Multiscale structural and thermal optimization towards 3D printable structures

†Chikwesiri Imediegwu, Ryan Murphy, Robert Hewson, Matthew Santer
Department of Aeronautics, Imperial College London, London, UK.

†Presenting author: chikwesiri.imediegwu14@imperial.ac.uk

Abstract

This work demonstrates a robust framework for the design of tailored structural and thermal properties. It exploits the high process flexibility and precision of additive manufacturing to the physical realization of complex microstructure of metamaterials by implementing a multiscale approach. Structures derived from such metamaterial exhibit potentially superior properties which differ from that of the constituent base material. We seek to efficiently optimize the distribution of the constituting microstructure parameters of such structures in an attempt to satisfy predefined functional objectives. We develop a periodic microscale model as a lattice system whose geometric parameterization enables smoothly changing properties and for which the connectivity of neighbouring microstructures in the large scale domain is always guaranteed by slowly changing large scale descriptions of the lattice system radii. We populate the structural and thermal property space by evaluating all achievable properties enabled by our microscale parameterization. A full factorial design of experiments (DOE) is implemented. By leveraging existing rotation and reflection symmetries in our microscale model, we reduce the number of valuation points by over an order of magnitude for computational efficiency. Each point within the property space is evaluated by the implementation of periodic boundary conditions (PBC), execution of strain deformation and thermal analyses and the implementation of compuational homogenization to derive average properties of the microstructures. The discrete population of the property space is transformed to hyper-surfaces generated by polynomial least square fits. These response surfaces (also known as metamodels) of the property space are directly integrated in large scale optimization problem formulations and are continuous functions facilitating lattice-based topology optimization which is implemented using the finite element method with sensitivities derived by the adjoint method. A large variety of optimization problems are formulated with objectives relating to optimal weight and stiffness under multiple load cases, target deformation due to structural and thermal loads. Re-engineered components are 3D printed and tested for validation to demonstrate superior mechanical and thermal properties, hence emphasizing the robustness of the derived framework.
Keywords: Topology optimization, Multiscale modelling, Response surface modelling, Homogenization

Introduction

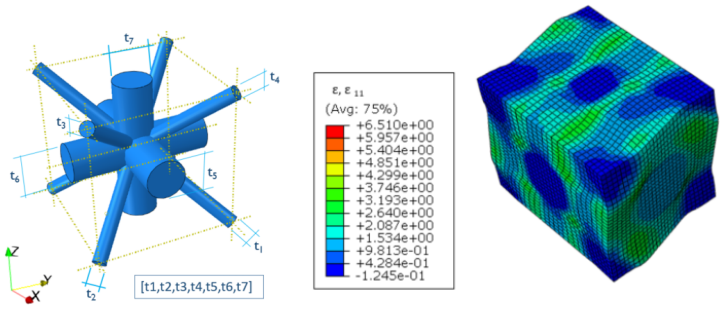
Conventional topology optimization answers the question of the optimal distribution of material within an established domain subjected to loads and boundary conditions to satisfy a functional objective[1][2]. Though the choice of these design objectives abound, the optimization process is constrained by a partial differential equation defining the physics of the problem and typically, limited material resources - a design cost. These constitute constraints on the problem that ensure the feasibility of the optimal design. A common approach to topology optimization is the Solid isotropic material with penalization (SIMP) method which implements a gradient based algorithm to determine the value of an artifical material density function within each element of the discretized domain. In SIMP, intermediate density values have no physical significance but a penalization parameter is employed to steer optimal material layout to a binary distribution that assigns material or void to every element. This penalization though esssential to the derivation of a physical optimal solution results in a loss in performance of the optimal design. Despite being the most orthodox approach to topology optimization, SIMP does not do well with multiple loading optimization problems and the final result is heavily mesh dependent and subject to checkerboarding, a computational problem abated by incoporating regularisation or sensitivity filters.

In this work, we extend conventional topology optimisation significantly taking inspiration from recent works of Xia et. al. [3] and Zhu et. al. [4]. We do not employ a fictitious density function as our control variable. Rather we take a multiscale approach [5] to derive a more robust optimization algorithm by implementing a metamodel that defines mechanical and thermal properties as functions of small scale design parameters. A direct consequence of the approach is that local intermediate material property values correspond to physically derivable microstructure and material distribution can be precisely tailored for optimal structural an thermal characteristics. A brief

description of our methodology follows.

Method

Our methodology spans over two scales coupled by computational homogenization of localized small scale properties to derive average macroscopic properties represented by response surface models in our optimization formulations .
On the microscale, we develop a material property model which is parameterized by the radii of members of a lattice system so that the structural and thermal properties of a periodic unit cell defined at this scale is a function of the parameters of the enclosed lattice system. Provided a significant scale seperation is applied, this parameterisation supports the implementation of periodicity and proffers smoothly changing geometry for smoothly changing perturbations of lattice parameters in the large scale optimisation. This property has inspired our choice of the lattice system. Ultimately, these lattice member radii constitute a vector of design parameters that fully define the mechanical and thermal properties of each microstructure. Fig. (1a) illustrates a typical microstructure with its vector of parameters. To reduce the number of simulations required, we leverage the existence of rotation

