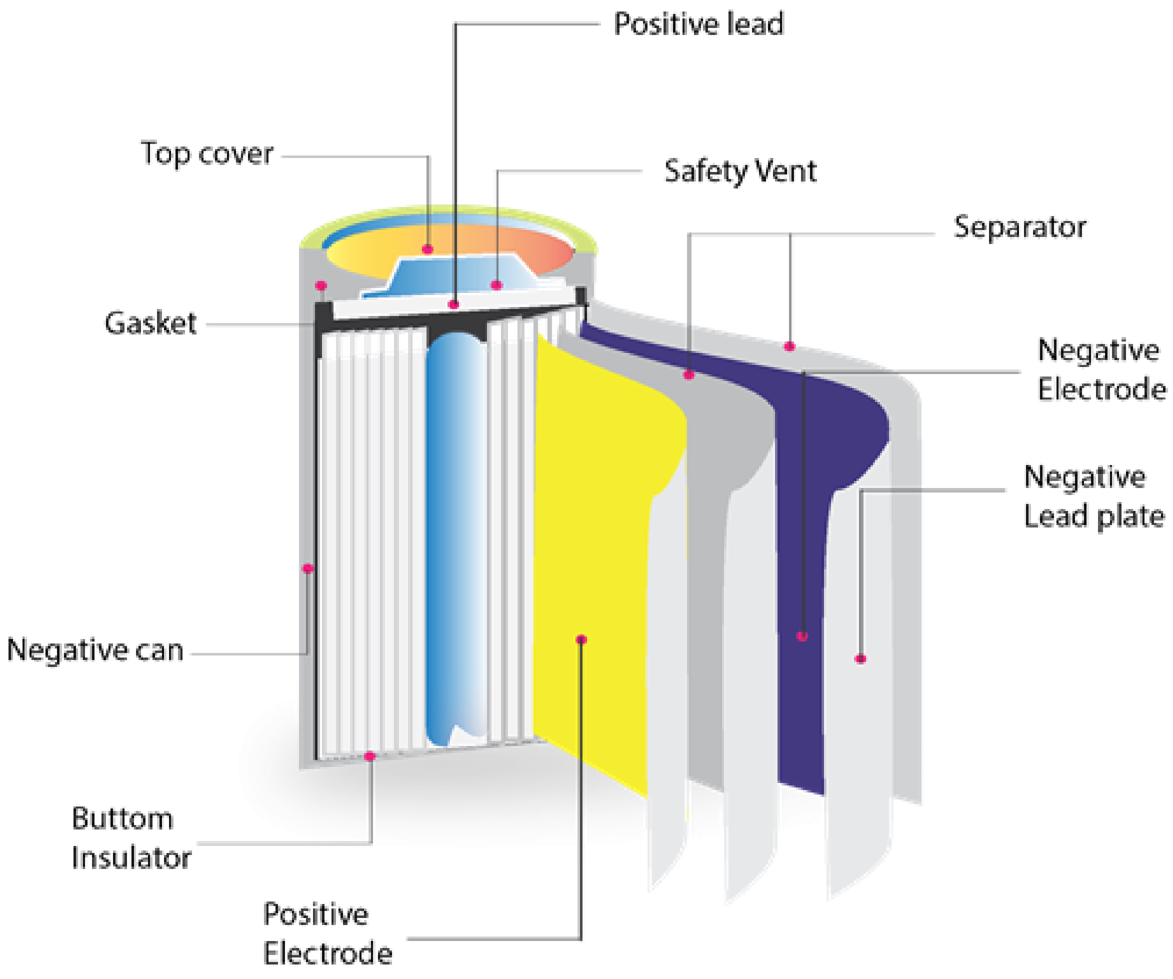
Inside Battery

Under the hood

Inside Battery

Components of Lithium-ion battery

- **Anode** is lithium storage when charged)
- **Cathode** is lithium storage when discharged
- **Separator** is an electric insulator
- **Electrolyte** is the lithium-ion carrier
- **Current collector** (not shown here) to collect electrons

