Efficient Mechanical Design of Lattice Metamaterials: a Multiscale Homogenization-based Approach

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EFFICIENT MECHANICAL DESIGN OF LATTICE METAMATERIALS: A MULTI-SCALE HOMOGENIZATION-BASED APPROACH

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Summary. Recent advancements in Additive Manufacturing have revolutionized mechanical component design. Lattice metamaterials, thanks to the possibility for effective control over their properties through the tuning of geometry layout, have gained great attention. However, the high computation time, required in all phases of numeric analyses is still a major challenge.

The homogenization-based multi-scale analysis is a computationally efficient numerical approach, able to extrapolate the macroscopic behavior from microscopic analyses of unit cells. Microscale properties are employed to model and simulate the metamaterial as a bulk domain, resulting in a substantial reduction in overall computation time.

This work introduces a comprehensive and universally applicable methodology, that provides essential mechanical data to evaluate component designs. Starting from the microscale with the homogenization, homogenized properties are employed in the simulation of the macroscopic component. Homogenized strain is then used to identify critical cells, that are then de-homogenized to retrieve microscale stresses, necessary to assess design constraints. The proposed framework is rigorously validated on a test case through the comparison between the numerical data obtained from homogenized component and its real counterpart.

1 INTRODUCTION

In recent years, Additive Manufacturing (AM) has emerged as a revolutionizing technology enabling the production of complex shapes, that were once deemed impossible to be manufactured through traditional processes. Among these groundbreaking developments, lattice structures have gained significant attention for their combination of strength, low weight, and highly customizable geometries. Lattice structures are also known as metamaterials, being their macroscopic properties dependent on the geometric layout. This allows their behavior to be tailored to the application they are designed for, and, therefore, they can be employed in a really wide range of applications, including lightweight structures, heat exchangers, energy absorbers, acoustic insulators and biomedical applications [1, 2, 4, 5, 6].

Although the Finite Elements Method (FEM) and Topology Optimization (TO) are well-established and powerful tools for the mechanical design of lattice metamaterials, numerical computations are often unfeasible due to the high computational time required to simulate even small components accurately, given the large number of mesh elements needed to model their complex geometry [3]. In this context, the multi-scale approach has emerged as a promising method to speed up simulations. It is based on homogenization, a numerical procedure able to retrieve the mechanical properties in the microscale of the smallest domain able to represent the behavior of the whole metamaterial, that is called Representative Volume Element (RVE). The equivalent mechanical properties can be used to model and simulate the whole lattice in the macroscale as a bulk material, allowing the generation of lighter meshes and, therefore, leading to a huge saving in computation time [7].

Homogenization was originally introduced to perform faster simulations of composites materials and several procedures have been developed since the end of the 20th century, ranging from analytical to numerical approaches. A comprehensive overview of homogenization algorithms can be found in Barbero [8] and Somnic et al. [9].

Homogenization procedures based on numerical FE simulation are founded on the satisfaction of Hill-Mandel's theorem, that ensures the energetic consistency between the real and homogenized microscale models. From this requirement, different types of boundary conditions (BCs) can be employed to retrieve the equivalent mechanical properties, such as uniform boundary conditions (UBC) [10] either in form of traction or displacements and periodic boundary conditions (PBC) [11]. Thus, several different algorithms originally developed for the homogenization of composite materials can be found in literature regarding the implementation of UBCs [12] and PBCs [13, 8].

