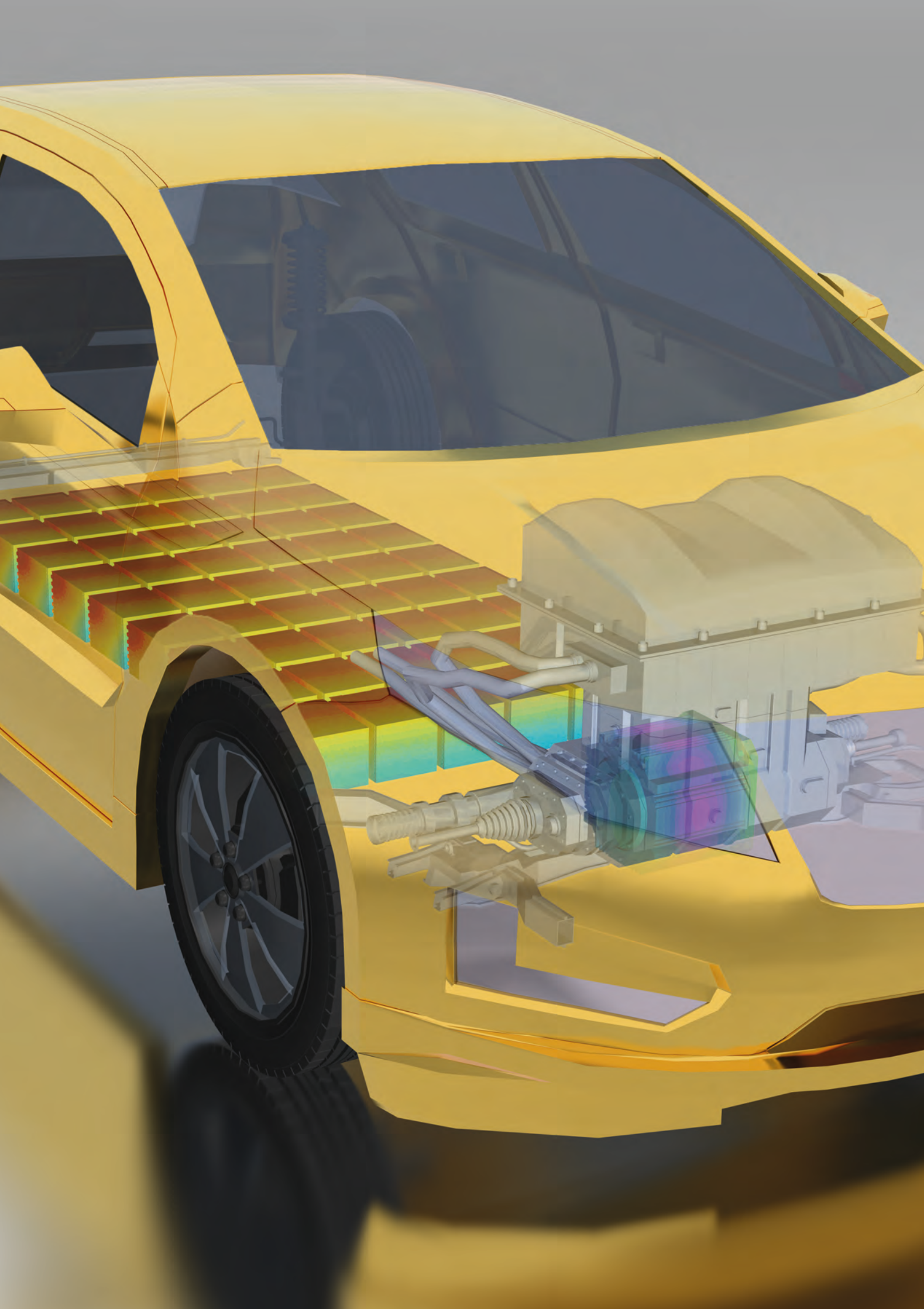


Driving battery innovation with CAE

Gaetan Damblanc – Siemens PLM Software

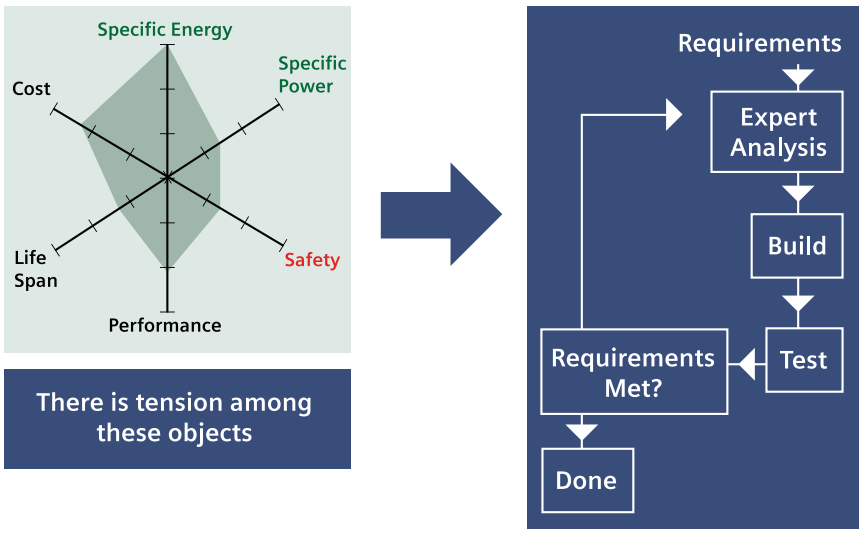


Figure 1: "Build and Break" conventional process to meet cell's requirements as seen on the spider chart

Introduction

The use of Lithium ion ("Li-ion") batteries is ubiquitous: they are used in phones, cameras, laptops, cars, watches, and more recently, hover boards. They are also used in larger systems, such as ships and airplanes. The demand for safe and high performance Li-ion batteries has never been higher.

Cell and battery pack manufacturers are continuously seeking higher energy density (or specific energy), higher power density (or specific power), safer products, longer lifespan and lower cost. Significantly improving a battery design across its whole operating range is a challenging task and involves the simultaneous optimization of numerous parameters. Large cell and pack producers know this very well: it is both cost and time-consuming to test and validate all the different material combinations. Accelerating the design process while reducing costs is an objective battery manufacturers are obsessed with and computer aided engineering (CAE) is part of the solution.

At the cell level, Battery Design Studio® (BDS), a powerful cell design software and cell testing platform, allows multiple cell designs to be assessed at a fraction of the cost and time usually required for experimental work. At the pack level, STAR-CCM+® Battery Simulation Module (BSM) predicts the complex electro-thermal behavior of the whole pack with high accuracy, a critical component for xEV powertrain design.