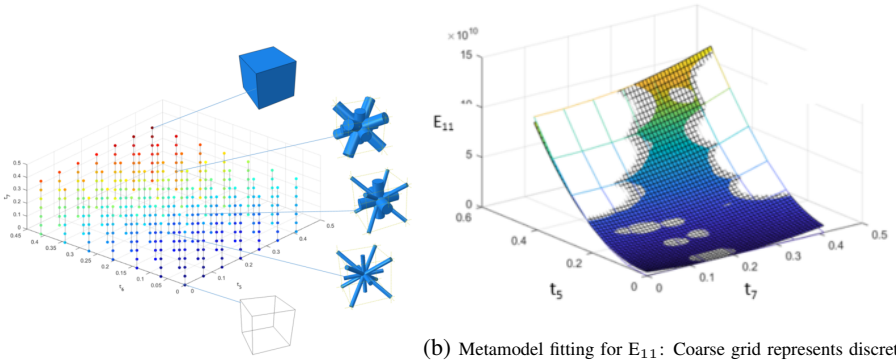


(a) Microstructure Parameterisation

(b) Typical strain deformation field for ϵ_{11} for stretch in x-direction (modelled in continuum)

Figure 1: Microscale Model Development

and reflection symmetries and develop an algorithm which sorts and classifies parent microstructures with their symmetry geometries. All symmetry geometry properties are derivable from parent microstructure properties by conventional mathematical rotation and reflection operations. By taking advantage of symmetries, we reduce simulations required by over an order of magnitude despite the implementation of full factorial design of experiments (DOE).



(a) Hyper-slice of 7-D property space

(b) Metamodel fitting for E_{11}: Coarse grid represents discrete property evaluations, fine grid represents generated response surface function ($R^2 = 0.9937$)

Figure 2: Response surface modelling of discrete valuation points

The process of property evaluations involve the implementation of periodic boundary conditions on a discretized unit cell as displacement constraint equations [6]. Next, a finite element solver is used to evaluate strain deformations in the principal and shear directions to determine the stress field. See Fig. (1b). A homogenization technique is applied to evaluate effective stresses and by implementing the constitutive equations in $\Re^3$, the stiffness tensor is derived [7]. In an analogous process, the microstructure thermal conductivity tensor is derived from Fourier's law

of conduction in steady state by applying temperature constraint equations on the unit cell, imposing temperature gradients in the principal axes and deriving effective heat flux by a similar homogenization technique.
These structural and thermal properties are evaluated for a large index of microstructures for which polynomial least square fits are generated as hyper-surface functions for each component of the stiffness and conductivity tensors. Fig. (2a) shows discrete valuation points in a hyperslice of one stiffness tensor component while Fig. (2b) illustrates a metamodel that converts discrete values to continuous functions. These continuous equations present a means to perform lattice-based large-scale structural optimization which is implemented using the finite element method with sensitivities derived by the adjoint method [8]. Our large scale optimization problem is set up as follows:

$$\begin{aligned} \text{minimize:} \quad & \mathbf{J}(u,\eta) \\ \text{subject to:} \quad & \mathbf{F}(u,\eta) = 0 \\ & V(\eta) \leq V_D \\ & a \leq \eta_e \leq b \end{aligned} \tag{1}$$

where $\mathbf{J}$ is the real-valued objective functional of choice that depends on the solution of a PDE that defines the physics of the problem and the vector of design parameters and $\mathbf{F} = 0$ stipulates that u satisfies the relevant equilibrium constraint. The cost constraint, $V \leq V_D$ puts an upper bound on the material volume of the optimal design and each component of the vector of design parameters, η_e has local bound constraints determined by the range of perturbations of the parameters for the microscale design of experiments. This eliminates the requirement for extrapolation on the generated response surface functions which could introduce inaccuracies to the macroscale solver.

Results and Conclusion

Several structural and thermal problems have been formulated and solved. We have extended the capability and efficacy of topology optimization for multiple loading linear elastic problems. Our framework shows great promise for a range of challenging applications where meta-materials can be tailored to predefined design requirements such as bend-twist coupling and global auxetic phenomena. Ultimately, re-engineered designs are physically derivable by additive manufacturing technology without a loss in precision of the tailored computational solution.

References

[1] *Bendsøe M.P., Optimal shape design as a material distribution problem, Structural optimization,* **1(4):***193-202 (1989)*

[2] *Bendsøe M.P., Sigmund O., Topology optimization: Theory, Methods and Applications, Springer-Verlag, Berlin (2003)*

[3] *Xia L., Breitkopf P., Multidisciplinary structural topology optimization with an approximate constitutive model for local material microstructure, Computer Methods in Applied Mechanics and Engineering* **286:** *147-167 (2015)*

[4] *Zhu B., Skouras M., Chen D., Matusik W., Two-scale topology optimization with microstructures, ACM Trans. Graph.* **36(5):** *17 pages (2017)*

[5] *Engquist, B., Lotstedt, P., Runborg. O., Multiscale Methods in Science and Engineering, Springer, Berlin Heidelberg, (2005).*

[6] *Xia, Z., Zhou, C., Yong, Q., Wang, X., On selection of repeated unit cell model and application of unified periodic boundary conditions in micro-mechanical analysis of composites. International Journal of Solids and Structures,* **43(2):***266-278 (2006).*

[7] *Kharevych L. Mullen P., Owhadi H., Desbrun M., Numerical coarsening of inhomogeneous elastic materials, ACM Trans. Graph. (Proc. SIGGRAPH)* **28(3):***51:1-51:8 (2009).*

[8] *Ghazlane, I., Carrier, G., Dumont, M., Aerostructural Optimization with the Adjoint Method in Proceedings of Conference Evolutionary and Deterministic methods for Design, Optimization and Control, Capua, Italy (2011)*