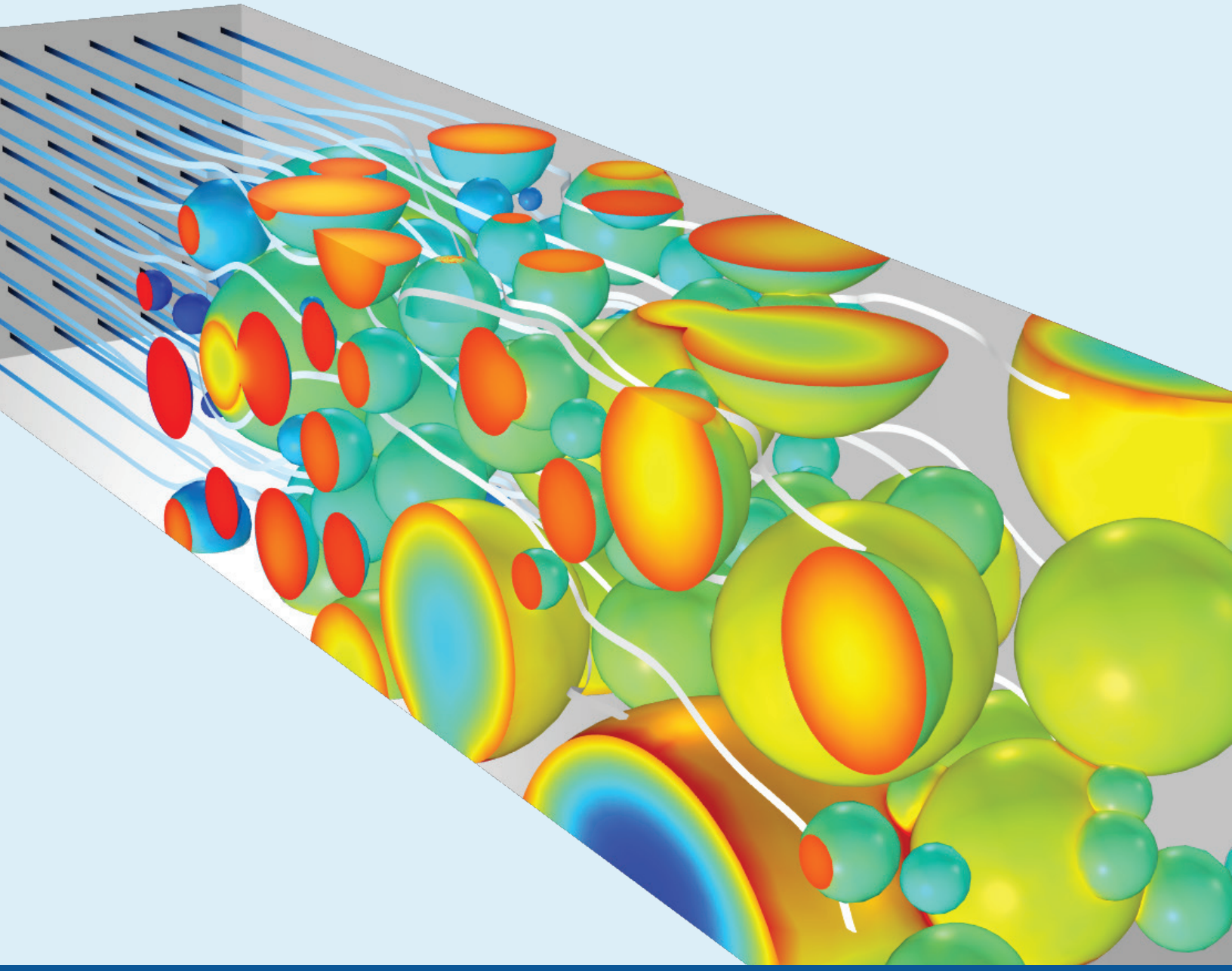


WHITE PAPER

Battery Modeling

By **HENRIK EKSTRÖM** and **ED FONTES**

COMSOL

TABLE OF CONTENTS

Further Resources

USER STORY GALLERY
https://www.comsol.com/stories

APPLICATION GALLERY
https://www.comsol.com/models

TECHNICAL PAPERS AND PRESENTATIONS
https://www.comsol.com/papers-presentations

COMSOL BLOG
www.comsol.com/blogs

Contact Information
For inquiries about how to use the numerical simulation and application design capabilities in the COMSOL® software for your unique application, visit comsol.com/contact.

