THE MULTI-SCALE CLOSED CHAIN OF SIMULATIONS – INCORPORATING LOCAL VARIATIONS IN MICROSTRUCTURE INTO FINITE ELEMENT SIMULATIONS

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Abstract

Numerical simulations of component behavior and performance is critical to develop optimized and robust load-bearing components. The reliability of these simulations depend on the description of the components material behavior, which for e.g. cast and polymeric materials exhibit component specific local variations depending on geometry and manufacturing parameters. Here an extension of a previously presented strategy, *the closed chain of simulations for cast components*, to predict and incorporate local material data into Finite Element Method (FEM) simulations on multiple scales is shown. Manufacturing process simulation, solidification modelling, material characterization and representative volume elements (RVE) provides the basis for a microstructure-based FEM analysis of component behavior and a simulation of the mechanical behavior of the local microstructure in a critical region. It is discussed that the strategy is applicable not only to cast materials but also to injection molded polymeric materials, and enables a common integrated computational microstructure-based approach to optimized components.

Introduction

In the automotive and transportation areas, the request and legislation demands for reduced emissions and fuel consumption drives the need for designing and manufacturing components with high mechanical performance and low weight. In this process, both materials with a low density, e.g. polymeric materials, aluminium and magnesium, and materials with higher density and higher strength, as e.g. cast irons and steel, has to be considered. A material with higher strength may compensate for its higher density by requiring a lower volume material, and a high density material may thus be found to be the optimal selection for producing a light component. Numerical structural analysis and optimization methods as FEM simulations, topology optimization and shape optimization has been proven to be important tools for finding the optimal geometry with respect to complex load cases, significantly reducing the weight of components while simultaneously maintaining or even increasing their mechanical performance in terms of e.g. stress distribution, fatigue life or damage. These numerical tools are typically based on the assumption that the material behavior throughout a given component is homogeneous. For many manufacturing methods, this is not in agreement with the underlying physics of the manufacturing process. For cast materials, as well as for many polymeric materials, the mechanical behavior and performance of the material is highly dependent on parameters as component design and manufacturing conditions. Here we study Spheroidal Graphite Iron (SGI), also known as ductile iron, a cast iron with more or less rounded graphite particles. The industrial request for SGI components is increasing, partly due to its highly attractive mechanical properties, as high strength

and ductility, in combination with excellent castability. This enables the production of products with high-performance and complex geometries near net shape in large series.
In SGI, the local mechanical response of the material is highly dependent on the microstructure formed during the manufacturing process [1]. The microstructure is here a complex combination of different phases, where the amount and morphology of the graphite particles [2] and the fractions of ferrite and pearlite and have been identified as important factors determining the mechanical performance of the material [1]. The formation mechanisms of these microstructural features are in turn highly dependent on several factors which are controlled by both manufacturing process parameters and component geometry, e.g. the local cooling rate which is controlled by both process-specific heat extraction conditions and the local section thickness [1]. These parameters all, to different extents, varies throughout the component and have complex interactions. This results in a variation in microstructure, and thus mechanical behavior, throughout a SGI component, which to a large extent is affected by the design of the component [3]. This needs to be considered in order to find the optimal geometry of a SGI component. The assumption of homogeneous behavior throughout the component will not provide an adequate description of the behavior of the material in the component [3]. Similar effects of process and design on material behavior are found in as well other cast materials, e.g. cast aluminium, but also in polymeric materials. Here the local material behavior depends on local microstructural features as e.g. crystallization, morphology, molecular orientation and reinforcement fiber orientation, which all in turn depend on both component geometry and injection molding process parameters [4]. For both these types of materials, there is a complex interaction between manufacturing parameters, component design and material behavior. From the industrial organizational standpoint, there is thus a mutual dependency between product design and production which needs to be considered to ensure a successful and efficient product realization process [5].

The closed chain of simulations for cast components

Two of the current authors, Olofsson and Svensson, have previously presented a simulation strategy to address this mutual dependency for cast components [6]. The simulation strategy is called the closed chain of simulations for cast components, schematically illustrated in Figure 1.

