**Original published:** S. Hannusch, R. Herzog, M. Hofmann, J. Ihlemann, L. Kroll, A. Meyer, F. Ospald, G. Rünger, R. Springer, M. Stockmann, and L. Ulke-Winter. Efficient simulation, optimization, and validation of lightweight structures. In *Proceedings of the 2nd International MERGE Technologies Conference for Lightweight Structures (IMTC 2015)*, pages 219–227. Verlag Wissenschaftliche Scripten, 2015. Best Paper Award.

# Efficient Simulation, Optimization, and Validation of Lightweight Structures

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**Keywords – lightweight structures, numerical simulations, injection molding, optimization, distributed computing, residual stresses, fiber Bragg grating sensors**

## *Abstract*

Multifunctional lightweight structures and their resource-efficient manufacturing are at the core of the research within the Federal Cluster of Excellence MERGE. As part of the interdisciplinary research area IRD F, we present an overview of the methods developed for the simulation, optimization, and validation of lightweight structures. The simulation approach considers both the manufacturing process and the subsequent load cases, thus leading to high computational demands. Two application examples for the optimization of fiber-reinforced plastics are presented. For the validation of the simulation results, a new approach for the analysis of residual stresses is described.

## *1 Introduction*

The interdisciplinary research area IRD F within the Federal Cluster of Excellence MERGE considers the use of advanced scientific simulations for the optimized manufacturing of multifunctional lightweight structures. The simulation approach includes the manufacturing process with composite materials and the subsequent characterization of mechanical properties with operating load cases. Both short fiber-reinforced plastics (SFRP) and continuous fiber-reinforced plastics (CFRP) are considered as composite materials. Special emphasis is given to the formation and the effect of manufacture-related residual stresses, which will also be investigated experimentally. The optimization goals for lightweight structures concern their mechanical properties, such as the strength, stiffness, or durability, as well as manufacturing quantities, such as the energy consumption or the operational costs. Due to the high computational demands of the simulation and optimization tasks, efficient computing strategies are provided to exploit distributed and high performance computing (HPC) resources.

The rest of this article is organized as follows. The simulation methods developed for lightweight structures are described in Sect. 2. This includes the computational fluid dynamics (CFD) simulation for the manufacturing process with injection molding, the finite element (FE) simulation for determining the mechanical properties of the resulting structures, and the efficient execution of these simulations on HPC platforms. Two application examples for the optimization of lightweight structures are presented in Sect. 3. We show first results for the optimization of the injection point for SFRPs and for the ply orientation of multilayer composites consisting of CFRPs. The steps towards the validation of the simulation results are described in Sect. 4. Especially, we present an approach for the measurement of residual stresses with a fiber Bragg grating sensor embedded in several plains. Sect. 5 concludes the article.

# *2 Simulation of lightweight structures*

For lightweight structures consisting of SFRP materials, the simulation approach includes applications for the manufacturing process and for the characterization of mechanical properties. In the following, the two simulation applications and their efficient execution on distributed computing resources is described.

## 2.1 CFD simulation of the injection molding process

Lightweight structures consisting of SFRP materials will be manufactured by injection molding, which represents one of the most economically important processes for the mass-production of plastic products. The parts are produced by injecting molten plastic with mixed in fillers, such as glass and carbon fibers, into a mold. Manufacturing parameters, such as the position of the injection point, influence the orientation of the fibers, which in turn determines the mechanical properties of the parts. Thus, simulating the injection molding process forms the basis for an optimization of lightweight structures for specific load cases. For the simulation, we developed a customized computational fluid dynamics (CFD) application based on OpenFOAM, a C++ library implementing the finite volume method [1]. Our OpenFOAM solver features a compressible two phase flow with heat transfer and fiber orientation calculation. The change of the fiber distribution caused by the flow is modeled by the Folgar-Tucker Equation [2]. The CFD application uses the structure geometry, the material properties, and the parameters of the injection molding process as input data. The simulation is complete when the mold is filled and leads to the fiber orientation and the temperature field within the structure.

## 2.2 FE simulation of cooling and load cases

The CFD simulation of the injection molding process is followed by the simulation of the cooling of the structure and the operating load cases. In addition to the structure geometry and the material properties, also the fiber orientation and the temperature field resulting from the CFD simulation are used as input data. More specifically, the random type material of the SFRP is described by the second order fiber orientation tensor. The simulation is done in two steps. First, the instationary cooling process of the freezed structure is simulated to obtain the residual stresses. Afterwards, these stresses are taken into account for the simulation of the operating load cases. The simulations are performed by solving the Lamé equation of linear elasticity, which means to find the displacement field $u$ over $\Omega$ with

$$\nabla \cdot \sigma\big(u(x)\big) = -f(x,T) \text{ for } x \in \Omega \ . \tag{1}$$

Here, $\sigma$ is the Cauchy-stress tensor, $f$ denotes the given loads and/or temperature influence, and $\Omega$ represents the structure. Equation (1) is approximately solved with the finite element method (FEM). Adaptive mesh refinement based on residual type error indicators is applied to achieve high precision solutions [3] and specific material laws are used to integrate the given fiber orientation and the properties of the SFRP [4]. The implementation is integrated into a Fortran-based in-house FEM application parallelized with OpenMP [5].

