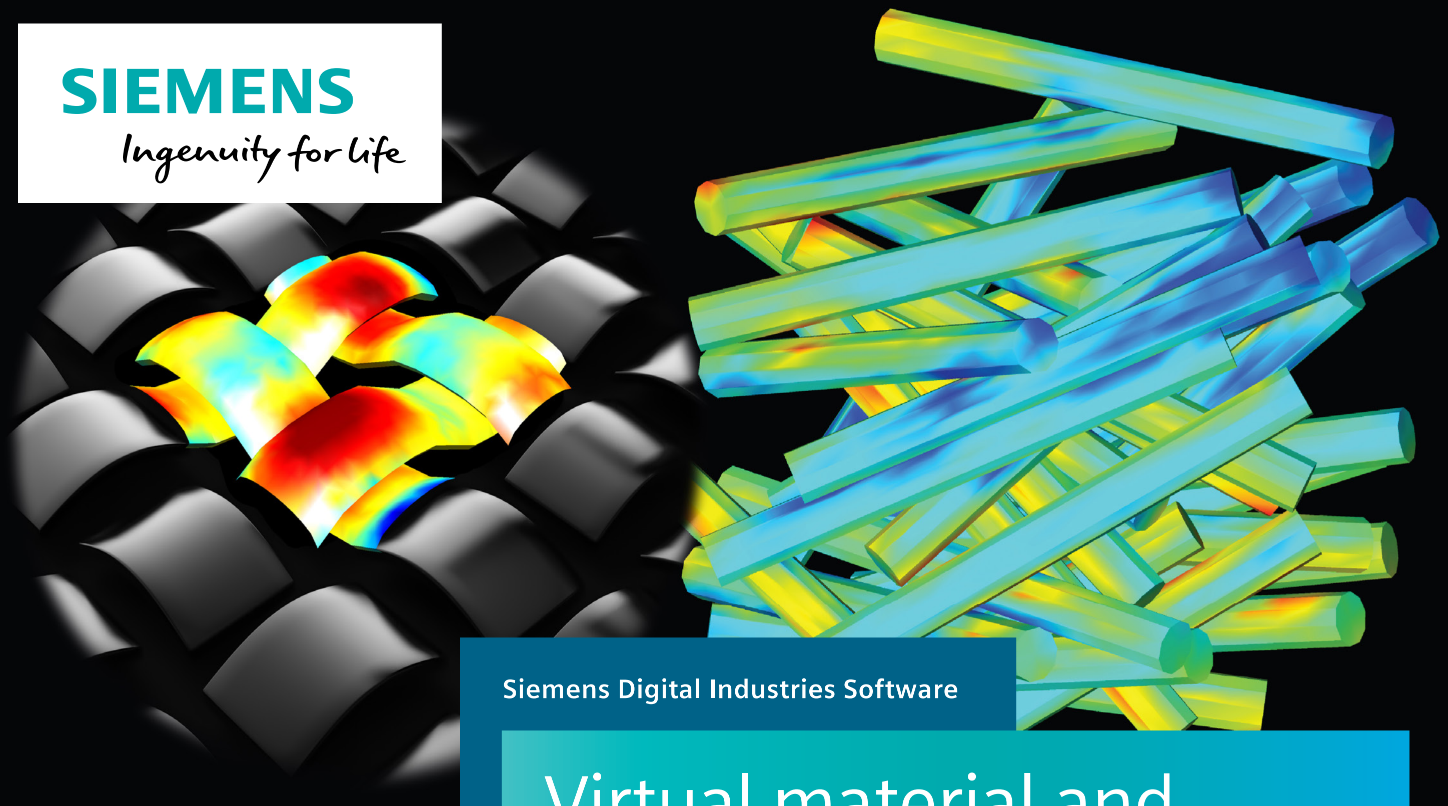

Siemens Digital Industries Software

Virtual material and product design

Simcenter 3D helps manufacturers comply with regulations and meet customer expectations

Executive summary

Materials innovation is critical for improving performance and reducing the cost of products. However, the amount of physical testing required to develop and certify new materials challenges the speed at which new materials innovation can be introduced. Due to recent advances, there is a reliable and efficient way to accurately predict behavior of complex multi-scale, multiphase material systems, enabling more efficient materials innovation in various industries. This white paper describes how new adaptive multiscale modeling technology, which is employed by Simcenter™ 3D Materials Engineering software, helps the virtual design of materials and complex products. Adaptive multiscale modeling facilitates speed without losing accuracy as compared to state-of-the-art 3D simulation methods based on the finite element analysis (FEA) method.

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Introduction

Today we see new materials being introduced to the market at unprecedented speed. Nearly 70 percent of product innovation relates to material innovation.[1] This can be the formulation of a new chemical, a new combination of existing materials, the enhancement of an available material or a new manufacturing method such as additive manufacturing. According to CIMdata,[2] two technologies that contribute to the innovative potential of generative design are additive manufacturing and advanced materials.

The global advanced materials market is expected to reach $2 trillion by the end of 2024,[3] with a compound annual growth rate (CAGR) of about 6 percent. The impact of new materials on the manufacturing industry production is factors larger, as the new materials enable lightweight, efficient and clean technologies to be used in products, thus impacting their compliance with regulations and customer expectations.

Huge costs and efforts are involved in materials design and development. An aerospace company may spend up to 10 years and $50 million (M) to develop a new material. However, this does not guarantee the new material will pass the physical testing and be certified for the aerospace sector. This underlines a clear need to virtually design and validate the performance of new materials as part of complex products. This drastically speeds up the design while lowering costs compared to a fully test-based approach, essentially a trial-and-error approach to manufacture prototype products and experimentally analyze them.

Simcenter 3D software, which is part of the Xcelerator™ portfolio, the comprehensive and integrated portfolio of software and services from Siemens Digital Industries Software, provides a response to this challenge with the new Simcenter 3D Materials Engineering module. It employs multiscale modeling technology that takes material information at the microscale into account along with the broader part model. This technology helps improve the virtual design of materials and complex products by delivering speed without losing accuracy compared to state-of-the-art 3D simulation methods based on the FEA method.