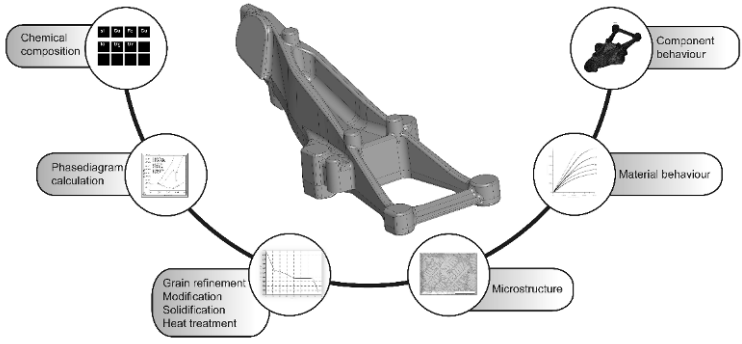

Figure 1. Schematic illustration of the closed chain of simulations for cast components [6]. Figure reprinted with permission from Elsevier.

The simulation strategy is based on a manufacturing process simulation, where in the case of casting the entire casting process, from chemical composition to mold filling, phase diagram calculations and models for solidification microstructure formation, is simulated. This simulation provides the local distribution of important microstructural features, e.g. the amount and morphology of the graphite and the local ferrite and pearlite content of the matrix. By using microstructure-based characterization models, the local elasto-plastic tensile behavior of the material can be predicted, e.g. using Hooke's law and the Young's modulus [2] for the elastic contribution and the Hollomon equation, $\sigma = K \times \varepsilon_{pl}^{n}$, for the plastic contribution [7]. This local material behavior is then implemented into the macro-scale FEM simulation of component behavior using element-specific material definitions [6]. Physical observations using Digital Image Correlation (DIC) [8] as well as numerical experiments [3] have been performed to verify the simulation strategy. Figure 2 shows the strain field during tensile testing of a cast aluminium sample observed using DIC, and a comparison with the FEM simulation results obtained using local material behavior and homogeneous material behavior. It is clearly seen that the local variations in microstructure causes a redistribution of strains within the sample that a homogeneous FEM model fails to predict. Using the closed chain of simulations and local material behavior, this effect is however very well predicted [8].

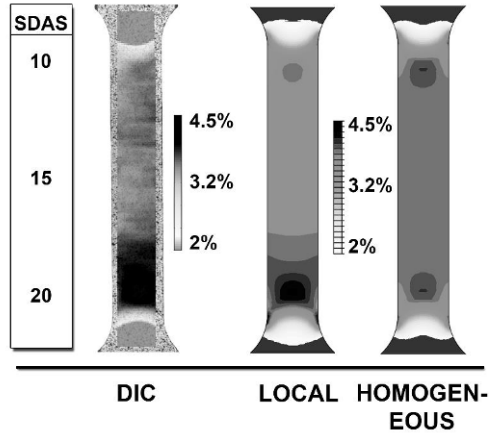

Figure 2. Comparison between strain fields observed using Digital Image Correlation (DIC) and FEM simulation results using local material behavior and homogeneous material behavior [8]. Figure reprinted with permission from Elsevier.

In a general perspective, each element of the FEM mesh is in the simulation strategy considered as a representative volume for the material contained in that specific volume, with its own unique elasto-plastic behavior based on the micro-structural characteristics within the volume. The general approach is applicable not only to SGI, but has previously been applied to cast aluminium components [9], and is also applicable to components in polymeric materials.

Micro-scale simulation of microstructure behavior

Typically, experiments are performed on a structural length scale to determine material properties as Young's modulus and yield stress of a specific material. These properties are most commonly used in FEM analyses to analyze structural performance of the product of interest. Furthermore, the material model is typically incorporated as an isotropic material model. However, in light of the demand of accuracy in virtual experiments of today, variations in the microstructure of the material has to be taken into account. One way of dealing with variations in micro structure is to divide the product in isotropic regions with whilst varying the material properties in each region, e.g. using the previously outlined simulation strategy by Olofsson and Svensson, *the closed chain of simulations* [6]. Extending the ideas of Olofsson and Svensson, critical regions of interest can be modeled by a semi-multiscale approach where the strain field from the structural simulation is used as a boundary condition of a unit cell of the actual microstructure to study events of e.g. crack initiation.

