Development of machine learning methods for the design of architectured materials: convolutional and Choquet capacity networks

1 Adam project: architectured materials with controlable properties

It has long been recognized that heterogeneous and architectured materials can achieve exceptional physical response. In optics, metamaterials, i.e. media with properties that go beyond that of their individual phases, may achieve negative refractive indices. In mechanics, auxetic materials, which present negative Poisson ratios, also exhibit interesting properties in plasticity [1]. Nowadays, additive manufacturing has opened ways to assemble materials with so-called "programmable properties". In the framework of the Adam project and of the Diadem "demonstrator", materials with tailored behavior are currently being investigated. These materials rely, for instance, on the onset of mechanical instabilities, that were ordinarily considered detrimental to the mechanical response, to control its mechanical response. These phenomena include elastic instabilities, buckling or plastic deformation mechanisms, and rely on the actuation and storage of elastic energy within the structure [2]. Investigating these problems and finding new materials requires, one the one hand, dedicated experimental devices [3] and, on the other hand, new modeling techniques. These techniques consist in predictive methods based on micro-mechanical computations, typically finite element, or FFT algorithms, but also on numerical tools that are able to simulate and explore the wide range of architectured structures and their mechanical responses.

So far, periodic arrangements or deterministic structures have been the topic of many (or most) studies undertaken, such as that devoted to structural optimization [4]. Nevertheless materials with *random* microstructures also present interesting features [2]. In particular, they are in general less sensitive to the presence of defects, such as the ones produced bu 3D printing techniques, and also exhibit improved mechanical properties with respect to failure.

To address the question of a random microstructure, a first step consists in developing techniques to simulate synthetic random structures that represent the materials of interest as well as numerical methods able to explore their mechanical properties. The present project aims to develop new modeling tools for studying random structures with improved mechanical response. To do this, machine learning techniques will be developed to generate materials with complex geometries, within mathematically well-defined classes of random microstructures. In practice, one must enforce geometrical constraints such as those that are suitable to 3D printing manufacturing [5].

2 Choquet networks

The Choquet-Matheron-Kendall theorem [6, 7] establishes that a random set with appropriate properties (stationarity, ergodicity) is fully characterized by its Choquet capacity [8]. The Choquet capacity functional can be seen as a convolution in the (max; +) algebra and can be compared to fuzzy measures in so-called fuzzy integral neural networks [9]. This max-plus convolution [10], or *dilation layer* [11] has been implemented in machine-learning layers, using the morpho-layers library. Preliminary results have shown that these machine leayers framework can be used efficiently to address classical problems in machine learning such as classification or regression, for point patterns [12]. Choquet networks offer perspectives as a way to provide *interpretable* kernels in machine learning methods, and also as a method for enforcing certain *geometrical constraints* on simulated structures. In the present project, we propose to use Choquet networks in addition to classical convolutional layers to simulate random structures.

3 Roadmap of the project

The project will be consist of the following indicative steps:

- *Simulation of random beam-lattice structures*. We will use models of random sets to generate 2D (and optionally) 3D structures resembling lattice beams that can be manufactured. To do so, we will use the following three steps: (i) a point process that serves to provide a set of vertices, (ii) a random graph connecting the vertices, (iii) an edge-valued function that can be used to represent the skeleton of a beams lattice. In steps (i) and (ii), we will use models of point process (Gaussian; Mattérn etc.) and lattice Gaussian Markov fields [13] generated from a mean and covariance function. The skeleton in step (iii) can be seen as the centers of maximal balls contained within the beams [14]. The generated sets will be used to populate a database of randomly-distributed virtual structures.

- *Generative based training* We will employ a machine learning framework to simulate microstructures that mimic beam lattices. Two types of generators (GAN or diffusion) will be considered that employ both classical convolutions and dilations, and the generator will be constructed to simulate points, making use of the representation of beam lattices as a set of connected vertices.

- *Constrained simulations* In addition to the above, we will perform simulations with constrained geometrical properties, such as a controlled density and maximum number of neighbours for each vertice.

- *Exploration of mechanical properties* FFT computations will be performed to simulate ground truth data on the local strain and stress distribution. The generative methodology detailed above will be employed to generate lattices with constrain ed strain and stress distributions.

Context The post-doctoral position will be part of the ANR demonstrator project "ADAM" as well as the ANR exploratory program "Diadem", with the collaboration of researchers from different laboratories including INSA Lyon (Simap-Mateis), Polytechnique (CMAP), Univ. Grenoble (3SR, LGP2), CEA (LIST, LITEN).

Supervision The post-doc work will be jointly supervised by François Willot, Paco Chinesta, Santiago Velasco-Forero and Jesus Angulo.

Duration 10 months.

Application We are looking for a junior researcher holding a PhD in image analysis and machine learning, especially in domains of applications related to engineering and material science, with excellent scientific background. Please include in your application submitted or published articles whenever possible. Send your full resume and application to `francois.willot@minesparis.psl.eu`, `francisco.chinesta@ensam.eu`.

Location CMM laboratory of Mines Paris (in Fontainebleau), regular visits to PIMM laboratory in ENSAM (Paris)

References

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