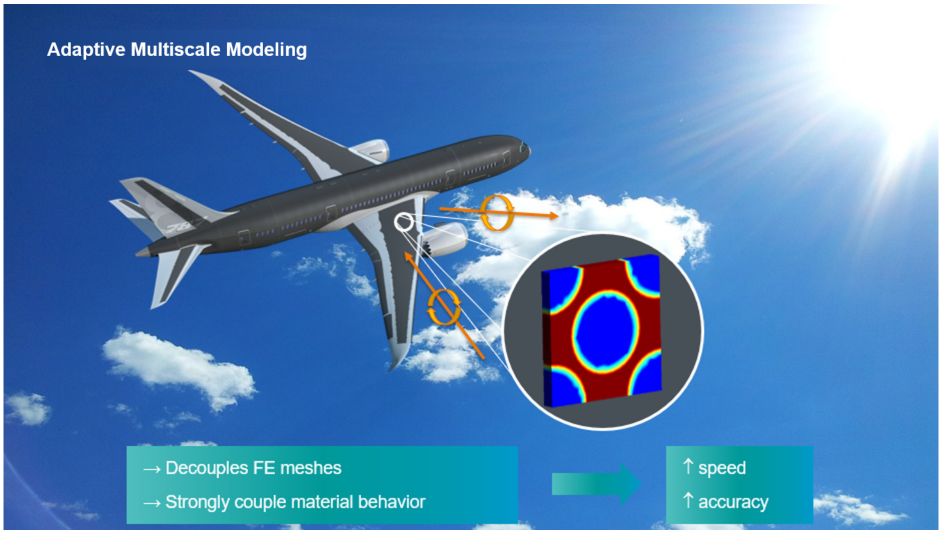


Figure 1. Adaptive multiscale modeling for product materials engineering and design.

Materials engineering challenges

Companies continue to look for ways to improve product performance and/or lower costs while ensuring business continuity and employee safety. Most companies are looking for disruptive technologies to set their business apart from competition. Innovation is key to the survival and growth of all companies. Product and materials innovation are closely linked, with product innovation relying almost 70 percent on materials innovation. Therefore, it's clear that developing new materials or innovative applications of existing materials are of paramount importance for the manufacturing industry. Digitalization is another booming trend, enabling manufacturers to virtually carry out ever more operational work and to deliver innovative services. Real progress is made where materials innovation meets digitalization.

Currently, materials innovation is inefficient, especially in adopting new materials. Developing and certifying new materials is a long and expensive endeavor. Part of this is due to extensive physical testing requirements, which are necessary as engineers often don't understand the failure mechanisms.

Computer simulation offers an efficient way to minimize the amount of required physical testing. However, traditional simulation technology has not been developed for complex multiscale multiphase materials. Materials innovation usually occurs at the microscale level by fine-tuning properties of individual constituents, changing their formulation or by reinforcing specific constituents with nanoparticles or fibers so they are multiphase materials.

Another important factor is the weakness of materials lies in existing manufacturing-induced defects; those defects are usually only noticeable at the microscale level. The material's microstructure is therefore its DNA.

A simulation model should hence take into account the material information from the microscale level upward, which results in prohibitively large models for traditional simulation technology. What is needed is a method that is fast enough for materials design engineering purposes without losing accuracy. Siemens presents a fully coupled and adaptive multiscale modeling technology for this purpose. This essential technology offers value for material and product manufacturers in four main use cases: (1) material design, (2) virtual coupon testing, (3) part design and optimization and (4) account for the effect of the manufacturing process on the structural performance.

Adaptive multiscale modeling technology is at the heart of the new Simcenter 3D Materials Engineering software, which enables multiscale modeling and simulation of failure in advanced materials in the Simcenter 3D environment. Using Simcenter 3D Materials Engineering, one can identify when, where, how, and why a material may fail at the microstructural level and subsequently predict how this will affect the performance of the overall part. Simcenter 3D Materials Engineering comes with a full suite of tools for fast and accurate modeling and simulation of the product performance using adaptive multiscale technology.

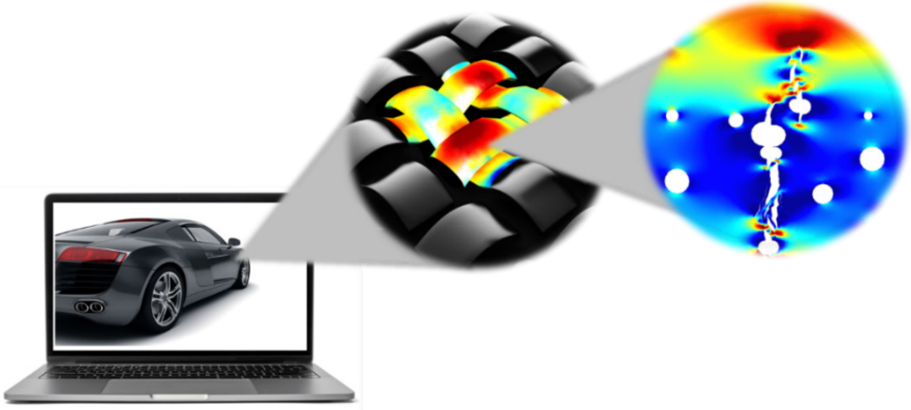


Figure 2. Failure starts at the microscale level and propagates to larger scales.

Materials engineering context

In industry, the development and adoption of new materials can be complex and time-consuming. Part of that is due to extensive physical testing required by a conventional approach,[4] see figure 3. The physical tests are needed because engineers often don't understand well enough how new materials will behave and fail.

Let's go into detail about what this conventional approach means for materials engineering challenges. The pyramid approach shown in figure 4 is valid for a wide range of materials applications.[5]

Materials engineers typically apply an iterative hybrid test simulation process that builds on the knowledge at the material level studied at the coupon stage. For the case of product design based on continuum fiber-reinforced composites (CFRC) materials, the largest number of tests are performed at the coupon stage. The aim is to generate a material database covering design-critical aspects such as stiffness, strength, manufacturing effects, variability and environmental effects. For experimental characterization of the basic mechanical behavior of CFRC and obtaining their material properties and allowable statistical ranges, a minimum of nine different coupon tests are required for each layup while treating a composite material as a homogenized laminate. The testing effort explodes once design factors are considered, such as damage tolerance or environmental aspects. For example, for two design factors and five stacking sequences with three repetitions, the total effort is equal to 270 mechanical coupon tests.

This conventional approach is prohibitively costly if one wants to explore new materials and optimize microstructural design variables that certain manufacturing methods allow us to control. It can take up to 10 years and $50M to develop a new material for the aerospace industry; and that does not include the original equipment manufacturer (OEM) investment to certify the new material and put it in an airplane. For other industries such as automotive, the cost is typically lower but still significant, with elapsed time ranging from months to years and the cost ranging from $500,000 up to millions of dollars.

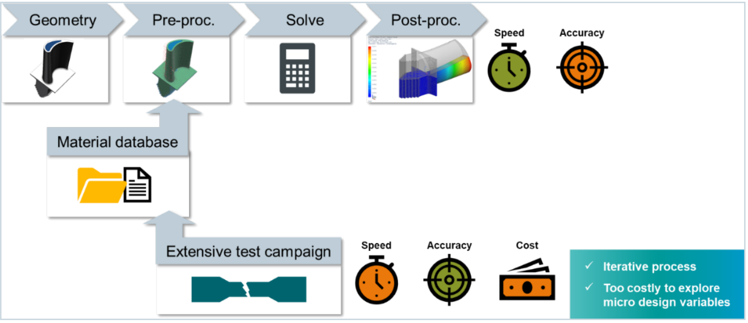


Figure 3. Conventional approach: structural performance simulation for materials engineering as part of product engineering.

