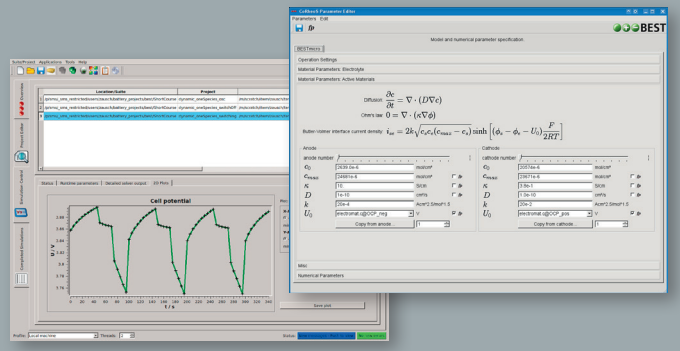

CONTACT

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Modular architecture

- Graphical User Interface
- **BESTmicro:** general microscale solver
- **BESTmicroFFT:** specialized, very efficient microscale solver
- **BESTmeso:** cell-scale solver
- Additional modules e. g. for thermal or mechanical coupling

Software architecture

- Qt-based graphical user-interface
- Simulation in high performance C/C++
- Thread-parallelization
- Input in CSV, GDT, TIFF
- Output in VTI/VTK, CAP, CSV

Coupling to

- GeoDict (Math2Market)
- FeelMath (Fraunhofer ITWM)

Requirements

- Windows/Linux
- PC/Computing cluster
- Intel Multi-Thread CPU (e. g. Core i7)
- 8 GB RAM

BEST

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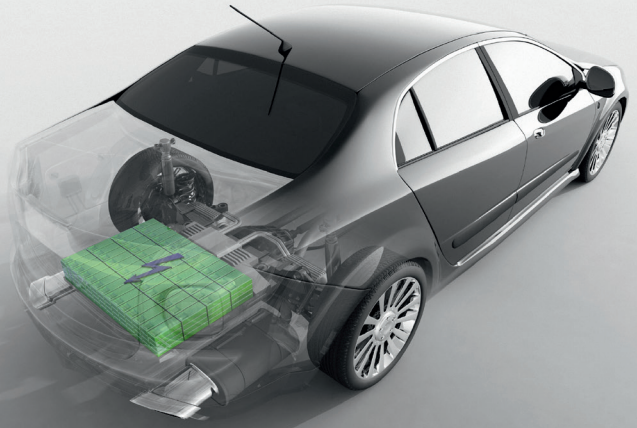
THE BATTERY AND ELECTROCHEMISTRY SIMULATION TOOL



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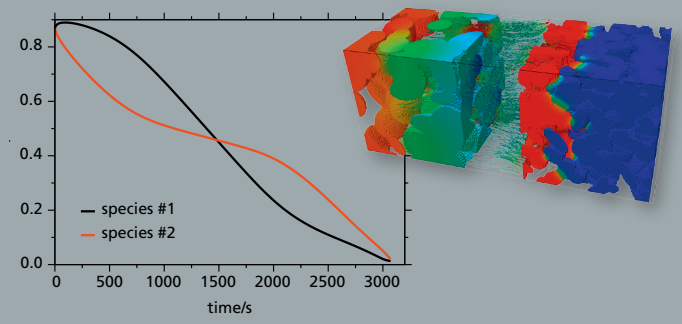

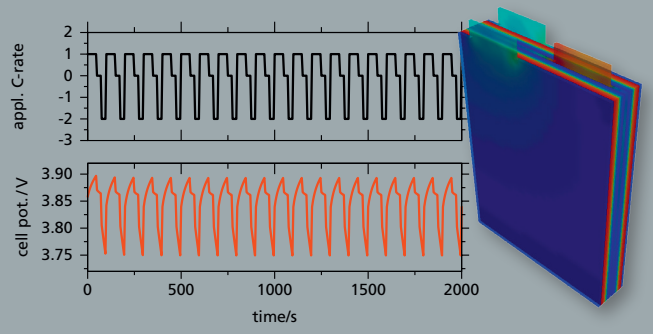

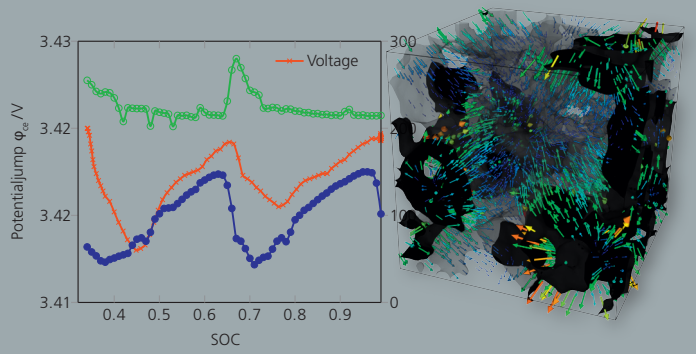

Computer-aided battery development

For increasing the share of renewable energy sources in the future energy mix modern energy storage technologies play a key role. In particular electro-mobility applications, where mainly lithium-ion batteries are employed, have high demands on capacity, power density, life-time and safety. The time-consuming and expensive experimental development of improved materials and cell designs is supported by computer simulations of the relevant phenomena. It is thus desirable to estimate the performance of a real battery by studying and modifying its virtual realizations. The simulation helps to better understand the reasons for a particular battery property.

Lithium-ion batteries consist of two porous electrodes that are electronically isolated by an electrolyte-filled separator membrane. During charging and discharging lithium ions are exchanged between the electrodes through the electrolyte. Our model describes the main properties lithium-ion diffusion and electric current as well as secondary effects like heat development, volumetric expansion or phase separation.

Battery simulation across the scales

In contrast to surrogate equivalent circuit models for battery simulations, **BEST** is based on a physical description that in principle requires no parameter fitting. As our simulation tool solely requires a set of physical material properties, the user can easily study for instance different geometries or load scenarios. Both galvanostatic or potentiostatic operation with time-dependent current or voltage is possible. By this, **BEST** enables the user to examine battery performance and supports the cell design process. Different length scales ranging from micrometer material scale up to cell scale are implemented in the soft-ware modules **BESTmicro** and **BESTmeso.**

With the microscopic transport model the material structure of the electrodes is spatially resolved down to micrometer scale. In such a geometry ion transport in electrolyte and active particles is explicitly computed. The detailed granular model allows for thorough analysis of the interplay between microstructural and electrochemical effects.

Our mesoscopic porous electrode model on the other hand employs volume averaging methods to obtain an effective description of ion transport. While this neglects some aspects of the microscopic detail of the electrodes, the relevant processes are captured and it allows for the efficient simulation of a full three-dimensional battery cell.

Model extensions

We aim to constantly improve our simulation and include latest scientific innovations and technological advances into our soft-ware. Recent extensions include:

Heat development

During operation a battery cell can heat up. For many applications it is important to estimate heat production and temperature distribution. **BEST** computes the local heat power and couples the temperature field to the electrochemical model such that the influence of temperature change on cell performance is taken into account.

Electrode expansion

For some electrode materials (e. g. silicone anodes), the intercalation of lithium ions leads to spatial expansions. The mechanical strains result in stresses on the battery structure, can damage the integrity and can lead to capacity loss or failure. Elastic models support design decisions and infer the influence of the microstructure on the mechanical stress.

Phase-separation

Certain electrode materials (e. g. $LiFePO_4$) show phase separation into lithium-rich and lithium-poor regions. This requires the application of generalized chemical potentials for the simulation of lithium-ion diffusion and electric currents.