This way, hundreds of designs can be tested at low cost. However, virtually building each cell/module takes time and requires continuous analysis for the design to be improved. This can be done automatically by coupling BDS and BSM to design exploration and optimizing software, such as HEEDS™.

This article will demonstrate how a well developed, commercially available cell can

Figure 2: Cell being dissected to study tabs and electrodes designs

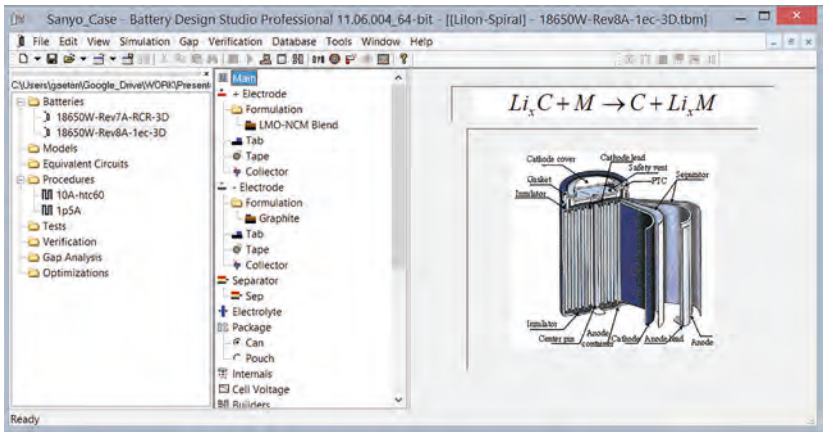


Figure 3: BDS user interface

still be improved by coupling BDS and HEEDS.

Cell description

The commercial cell considered in this study is a cylindrical cell of Type 36650, which means it measures 3.6 cm in diameter and 6.50 cm in height. It is a high power cell and the chemistry used for the cathode is a blend of Nickel Cobalt Manganese (80 percent) and Lithium Manganese Oxide (20 percent). The anode is made of graphite.

Because it is a high power cell, it can operate at very high current while still retaining most of its available energy. Typically, the power capability and the available energy are referred to as power density and energy density. These are the power and energy available per mass unit and are expressed in W/kg and Wh/kg, respectively. Battery cells are systems that cannot provide high power density with high energy density, one of the trade-offs in cell design. However, it is still possible to optimize the amount of energy such a high power cell can contain, which is the objective in this example.