Recently, homogenization has also been applied to lattice metamaterials to both evaluate their mechanical properties and develop fast performing TO frameworks [14, 15, 16]. Generally, in optimization workflows the fulfillment of mechanical design constraints, like yield or ultimate strength, is performed through the FEA of the final optimized component. However, this implies a direct modeling and simulation of the full macroscale lattice component, that, as it has been said previously, is computationally demanding or even unfeasible. Few researches have proven the validity of the homogenized model to accurately simulate the real macroscale displacement of the full-scale model [17]. However the development of a procedure, able to detect the critical zones within the homogenized lattice domain and compute the real stress field, would make the evaluation of each design within the optimization cycle more complete, as the design constraint on admissible stresses would be evaluated at each iteration. Montoya-Zapata [18] presented a methodology, that combines material homogenization and Design Of Experiments (DOE) to estimate the stress–strain response in large lattice domains for lesser computational demands in comparison to FEA. The results on stress were reported to be not sufficiently accurate, being the error in the order of 50-100 %, and, therefore, that procedure should be used only for pre-evaluation designs. More recently, Coluccia et al. [19] presented an homogenization-based framework to estimate the fatigue life of strut-based lattice structures. It involves a de-homogenization phase, in which the most critical zone is identified through the evaluation of the homogenized strain field of the homogenized macroscopic lattice and simulated to retrieve the maximum stress within the whole lattice domain. However, the procedure was not validated through comparison with a full-scale real model of the lattice component.

Taking inspiration from the above-mentioned procedure, this work aims to provide a com-

plete, unified and validated multi-scale homogenization-based workflow for fast and reliable FE simulations of lattice structures, providing all the essential data for the evaluation of components designs. In the first part of this work basic theoretical notions on the multi-scale approach, homogenization and the most used algorithms along with their implementation are provided. Then, the workflow developed in this research is presented and tested on case study. Its validity is proven through the comparison of the numerical data with those obtained through direct numerical simulation (DNS) of the full-scale real model. Finally, possible critical issues are highlighted as well as the way to overcome them.

2 TOWARDS AN EFFICIENT PROCEDURE: THEORETICAL CONCEPTS

In this section few key theoretical notions about the multi-scale approach, homogenization basis and algorithms are presented.

2.1 Multi-scale modeling fundamentals

Multi-scale modeling refers to an approach in which the mechanical response of the material is studied at one length scale, but the outcomes of the analysis are referent to several properties at another one [16]. Homogenization is a technique for evaluating the equivalent macroscale properties of a complex metamaterial with a periodic structure and it can be either performed through experiments or virtual tests based on numerical simulations. Being the FEA of a whole lattice structure high demanding and often unfeasible due to the high number of mesh elements, numerical homogenization techniques have been developed and proven to lead to huge time saving in the simulation of complex lattice structures composed of hundreds or even thousands of repeated unit cells [8].

The homogenization approach was born to model composite materials, but can be effectively used also for lattices: the dual fiber-matrix phase composition of composites is replaced with the solid and void phases in lattices. The final goal of the procedure is to transform a porous periodic lattice structure into an equivalent solid material with homogenized properties, that make it behave as if it were a true lattice domain [13]. A fundamental problem that has to be solved to homogenize a lattice material is the definition of the minimum sufficient representative volume, so that the boundary conditions effects are minimized. To address this issue the concept of RVE was introduced [20]. The Representative Volume Element (RVE) is a region much smaller than the entire lattice structure. It possesses the same mechanical characteristics and behavior as the lattice, and its properties do not depend on boundary conditions.

Sub-scale modeling is energetically consistent, only if the deformation energy at the macroscopic level is equal to the volume average of the microscale stress work. Thus, at any equilibrium state of the RVE, characterized by the stress field σ and the strain field ε, the following equation must be satisfied [21]:

$$\bar{\sigma}_{ij}\bar{\varepsilon}_{ij} = \frac{1}{V_{RVE}} \int_V \sigma_{ij}\varepsilon_{ij}\,\mathrm{d}V \tag{1}$$

where $\bar{\sigma}$ and $\bar{\varepsilon}$ are the average stress and strain tensors, V_{RVE} is the total volume of the RVE and the indexes i, j represent the principal directions. The average stress and strain are defined as [22]:

$$\bar{\sigma}_{ij} = \frac{1}{V_{RVE}} \int_V \sigma_{ij}\, dV \qquad (2)$$
$$\bar{\varepsilon}_{ij} = \frac{1}{V_{RVE}} \int_V \varepsilon_{ij}\, dV.$$

In absence of body forces, using the averaging theory (Eq. 2) and the equilibrium condition of the RVE ($\nabla \cdot \sigma = 0$), the Hill-Mandel principle can be rewritten in the more convenient form:

$$\oint_{\delta V} (t_i - \bar{\sigma}_{ij} n_j)(u_i - \bar{\varepsilon}_{ik} x_k)\, \mathrm{d}S = 0 \qquad (3)$$

where t and u are the traction and displacement at the boundary of the RVE, x and n are the coordinate and the normal of the surface $\mathrm{d}S$ where the integral is currently evaluated.