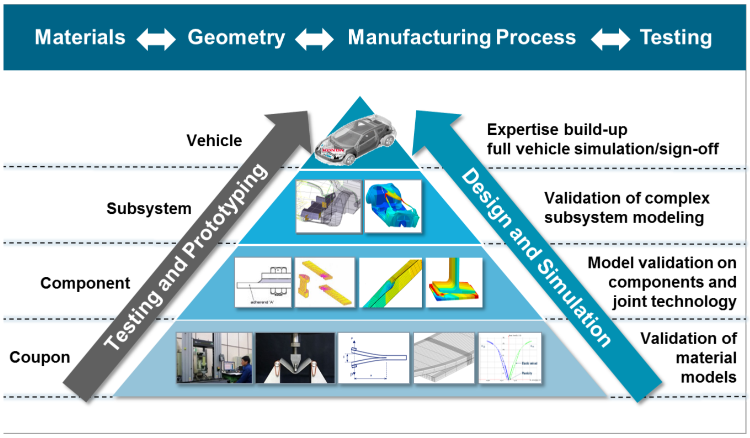


Figure 4. The pyramid approach to multiscale modeling and validation testing for automotive structures applications.

Using digitalization to accelerate materials innovation

Clearly, industry needs to be able to accelerate innovation and adoption of advanced materials. Digitalizing and virtualizing materials innovation is essential for this. This trend is ongoing and it can be accelerated by increasing the trust in modeling, providing more accurate models and advancing verification and validation procedures and data.[6]

Looking closer at smaller length scales (see figure 5), it becomes clear there are many complex mechanisms at play: for example, voids may be created during manufacturing; cracks may initiate and propagate in the fiber, matrix or fiber/matrix interface; fibers can exhibit anisotropic nonlinear behavior and matrix materials are typically time- and temperature-dependent. In such materials, each individual constituent has unique behavior, and on top of that the geometric architecture plays an important role.

In the end, it is a similar problem that engineers faced about 60 years ago with the design of complex geometries, which resulted in the invention of the finite element method (FEM).[7,8] However, for addressing the advanced materials engineering challenges of today and tomorrow, something other than standard FEM is needed, which is fully adapted to including material behavior at smaller length scales. For this purpose, Siemens offers an FEM-based solution to model the microstructure of the material, which can be applied to virtually any type of material. To accelerate the workflow, an automatic generator of microstructures is provided for a variety of architectures, including continuous and chopped fibers, particulates, shells, voids, textiles, etc. The list keeps expanding as more and more applications for the technology are identified. However, with the capability to model various complex microstructural behavior, a bigger challenge should not be forgotten: How do we link the microstructure to the product length scale?

Even though it would be interesting, modeling microstructural details explicitly in the part-level finite element (FE) mesh is not feasible. Instead, we use homogenization techniques to decouple the different length scales: Use smaller representative models of the microstructure, but still strongly couple the material constitutive behavior.

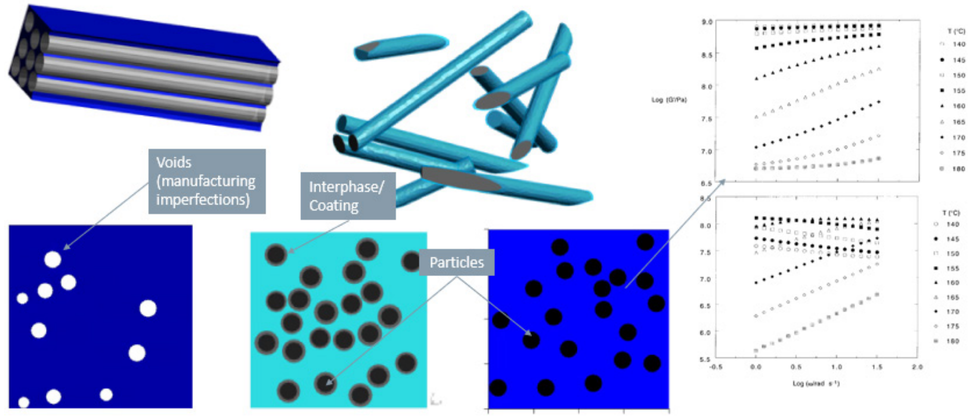


Figure 5. Looking closer at CFRC – complex geometry and behavior: fiber, matrix, coating, interfaces, etc.

Siemens Digital Industries Software uses FE technology as a basis for modeling the microstructure[9] for the adaptive multiscale approach, adopting an approach that is both efficient and accurate. This innovative technology is the core of the new Simcenter 3D Materials Engineering solution, which was enabled by Siemens' acquisition of MultiMechanics.[10] By embedding accurate virtual coupon testing and adaptive multiscale modeling in the materials engineering workflow (see figure 6), microstructural design variables can be embedded naturally, which is a crucial factor for materials innovation. The new workflow enables the optimization of material and product part at the same time.

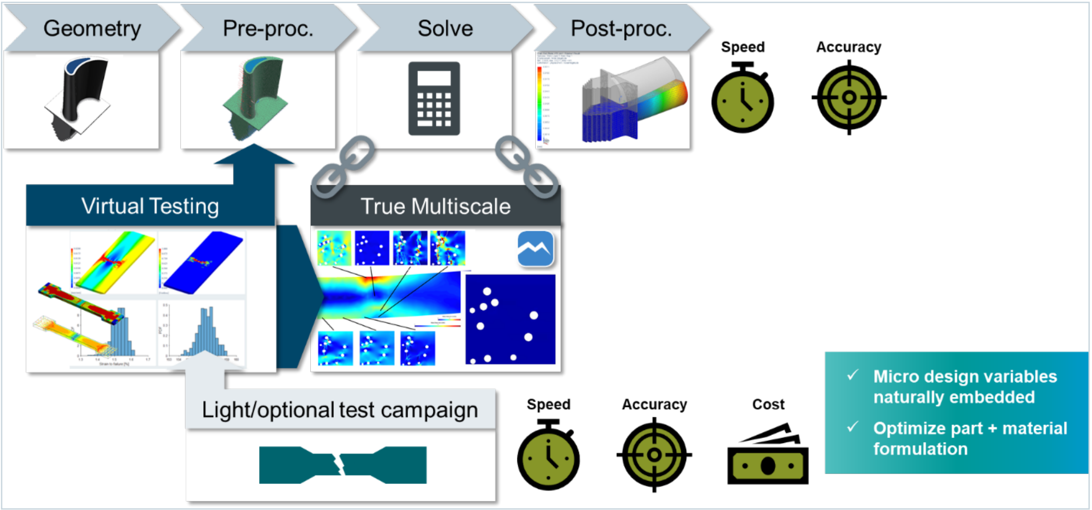


Figure 6. New Simcenter 3D Materials Engineering workflow.