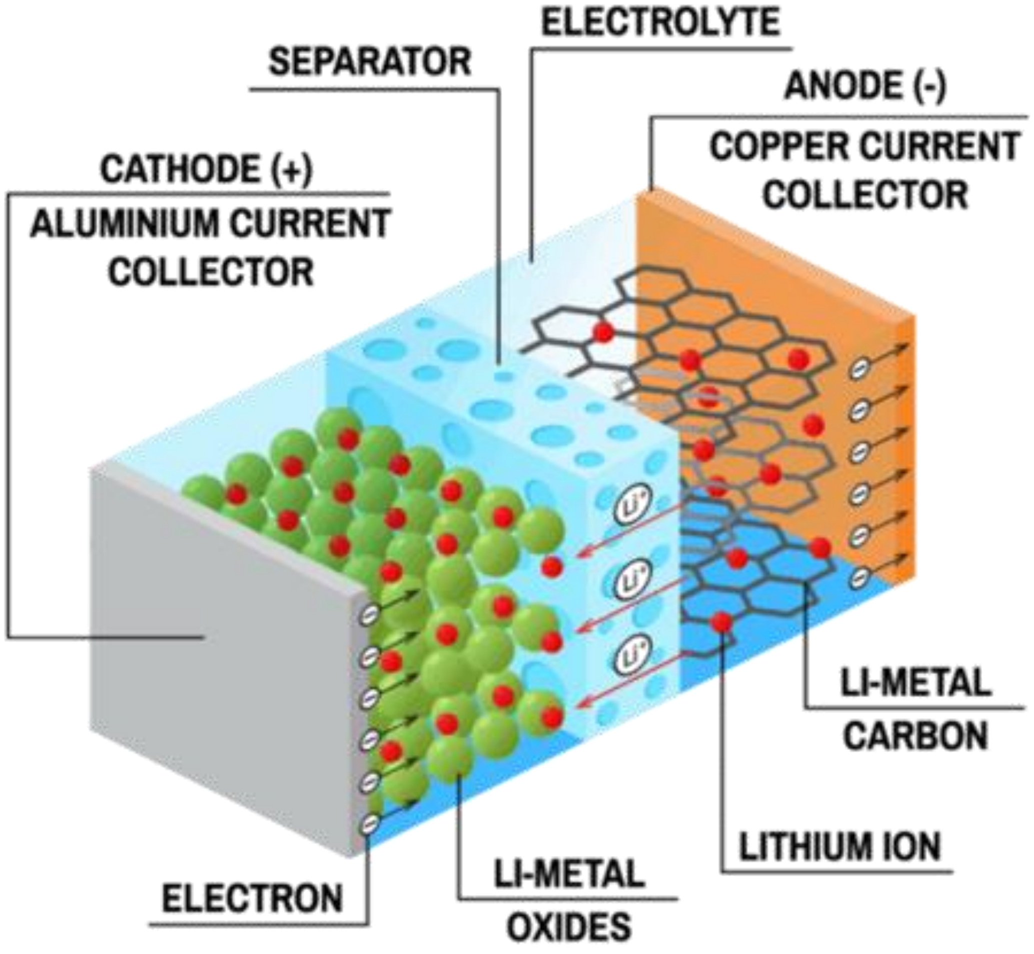


www.batterypowertips.com

Inside Battery

Charging and discharging physics

- Discharging (charging vice versa)
  - **Electrolyte carries positively charged ions** from anode to cathode through separator
  - The **separator, as an electric insulator**, only allows for the lithium ions to pass
  - The newly created **free electrons are forced through an electric conductor**
  - Thereby, powering an electric device

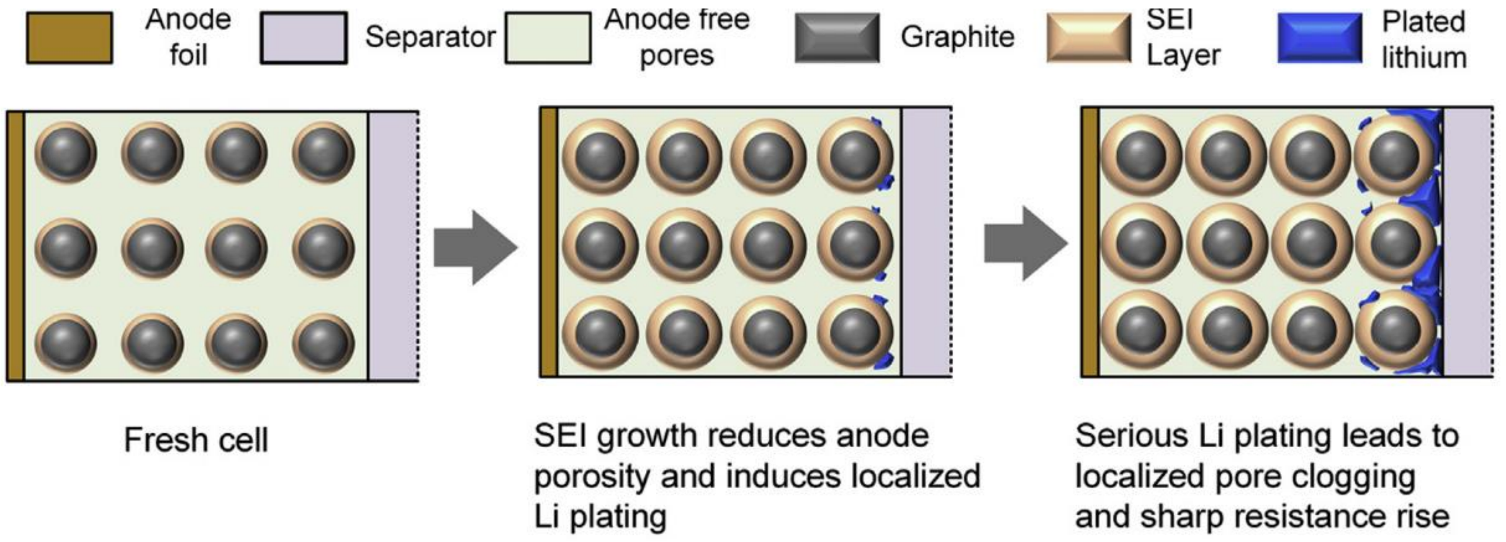


sivVector/Shutterstock.com

Inside Battery

Ageing

- Ageing is a result of **parasitic side reaction** while charging/discharging
  - Formation of **solid-electrolyte interface** (SEI) due to consumption of electron/lithium-ion
  - Deep charging **gather too many lithium on cathode**, thereby permanetly bounding them
  - **Drop in diffusion porosity** due to clogging



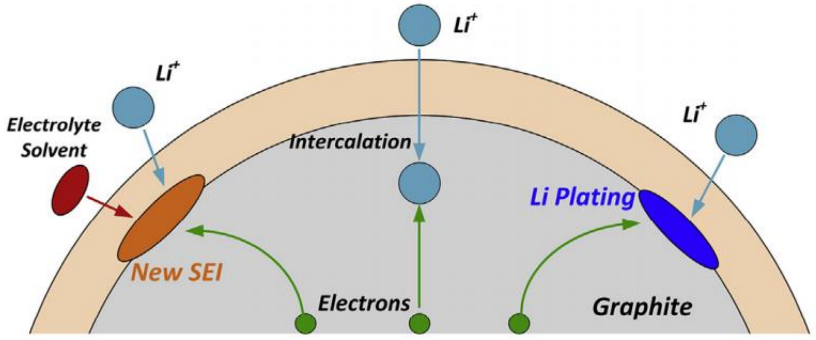


Fig. 1. Schematic illustration of the electrochemical reactions occurring in the anode during cell charging. The main reaction is intercalation of lithium, but lithium can react with solvent molecular to form new solid electrolyte interphase (SEI), or be deposited onto the graphite surface to form metallic lithium.

