Data driven Computational Mechanics at EXascale

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REPORT ON THE DCoMEX – OPTIMAL MATERIAL COMPOSITION

DELIVERABLE D7.6

Version No 1

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Contents

1 Introduction

This report presents a detailed description of Deliverable 7.6, which pertains to WP7 "Applications" of the DCoMEX project and it is related to DCoMEX-MAT (Deliverables 7.3 and 7.4). The focus is the development of the appropriate computational machinery for optimizing material compositions and achieving targeted mechanical properties and responses in contemporary composite materials. Specifically, a model of CNT-reinforced concrete is analyzed, with optimal structures identified through topology optimization. To accurately simulate the complex behavior of this nano-composite material, a concurrent multiscale modeling technique is employed. The topology optimization is carried out using the BESO algorithm, a well-established method known for delivering reliable results. The analysis was performed on MELUXINA, the supercomputer located in Luxembourg, designed to provide energy efficient high-performance computing (HPC) capabilities for research, innovation, and industrial applications.

2 Application

2.1 CNT-reinforced concrete multiscale model

Predicting the behavior of CNT-reinforced concrete is a complex challenge due to the physical mechanisms that occur across multiple length scales, all of which significantly influence the material's macrostructural response. To closely replicate real-world behavior, a multiscale modeling strategy is applied. This model incorporates four distinct length scales, with their interactions captured through a nested computational homogenization scheme. For a more in-depth explanation of the underlying theory and description of the multiscale model solution pipeline, the reader can refer to the report in Deliverable 7.4 (theory manual). The application under study for topology optimization is the cantilever, as shown in Fig. 2.1. The geometric specifications of the investigated cantilever are length $L = 40m$, height $H = 10m$ and width $W = 10m$. The discretization of the model with finite elements is defined as $Nx = 10$, $Ny = 10$ and $Nz = 40$, where the x and y directions refer to the width and height respectively, while the direction z corresponds to the length of the cantilever. A vertical load is applied on point A, with coordinates (5,5,40), as seen in Fig. 2.1 with a magnitude of $F_A = -0.5GPa$

2.2 Topology optimization with BESO

The Bi-directional Evolutionary Structural Optimization (BESO) method, that was employed in this study, like its predecessor ESO, is a combination of gradient-based and heuristic algorithm aimed at optimizing structural layouts. Initially proposed by Querin et al. (1998, 2000), BESO extends the ESO approach by allowing the removal of inefficient material (low-stress elements) while also enabling the addition of material near high-stress regions during the iterative process.

The objective function in BESO is typically the minimization of mean compliance, which represents structural stiffness. The objective function is expressed as:

$$C = F^T u \tag{2.1}$$

where C is the global compliance, F is the global load vector and u is the global displacement vector.

Sensitivity analysis, based on elemental strain energy values, is employed to guide the addition or removal of material by identifying high and low-sensitivity elements. The gradient based sensitivity is quantified as:

