# Data Driven Material Design at Exascale

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**Keywords: Computational homogenization, FE$^N$, deep neural networks**

The need for advanced high-performance materials is undoubtedly one of the main drivers of today's innovation in industry and research. Over the past decades, several new technologies have emerged for the development of composite materials with enhanced properties (mechanical, thermal, electrical) based on appropriate modifications of their composition in finer scales. As an example, carbon-based nanomaterials such as graphene sheets and carbon nanotubes (CNTs) are considered to be among the most promising fillers for the development of next-generation composite polymeric materials.

The resources required to experimentally study the behavior of advanced nanocomposites greatly slow down progression on this field. A promising alternative is to use multiscale computational approaches that enable to study a large number of material combinations and microstructural configurations at a low cost. According to these, the system is decomposed and defined in a number of distinct length scales (e.g. nano-, micro-, mesoscale), with each of these scales having its own material 'genome', i.e. individual topological, geometrical and physical properties. The material 'genomes' can vary significantly between scales and accordingly dissimilar and scale dependent physical phenomena can emerge. The concept of multiscale mechanics, then, consists in identifying appropriate regions to bridge the various length scales and quantifying these dependencies. With this approach, information from the lower scales passes to the upper scales, usually by applying averaging theorems on a Representative Volume Element (RVE) [1,2]. Despite the high accuracy and modeling capabilities that computational homogenization offers, it requires however immense computational resources, especially in non-linear analyses, which renders it in many cases unrealizable.

In this presentation, we demonstrate a surrogate modelling strategy designed to accelerate the analysis of structural systems composed of materials with microstructure, in the context of FE2 computational homogenization. In particular, the main idea is to replace finite element analysis of parameterized RVEs using customized neural networks architectures to emulate the stress-strain relation of the RVE. With this approach we can achieve a tremendous speed up in computational cost, which in turn enables us to tackle highly challenging problems. To demonstrate this framework, we first apply it in a stochastic optimization problem of car bumper made up of CNT-reinforced polymer with the aim of increasing the part's crashworthiness during crash simulations (Fig. 1). Here, we used a contact FE formulation to simulate impact, along with a nonlinear constitutive law for the polymer material and sought for the optimal CNT weight fractions and orientations at different locations of the car bumper.

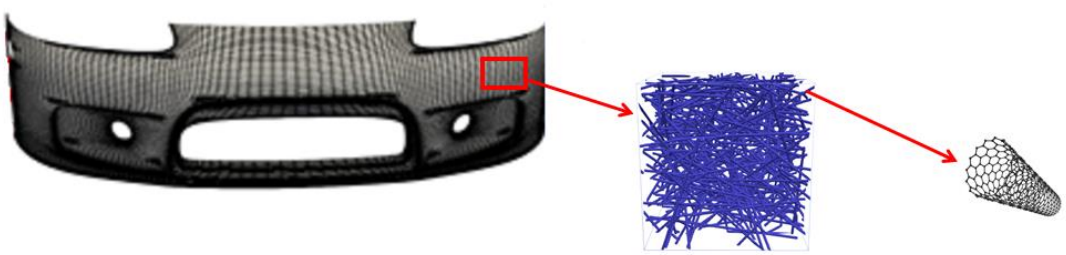

*Fig. 1 – Multiscale model of a car bumper made up of CNTs-reinforced polymer.*

Next, we extend the previous idea to multiscale problems with N>2 scales. The proposed strategy is to employ a sequence of neural networks that represent the hierarchy of the separate scales in the multiscale problem, with each neural network of a finer scale being contained in the neural network of the successive, coarse scale. At the end of the training process, a single deep network is produced which emulates the macroscopic behavior by incorporating all physical mechanisms arising at each of the problem's finer scales. This approach takes full advantage of the accuracy and modelling capabilities that $FE^N$ schemes provide, while at the same time overcomes their immense computational requirements. It is demonstrated on the analysis of a large-scale building made of CNT-reinforced concrete material, as shown in figure 2.

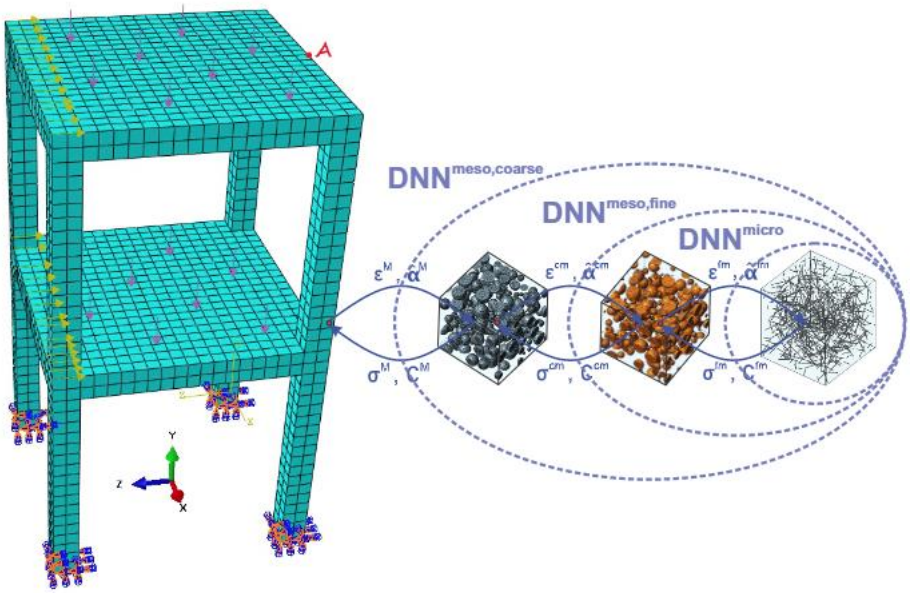


*Fig. 2 – Multiscale model of a CNT-reinforced structure. Each Gauss point of the macroscale is associated with a constitutive law delivered by the DNN hierarchy*

The previous applications illustrate the capabilities of surrogate modelling in accelerating the solution of complex engineering problems that would otherwise be unapproachable. However, despite one's best-efforts surrogate models can never be exact. In the last part of this talk, we attempt to address this issue with a newly developed methodological framework, termed AI-Solve, which combines machine learning algorithms with algebraic solvers and is capable of achieving user-prescribed levels of accuracy with significantly faster convergence rates than conventional solvers.

**References**

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