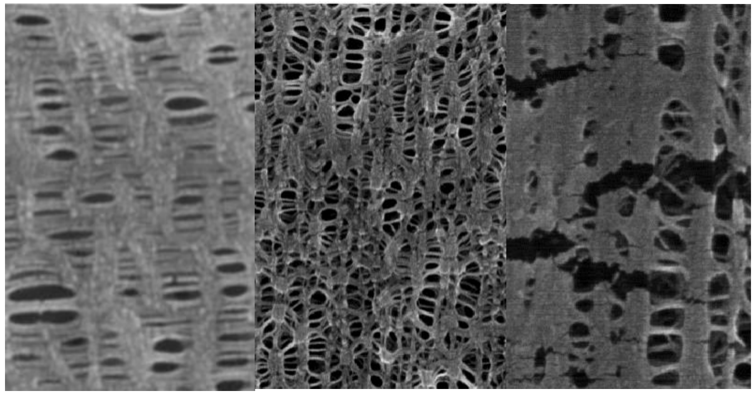
Yang et al. 2017

Inside Battery

Abuse

Mechanical

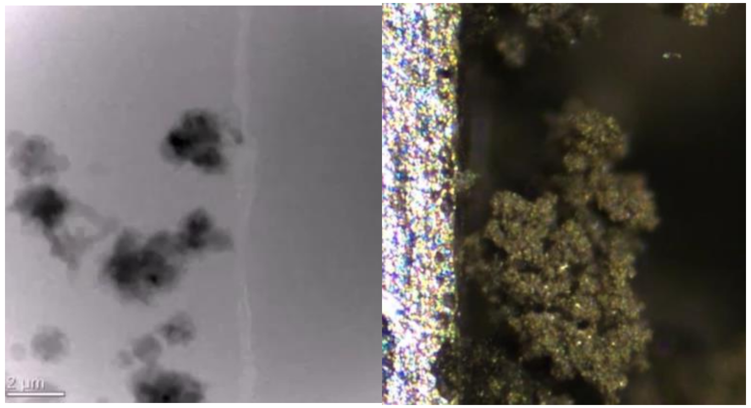
- Excessive deformation may cause separator rapture



Initial, deformed and ruptured separator
[Kalanus et al.]

Electrical

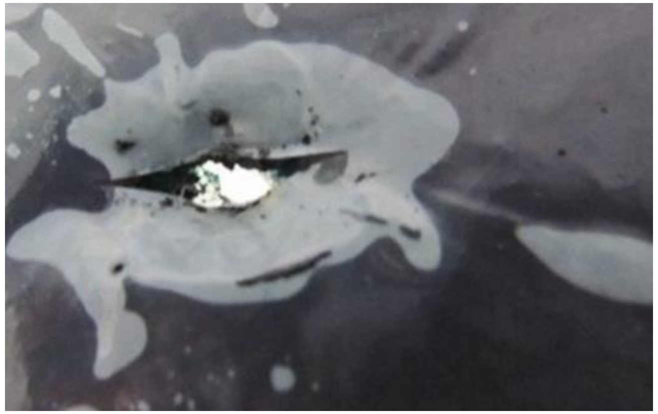
- Dendrite growth causes separator piercing



Dendrite growth
[Oak Rdige National Lab]

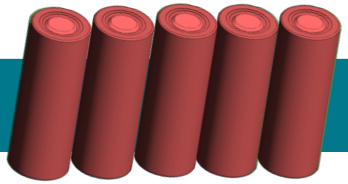
Thermal

- Excessive temperature causes separator collapse



Molten separator at 170°C
[Dreamwaver International]

Internal short to **thermal run-away** to **chainreaction on neighbouring cells**

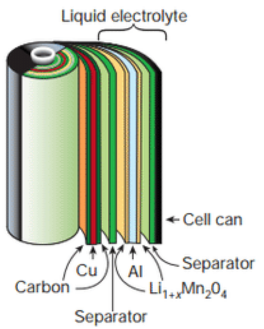


Inside Battery

Cell-housing geometries

Cylindrical cells

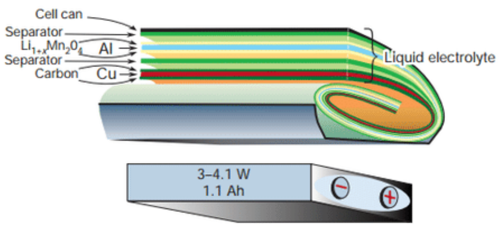
- Anodes, separators and cathodes are **sandwiched and rolled up**



- Well suited for automated mass production
- High tolerance for internal pressure
- Low energy density as pack

Prismatic cells

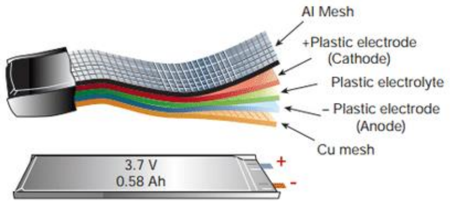
- Sandwiched components are rolled up or stacked, and **pressed into cubic case**



- High energy density as a pack
- High stress on corners at internal pressure
- Challenging thermal management due to smaller space cavities

Pouch cells

- Anodes, separators and cathodes are often stacked and **sealed by a flexible foil**



- Lightweight container
- Space to surrounding structure needs to allow for swelling

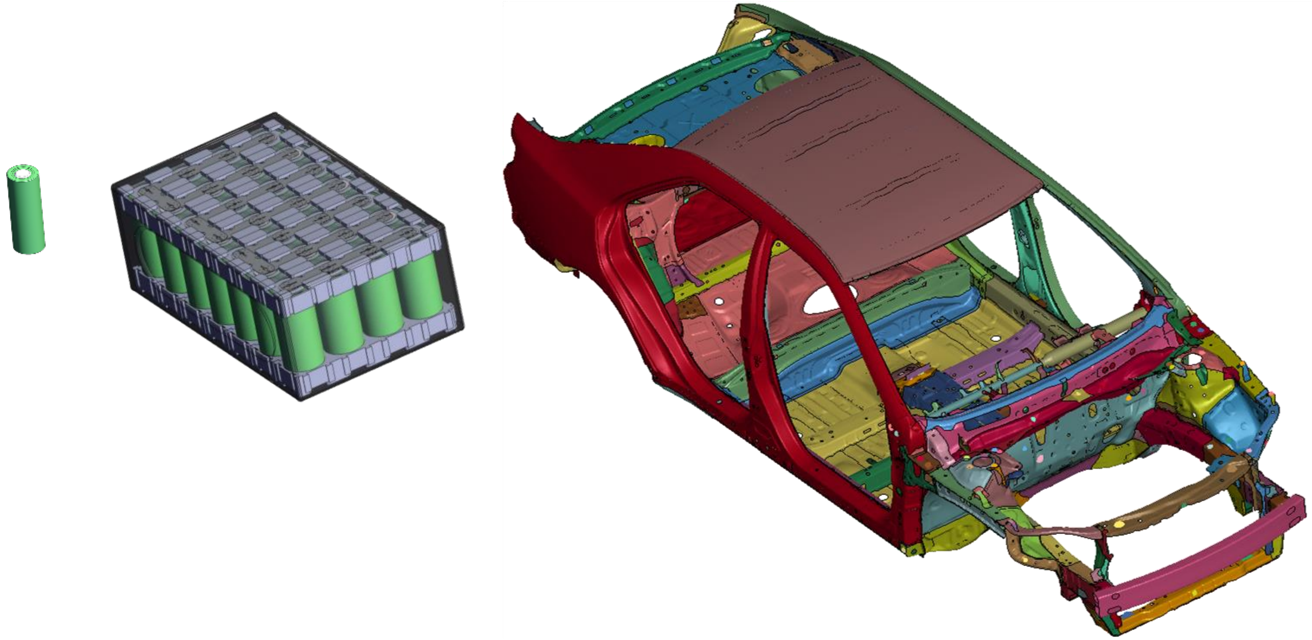
www.flashbattery.tech
[Mekonnen et al.]