The Hill condition guarantees that the effective modulus of the RVE calculated by energy and direct approaches are the same and it is satisfied by for different types of BCs:

- *Dirichlet or kinematic* (displacement controlled)

$$u_i = \varepsilon^0_{ij} x_j \qquad (4)$$

- *Neumann or natural* (traction controlled)

$$t_i = \sigma^0_{ij} n_j \qquad (5)$$

- *Mixed*: obtained through the combination of Eqs. 5 and 4

$$(t_i - \sigma^0_{ij} n_j)(u_i - \varepsilon^0_{ij} x_j) = 0 \qquad (6)$$

- *Periodic boundary conditions (PBCs)*

$$u_i(x + L) = u_i(x) + \varepsilon^0 L \qquad (7)$$
$$t_i(x + L) = -t_i(x)$$

where σ^0_{ij} and ε^0_{ij} are the uniform applied stress and strain, respectively, and L is the dimension of the RVE. Dirichlet and Neumann BCs are both kinds of UBCs.

2.2 Homogenization: computation of the homogenized elasticity tensor

Homogenization is an iterative procedure that requires the application of six independent loading conditions. This work focused on the study of UBCs and PBCs both in term of displacement constraints, thus, each loading condition consist in a specific displacement field with all but one null entries of the strain tensor. Recalling the Hooke's law

$$\{\sigma\} = [E]\{\varepsilon\} \qquad (8)$$

where $\{\sigma\}$ and $\{\varepsilon\}$ are the stress and strain tensors, respectively, and $[E]$ is the stiffness matrix of the material, taking for example the first iteration of the procedure, whose homogenized deformation state is:

$$\{\bar{\varepsilon}\} = \{\bar{\varepsilon}_{11},\ 0,\ 0,\ 0,\ 0,\ 0\}^T \tag{9}$$

plugging it into Eq. 8, it is possible to compute one column of the homogenized elasticity tensor at a time:

$$\{\bar{\sigma}_{11},\ \bar{\sigma}_{22},\ \bar{\sigma}_{33},\ \bar{\sigma}_{12},\ \bar{\sigma}_{23},\ \bar{\sigma}_{31}\}^T = \{\bar{C}_{11},\ \bar{C}_{22},\ \bar{C}_{33},\ \bar{C}_{12},\ \bar{C}_{23},\ \bar{C}_{31}\}^T \tag{10}$$

The components of the homogenized stress tensor can be retrieved from the FEA of the RVE with the prescribed BCs using either of the following approaches:

- *Reaction forces*:

$$\bar{\sigma}_{ij} = \frac{F_{ij}}{S_i} = \bar{C}_{ij} \tag{11}$$

  where F_{ij} is the total reaction force on the RVE face S_i with normal in the i-direction and along the j-direction.

- *Microscale stresses*:

$$\bar{\sigma}_{ij} = \frac{1}{V_{RVE}} \sum_{e=1}^{n_e} \sum_{I=1}^{n_{int}} \sigma_{ij}(\mathbf{r}_I) w(\mathbf{r}_I) J(\mathbf{r}_I) = \bar{C}_{ij} \tag{12}$$

  where n_e is the number of element of the mesh, n_I is the number of integration points of each element, w, J and $\mathbf{r}$ are the weight, determinant of the jacobian and position of the integration point I, respectively and V_{RVE} is the total volume of the bounding box containing the RVE.