Contact technical support at: comsol.com/support

Original publication: *Tech Briefs* - February 2021 - Vol. 45 No. 2, *Battery Technology* Pages 8–11.

About the Authors

Henrik Ekström, COMSOL, www.comsol.com
Henrik Ekström works at COMSOL and has a Ph.D. in Applied Electrochemistry from The Royal Institute of Technology (KTH), Stockholm. As the technology manager of electrochemistry at COMSOL, he is responsible for the development of various simulation and modeling solutions for batteries, fuel cells, corrosion, electrodeposition, as well as general electrochemistry applications.

Ed Fontes, COMSOL, www.comsol.com
Ed Fontes is Chief Technology Officer at COMSOL and has a Ph.D. in Applied Electrochemistry from The Royal Institute of Technology (KTH), Stockholm. He has been the lead developer for the chemical engineering, CFD, and heat transfer product lines at COMSOL. He is responsible for technology development at COMSOL.

INTRODUCTION

When it comes to the research and development of batteries, modeling and simulation (M&S) provide an efficient and low-cost approach.

The use of M&S is always combined with experimental investigations, where the first step is to develop and validate the models. Validated physics-based models can be used to make predictions within the range of the theory, which is usually beyond the range used for validation of an individual model.

Throughout the R&D process, researchers and engineers can use models to run thought experiments and virtual experiments. These "what if" studies lead to a deeper understanding of the battery system under investigation — and can even help foster new ideas. The models can be used for predictions, design, optimization, and control of the battery system.

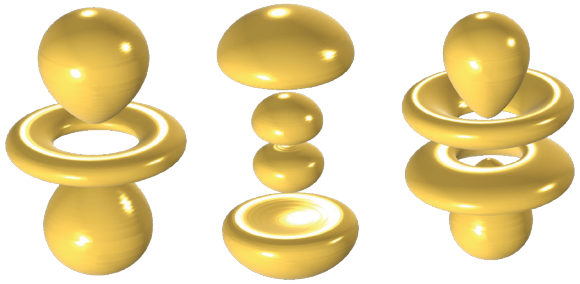
Battery systems are investigated by a variety of stakeholders with different goals and purposes. For example, in an electric vehicle, aspects of the battery system, such as energy density, power density, life, cost, and sustainability, may determine the technical bounds and the goals for all stakeholders.

Universities, research institutes, and national labs often have research programs that aim to fundamentally understand all aspects of battery usage. Research topics can include materials research on new battery chemistries; design of battery cells and battery systems; and life-cycle assessment (LCA), including the process of raw material extraction, disposal, and recycling of battery systems. Battery manufacturers have to investigate similar aspects but with a larger focus on manufacturability, implementation, and use. Original equipment manufacturers (OEMs) are usually involved in the aspects that relate to battery cell and battery system design, with a stronger focus on use, but also on aspects of LCA.

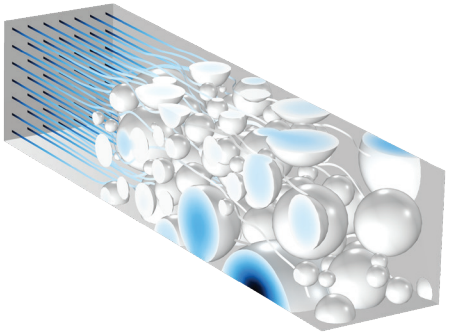
MODELING SCOPES

Depending on the stakeholder and the purpose, M&S projects can be carried out with different scopes. This may involve modeling processes at the molecular, microscopic, battery module, and battery stack scales. Aspects of material extraction, disposal, and recycling also have an impact on the modeling projects. These aspects indirectly determine the range of properties of battery cells, modules, and packs.

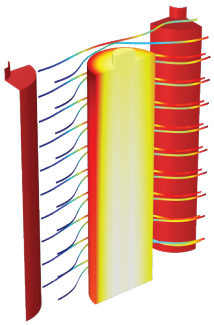
Material scientists, electrochemists, and physicists researching new battery chemistries may use molecular dynamics models to simulate and predict the behavior of possible new materials and chemistries for batteries. This type of research is usually done at universities, research institutes, national labs, and at battery manufacturer's R&D labs.