Established approaches for materials modeling

Multiscale modeling

Multiscale modeling is a broadly used term to describe any situation where a physical problem is solved by capturing a system's behavior and important features at multiple scales, particularly multiple spatial and/or temporal scales. Applications for multiscale analysis include fluid flow analysis, weather prediction, operations research and structural analysis, to name a few.

For advanced materials modeling, a predictive simulation software must be used to account for all microstructural details in a realistic manner. The software must also be used to link the microstructure behavior back to the product performance. Moreover, the product design and material microstructural behavior must be tightly coupled. Even though some analytical solutions exist for problems involving heterogeneous media, they exist only for simplified geometries and material behavior so numerical solutions are often necessary. However, it is typically not justified to perform direct numerical simulations that account for all heterogeneities, as this necessitates an unreasonable amount of computer power.

These limitations have led researchers and engineers to seek alternative approximate approaches that can account for the hierarchical structure of heterogeneous materials without having to model every microstructural detail. One of the most promising approaches is multiscale modeling, aimed at calculating material properties or system behavior on one level using information or models from different levels. This partly overcomes the computational issue of modeling all heterogeneities at once, thanks to decoupling widely separated length scales. The microstructural features must be small in comparison to the smallest characteristic length scale of the product in order for the homogenization assumptions to be satisfied. Fortunately, that condition is usually met for fiber reinforced composites, and many other advanced materials.

Impossible to consider the fibers in a **single scale mesh**

- How long to mesh?
- How long to solve?
- How much memory?
- How many CPUs?

Figure 7. Too many details for a single FE model, elaborating the need for multiscale modeling and simulation.

Multiscale modeling in practice: RVE and homogenization step

The most efficient structural analysis solution of a complex mechanical structure is to use multiscale FE analysis to divide and conquer the problem. To accomplish this, a local scale model of the material microstructure – the representative volume element (RVE) – is embedded within the global scale FE model of the entire structure. The different scales are analyzed simultaneously and the behavior of one level affects the behavior of the other. This involves a detailed calculation of the RVE model, and a homogenization step to obtain the mechanical properties that are used at the higher level.

The goal of homogenization is to obtain the overall material behavior for a RVE by satisfying the Hill-Mandell energy consistency condition,[11] which requires that energy is conserved across scales. The RVE is defined as the minimum material volume for which one can capture the relevant overall material behavior. In other words, an RVE must be statistically homogeneous.[11] From the practical point of view, one must also accept approximations to allow smaller RVEs to gain in computational efficiency. The assumption of separation of length scales comes down to a practical definition that allows one to apply uniform boundary conditions to the RVE that satisfies the Hill-Mandell condition. Therefore, the RVE size may be similar, or a few times smaller, than the product length scale.

Although the classical homogenization theory aims to determine the homogenized constitutive behavior of heterogeneous materials a priori, the purpose of concurrent multiscale methods[12,13] is to perform simultaneous analyses on all length scales. The material overall properties are calculated a priori without knowing the loading history. Therefore, in cases where the microstructure does not change and its behavior does not depend on the loading history so the effective constitutive properties need to be determined only once, spatially and in time, the classical homogenization theory is more cost-effective.

Multiscale models are particularly advantageous for problems with evolving microstructure, especially when formation, crack growth and/or rate- and time-dependent behavior is considered, as the microstructure evolution is both spatially and time dependent,[13] which poses a big challenge.

Finite element squared methods

Finite element squared (FE^2) methods can be used for the analysis of heterogeneous materials at the continuum macroscale, while simultaneously accounting for the microstructural details.[14] FE^2 is a concurrent multiscale approach, with analyses comprising two levels of FE simulations that are performed concurrently. The behavior of heterogeneous structures is described with FE models at both the macro and micro scales (this is the origin of the name FE^2). At each integration point on the macroscopic scale, an RVE is assigned and a separate finite element computation is performed simultaneously. The macroscopic behavior is thus deduced from the nonlinearities in the behavior of the associated microstructure.[15, 16] The model is built using three main ingredients:

1. The mechanical behavior at the lower scale (the RVE).
2. A localization rule, determining the local solutions inside the unit cell for any given overall strain.
3. A homogenization rule, yielding the macro-level stress tensor from the micro-level stress rate.

Because the microstructure is an FE mesh, all standard analysis techniques, failure theories, constitutive models, etc., can be easily applied. For this reason, FE^2 is known to be flexible and highly accurate, but is often regarded as too expensive to be practical in full component designs and optimizations. In cases where nonlinearity is modeled, it is as if the number of computations required for standard FE analysis is being squared.

FE^2 and other concurrent multiscale approaches attach one RVE to the integration points of selected finite elements, usually in the regions more prone to damage. Industrial applications may require up to millions of independent RVEs to realistically predict failure. The FE^2 method can reach the required accuracy in the analysis, but for complex mechanical structures, the data and central processing unit (CPU) requirements become excessive.

The core of Simcenter 3D Materials Engineering

Adaptive multiscale modeling methodology

Thanks to significant improvements in computer capacity and to the development of a new mathematical framework[17,18,19] and adaptive multiscale schemes[4,20] tailored for this type of analysis, it is possible to solve industrial-scale problems with a concurrent multiscale FE approach.

The adaptive multiscale modeling approach is brought to market exclusively by Siemens. It retains the accuracy of FE^2 with much higher computational efficiency. It has been shown this approach can be as accurate as FE^2, while up to 1,000 times more efficient than traditional FE^2.

Just as in FE^2, the multiscale modeling approach allows materials and product engineers to explicitly model microstructural details, capture local progressive damage and show the fusion of local scale phenomena into global scale phenomena. The adaptive multiscale modeling approach naturally has the same amount of flexibility and accuracy found in the widely accepted FEA and FE^2 methods. With this approach, engineers are able to perform component and subcomponent designs with production-quality run times and put the accurate and efficient model in a loop to perform optimization studies.

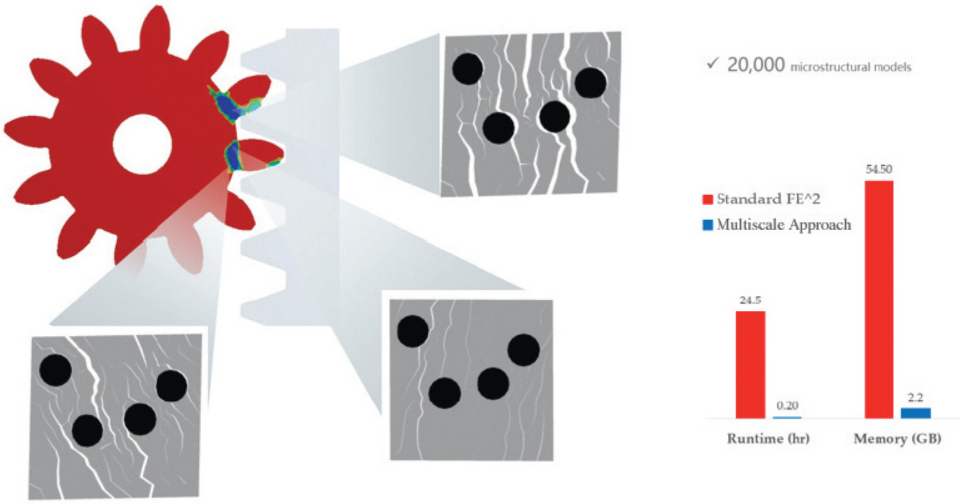


Figure 8. Performance benchmark for a cast iron gear with microscale impurities. Multiscale simulation performed coupled: gear FE model solved and microstructural FE models solved by a multiscale approach.