- *Energy*:

$$\bar{C}_{ij} = \frac{2\,U}{\left(\bar{\varepsilon}^0_{ij}\right)^2 V_{RVE}} \tag{13}$$

  where U is the elastic energy stored inside the RVE, that can be computed through one of these three equivalent equations:

$$\begin{gathered} U = \textstyle\sum_{e=1}^{n_e} U_e V_e \\ U = \frac{1}{2} \textstyle\sum_{e=1}^{n_e} \sum_{I=1}^{n_{int}} \sigma^T(\mathbf{r}_I)\, \varepsilon(\mathbf{r}_I)\, w(\mathbf{r}_I)\, J(\mathbf{r}_I) \end{gathered} \tag{14}$$

  where U_e is the element energy density and V_e is the volume of the mesh element.

2.3 Homogenization: algorithms

In this section a quick overview on the homogenization algorithms investigated in this work and their implementations are presented. A summary, containing the type of BCs employed for each of the different approaches, their pros and cons and a quick reference for the complete explanation of their implementation can be found in Table 1.

Steven's algorithm relies on a reformulation of the classic implementation with UBCs and it is a very simple and straightforward homogenization algorithms. PBCs with either relative or absolute coupling of nodes on opposite faces to reference points (RPs), which are used to apply the displacement BCs to the RVE, require periodic meshes. Those are special kind of meshes that have the nodes on opposite faces of the RVE in the same location. Creating periodic meshes is not always simple, because a dedicated meshing algorithm is required, especially in automated frameworks. Therefore, the formulation of PBCs with interpolation overcomes this issue by using a generic mesh and interpolating the displacement of the virtual node on the opposite face form the surrounding ones, since it not guaranteed that two nodes located on two opposite faces of the RVE are in the same location. All the algorithms with PBCs require a pre-processing phase for the node coupling, that can be quite time consuming especially for larger meshes.

Algorithm	BCs	Notes	References
Steven	UBC	$\oplus$ Easy implementation $\oplus$ Generic mesh	[12]
PBC Abs	PBC	$\oplus$ Absolute node coupling to RPs $\ominus$ Periodic mesh $\ominus$ Pre-process for node coupling	[23, 8]
PBC Rel	PBC	$\ominus$ Periodic mesh $\ominus$ Pre-process for node coupling $\ominus$ Relative node coupling to RPs	[23, 24]
PBC Interp	PBC	$\oplus$ Generic mesh $\ominus$ Complex pre-process for node coupling $\ominus$ Requires finer mesh	[13, 21]

Table 1: Overview of the homogenization algorithms investigated in this work.

3 AN EFFICIENT PROCEDURE FOR FAST FEA OF LATTICE STRUCTURES

This section presents the complete workflow aimed at the simulation of lattice components composed of a high number of unit cells repeated periodically throughout the domain space (Fig. 1). The procedure presented in this work not only leads to a great reduction in the overall computation time, but also provides detailed and accurate information about global displacement of the macroscopic component and microscopic stresses of the most loaded portions, allowing the designer to check the fulfillment of the mechanical design constraints.

The first phase of the workflow consists in the computation of the equivalent properties of the lattice structure through homogenization. A convergence study on mesh size and dimensions of the RVE should also be performed to compute the true and effective homogenized elasticity tensor. From now on, the lattice domain can be replaced with an equivalent bulk material, that mechanically behaves like the original lattice structure.

The second stage consists in the FE simulation of the whole component, substituting the lattice domain with the homogenized bulk material. In the material assignment phase, the original

