Inverse Homogenization-Based Design of Canonical Microstructures

Jakub Rainer[1,*], Damian Stefaniuk[2] and Dariusz Łydżba[3]

[1]Faculty of Civil Engineering, Wrocław University of Science and Technology, Wrocław, Poland
e-mail: jakub.rainer@pwr.edu.pl

[2]Department of Civil and Environmental Engineering, Massachusetts Institute of Technology, Cambridge, MA, USA
e-mail: dstefani@mit.edu

[3]Faculty of Civil Engineering, Wrocław University of Science and Technology, Wrocław, Poland
e-mail: dariusz.lydzba@pwr.edu.pl

KEYWORDS: *inverse problem, canonical microstructure, homogenization theory, numerical simulation*

Inverse problems in homogenization theory have recently attracted considerable attention, particularly in the context of optimal design of multifunctional materials. In this context, one seeks to determine a microstructure that realizes prescribed effective (homogenized) properties, i.e., to reconstruct a spatial distribution of phases such that the corresponding homogenized response matches given target data.

In this work, we consider the problem of reconstructing the microstructure of a two-phase composite from a sequence of macroscopic measurements. The analysis focuses on effective properties associated with heat flow problem in a heterogeneous medium. The inverse problem is formulated as the minimization of a cost functional defined as the mismatch between target and computed effective responses. The optimization is carried out using a simulated annealing (SA) algorithm, in which the design variables correspond to phase indicators at the pixel level. The microstructure is iteratively updated by modifying the phase assignment of individual pixels, and convergence is assessed through the evolution of the cost functional.

Due to the non-uniqueness of admissible solutions, the problem is inherently ill-posed, exhibiting both non-uniqueness and instability. To address this issue, a regularization term is incorporated into the objective functional, penalizing the interfacial measure (specific surface area). This promotes geometrically simpler configurations and imposes additional structural constraints. Numerical results indicate that, across a broad class of microstructural types, the reconstructed microstructures converge toward configurations consisting of a single irregularly shaped inclusion embedded in a matrix phase. This observation motivates the introduction of the concept of a *canonical microstructure*, defined as a reduced representation that is macroscopically equivalent—within the homogenization framework—to more complex heterogeneous media. Within this framework, the canonical microstructure acts as an effective surrogate for the underlying heterogeneous material, allowing for a substantial reduction in geometric complexity while preserving the essential macroscopic response.

The results suggest that, under suitable regularization, complex multi-inclusion microstructures can be effectively replaced by a single connected inclusion without significant deviation from the target effective properties. This finding sheds light on the structure of solutions to inverse homogenization problems and points toward reduced-order representations in material design. This is particularly relevant in the context of additive and advanced manufacturing technologies, where simplified geometries are advantageous for fabrication and optimization.