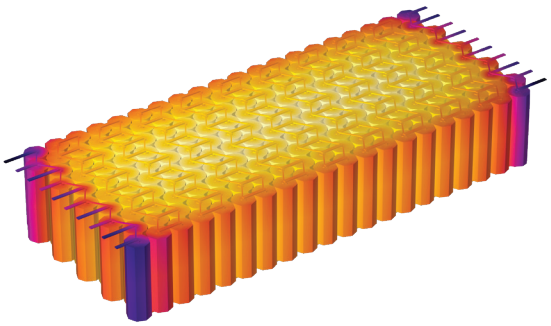
Molecular scale ⟼ 0.5 Å



Microscopic scale ⟼ 5 µm



Battery cell scale ⟼ 2 mm



Battery pack and module scale ⟼ 2 cm

FIGURE 1 The modeling scales span from Ångström ($1 \cdot 10^{-10}$ m) up to the module scale (1 m). Here, the scales are exemplified with a cylindrical Li-ion cell and a battery pack of cylindrical cells.

The microscopic structure and the physical properties for a battery material are interesting for all stakeholders, including the OEMs. The design of the electrodes, the electrolyte, separator, and current collectors in a battery cell are also interesting for all stakeholders. M&S in these projects is crucial for the understanding of the factors that determine a good battery cell design for a specific application.

Battery systems for electric vehicles consist of battery packs and battery modules. The design of the modules and packs are of great interest for both battery manufacturers and OEMs. National labs and research institutes are often involved in these types of research, usually for aerospace and defense applications. Modeling is then focused on the understanding and design of system performance (energy density and power density), thermal management, safety, and battery life.

MULTIPHYSICS MODELING

Microscale

Modeling a battery at the microscopic scale involves the chemistry, physical properties, and detailed geometry of the porous structure and the pore electrolyte. Molecular modeling may generate the input data to the microscopic models. Examples of such inputs include rate constants, electrode potentials, transport properties, and other chemical and physical properties of the materials in a battery.

Models at the microscale have to account for the electric potential of the electronic conductor (the electrode), the ionic potential of the pore electrolyte as well as the free electrolyte, the concentration of ionic species and neutral species, the electrochemical and chemical reactions, the temperature distribution, and the mechanical displacements due to thermal expansion or expansion caused by the transport of chemical species. In other words, several physics phenomena are involved in an accurate description of a battery material.

A very important aspect of the output of such modeling projects is the deep understanding of the basic mechanisms that determine battery performance and life. The models also allow us to make accurate quantitative estimates about absolute limits for performance (energy density and power density), impact of material and design parameters, distribution of the electrochemical reactions, temperature distribution, risks for short circuits and premature failure, formation of harmful byproducts, risks for fatigue and failure, and other quantitative estimates that may determine the performance and life of a battery. In addition, the models make it possible to develop methods for detecting and evaluating the state of health of a battery. Performance decay and failure is almost always manifested on phenomena at the microscopic scale first — long before health becomes obvious in the overall performance of a cell.