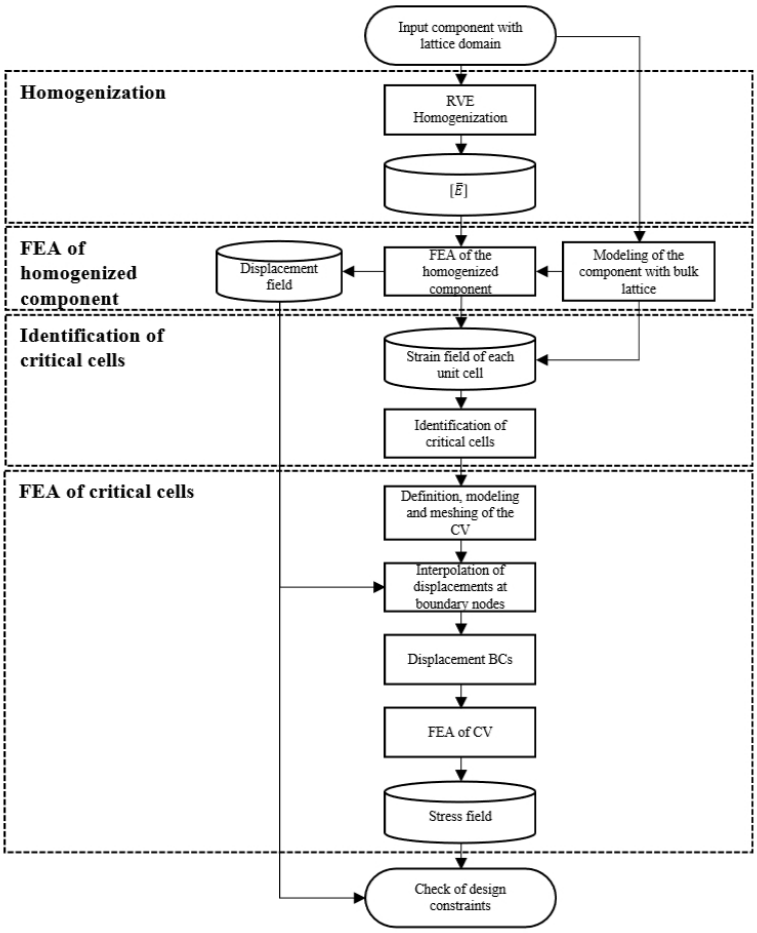

Figure 1: Flowchart of the procedure for fast FEA of lattice structures.

material is applied to all the bulk parts, while the homogenized equivalent material properties in form of the elasticity tensor computed in the previous phase of the procedure is applied to the lattice domain. Then the prescribed boundary conditions, loads and displacements, are applied to the FE model and the simulation can be performed.

Once the numerical computation is completed, the macroscopic displacement field is retrieved and reflects the real behavior of mechanical component under test, while only a "mean" stress field can be computed. Therefore, at this stage it is not possible to evaluate the real mechanical strength of the component and to check the fulfillment of the mechanical design constraints. However, even if the values of stress of the homogenized lattice and those of the real one do not match, the spatial distribution of the strain field is the same, i.e. the most stressed areas are the same.

For that reason, the third stage of the workflow is aimed at the individuation of the most stressed cells of the lattice. First of all, the geometrical topology of the lattice has to be created. Cells are divided into two categories: boundary cells and inner cells. The former group is composed of the cells that have at least one boundary face that is either free (not attached to any other cells) or to the bulk material of the component. The latter group includes all the

cells that are fully surrounded by other cells. This distinction is useful to analyze both the most stressed cells of the inner domain of the lattice and those that are at the interface with the bulk material, where high stresses are usually present due to the abrupt transition from solid to lattice. Then the homogenized strain at each integration point of the lattice domain, taken from the FEA of the homogenized component, are assigned to the cell the node under exam belongs to. Once all integration points are processed, for each unit cell the mean and maximum Von Mises strain values are computed. This allows the identification of the most critical cells of each group.

The final stage of the workflow is dedicated to the de-homogenization of the critical cells. The domain of each critical cell is modeled using CAD tools and meshed. The nodes that lie on each of the six boundary faces of the control volume are identified and their coordinates recorded. Then, the displacements along the three principal directions of each boundary node are computed through linear interpolation from the displacement field of the homogenized component and applied as displacement BCs. Once all boundary nodes are processed, the real microscopic stress field can be computed through FEA. Now all the necessary data to evaluate the design of the mechanical component are available.