The identification of microstructures have been proven useful when determining volume fractions for different phases. Commonly the volume fractions are measured by means of image processing of SEM images on the surface of the specimen. Velichko et al. [10] used SEM images in combination with Focused Ion Beam (FIB) slicing to generate 3D microstructural cells to identify the volume fractions. In order to use the 3D structures in FEA, a huge number of finite elements have to be used to obtain the resolution needed. This motivates the choice to in the current work use SEM images of the surface of SGI to do the analysis on. Nevertheless, in order to get an idea about the complexity of the SGI we have used 3D X-ray tomography to capture the volume fraction of each individual phase, i.e. pearlite, ferrite and graphite. The Representative Volume Element (RVE) finite element model, see Figure 3, is then generated where the volume fraction of the RVE is chosen so that it corresponds to the 3D microstructure. The numerical model is utilized to reverse engineer the material properties of the different phases within the microstructure, and is correlated with experimental data on a structural scale, see Figure 4. The process of identifying the material properties of the individual phases is vital when determining e.g. crack initiation or properties of heat transfer within the alloy.

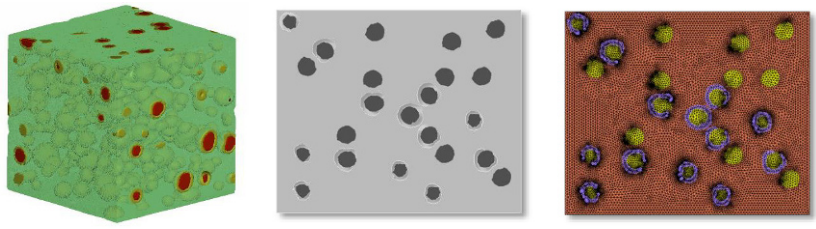

Figure 3. The microstructure of the SGI alloy (left), 2D representation of the microstructure (middle) and the RVE finite element model (right).

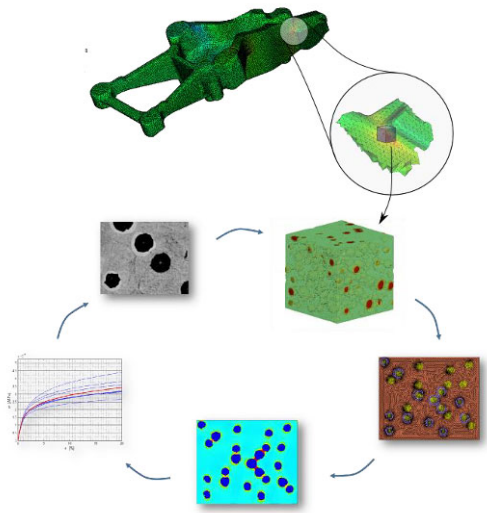

Figure 4. Schematic cycle of the reversed engineering strategy applied on a critical microstructural region identified from the macro-scale FEM simulation performed using microstructure-based mechanical behavior.

Since the homogenized behavior of the RVE depends on the choice of material properties within each phase, it is essential that an approximate material model is chosen to which a reversed engineering scheme can be applied. In the current work, we have chosen to use the Ramberg-Osgood material model, see Eq. 1, for the pearlite. An example of the plastic strain distribution in the pearlite can be seen in Figure 5. For simplicity, the ferrite and the graphite phases are initially assumed to be elastic.

$$E\varepsilon = \sigma + \alpha \left(\frac{|\sigma|}{\sigma_Y}\right)^{n-1} \sigma \tag{1}$$

In Eq. 1, σ is the Cauchy stress, σ_Y is the yield stress, E is the Young's modulus, ε is the strain and α and n are material specific constants.
The reversed engineering strategy is based on minimizing an objective function in the form of a fitness functional according to Eq. 2. As consequence of the chosen material model to approximate, there are three variables in the objective function, namely σ_Y, α and n.

$$f_j\left(\sigma_{Y_j}, \alpha_j, n_j\right) = \sum_i^k W_i ||\sigma_i^{\text{sim}} - \sigma_i^{\text{exp}}|| \tag{2}$$

Here σ^{sim} is the simulated homogenized stress on the top boundary of the RVE, see Figure 5, and the corresponding experimentally measured stress is given by σ^{exp}. The L_2-norm is denoted by $||\ldots||$ and W denotes a weight factor.