$$a_e = \frac{\partial C}{\partial x_e} \tag{2.2}$$

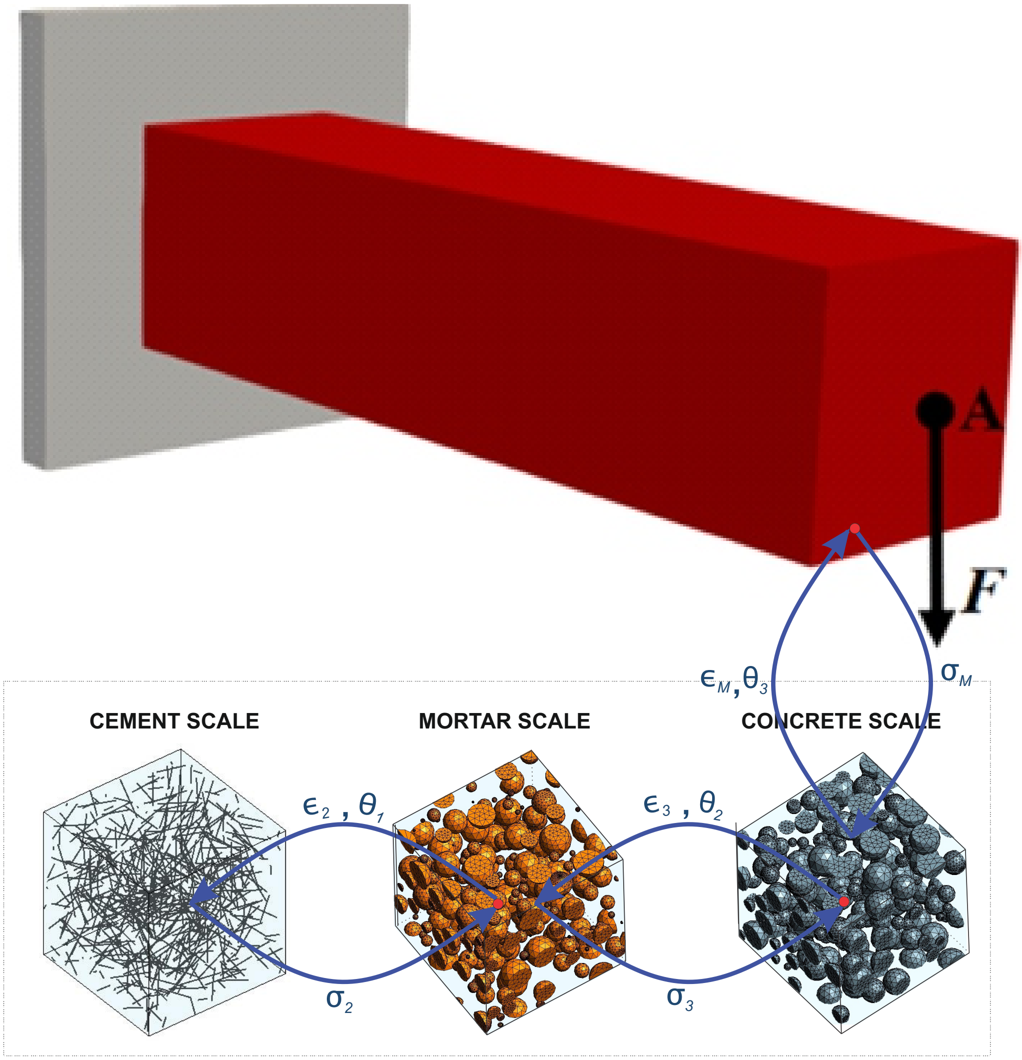

Figure 2.1: CNT-reinforced concrete cantilever model

where a_e is the sensitivity of the objective function to changes in element e's material and x_e is the material density of the element e.

This process continues until a specified volume constraint (Vc) is satisfied, with the volume evolution rate (ER) controlling the material adjustments in each iteration. The Vc has the following form:

$$V = \sum_{e=1}^{n=1} x_e V_e \leq V_c \tag{2.3}$$

while the ER of the volume is postulated as:

$$N_{remove} = ER \times N_{total} \quad \& \quad N_{add} = ER \times N_{void} \tag{2.4}$$

where N_{remove} and N_{add} is the number of elements where material will be removed and added respectively, while N_{total} is the total number of elements currently in the structural model and N_{void} is the number of elements in void regions that are capable of having material added to them.

Based on the above the following update rule is used by taking into consideration the evolution rate:

$$x_e^{new} = \begin{cases} 1, & if \quad a_e \geq T_{add} \\ 0, & if \quad a_e \leq T_{remove} \\ x_e^{old}, & otherwise \end{cases} \tag{2.5}$$

where T_{add} and T_{remove} are thresholds for adding and removing material, respectively.

BESO is applied towards the identification of the optimal topological structure of the studied structural application shown in fig. 2.1.

2.3 Numerical results

To perform the BESO optimization the target volume constraint is chosen as $Vc = 0.5$ and the evolution rate as $ER = 0.01$. Additionally, to prevent numerical issues and achieve a physical meaningful design a smoothing is applied with a filter radius of $R = 1.25$. The material density distribution and the final form of the optimized structure are presented in figs. 2.2 and 2.3, respectively.