4 CASE STUDY

This sections presents the application of the complete procedure for the efficient and fast FEA of lattice structures, presented in Section 3, to a sample study. The aim of the study was the numerical computation of the macroscopic displacements and microscopic stresses of the most critical zones of the mechanical component, that represent the most important data for the mechanical design of components. Results were also compared to the outcomes of the FEA of the real lattice components to prove the validity of the presented method.

The mechanical component under study is a beam made of AlSi10Mg aluminum alloy with a reinforcing prismatic lattice domain composed of the so-called tetra cells, that are obtained through the combination of a cubic and a BCC cell. The dimensions of the beam are 100 $\times$ 24 $\times$ 12.5 mm and those of the back plate are 50 $\times$ 40 $\times$ 5 mm. The unit cell has got side length 6 mm and strut diameter of 0.75 mm. The mechanical component is restrained on the back plate and a force of 500 N is applied on the tip of the beam. The base constituent aluminum alloy was modeled as an isotropic elastic material with the following mechanical properties $E = 70$ GPa, $\nu = 0.33$.

Geometric modeling and meshing were performed using the free and open source software Gmsh, while numerical computations were carried out with the FE software CalculiX. All the pre and post-processing activities as well as the orchestration of the complete automated framework were performed using a self-developed Python program.

4.1 Results and discussion

In the first phase of the framework the RVE of the lattice was homogenized. Strut-based cells like the tetra cell can be modeled as orthotropic materials with cubic symmetry. Thus, the elastic constitutive law of the material can be described using only the three independent parameters: the in-plane elastic constant C_{11}, out-of-plane elastic constant C_{12} and shear component C_{44}. This allows the full characterization of the homogenized material performing only two out of the six simulations. After having performed a convergence study on mesh size and RVE dimensions,

Steven's approach was selected, as it provided almost the same results as PBCs. Moreover, for this type of cell the convergence on results was achieved after 30000 elements per unit cell and the number of unit cells within the RVE did not influence the outcomes.

The homogenized elasticity constants were identified as $C_{11} = 1.81$ GPa, $C_{12} = 0.811$ GPa and $C_{44} = 0.731$ GPa and were then used in the FEA of the homogenized macroscopic components. The BCs described in the previous section were applied to the model and the simulation was run. Fig. 2 depicts the comparison between the macroscopic displacement obtained through the direct and homogenized simulation. As it can be seen from Table 2, the agreement between those data is almost perfect, but as already said, the stress field computed through the homogenized FEA does not reflect the true behavior of the lattice domain, because the equivalent bulk material does not present any stress concentration point.

Displacement data			
	Real	Homo	Difference [%]
Max disp. [mm]	0.59	0.59	0
Disp. at tip [mm]	0.59	0.59	0
Max stress [MPa]	268	3.78	-98
Computation time	2.5 hrs	20 s	-99.9

Table 2: Comparison between real and homogenized displacement and stress data.

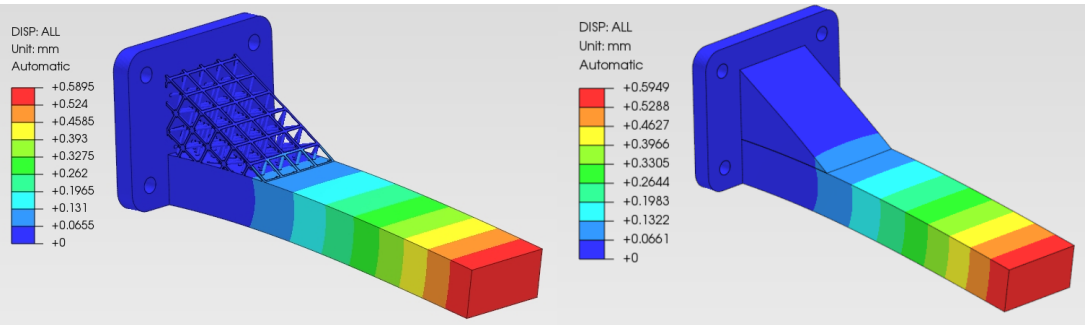

Figure 2: Comparison between the displacement field obtained through direct and homogenized simulation.