Before starting the optimization, it is important to accurately characterize the reference cell in BDS, for example, specify the geometrical dimensions of each part, such as electrodes, coating, tabs, etc., as well as the physics-based performance model in order to predict the cell behavior. Additionally, tab design, electrode dimensions and coating formulations can be easily input in BDS' user-friendly interface.

Optimization 1: Energy density

With this reference cell built, the optimization work can start. Since the objective is to maximize the energy density (Wh/kg), the changes will be focused towards weight reduction and increasing the coating length in order to add more active material in the cell and therefore more energy.
The following design variables were selected for the study:

- Positive electrode: Length, number of tabs and current collector thickness
- Negative electrode: Length, number of tabs and current collector thickness
- Positive tabs: Width
- Negative tabs: Width

Each of these design variables evolve within relevant constraints so that they make both physical and manufacturing sense. The design exploration study will perform an analysis of 100 designs.
The results show a significant energy density increase, approximately 60 percent compared to the reference case (figure 5).

HEEDS has useful outputs to easily visualize the different parameter changes and highlight combination trends which give best results. This can be seen on a "Parallel Plot" like in figure 6. Highlighted by the green curve are the designs that achieve the highest energy density. The best results are achieved with low current collector thickness (Neg_CC_T, Pos_CC_T) and a high tab count (Pos_Tab_Num, Neg_Tab_Num). The yellow curve shows the combination for the best design, where it can be seen that energy density is much higher than that of the reference design highlighted in gray.

However, it can be seen that the best design has a higher material cost than the reference design. It would be ideal to have the best of both worlds, which is increasing the energy while reducing the cell material

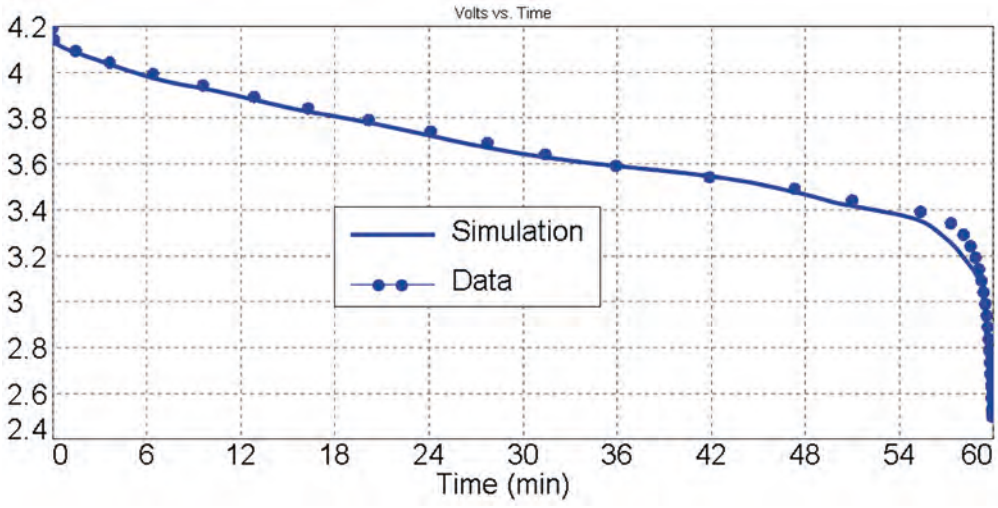


Figure 4: Cell voltage evolution during 1C discharge: comparison between simulation (solid) and experiment (dots)