Inside Battery

Battery integration - example on electric vehicles (EV)

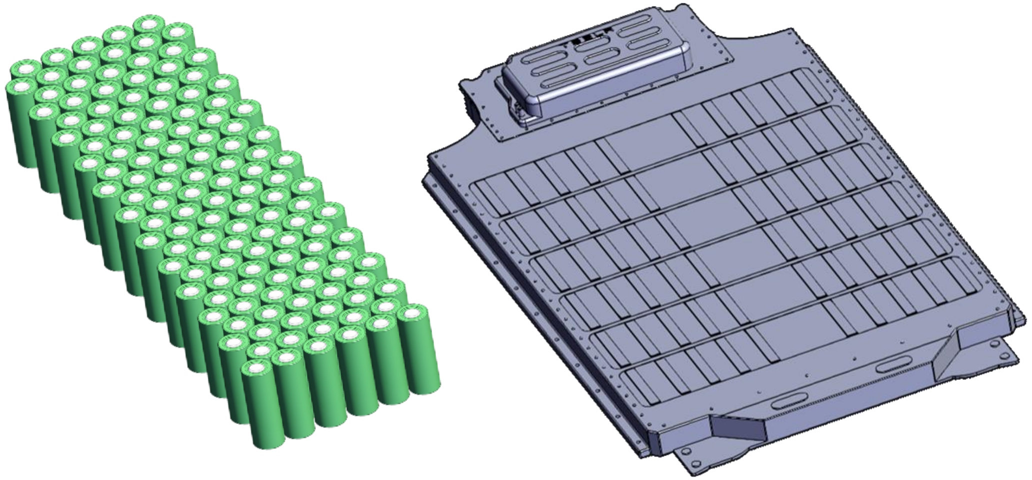
Early EV design

- Battery retrofitted into internal-combustion-engine (ICE) constructions
  - Low energy density per volume
  - Heavy and likely redundant construction



Current/upcoming EV design

- Battery is an essential structural part of the body
  - Lightweight construction
  - High energy density per volume
  - However, detailed knowledge of the battery cells mechanical behavior is needed



Users of www.grabcad.com

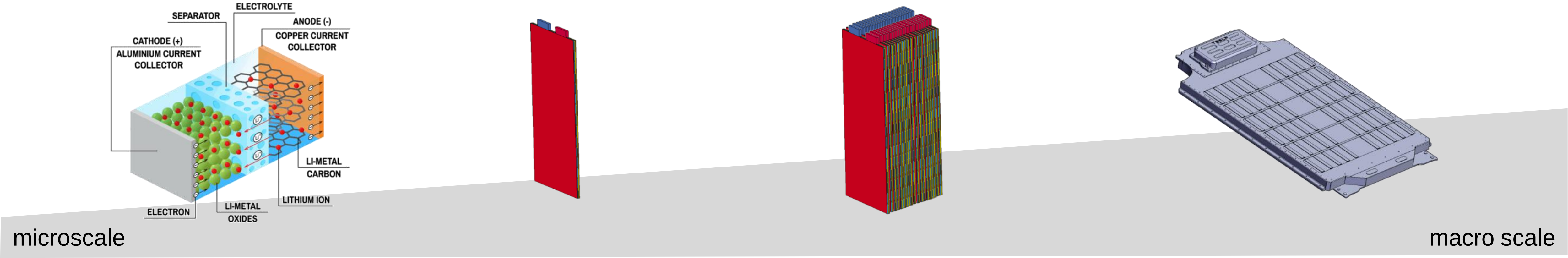
Numerical Simulation

Facing the challenge

Numerical Simulation

Multiscale and multiphysical challenge

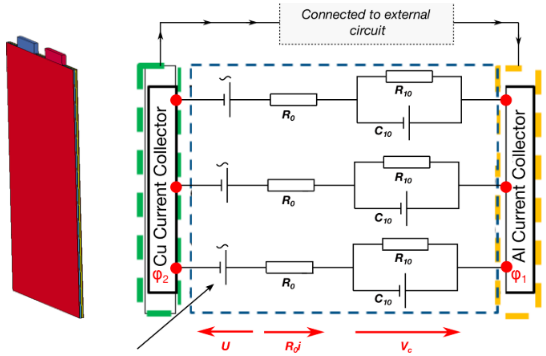
- Multiphysic coupling
  - **Chemical reactions** at anode and cathode
  - **Ion diffusion** as porous-media-like problem
  - **Heat generation** and transport
  - **Structural deformation**, e. g. swelling or external loading
  - **Gas generation** during thermal runaway
- Individual physics act on **different scales in time and space** → multiscale problem



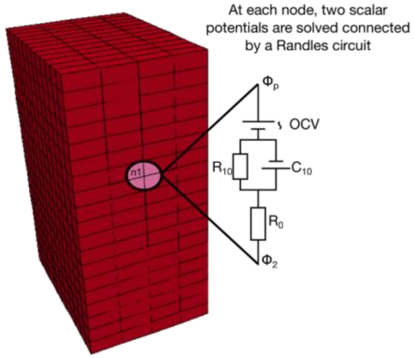
Numerical Simulation

Ingredients to an efficient simulaition

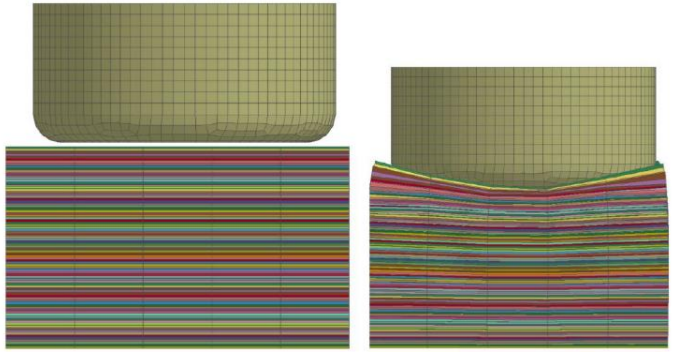
- Scale-dependent solution approach
- Physic-dependent approach
- Underlying physics are often described by abstract representative models, e. g.,
  - Charging/discharging via, **equivalent circuit models (ECM) / Randle Circuits (RC)**
  - For thermal management, battery **soley as a heat source**
  - For structural mechanics, battery as a **composite material**