However, as it can be seen in Fig. 3, from the analysis of the homogenized strain field, the most critical zones of the real lattice component can be effectively identified. Once the critical cell was identified a control volume, containing the cell itself was modeled, meshed and simulated applying to the boundary nodes the displacement interpolated from the homogenized displacement field. Control volumes with increasing dimensions (1 cell, 1.5 and 3 cells per side) were simulated to investigate the effects of BCs on the outcomes of the simulation. Table 3 reports the comparison of the obtained stress data through direct numerical simulation and the de-homogenization procedure. As it can be clearly seen, the analysis of the homogenized strain field correctly identifies the most critical cell of the lattice. As the dimensions of the control volume get bigger, the error on the maximum stress within it decreases and approaches

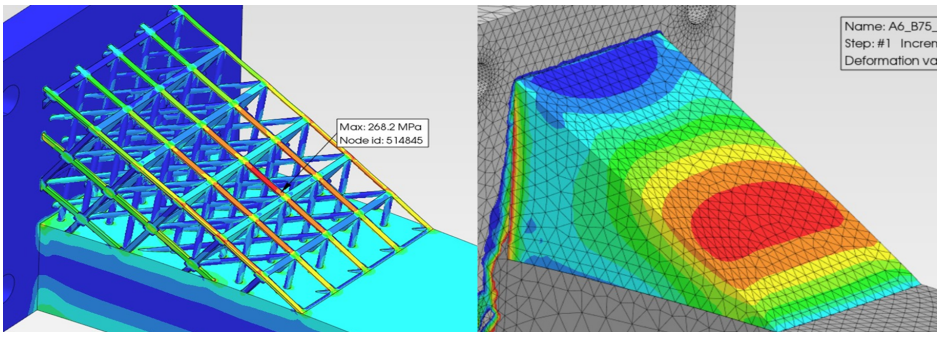

Figure 3: Real stress field and homogenized strain field.

the true maximum stress inside the lattice domain. The stresses computed through the de-homogenization procedure seem to be always higher than the true ones, so it is a conservative approach.

In conclusion in less than three minutes all the relevant data for the evaluation of the design of the mechanical component under test were retrieved with a very high fidelity.

Stress data							
		1 cell		**1.5 cells**		**3 cells**	
	Real [MPa]	Homo [MPa]	Err [%]	Homo [MPa]	Err [%]	Homo [MPa]	Err [%]
Max stress [MPa]	268	320	19	294	10	278	4
Mean stress [MPa]	29.0	66.4	129	46.5	60	30.4	5
SD [MPa]	25.3	50.3	99	44.0	74	25.9	2
Computation time		10 s		24 s		85 s	

Table 3: Comparison between real, homogenized stress data and computation time in dependence of the dimensions of the control volume.

5 CONCLUSIONS

Despite lattice structures have shown big potential for their outstanding mechanical properties, low weight and the possibility to finely tune their behavior depending on the application, however, their numerical design and optimization are strongly limited by the high computation time required in every phase of Direct Numerical Simulations (DNS). Therefore, this research aimed to provide a procedure able to reduce the overall computation time, while still providing all the necessary data for the evaluation of the mechanical designs.

A multi-scale framework based on homogenization was presented and tested on a case study to compare the results to those obtained through DNS. Using the homogenized properties, the simulation of the mechanical component with lattice domain could be speeded up by more than 99% and the macroscopic displacement field matched with that coming from DNS. Since the stress field did not reflect the true behavior of the lattice, a de-homogenization was required. The most critical cell were identified analyzing the homogenized strain field inside the lattice domain and then simulated by applying the homogenized displacement to the boundary nodes. It was found that the error on the maximum stress between the de-homogenized critical cell

and the DNS becomes smaller, as the control volume involved in the sub-modeling gets bigger, because the boundary effects are minimized.

The presented procedure was proven to be reliable and to reduce the overall computation time. Thus, it can be employed in optimization framework to evaluate each design online in just few seconds. Future research will be oriented at extending the procedure to study the dynamic response of mechanical components with lattice domains.

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