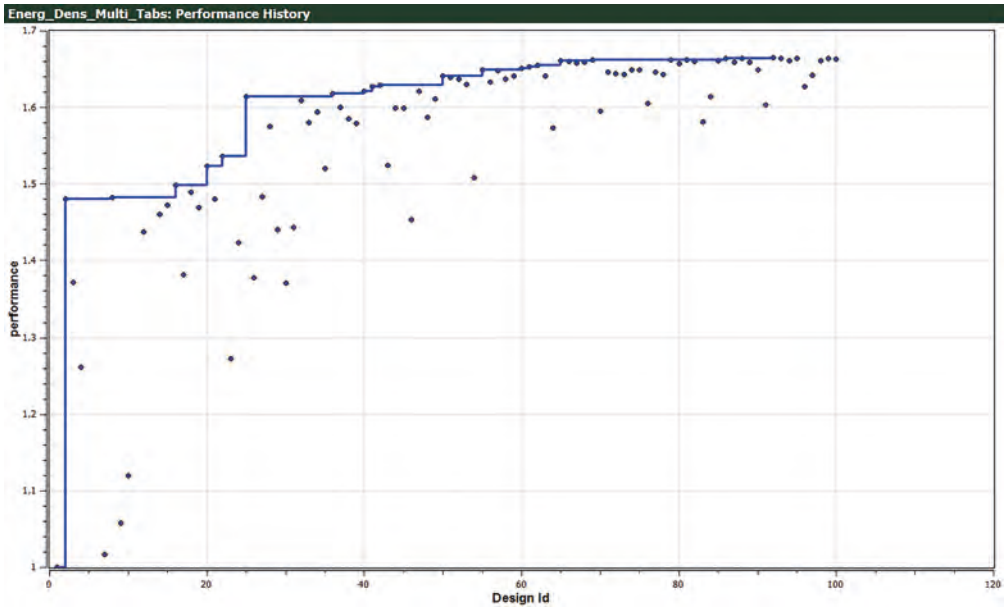
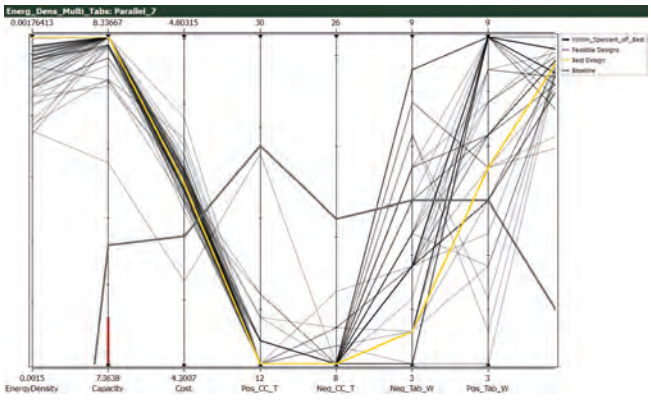


Figure 5: Performance (energy density) for each design

"The ability to automate the simulation set-up and computations brings a significant gain in productivity; the entire cell design exploration study was conducted in one day."



Designs	Energy density improvements (%)	Cost ($)	Capacity (Ah)	Pos_CC_T (mm)	Neg_CC_T (mm)	Neg_Tab_W (mm)	Pos_Tab_W (mm)	Pos_Tab_ Num	Neg_Tab_ Num
Baseline	-	4.49	7.71	24	16	6	6	4	4
85	60	4.4	7.71	30	10	5.4	8.4	24	15
119	31	4.32	7.79	28.7	8	5.4	8.4	24	5

Figure 6: Parallel plot - The three left parameters are inputs, the rest are responses. Gray is reference design, yellow is best design (top left)

Figure 7: Pareto front plot - This graph plots the set of optimum designs as a tradeoff between energy density and cost. The black line serves only as an indicator to show the Pareto front. The gray square is the reference design. Circled in blue are designs 85 and 119 discussed here (top right)

Table 1: Best designs from Pareto front analysis

price at the same time. This is the objective of the next optimization study.

Optimization 2: Material cost versus energy density

For the second study, in addition to the inputs of the previous study, the material cost is also incorporated, something which can be handled by BDS. The design exploration study becomes a multi-objective study in which energy density will be maximized while cost is minimized. The optimal result will not be one single best design but a set of best designs. This will yield a Pareto front showing a trade-off of optimum designs between energy density and cost.

From this Pareto front two designs were selected (out of nine) that match both requirements in terms of energy density and cost as seen in table 1.

Designs 85 and 119 both show increases in energy density compared to the baseline design. Design 85 is closest to the best design in the previous study in terms of energy density but shows a $0.09 material cost reduction. It may appear as a small improvement, but when multiplied by hundreds of thousands or millions of cells produced, this has an impact. Alternatively, if one is looking at higher cost savings, design 119 is a good choice with $0.17 cost reduction, but still offering a 31 percent energy density increase.

Conclusion

Improvements into modeling of Li-ion cell behavior have made associated CAE a powerful design tool. It allows for a tight coupling between the electrochemical and thermal problem which provides great accuracy in predicting these complex systems.

The ability to automate the simulation set-up and computations brings a significant gain in productivity; the entire cell design exploration study was conducted in one day. Design exploration using BDS and HEEDS enables optimized cell performance by incorporating both physical and cost performance objective analysis, resulting in better designs, faster based on a number of related parameters that would be time-consuming to achieve in a manual approach. This demonstrates that CAE software is a powerful tool to design and size cells and packs, not only because of the tight coupling between the electrochemical and thermal aspects of the problem at hand in these complex systems, but in the way design exploration studies can be used to rapidly analyze the design space.