RC of a unit cell [LST EM class notes]



BATMAC of a cell stack [LST EM class notes]



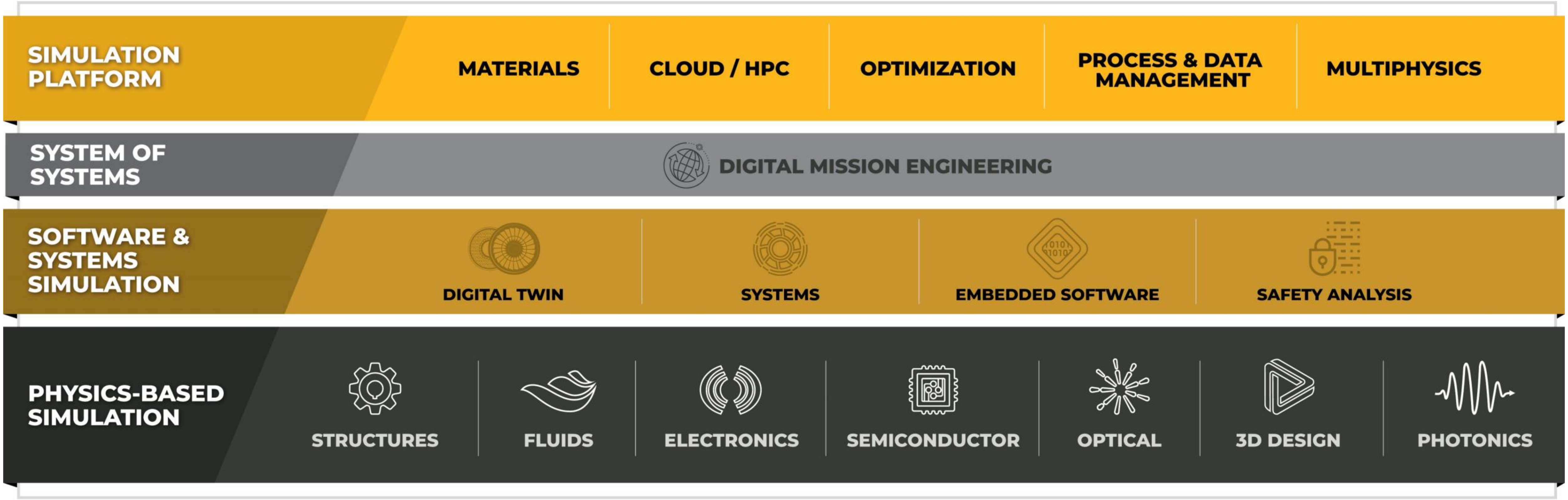
Layered structural battery model

Solver

What to use

Solver

Ansys multiphysic environment



- Portfolio comprised of 85 Ansys products, incl. e. g. LS-DYNA, Fluent, Ansys Mechanical
- Integration with partner and competitor products

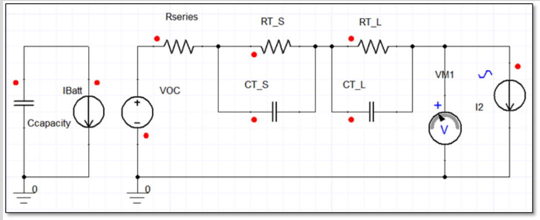
Courtesy of Ansys, Inc.

Solver

Battery simulation with Ansys product portfolio

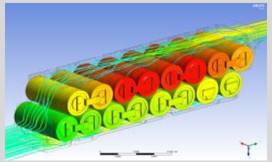
Solutions to meet the different requirements at different stages of the development process

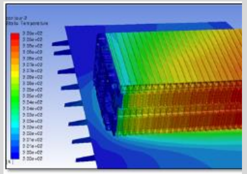
Cell
Electrochemistry, materials, characterization

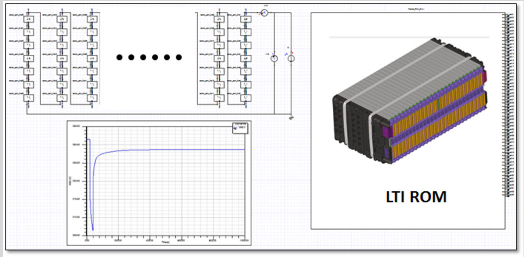


- Fluent
- Twin builder

Module
Thermal, structural

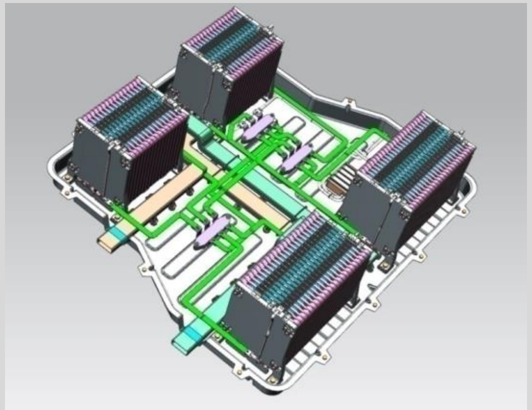






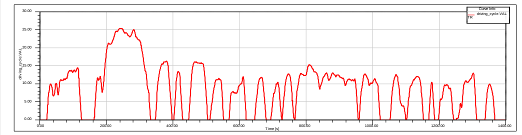
- Fluent
- Mechanical
- Twin builder
- **LS-DYNA**

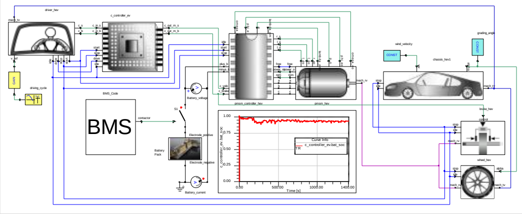
Pack
Thermal, electrical, structural, crash