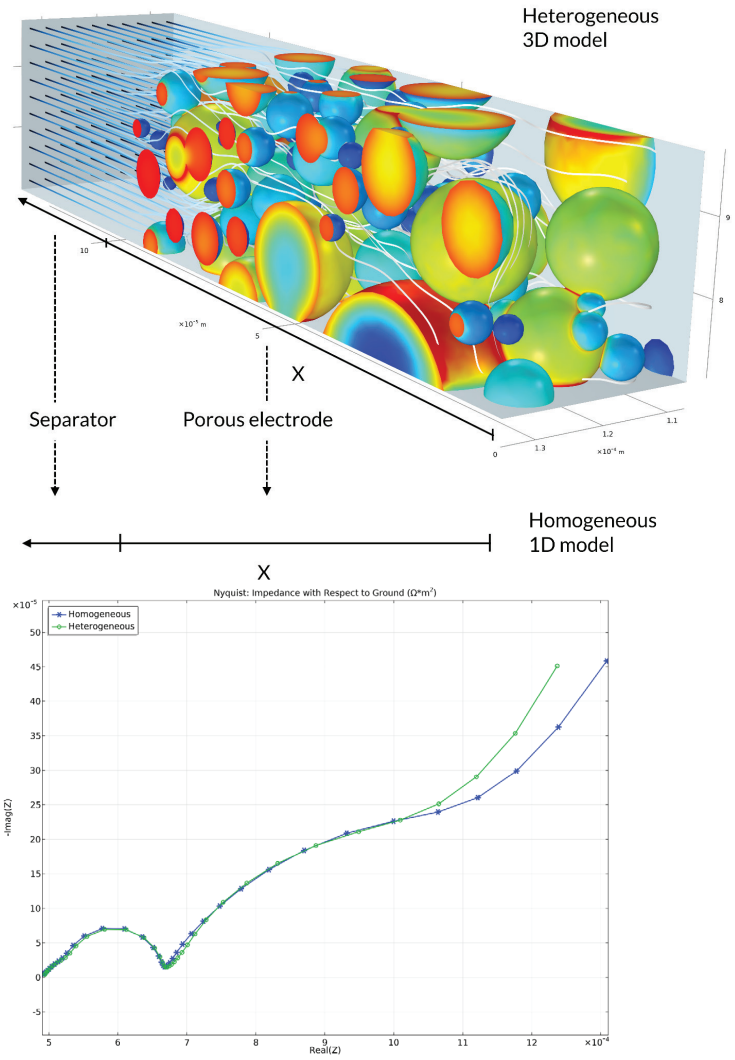


FIGURE 2 The heterogeneous electrode model contains a 3D description based on spherical particles obtained from treatment of micrographs in a lithium-ion battery electrode. The heterogeneous model can then be used to compute porosity, specific surface area, and other effective properties. These properties can be used in a homogenized 1D Newman model where the electrode is described as a homogeneous slab (top). The Nyquist plot shows that the results of the detailed heterogeneous model and the averaged heterogeneous model are in very good agreement, especially at high frequencies. In this case, the heterogeneous model validates the homogeneous model (bottom).

Battery Cell Scale with Porous Electrode Theory

The next scale from the microscopic scale is to look at the battery cell scale. The porous electrodes are then described as homogenized slabs, where the pore electrolyte and the electrode materials are defined in the same point in space in the model, see Figure 2 (top) above. This means that the structure of the electrode is described using effective parameters such as volume fraction of pore electrolyte, volume fraction of electrode, and tortuosity. These models make use of the so-called porous electrode theory as devised by Newman et.al., which form the basis of battery modeling at a scale just above the microscale.

The investigations at this scale involve similar aspects as the microscale, but for one or maybe several battery cells. Typical studies would involve the impact on the performance and life of different materials and chemistry; porosity of the electrodes; specific surface area of the electrodes and the different electrode materials (if there are several in the same electrode); thickness, length, and width of the current collectors, electrodes, and separator; mechanical loads on the battery cell imposed by the geometry and expansion during discharge and recharge; impact of the thermal management system; and other parameters that may affect the battery cell.

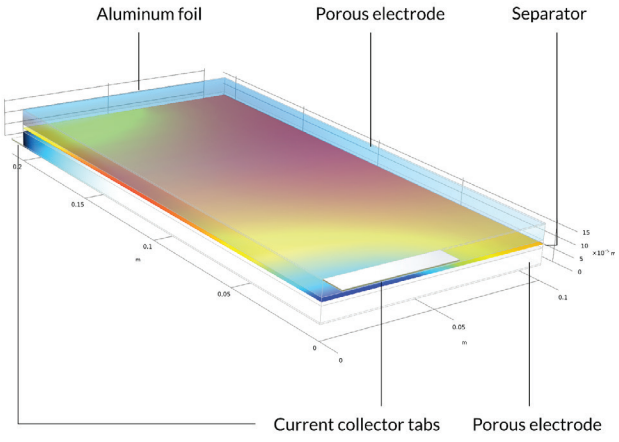


FIGURE 3 Current density distribution in the middle of the separator obtained using a 3D Newman model of a lithium-ion battery pouch cell. The model applies porous electrode theory and includes effects of aging, such as the growth of a solid electrolyte interface (SEI). The cell consists of two aluminum foils at the top and bottom of the figure, two porous electrodes (one positive and one negative), and a separator between the electrodes. The aluminum foils have a tab each to connect to the outer circuit. This is a typical high-fidelity model at the battery cell scale.