The adaptive multiscale modeling methodology is based on two breakthrough innovations, which are combined into a multiscale solver that provides unprecedented speed without sacrificing accuracy. Additionally, the solver is fully parallelized across threads and CPU cores to achieve even higher gains in performance. The two breakthrough innovations are:

- **A new mathematical formulation**[18]**:** The key outcome is that no load case has to be evaluated in order to calculate the RVE model for obtaining the relevant material properties, whereas FE^2 requires that six load cases are evaluated. This accounts for a six-time speed up of multiscale modeling (compared to FE^2) without accuracy loss.
- **An adaptive multiscale algorithm**[4,20] **:** This is a proprietary new algorithm, which makes the multiscale modeling technology another 100 to 200 times faster than FE^2, depending on the model of interest. An accuracy tolerance can be specified by the user, allowing him/her to balance accuracy versus speed.

The goal of adaptive multiscale modeling is to deliver speed without losing accuracy.

Fully coupled adaptive multiscale modeling is an extension of FE^2 (making FE^2 fast enough for industrial applications).

Adaptive multiscale modeling example: gear model

For a cast iron gear example case, the aim is to evaluate the effect of impurities in the cast iron, as shown in figure 8. The gear model has 35,142 degrees-of-freedom; each of the microstructural FE models initially had 944 degrees-of-freedom, which results in a total of nearly 19 million degrees-of-freedom for the entire simulation. Note the various independent cracks automatically inserted into the FE models – so the number of degrees-of-freedom in each microstructure increases as the simulation progresses.

This model has been used as a benchmark simulation case with 20,000 independent microstructural FE models attached to integration points of the product's FE mesh. It solves in less than 11 minutes using 2.2 gigabytes (GB) of memory on a 3.5 gigahertz (GHz) Intel i7 laptop computer running on a single CPU core (the software is fully parallelized for clusters and multi-threading). The error due to adaptive multiscaling was within 5 percent.

The two-way coupling between micro and macro scales is critical for highly nonlinear problems because the loading history may induce microscale damage and reduce material stiffness, which in turn will redistribute the loads at macroscale and change the loading history in the next solution step. It is the continuous communication between the scales that brings unprecedented accuracy to the model.

Fully integrated simulation platform

Simcenter 3D is a fully integrated simulation platform for modeling, simulating and analyzing complex engineering products. It combines the legacy strengths of the LMS, Samtech and NX™ CAE software products in one platform, offering the leading structural FE solvers Simcenter Nastran® software and Simcenter Samcef® software, and new capabilities as the electromagnetic simulation solution from Infolytica Corporation, part of Mentor Graphics, acquired by Siemens in 2017.[20] Simcenter 3D also links to third-party solvers such as Abaqus, Ansys and LS-DYNA.

Siemens is the only computer-aided engineering (CAE) software provider that supports FE^2 with high computational efficiency and accuracy for all major FE solvers, enabled by the Simcenter Multimech adaptive multiscale technology, which is now the key part of the Simcenter 3D Materials Engineering solution of Siemens.[10] Simcenter 3D Materials Engineering[21] consists of a unique multiscale FE software platform that extends the flexibility and robustness of the FEM down to the microstructural level, strongly coupling the part (macro) and material (micro) length scales response and integrating key material design variables with part design, making materials act like a degree-of-freedom.

The core FE solver is called Simcenter Multimech, a full-featured nonlinear finite element solver capable of performing two-way coupled adaptive multiscale analyses of parts and streamlined virtual testing of material microstructural models, as shown in figure 9. The Simcenter Multimech multiscale solver technology is based on the two breakthrough innovations – the new mathematical formulation and the adaptive multiscale algorithm, which together provide unprecedented speed without sacrificing accuracy.[9,22] It is fully parallelized across threads and CPU cores to yield even higher gains in performance. Simcenter Multimech can be coupled with Simcenter Nastran and Simcenter Samcef as well as third-party FE solvers.

Simcenter 3D Materials Engineering allows accelerating the product development lifecycle by accurately accounting for microstructural details, defects and manufacturing-induced variations, as well as predicting failure in advanced materials. It enables manufacturers to implement advanced materials in their designs and make their products lighter, stronger and more durable. Simcenter 3D provides a complete set of features and digital workflows for multiscale modeling and simulation capabilities, thus enabling it to identify the root cause of failure in advanced materials by zooming into the materials microstructure. It is used by companies working with novel materials to reduce development time and costs by virtually testing how damage at the microstructure could lead to part failure and learning how controllable manufacturing conditions can lead to performance improvements. Simcenter 3D also helps streamline the simulation process of structures made from laminate composite materials.

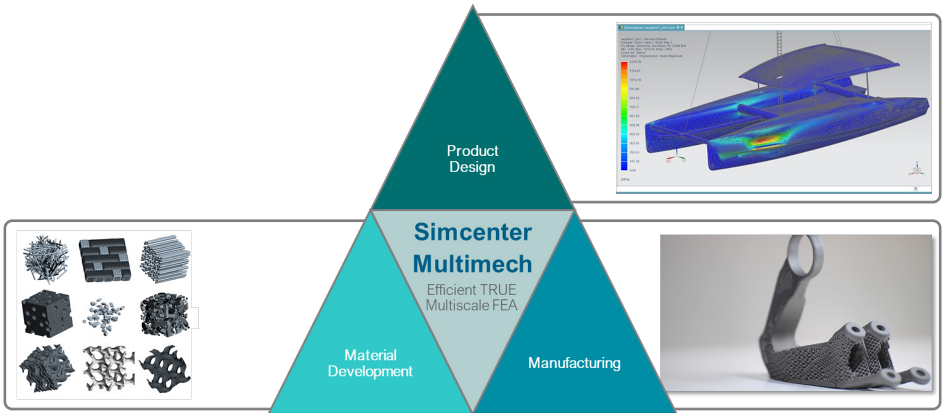


Figure 9. Simcenter 3D Materials Engineering and Simcenter Multimech: Taking into account manufacturing process variations into the materials models and performing enhanced structural analysis using homogenization and efficient two-way coupling.

