Data-driven multiscale framework for architected cellular materials

Key words Data-driven, model-free, computational mechanics, material database, multiscale, finite element analysis, computational homogenization.

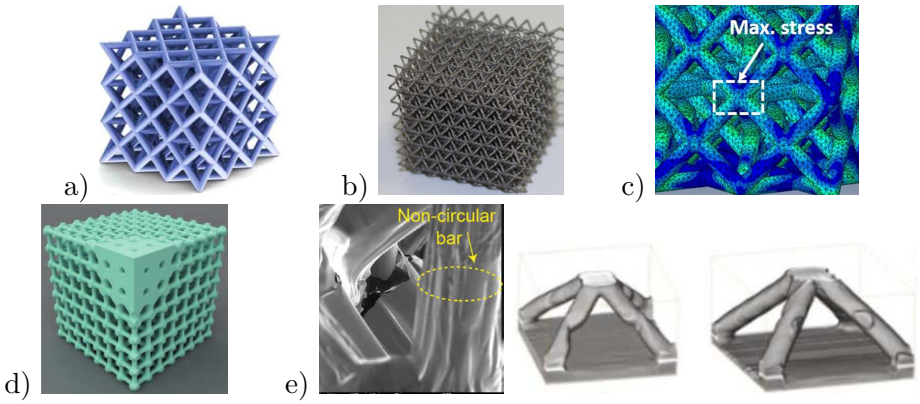

Figure 1: Architected, latice-type cellular material a) CAD model, b) manufactured lattice, c) three-dimensional FE analysis of the lattice, d) example of the location specific cellular structure, e) example of the truss ligament defect (non-circular shape).

1 Context

In this research project we will study lattice-type, cellular materials (Fig. 1). The advances of these materials parallels the rapid progress in additive manufacturing (*e.g.* Electron Beam Melting (EBM) and Selective Laser Melting (SLM) for metal lattices). 'Printing' a material with the chosen lattice architecture leads to high structural efficiency where strength and stiffness scale proportionally with the solid volume fraction. Principal application is in transport and industry with the most stringent criteria related to mass reduction, energy absorption (crash) and thermal management.

The tendency to shift towards cellular materials in lightweight application however requires a dedicated tool for material design and prediction of the specific material behavior. Classical computational tools based on finite elements (FE) together with high-fidelity models leads to time-consuming simulation on the structural scale. Using a reduced model of the cellular structure can speed-up the computation, however it is inappropriate for describing accurately the local behavior (related to damage, plasticity and buckling) leading to introduction of safety factors and lack of confidence in the design.
A multi-scale (MS) modeling [1] permitting to obtain the material behavior on the macro-scale from the simulation of the representative part of the high-fidelity micro-scale is a promising alternative. The principal downside of MS modeling based on the computational homogenization [4] is that the micro-simulation with fine FE mesh has to be run for every macro load step and integration point leading to tremendous repetitive computations.

One of the possible solutions for the problem of repetitive and never re-used computations is proposed recently [6, 2] and resides on combining so called *data-driven approach* (DDA) [3] and computational homogenization in order to decouple the MS problem in two single-scale problems, as follows:

1. **Material database genome.** One firstly performs numerous, but usually off-line, micro-simulations for a chosen set of macroscopic deformations as input. The microscopic system modeling exactly the lattice structure will be solved using FE method and existing commercial code (*DS Abaqus*).

The homogenized micro-scale stress together with the input deformation is collected and stored in the material database.

2. **Material data drives macro-scale.** Having a material database at hands, the macroscopic problem turns to DDA which aims to replace the constitutive model in favor of the material database. In particular, within DDA the solution is sought in the set of mechanically admissible states by minimizing the distance to the material data set.

Within this framework once the material database is properly sampled, no 'online' constitutive model nor micro-simulation is needed. Moreover, microscopic information in the database can be called at any time (re-usage of data!) making **data-driven MS** simulation computationally less demanding since searching a material database is typically much faster than a new high-fidelity calculation. However, the *computational cost* in the 'off-line' stage of the creation of the material database genome is *still very high*. The key challenge is how to efficiently sample the data base using micro-scale computations and, first and foremost, in the case of varying micro-scale geometry. Varying micro-scale geometry occurs in two situations: (i) Intenionally – to have a location specific cellular structure, depicted on Fig. 1 d); (ii) accidentally – defects related to the limitations of the manufacturing process [5], depicted on Fig. 1 e).
In the proposed project we will deal with the defects, which inevitably form during material layer deposition and together with the cell topology govern the overall lattice behavior.

2 Objective, program and outcome

To alleviate the principal obstacle of the DD-MS framework the objective of this project is the development of the algorithm that efficiently morphs the material database of ideal (CAD) lattice architecture Fig. 1 a) to adapt to the real (manufactured) architecture Fig. 1 e) with varying geometry and material.
To that end, the envisaged work of the student considers:

- The development of the framework for the parallel computing and computational homogenization of the large number of high-fidelity simulations. The parallel computing incorporates the usage of *DS Abaqus* and *CALMIP* computational platform.

- The modeling and development of the synthetic defects and the study of the influence of the manufacturing imperfections on the mechanical response and failure mechanisms. The classification of the defect's morphology and the development of the compact parametrization of geometry variations together with the scheme to incorporate geometric imperfections into the computational models.

- The development of the algorithm able to learn the material database variations as a function of the parametrized geometry variations.

- In the second step the student will work on the data-driven MS approach using the in-house *python* code developed in the laboratory.

The internship is taking place at Institut Clément Ader (ICA), Toulouse within the project "DataARC-en-CELL" in the frame of the program Interdisciplinarité et Émergence 2022, INSA-Touluse.

The result of the project is a scientific article written and submitted for review to one of the international journals. Moreover, this internship is considered as the preparation period for the PhD thesis funded by doctoral school of Mechanics, Energetics, Civil & Process Engineering (MEGeP) which follows the internship.

3 Candidate profile

Highly motivated candidate with the applied mathematics or mechanical engineer profile and the interest for the computational mechanics is welcome to apply. The experience in finite elements and *python* programming is required.
The candidates should send their CV and motivation letter to the internship advisors:
Eduard MARENIC (ICA) : `marenic@insa-toulouse.fr`
Jean-Charles PASSIEUX (ICA) : `passieux@insa-toulouse.fr`

Institution Institute Clément Ader (ICA), Université de Toulouse,
CNRS UMR 5312 INSA-ISAE-Mines Albi-UPS, 3 Rue Caroline Aigle, 31400 Toulouse, France.
Duration The duration of the internship is 6 months with a start in March or April 2022.
Gratification Standard internship about 600 EUR/months.

References

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