Internship proposal

Contacts

- Jonàs Martínez (jonas.martinez-bayona@inria.fr)
  `https://sites.google.com/site/jonasmartinezbayona/`
- Monique Teillaud (monique.teillaud@inria.fr)
  `https://members.loria.fr/Monique.Teillaud/`

INRIA Nancy - Grand Est.

Title

Inverse homogenization of implicit functions.

Context

Additive Manufacturing (AM) technologies are now capable of fabricating microstructures at the scale of microns, therefore enabling to precise control of the macroscopic physical behavior. This control empowers a wide range of industrial applications by bringing high-performance customized materials.

The design of microstructures with tailored macroscopic properties was introduced in the 1990s [12]. A key challenge is to relate the parameters of the microscopic structure to the macroscopic physical behavior. Homogenization methods [1] have been extensively used to predict the homogeneous physical behavior of heterogeneous materials (see Figure 1). Conversely, inverse homogenization [14] methods seek to find a microstructure with a prescribed macroscopic physical behavior. State of the art methods consider periodic microstructures [14, 12, 13] (see Figure 2), offering compact storage, efficient display, and simulation of the macroscopic physical behavior.

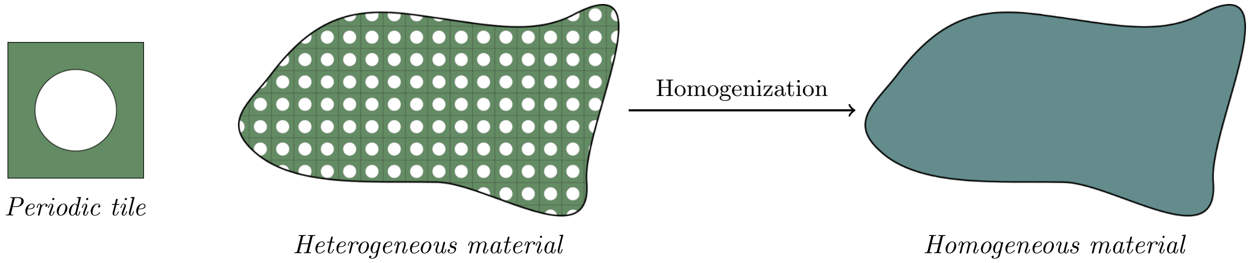

Figure 1: A periodic tile characterizing a heterogeneous material. Periodic homogenization derives a homogeneous material, that effectively represents the heterogeneous one.

Microstructures for AM will play a decisive role in the factory of the future, but several challenges remain aside [4]. The dimension of the objects being printed increases, and concurrently, the available printing resolution becomes finer. Thus, the geometry size of microstructures is drastically escalating.

We are particularly interested in two-phase microstructures defined by an implicit function $\mathcal{F} : \mathbb{R}^n \rightarrow \{0, 1\}$ (0 being void, and 1 solid matter) which is evaluated at every point in space, at the desired resolution, in constant time and constant memory computational complexity. The time/space complexity quantifies the amount of time/space taken by an algorithm to run as a function of the length of its output. In other words, having a constant factor implies that the algorithm complexity is independent of the output size. Thus, an implicit function will scale with future additive manufacturing technologies, as it is algorithmically independent of the output microstructure geometry size and complexity.

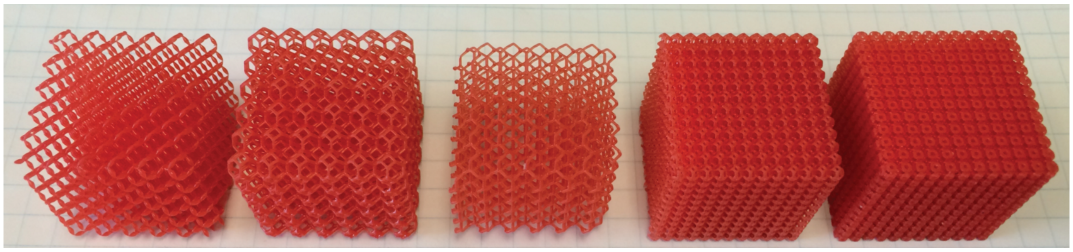

Figure 2: Additively manufactured periodic microstructures [8].

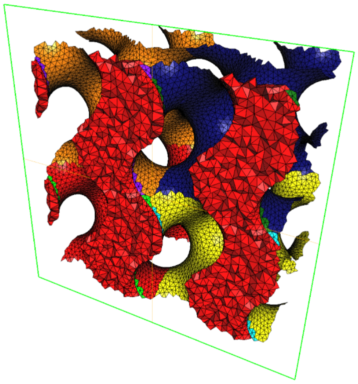

Figure 3: Tetrahedral mesh defined by an implicit triply periodic minimal surface (gyroid) [10].

Subject

The objective of the internship is to perform inverse homogenization of periodic microstructures defined by an implicit function. Specifically, we aim to study implicit functions defined by **skeletal structures**. Skeletal structures are a powerful tool used in a broad number of scientific fields [11]. Skeletons reduce the dimension of shapes, capture their geometric and topological properties, and seek to understand how these structures encode local and global features. The above properties provide a tight control of the topology and the geometry, which turns out to be crucial for enforcing fabrication constraints for AM.

The overall gradient-based inverse homogenization process can be summarized as:

1. (Meshing) Compute a 3D periodic mesh given by the implicit function $\mathcal{F}$.
2. (Optimization) Compute the inverse homogenization gradients of the tetrahedral mesh with respect the parameters of $\mathcal{F}$, and update $\mathcal{F}$ accordingly.
3. Loop to Step 1 until optimization convergence is reached.

This optimization procedure is in line with recent work on microstructure design [7]. Step 1 will involve to run the 3D periodic mesh generator or the CGAL library (`https://www.cgal.org/2018/09/10/Periodic_Mesh_Generation/`) on the implicit function $\mathcal{F}$ [9, 3, 2]. Step 2 will require to relate the inverse homogenization gradients (computed with FEM from the tetrahedral mesh) with the parameters of $\mathcal{F}$. Once the above pipeline is completed we will use it to optimize for implicit functions based on our recent research on skeletal microstructures [6, 5], as well to explore which type of physical properties it can optimize for (e.g. rigidity, heat conduction, conductivity). Apart from gradient-based optimization, other optimization schemes could be evaluated.

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