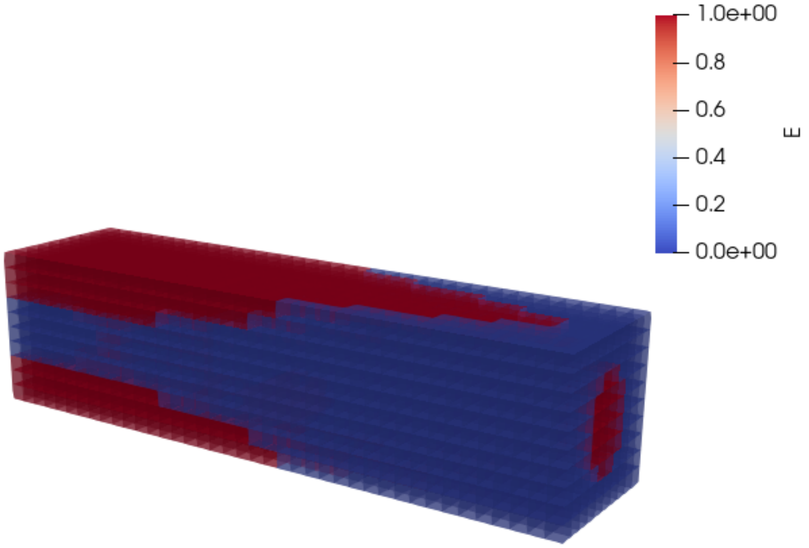

Figure 2.2: Material density of all the elements of the discretized model

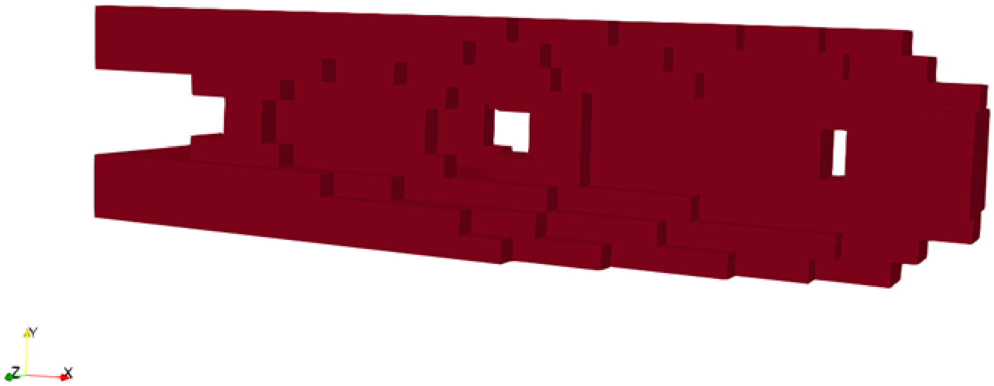

Figure 2.3: Final form of the optimized cantilever

To evaluate the influence of CNTs on the optimized configuration of the cantilever, two analyses were conducted. In the first, the multiscale model depicted in Fig. 2.1 was examined without the inclusion of CNTs (0% weight fraction). In the second analysis, a 3% weight fraction of CNTs was incorporated at the cement scale. The vertical displacement observed at point A (refer to Fig. 2.1) is compared in Fig. 2.4.