The output of M&S at this scale are quantitative estimations of performance, performance limitations, and life. These estimations can be obtained from results such as current and potential distribution, temperature distribution, metal deposition and short circuiting, fatigue and cracking in the electrodes due to expansion during charge and discharge, and formation of byproducts and occurrence of side reactions that lower life. The features and properties as well as the quantitative predictions of these models can be further validated using the detailed microscopic models. The battery cell models may link back to the detailed microscopic properties of the battery.

Battery Module and Battery Pack Scale

The individual battery cells may be part of a battery module or a battery pack. These modules may consist of tens to hundreds of battery cells. This means that we are not able to model each battery cell in 3D using the porous electrode theory. Instead, lumped 0D and 1D models are used for the electrochemical behavior of each of the battery cells. These models may be validated and link back to more detailed battery cell models. The 3D geometry of the battery module or pack is used for computations such as thermal management, external current conduction systems, and macroscopic mechanical analysis of the battery system. The electrodes and separators are described as homogeneous materials with effective mechanical and thermal properties.

The M&S projects at this macroscale focus on the impact of module and pack materials, geometry, operating conditions, thermal management systems, macroscopic mechanical designs, and other design parameters.

Typical outputs from such models include temperature distribution; distribution of current and potential between individual cells; effects of temperature, charge, and discharge on the mechanical expansion of the different cells; effect of expansion as well as mechanical design on the mechanical integrity of the battery module or pack; temperature distribution as a result of the thermal management system with cooling and heating channels in the cell; impact of the design of the external current conduction system; and other aspects that may influence the battery module or pack. The models may also be used to design early warning systems of battery cell failure and thermal runaway in a battery system.

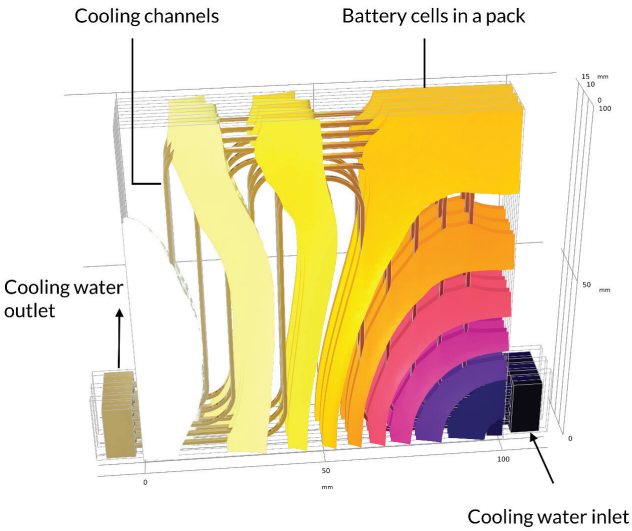


FIGURE 4 Section of a battery pack consisting of lithium-ion planar cells. The cooling channels are incorporated in the pack. The flow field and the temperature distribution in the pack is coupled to the electrochemistry for each of the cells. The electrochemistry for each cell in the pack is described with a 1D homogeneous model as described in Figure 2 (bottom). The 1D model for each cell is coupled to the heat transfer model in 3D. The pack model links back all the way to the detailed microscopic model through validation and parameter estimation.

TRENDS AND CONCLUDING REMARKS

The level of sophistication in a battery system model depends on the purpose of the battery system itself. Microscopic models are highly sophisticated and aimed at detailed understanding of the heart of the battery. A model used for the control of a battery pack as a part of an electric vehicle drivetrain may not and cannot have the same degree of sophistication. Instead, these may be lumped models that do not really describe the physics of the battery system.

However, even for large battery systems, there needs to be sophisticated methods for early detection of failure and for measuring state of health. These methods may be based and linked all the way from the lumped models to the microscopic model, where the high-fidelity models may be part of a central digital twin, residing in a central server, for that specific battery pack. The reason is that we want to be able to explain performance deterioration and we need to detect this, even if it is small, long before failure. It has to be possible to physically explain the reason for failure and performance decrease so that the detection, design, control, and operation of a battery system can be improved. Multiphysics M&S offers an unbroken chain of qualitative and quantitative validation of a battery system from its macroscale properties to the heart of the battery at the microscale.