- Mechanical
- Fluent
- **LS-DYNA**
- Twin Builder

System + BMS
Control logic, software,Functional Safety, Lifing





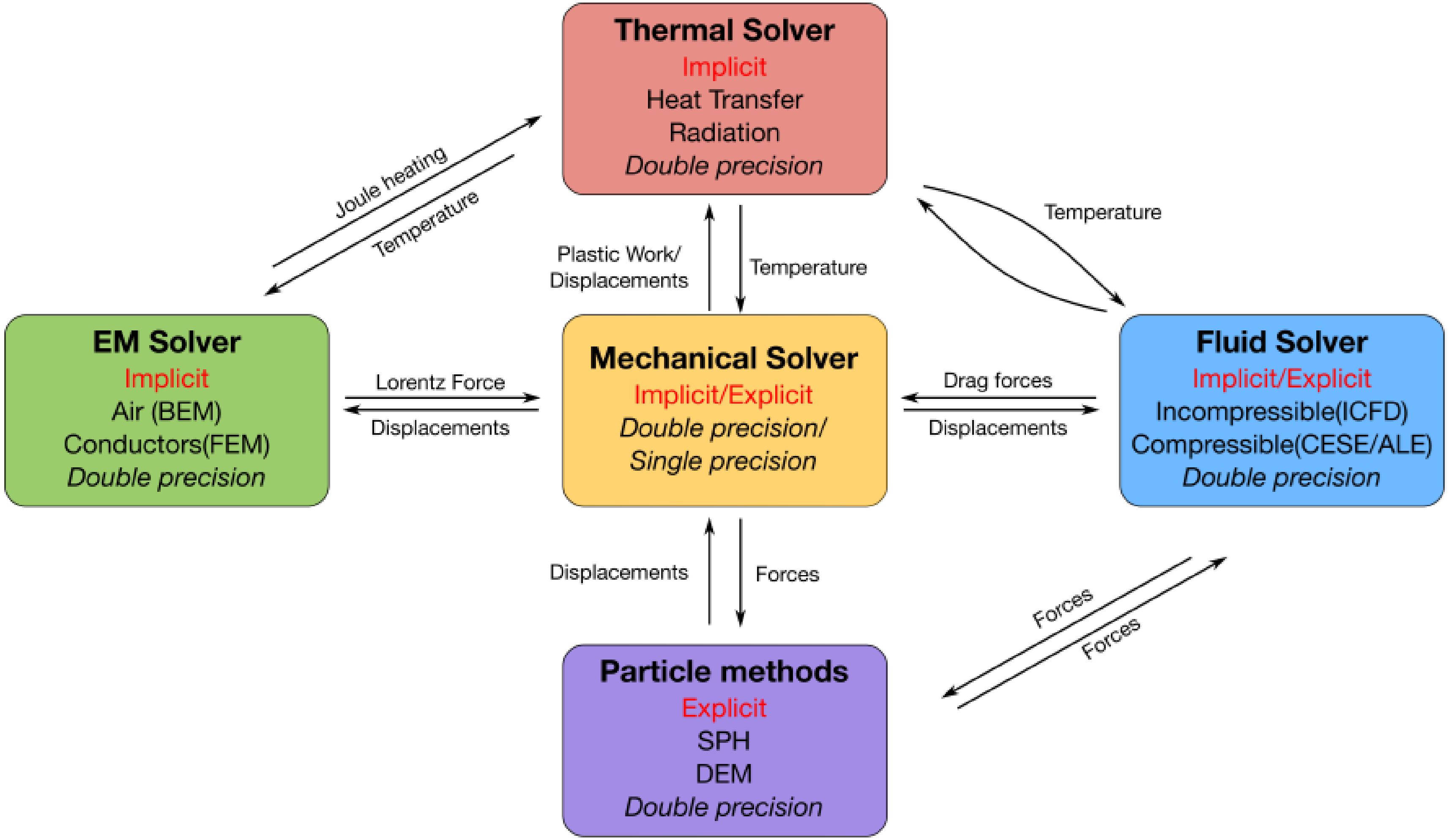
- Twin builder
- SCADE
- medini

Courtesy of Ansys, Inc.