## 2.3 Efficient computing strategies

The CFD and FEM simulations are compute-intensive applications that need to be executed on parallel computers, such as multi-core clusters. Furthermore, for the optimization of lightweight structures, the simulations have to be performed several times with different configurations for the optimization parameters. To achieve an efficient utilization of distributed computing resources as well as a transparent data exchange between the applications, the newly developed Simulation Component and Data Coupling (SCDC) library is used [6]. This communication library implements a service-oriented approach for the data coupling of independent software components that are executed on various computing platforms, such as laptops, desktop PCs, dedicated servers, and HPC clusters. For the simulation and optimization of lightweight structures, the software components include computationally intensive numerical simulations, control applications for implementing the optimization process as well as data-oriented applications for the generation, management, and visualization of the simulation data. The SCDC library is an integral part of a novel methodology for the building of complex simulation programs for distributed computing systems [7].

# *3 Optimization of lightweight structures*

Both the specific design and the manufacturing parameters of lightweight structures can have a strong influence on their resulting mechanical properties. In the following, an application example for the optimization of the injection point of SFRPs and a method for the optimized design of CFRPs with multiple layers is presented.

## 3.1 Injection molding optimization

The optimization of SFRPs is performed with a dedicated software program called Injection Molding Process Optimization Tool. The tool provides a graphical user interface to support the configuration of optimization problems and parameters, the selection of optimization algorithms, simulation applications, and computing resources as well as the evaluation of the optimization results. As an application example, we consider a plate with a hole produced from Polypropylene with glass fiber fillers. The plate is clamped on both sides and a circular surface load is applied as shown in Fig. 1 (left). The deflection in force direction depends on the local fiber orientation in the structure, which in turn is influenced by the position of the injection point. Thus, the optimization uses an objective function that minimizes the maximal deflection of the structure in force direction. We employ a Kriging-based optimization algorithm starting with a design of experiments for the injection point. Then for each initial design point, the expected improvement of the objective is maximized and a number of candidate points are chosen for the next evaluations. The search for an optimal solution is then continued recursively in the vicinity of each of these candidate points. Throughout the optimization, an interpolation based surrogate model is created, as shown in Fig. 1 (right). The optimal injection point determined is shown in both figures.

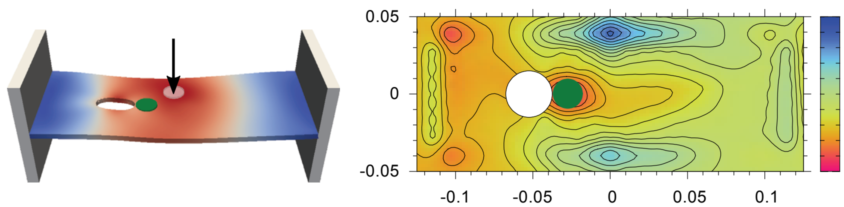


**Figure 1: Left: Clamped plate with hole, applied surface load (arrow), and optimal injection point (green). Right: Contour plot of the objective function obtained by the Kriging interpolation including the obtained minimum (green).**

## 3.2 Optimization of multilayer composites

As an application example for CFRPs, we consider the optimization of ply orientations in multilayer composites consisting of carbon fibers. Figure 2 (left) shows a symmetrical three-layer composite with two independent ply orientations $\Phi_1$ and $\Phi_2$. The objective function considered maximizes the component minimum reserve factors [8] for a given exemplary multi-axis load case (max-min problem). Because of the need of polar transformations for the material properties, the fracture functions are not convex. Furthermore, since the objective function is only $C^0$-continuous, derivation-based optimization algorithms can not be applied. Figure 2 (right) shows the surface of the objective function depending on the ply orientations. In addition, several solutions determined with the derivative-free Nelder-Mead algorithm for runs with varying initial ply orientations are shown [9]. The results show that this deterministic optimization algorithm mostly only leads to local maximum solutions. To solve the corresponding non-convex optimization problems, we have implemented various nature-analogous optimization algorithms, such as Particle Swarm Optimization and Ant Colony Optimization [9]. Furthermore, by supporting also discrete optimization parameters, additional manufacturing constraints, such as material combinations, allowable ply orientations, and individual ply thicknesses, can be considered.