Case study 1: CMC material design at DLR

Challenge

Ceramic matrix composites (CMCs) consist of fibers embedded in a ceramic matrix. The fibers can consist of carbon fibers or be made of ceramic material. CMCs have been designed to overcome the problems associated with conventional ceramics such as alumina, silicon carbide and aluminum nitride, which fracture easily under mechanical or thermomechanical loads due to cracks that are initiated by scratches and other small defects (see figure 10). CMCs are used in challenging operational environments, including high thermodynamic loads in energy and aerospace applications. This first case study is taken from the daily practice at DLR – the German Aerospace Center. The team wanted to understand how temperature change would affect the material microstructure and consequently the material behavior.[23] The initial problem was modeling cracking, which typically occurs during manufacturing due to a fast drop in temperature. To investigate this, DLR models the process of pyrolysis, an intermediate step in production of ceramic matrix composites. Key material design questions are:

- Determine how to optimize fiber/matrix interface properties
- Determine which manufacturing conditions would be acceptable to avoid early micro-cracking

Solution

Adaptive multiscale modeling technology has enabled DLR to design the right CMC material with favorable thermomechanical properties. Our automatic cracking approach combined with stochasticity embedded in the Simcenter Multimech solver has enabled DLR to answer material design questions. This allowed DLR to model microstructural cracks and determine how they would affect the overall part[23].

Results and benefits

A visual correlation between scanning electron microscope (SEM) images and simulation results determined that Simcenter Multimech accurately characterized the trend in crack area and frequency in these CMC materials. This trend was even captured for fibers and matrices with different interfacial strengths. The newly designed material has resulted in a 30 percent increase in productivity, with an estimated 50 percent time and cost saving. Also, by using accurate virtual material characterization, the DLR team has been able to significantly narrow down the number of material combinations needed to be physically prototyped. In one example, they only selected the three best candidates out of 30 possible combinations of fibers, matrices and manufacturing conditions.[4]

This is a great example of accelerating materials innovation with predictive simulation! Overall, material design with Simcenter 3D Materials Engineering has been proven to be crucial for future CMC components produced by DLR, including nozzles for rockets and thermal protection systems for re-entry vehicles amongst other applications.

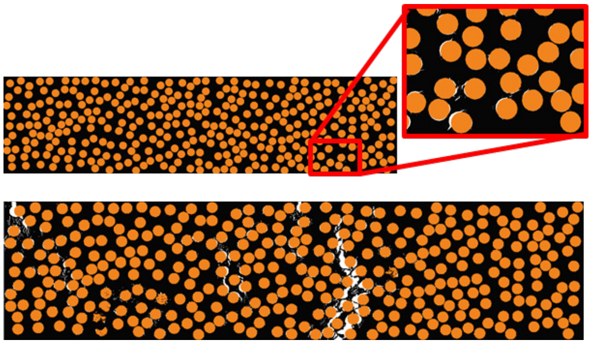


Figure 10. Example of CMC material: matrix and fiber detail (top) with crack growth result (bottom)

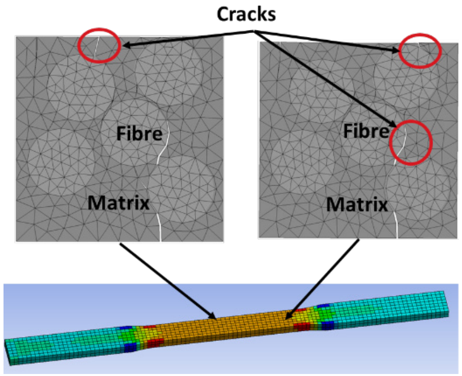


Figure 11. Multiscale analysis correctly predicted composite properties when altering interfacial strength of the fiber and ceramic matrix.

Case study 2: Virtual coupon testing at Solvay

Challenge

Recall that developing advanced aerospace materials can take five years and costs material suppliers up to $50M. This is partly due to the cumbersome material testing process, resulting in stagnation of new material development for the entire industry. Replacing testing with computational analysis is a goal for many, but it is complicated by the unique behavior and challenges of composites.

Scientists at Solvay knew that simulation would be crucial for getting new materials developed faster and at lower cost. They needed a platform to process inputs such as fiber volume fraction, fiber orientation, interface effects, resin ductility and material variability, in order to properly define and test their new materials. Furthermore, Solvay needed a tool to quickly provide insight on how changes at the constituent material level affect the overall mechanical performance at the composite level. Physical testing of new composite materials is often cumbersome, and most new material designs do not behave as intuitively expected during physical testing due to competing mechanisms and complex failure modes.[24]

Solution

With its integrated Simcenter Multimech solver, Simcenter 3D Materials Engineering enabled the team to test the effect of inputs they changed during the material development process. It accurately predicted composite failure by accounting for multiple competing damage mechanisms such as fiber rupture, resin cracking and fiber-resin debonding. The rate dependency of materials was also captured, allowing Solvay to fine-tune a given material to perform as expected under distinct loading scenarios. Most importantly, the team obtained insight not only into when the material would fail, but also why. Engineers can successfully create new materials as well as improve them over time. The software provides the required understanding of when, how and why materials fail, and helps mitigate it.[25]

Results and benefits

As shown in figures 12 and 13, the 10-degree tensile test simulation demonstrates matrix shear failure. With visual failure analysis of experimental specimens and correlation with stress-strain data, this model demonstrates high efficacy and accuracy. The other standardized tests, including longitudinal and transverse, also show this agreement of failure modes.

Solvay has been using the core Simcenter Multimech solver technology and platform for years with the main goal of reducing the time and cost to develop and certify new materials, especially fiber-reinforced polymers. Solvay reports they have gained valuable insight into how their materials behave from a microstructural perspective and how damage at the microstructural level links to overall part or system behavior, estimating 40 percent time and cost reduction when applying multiscale simulation workflows.[4]

“The accuracy and speed afforded by Simcenter Multimech is changing the way we develop new materials and interact with our customers,” says Nicolas Cudré-Maurpoux, chief technology officer (CTO) at Solvay.

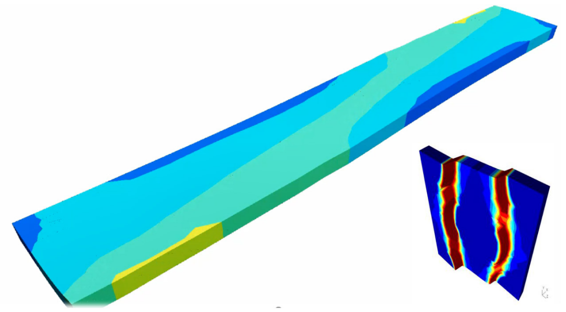


Figure 12. Virtual results for a 10-degree standardized composite coupon test with the RVE (right) undergoing severe in-plane shear damage.

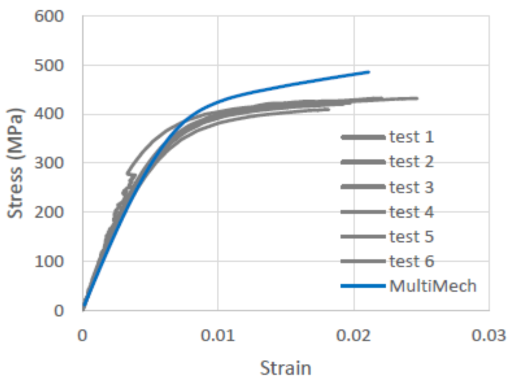


Figure 13. comparing Simcenter Multimech with multiple experimental tests.