Solver

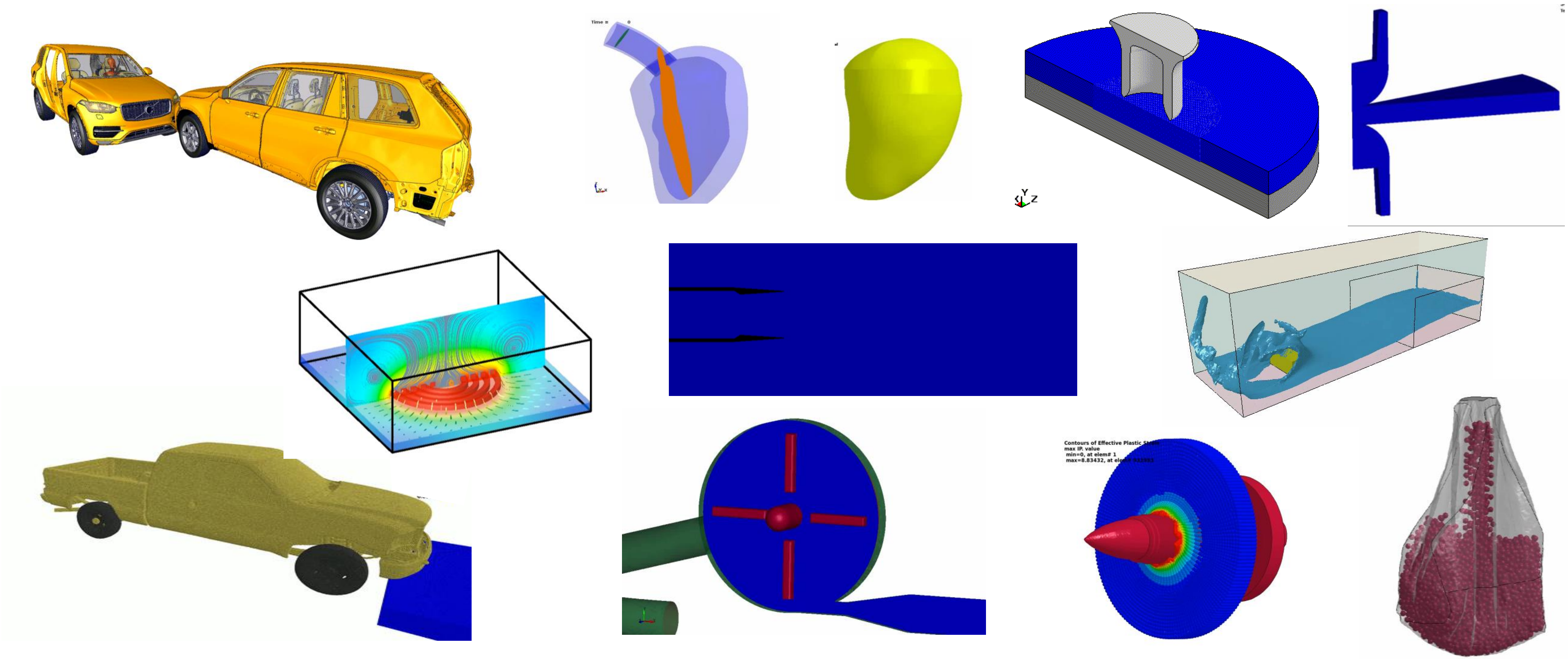
LS-DYNA multiphysic solver

- One-code strategy
  - Fluid mechanics
    - Incompressible (ICFD)
    - Compressible (CESE)
    - Chemistry (CESE)
  - Electromagnetics
  - Particle methods
  - Thermal
  - Mechanics



Solver

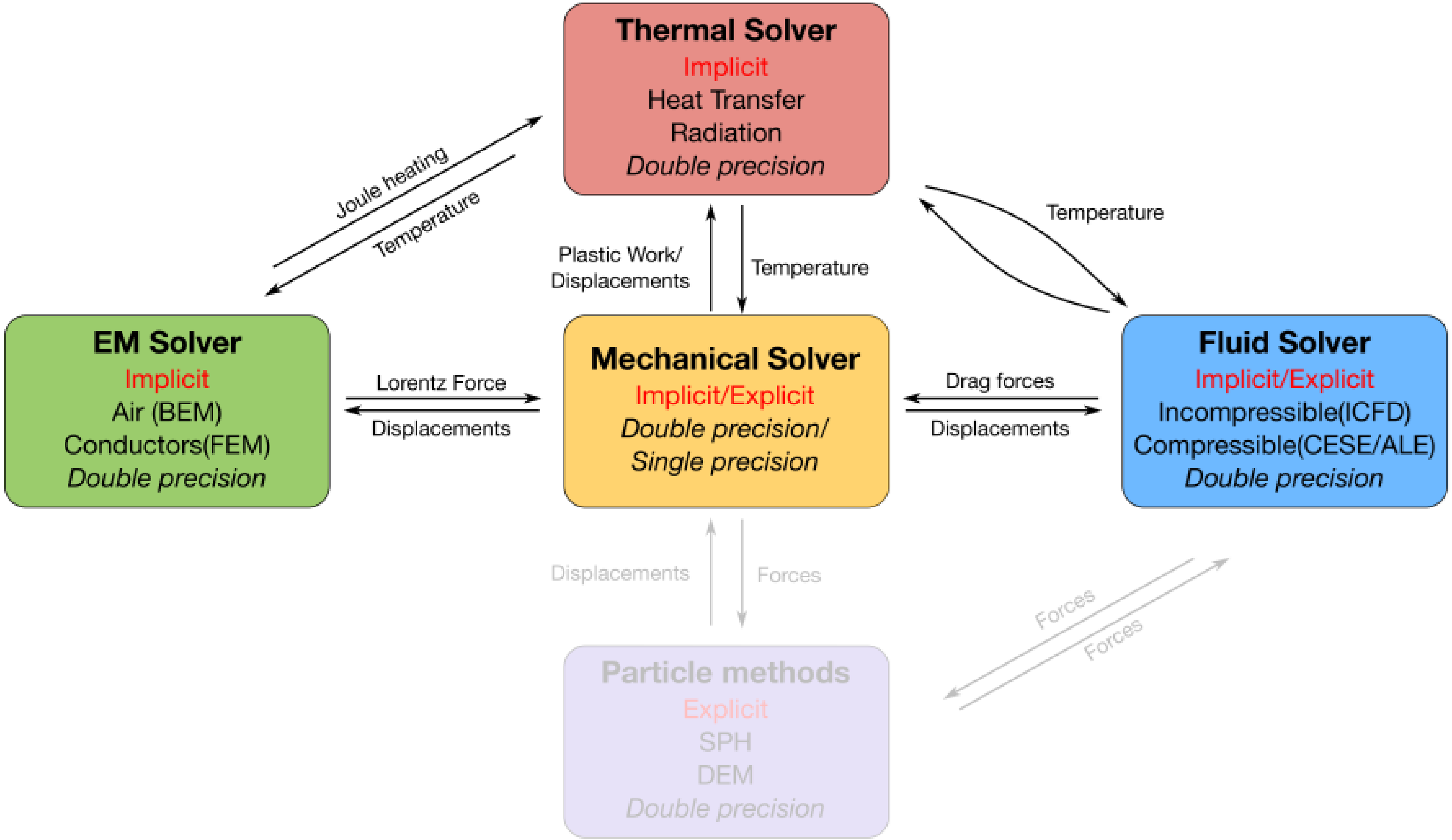
LS-DYNA application examples



Solver

Battery simulation with LS-DYNA

- Fluid mechanics
  - Incompressible (ICFD)
  - Chemistry (CESE)
- Electromagnetics
- Thermal
- Mechanics