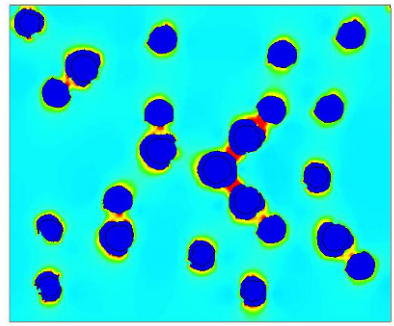

Figure 5. Example of the plastic strain distribution in the RVE.

As is seen in Eq. 2, the difference between the numerical and experimental stress-strain relations will provide the fitness response for each combination of variables. A composite Design Of Experiment (DOE) scheme is used to initiate the optimization process by providing combinations of variables. In order to reduce the number of simulations needed to find an optimal set of variables, a surrogate model is generated by use of a Radial Basis Function (RBF), see e.g. the work by Amouzgar and Strömberg [11]. The RBF is in the form of

$$f(\tilde{x}) = \sum_{i=1}^{n} \lambda_i A_{ij} + \sum_{i=1}^{n} \beta_i B_{ij} \qquad (3)$$

where the first term is the RBF and the second term is the augmented bias. The optimal point of the surrogate model generated from the first set of DOE is established by the Hooke and Jeeves pattern search method and is then used as input to the next set of DOE:s in an iterative manner, thus localizing as well as increasing the accuracy of the response surface. Figure 6 shows an example of the surrogate model using RBF.

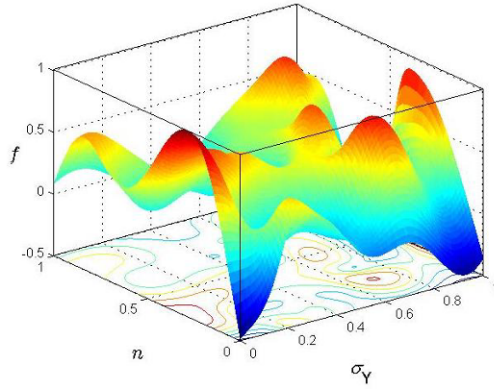

Figure 6. Example of the surrogate model using RBF with *a priori* bias.

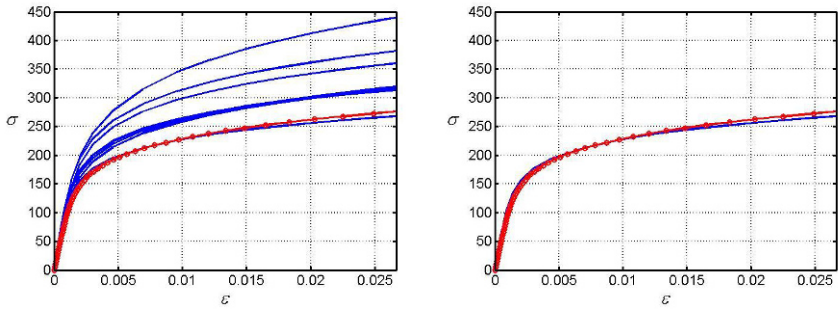

Figure 7. Stress (MPa) as a function of strain (-). The blue curves correspond to simulated results and the circle marked red curves corresponds to experimental data for (a) initial iterations and (b) the converged result.

Figure 7 illustrates the optimization process. In Figure 7b, the converged simulated stress-strain curve is shown together with the corresponding experimental curve. As is seen, the structural behavior on a macroscopic length scale is well captured by an optimization of an approximated material model for the pearlite on a microscopic length scale. It should be noted that the ferrite and graphite are in this example modeled as elastic. However, the implementation of a non-linear ferritic phase and/or non-isotropic graphite phase into the present methodology is straight forward.

Conclusions

We have presented a framework for a multi-scale closed chain of simulations to predict the structural behavior of cast iron components with microstructure-based mechanical behavior. In essence, the framework enables microstructural design to obtain specific properties for special purpose products. Even though the framework in the present study is applied on cast iron components, it can also be applied to e.g. aluminium components or fiber reinforced plastics products as well. The approach is thus highly applicable to approach the dependency between product development and manufacturing aspects of the microstructure-based mechanical behavior and performance for a wide range of industrial components. By adopting a common and general perspective on microstructure-based product behavior of components, new aspects of geometry and material optimization methods can be revealed. Future work in this area will be aimed at exploring further aspects of microstructure-based product performance and optimization.

Acknowledgements

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