Case study 3: Using HEEDS to optimize the lattice structure

Challenge

Additive manufacturing facilitates design freedom for optimizing the structural and thermal properties of 3D printed parts. One design concept, repeating lattice structures, assists in light-weighting components in areas with low structural loading.[27] Predicting part performance of a component that comprises hundreds or thousands of lattice structures, however, is difficult due to the complexity and refinement of the shapes. One method for analyzing structural performance is directly modeling every detail of these structures, which can result in enormous models that require a lot of memory and time to run. For a design exploration study, excessively large models will not allow for a large enough design space for optimizing or creating Pareto fronts. Other methods for optimizing lattice structures involve topology optimization techniques.[28] These methods, although fast, have the risk of overgeneralizing the properties of lattice structures.

With an endless combination of materials, lattice topologies and relative volume fractions, it is important to rapidly and accurately iterate many different designs to realize the full potential of additive manufacturing.

Solution

Fully coupled multiscale analysis facilitates treating the lattice regions as a continuous domain of lattice meta-material. This method enables a coarser meshing at the macro scale since the features of the lattice structure are captured within an RVE. With the lattice RVE determining the properties of the lattice region (which can sometimes be highly anisotropic), the global model retains accuracy without long run times or extensive memory use.

Having established an efficient method for simulating the lattice domain, one can turn the problem around and find which is the optimal lattice design that meets a part scale structural requirement. To find an optimal lattice structure geometry and relative volume fraction, we used HEEDS™ software,[29] a powerful tool for exploring the design space and Simcenter Multimech for the virtual characterization of the lattice material for every iteration. Using HEEDS enables the automatic creation of a finite element model based on parameters of interest, performs the calculation and records the results and adjusts the parameters to optimize a design according to one or multiple objectives and constraints. The HEEDS flexibility allowed for parameterization of the Simcenter Multimech microstructure models and automated over 200 multiscale simulations.

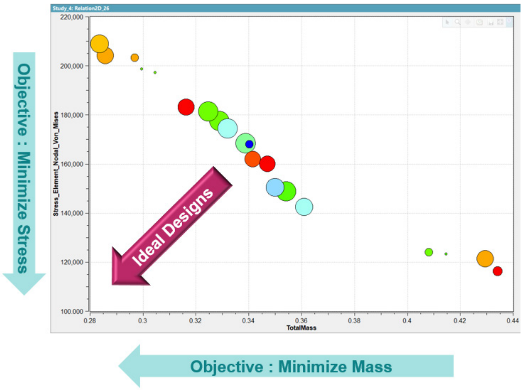
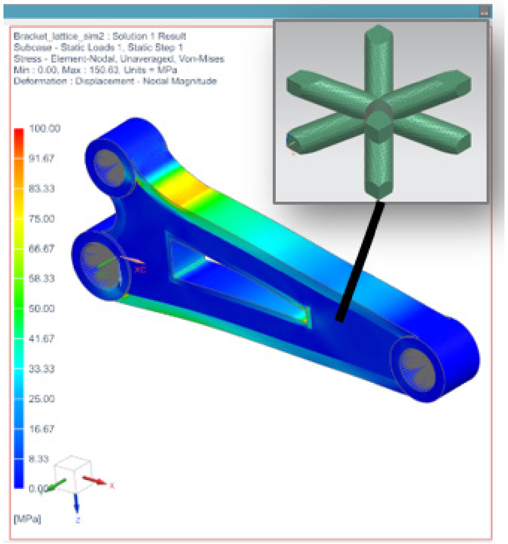


Figure 14. Pareto front of optimal designs demonstrating the trade-off between weight and maximum stress.



Bracket_lattice_sim2 : Solution 1 Result
Subcase - Static Loads 1, Static Step 1
Stress - Element-Nodal, Unaveraged, Von-Mises
Min : 0.00, Max : 150.63, Units = MPa
Deformation : Displacement - Nodal Magnitude

Figure 15. Bracket model stress results for an individual design from the design study.

Results and benefits

Case study 3, as depicted in figure 15, is a bracket with a center slot designed for mechanical loading. To make this part lightweight, the region joining the slot and the other boundary is filled by body centered cubic (BCC) lattice structures. The goal is to ensure the part will not yield for three different load cases, while optimizing for the lightest possible design. There are six design parameters: four bracket shape parameters and two lattice shape parameters, bar thickness and repeating unit cell (RUC) aspect ratio.

After 200 simulations, the HEEDS optimization algorithm was used to construct a Pareto front that shows the design trade-offs for an optimized structure, as shown in figure 14. One can see the trade-off between mass and stress, with an obvious relationship between the two objectives. The design points on the right side of the plot are risk-averse designs with minimal stress, whereas the design points on the left focus on cutting as much weight as possible, edging toward the maximum allowable stress. An engineer designing this part can use this information to make a rational and virtual evidence-based decision on preferred product performance. Once the optimum has been located, it is still possible to explore the nearby design space to evaluate the effect of other parameters on product performance.

Case study 4: Accounting for manufacturing-induced variations

Challenge

To reduce carbon dioxide (CO^2) emissions, the manufacturing industry works hard to design lightweight parts that maintain the structural integrity and performance of the part. The use of short fiber reinforced composites (SFRC) contributes to this objective. SFRC is an attractive material for industrial applications because they are easy to manufacture and provide favorable performance properties at low weight.

An important prerequisite for industrial deployment is the parts can be properly designed, studied and optimized virtually in terms of structural and durability performance, yielding a high-performing product. The challenge is SFRC parts have a variable local statistical distribution of fiber orientations, leading to different material properties and mechanical behavior at different locations.[30] For SFRC composites, due to the local inhomogeneity (lack of uniformity), it is necessary to take the local microstructure into account, as it defines the basic structural behavior.[31] For injection-molded short fiber reinforced composites, the local distribution of the fiber orientation directly influences the (anisotropic) local stiffness of the structure, and it also defines the damage behavior.

Solution

Manufacturing-induced variations, from manufacturing simulation software or from imaging techniques such as a CT scan, can be naturally accounted for by the adaptive multiscale approach. Variations in fiber orientation, volume fraction, porosity, among others, can be used to generate material microstructural models accordingly, which in turn is connected to part simulation software through various workflows: the simplest one-way homogenization and dehomogenization of critical hot spot locations, or a fully coupled multiscale modeling approach. Thanks to these connections, accurate predictions of material property variation across the parts can be obtained so achieving cost and time reduction becomes a reality for injection-molded short fiber composites.[32]

Results and benefits

Figure 16 shows a case study taken from[30] a demonstrator for the design freedom of injection molding, with complexity that can be compared with a consumer electronic device or any other project with body housing. The case study is called “Pinocchio,” owing to its resemblance to the famous Italian cartoon character by the same name.[30] The dimensions are 130 millimeters (mm) long, 84 mm wide and with a depth of 32 mm.