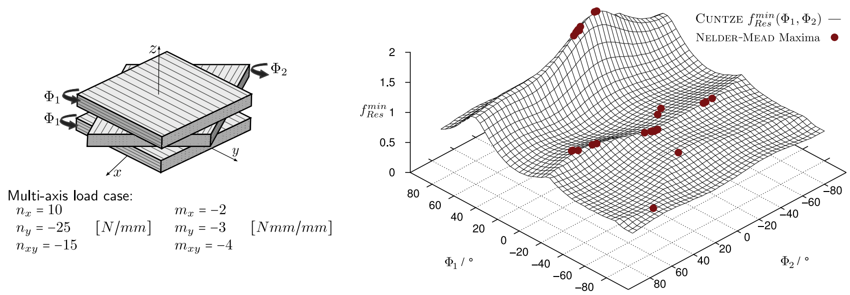


**Figure 2: Left: Symmetrical three-layer composite with two independent ply orientations and multi-axis load case. Right: Minimum reserve of a multi-axis load case and local maxima determined with the Nelder-Mead algorithm.**

# *4 Experiments and validation*

Residual stresses resulting from manufacturing processes, such as injection molding, can lead to distortions of the structures and influence their mechanical properties. The hole-drilling method [10] represents a well-investigated method for the measurement of residual stresses: By drilling a hole into the specimen, the stress state is varied and the resulting deformations are measured. Strain gauge (SG) rosettes measure the strains solely on the surface while changing the stress state. Thus, they provide only limited information on the progress of residual stresses in the material. To enable the measurement of deformations in several depths, we embed a fiber Bragg grating (FBG) sensor in several plains of the structure. Figure 3 (left) shows the design of the specimen used for the following experiments. Three epoxy plates are joined with epoxy glue to embed the FBG sensor in the glue layers. The FBG sensor is applied in tangential direction to exploit the utilization of several measurement points within a single fiber. An additional electrical strain gauge rosette is applied on the surface and a fixed pressure load is generated at two sides of the specimen in the *y*-direction to provide a known stress state. A 2-blade face cutter drills a hole with a diameter of 5 mm until 9 mm depth. After each drilling step of 1 mm, the specimen is untouched for 30 minutes to eliminate the effects of the pressure load by the cutter and the heating by the drilling. Figure 3 (right) shows the measurements with the SG rosette. The results show an expected progress of the strains as they approach a constant value after a small drilling depth. The expected symmetric results of SG A and SG C can also be seen, whereas their differing values might be caused by a rotation of the rosette and by the drilling hole being not exactly centered in the rosette. Additionally, first results for the FBG sensor in the first plain are shown. As expected, the measured tangential strains are significantly smaller than the radial strains observed with the SG rosette. A further quantitative comparison will thus require an appropriate converting into related residual stresses based on a mathematical model.

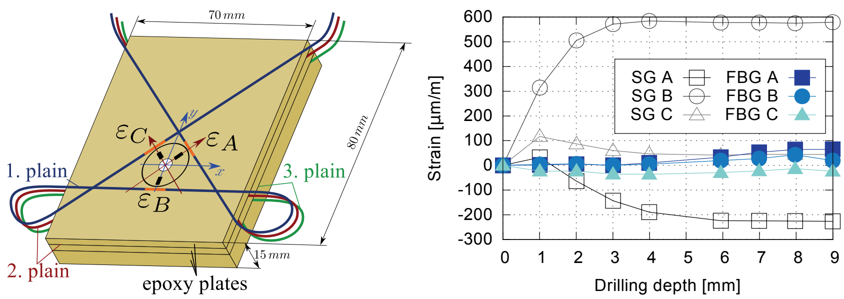


**Figure 3: Left: Experimental set-up for the hole-drilling method with epoxy specimen. Right: Results with SG rosette and FBG sensor.**

## 5 Summary and outlook

In this article, we have presented different approaches and first results for the simulation and optimization of lightweight structures consisting of fiber-reinforced plastics. The simulation of SFRPs is already based on HPC applications that will be extended in future developments, for example, by integrating advanced material laws for large deformations. The presented optimization of multilayer composites is based on an analytical approach, but will also be coupled with numerical FE models and appropriate solvers to exploit HPC resources. The novel approach for measuring strains in several plains forms the basis for validating the simulation and optimization results. Due to the measurement of tangential strains, a new mathematical model has to be developed for the stress analysis.

## Acknowledgment

This work was performed within the Federal Cluster of Excellence EXC 1075 "MERGE Technologies for Multifunctional Lightweight Structures" and supported by the German Research Foundation (DFG). Financial support is gratefully acknowledged.

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