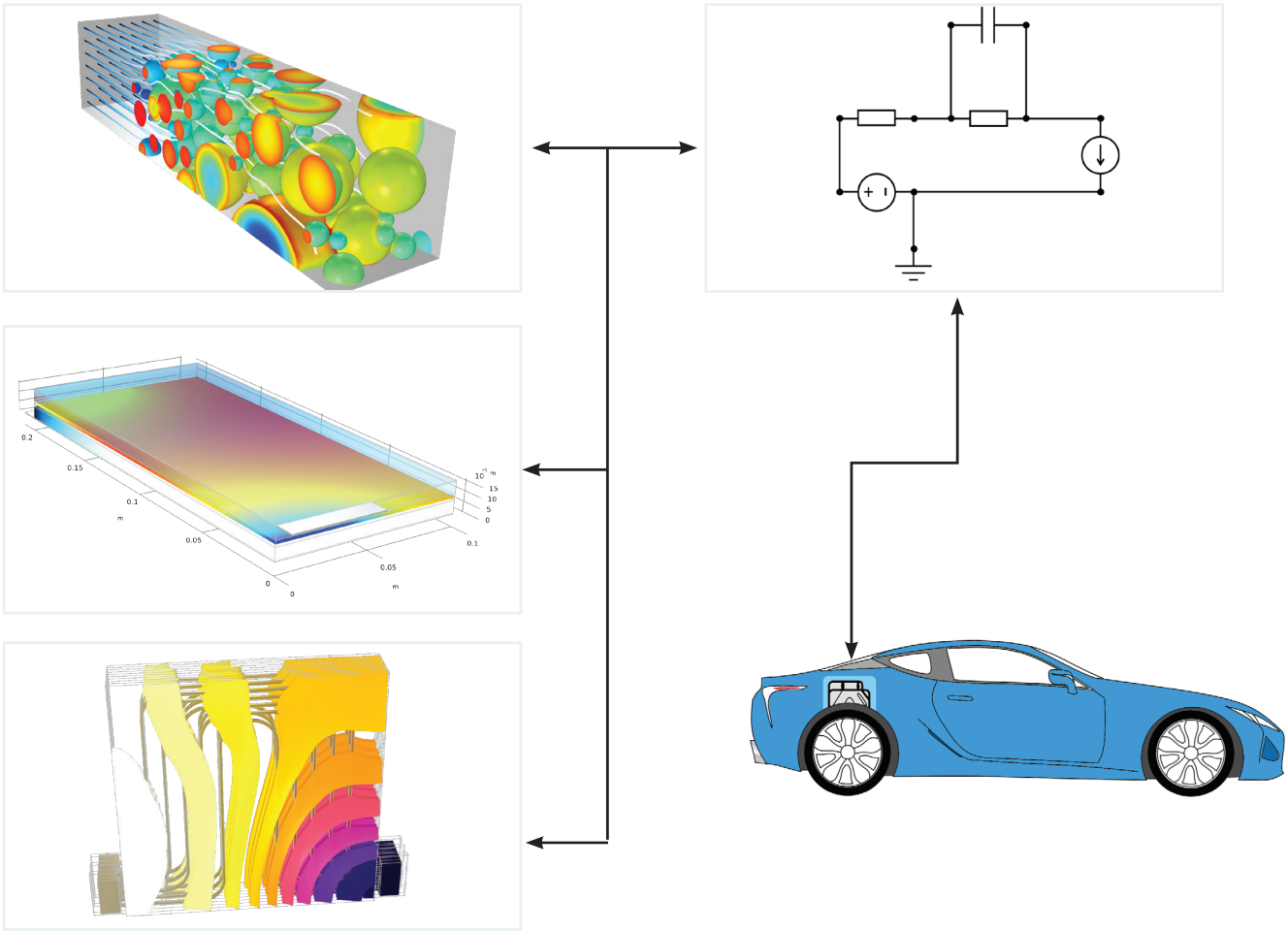


FIGURE 5 All levels of sophistication have to in some way be incorporated into the model of a battery pack in an electric or hybrid vehicle. This could be through validated lumped models that link back all the way to the fundamental properties of the battery cells, where the sophisticated models are part of a digital twin residing in a central server. The lumped model is in this case exemplified with an equivalent circuit but it may also be an advanced table look-up type of model obtained using machine learning techniques.

www.comsol.com

COMSOL