The fiber orientation is imported from Moldflow, which in turn is used by Simcenter Multimech to automatically generate different microstructural models. The central picture shows the fiber orientation mapped onto the structural mesh. The principal orientation and degree of alignment of fibers are driven by the imported orientation tensor. Subsequently, the spatial variation of homogenized properties is obtained for each location in the part based on their corresponding microstructural model.

The part model has about 140,000 elements, each microstructural model has about 11,000 elements and the simulation is subdivided into 40 timesteps. The total runtime was 13 minutes using eight CPU threads and consuming 1.8 GB of random access memory (RAM). Figure 17 shows the homogenized properties varying in space and time, which is a function of the fiber orientation and material failure. The Simcenter Multimech results correctly predict the location and load of failure for the part.

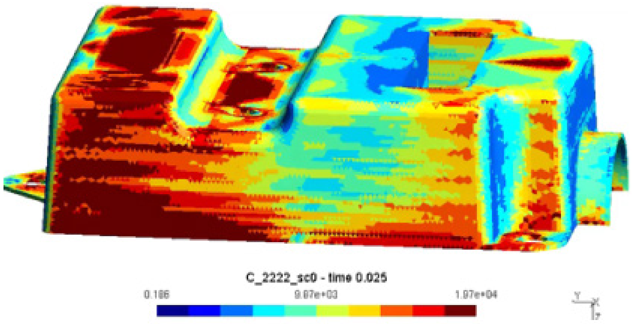


Figure 16. Adaptive multiscale modeling of “Pinocchio,” a short fiber composite case: imported fiber orientations, generating RVEs for defining the local material properties.

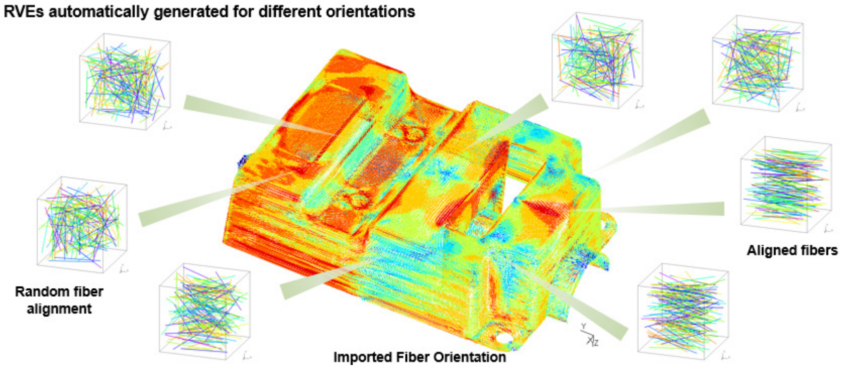


Figure 17: Results for “Pinocchio”: the homogenized properties varying in space and time as the material fails.

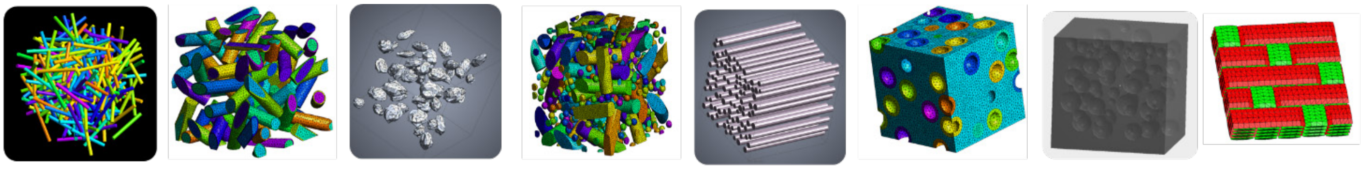
Conclusion

Materials innovation is critical for improving performance and reducing the cost of products. Given the slow adoption of reliable physics-based simulation tools capable of being used to accurately model complex microstructural features, the big challenge is the amount of physical testing required to develop and certify new materials. With the recent advances in multiscale computational methodology, a major reduction in computational requirements is achieved, thanks to the combination of a new mathematical formulation and adaptive multiscale algorithms. Multiscale modeling has thus become a reliable and efficient way to accurately predict the behavior of complex multiscale multiphase material systems, enabling more efficient materials innovation in various industries.

The adaptive multiscale modeling approach offers speed without losing accuracy, enabling fast and accurate materials modeling and simulation that can be used for materials design, virtual coupon testing, part design, validation and optimization and accounting for the manufacturing process effects on part performance. This solution is brought to market as Simcenter 3D Materials Engineering software, with the underlying Simcenter Multimech solver that captures the innovative methodology know-how and delivers big value to the end users. With the ability to connect material development, product design and manufacturing, an Integrated computational materials engineering (ICME) approach[33] becomes a reality.

Simcenter 3D Materials Engineering solution, which is empowered by the adaptive multiscale modeling approach, enables the user to:

- Combine the accuracy of FE^2 method with speed using a new mathematical formulation and a proprietary adaptive multiscale technology
- Facilitate accurate homogenization of a mix of constituents into part-scale composite properties
- Accurately predict the material failure by accounting for multiple competing damage mechanisms, including fiber rupture, resin cracking and fiber-resin debonding
- Predict not only when the material will fail, but it also provides insight why. While most other tools simply approximate results, Simcenter 3D Materials Engineering gives unique, accurate insight into exactly why damage will occur. This gives engineers the ability to not only successfully mitigate failure, but also create new materials and improve existing materials over time
- Account for manufacturing variability and imperfections to maximize product reliability
- Provide an open platform solution linking to a wide range of Siemens solvers as well as third-party solutions
- Combine with HEEDS to accelerate product innovation by automating design space exploration and optimization



1D Chopped Fibers | **3D Chopped Fibers w/ coating** | **Irregular Particulates** | **Combine different inclusions** | **Continuous Fibers** | **Shell spheres (*self-healing*)** | **Porous Materials** | **Woven Textiles**

Figure 15. Simcenter 3D Materials Engineering enables automatic generation of microstructures for any material.

Acknowlegements

Siemens acknowledges the research project, “ModelSteelComp,” which fits in the SIM NANOFORCE research program, coordinated by Bekaert (Belgium, until 2015) and ABV (Belgium, since 2016), and has been funded by Strategic Initiative Materials (SIM) in Flanders and VLAIO, the Flemish government agency Flanders Innovation & Entrepreneurship (VLAIO).

Siemens further acknowledges the twin projects SBO and ICON “M3Strength” and the ICON project “FATAM,” which fit in the MacroModelMat (M3) research program (see https://www.sim-flanders.be/research-program/m3), coordinated by Siemens (Siemens Digital Industries Software, Belgium) and funded by SIM and VLAIO.

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