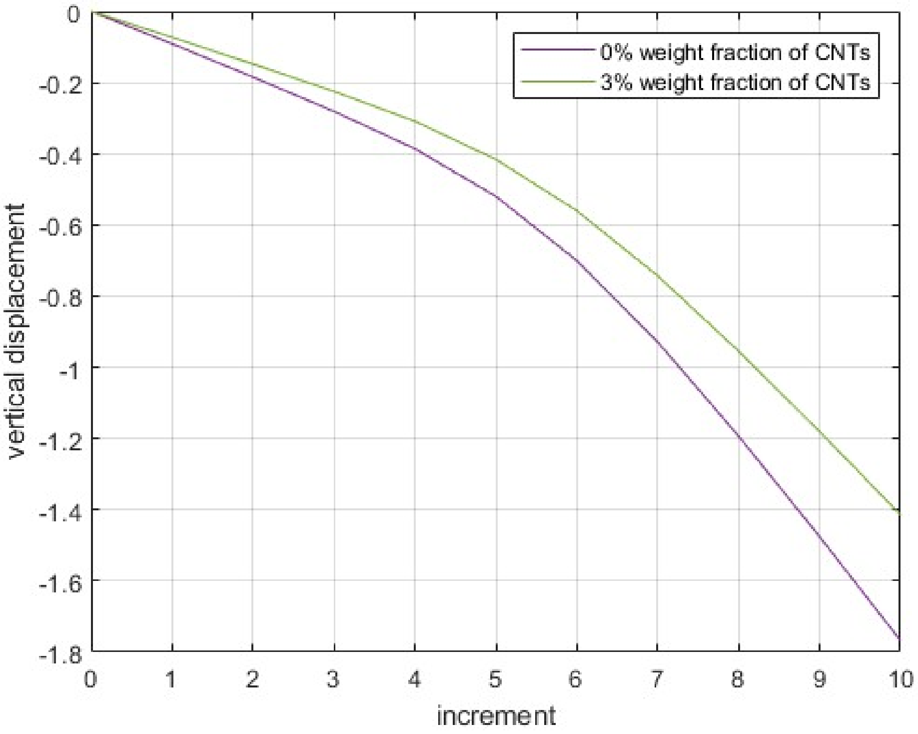

Figure 2.4: Vertical Displacement at point A for the cases of 0% and 3% CNT weight fraction

As shown in Fig. 2.4, the incorporation of CNTs significantly enhances the overall stiffness of the structure.

Moreover, the displacement fields from both analyses are presented in Figs. 2.5 and 2.6.

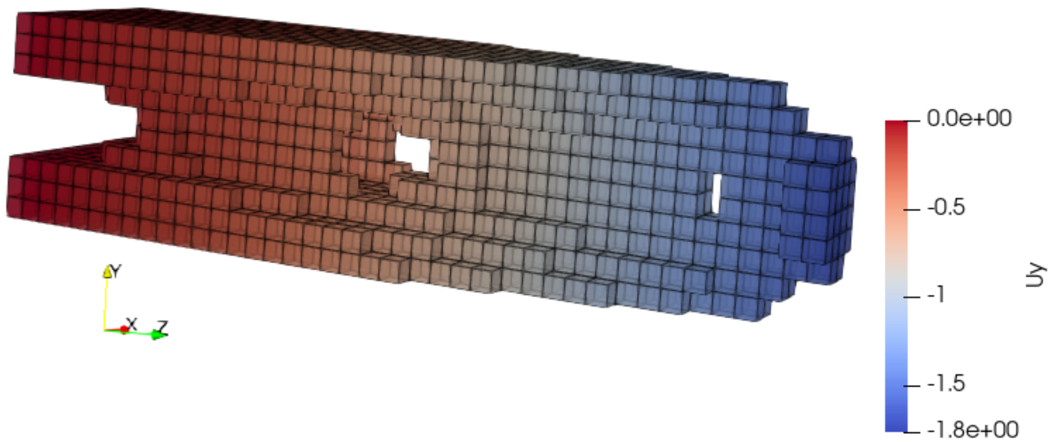

Figure 2.5: Vertical displacement field for the case of 0% weight fraction of CNTs

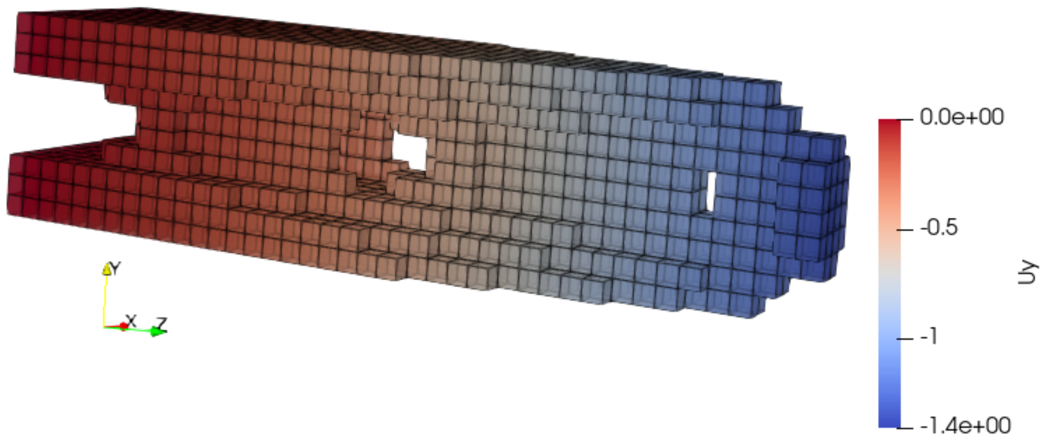

Figure 2.6: Vertical displacement field for the case of 3% weight fraction of CNTs

Similar to our previous conclusion, the displacement fields shown in Figs. 2.5 and 2.6 demonstrate that CNTs significantly enhance the structural stiffness. This influence has the potential to effectively reduce the displacements along the length of the deformed cantilever. To further quantify the benefits of CNT reinforcement on concrete-based structural, the Energy Dissipation (ED) is measured. The energy dissipated by the structural system during deformation is calculated as:

$$ED = \int_V \int_0^{e^p} \sigma d\varepsilon^p dV \tag{2.6}$$

where V is the total volume of the structure and ε^p is the plastic strain.