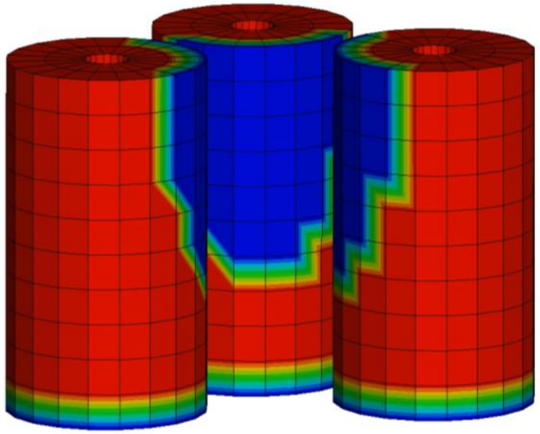


Solver

Battery simulation with LS-DYNA I

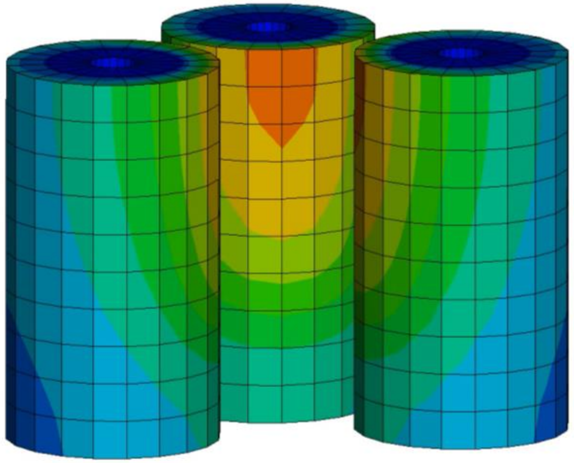
Electromagnetics

- Resistive heating solver of EM module by
  - Laplace equation
  - Electric field
  - Current density
  - Joule heating
- Computes, e. g.
  - State of Charge (SOC)
  - Joule heating



Thermal problem

- Heat transport problem by
  - Energy balance
  - Heat conduction (Fouriers Law)
- Computes
  - Temperature field (in solid)

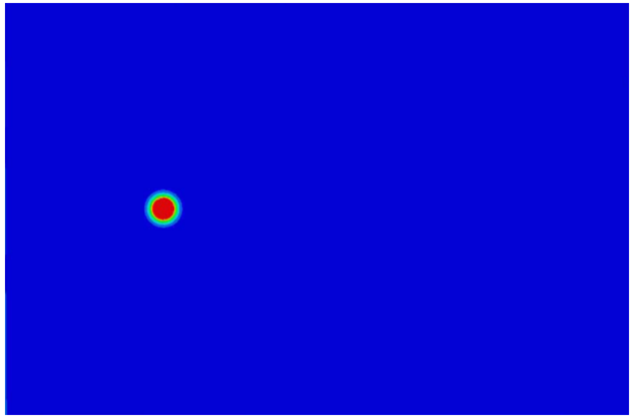


Solver

Battery simulation with LS-DYNA II

Fluid dynamics

- Incompressible flow by
  - Navier-Stokes equation
  - Volume balance
  - Energy balance
- Computes
  - Fluid temperature
  - Fluid velocity
  - Pressure



Chemistry

- Chemical kinetics by
  - Reaction equation
  - Consumption rate
- Computes
  - Molar species concentration
  - Electric potential

Remarks

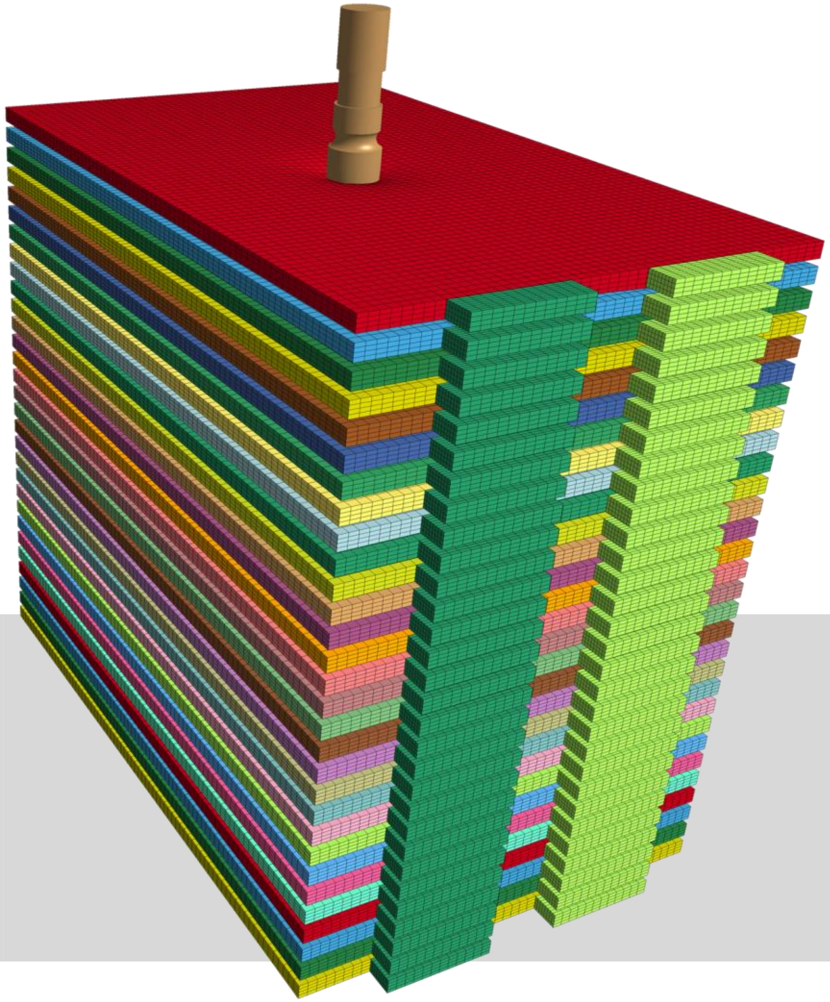
- Based on CESE chemistry module
- Ansys CHEMKIN input style
- LS-DYNA R13 or later
- **Highly experimental**

Solver

Battery simulation with LS-DYNA III

Structure

- Structural deformation by
  - Momentum balance
- Computes
  - Deformation, strains and stresses



Various modelling approaches on different scales, e. g.

- Pouch cells via shells, beams and airbag model
- Honeycomb model
- Composite-like layered models

Outlook

What to expect from today

- Battery simulation is challenging
  - **Multiphysical coupling**
  - **Different time and length scales**
  - **Abstract representations**
  - Currently under heavy research
- Current state-of-the art
  - **Testing/model calibration**
  - **Electromagentic-thermal coupling**
  - **Thermal-fluid coupling**
  - **Structural mechanics**
  - **Structural integration**
  - **Battery management**

Lets get started

DYNAmore GmbH
Industriestr. 2
70565 Stuttgart-Vaihingen
Germany

Tel.: +49 - (0)711 - 459 600 0
Fax: +49 - (0)711 - 459 600 29
info@dynamore.de

www.dynamore.de
www.dynaexamples.com
www.dynasupport.com
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