The ED is analyzed for two different material compositions: 0% and 3% weight fraction of CNTs. The results are presented in Figure 2.7. It is evident that the incorporation of CNTs significantly enhances the total ED of the structural system.

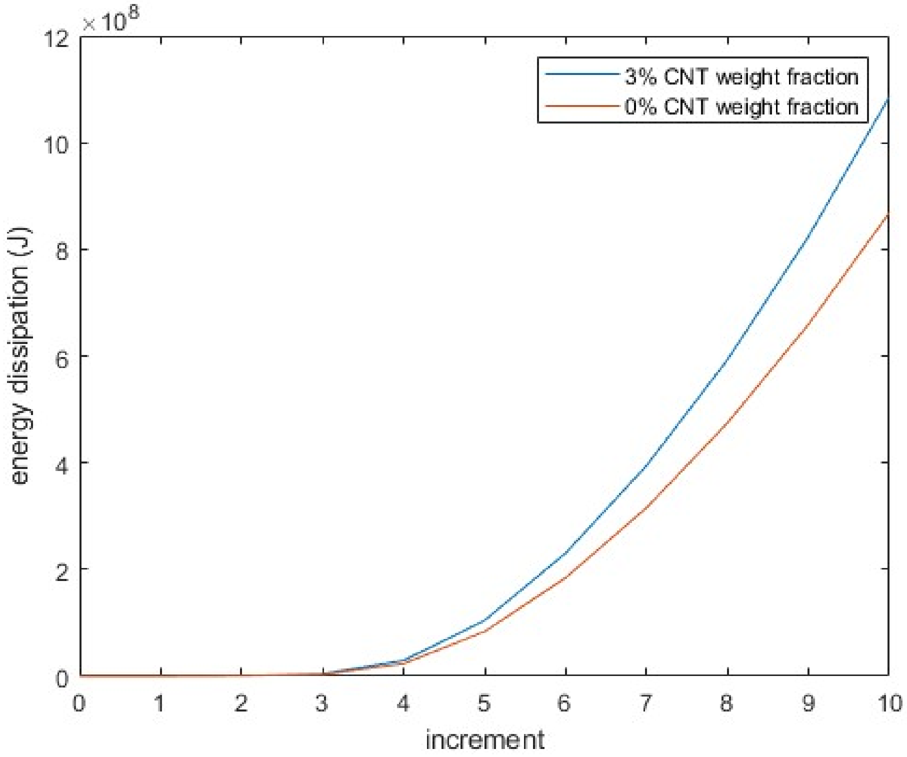

Figure 2.7: Energy Dissipation for the cases of 0% and 3% CNT weight fraction

Details regarding the performance evaluation of the DCoMEX-MAT applications can be found in the respective part of the report of Deliverable 8.2.

2.4 Conclusions

This report introduces a framework for recovering optimal structural configurations in models composed of advanced nanocomposite materials. The approach leverages a multiscale modeling technique, beginning with a preprocessing phase where a hierarchy of deep neural networks was developed to generate an efficient and cost-effective constitutive law. This strategy successfully bypasses the need for the computationally expensive homogenization analyses typically required in such complex systems (refer to Deliverable 7.4 (theory manual) of DCoMEX-MAT for more details). By employing surrogate modeling techniques, and harnessing the high-performance computing capabilities of the MELUXINA supercomputer, the framework achieves rapid solutions to computationally demanding topology optimization problems within multiscale material systems.

A case study is also presented, focusing on the optimization of a CNT-reinforced concrete cantilever structure. The results demonstrate substantial improvements in both structural stiffness and energy dissipation, owing to the integration of CNTs, which play a pivotal role in enhancing the overall performance of the optimized structure. These findings underscore the potential of CNTs in revolutionizing material behavior, particularly in structural applications where advanced mechanical properties are essential.