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Asymptotic expansion homogenisation and topology optimisation of cellular materials

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Abstract

Topology optimisation defines a set of tools associated to the modelling of an effective material domain within structural optimisation. Based on this type of optimisation, it is possible to obtain an optimal material distribution for several applications and requirements. Cellular materials are part of the most prominent materials today, both in terms of applications, and in terms of research and development. However, their potentially complex and heterogeneous structures carry some complexities, associated to the prediction of effective constitutive properties and to its design. Homogenisation procedures can provide answers for both cases. On the one hand, the asymptotic expansion homogenisation can be used to determine thermomechanical effective properties for these materials through the detailed modelling of representative unit-cells, in a flexible and accurate fashion, regardless of the type of constituent distribution. On the other hand, this homogenisation technique integrates a localisation procedure, able to obtain detailed information on the behaviour of the material within the unit-cell, giving way to local sensitivities that can be used to control optimisation procedures. This leads to a material topology optimisation approach, perfectly suited for the design of this type of material. Within this scope, this work focuses on the analysis of effective thermomechanical material properties of cellular materials designed with topology optimisation procedures.

Keywords: representative unit-cell; homogenisation; effective properties; optimisation; cellular materials.

1. Introduction

The methods presented in this work are primarily developed for complex materials with periodical material distributions. Cellular materials, namely metallic foams, are commonly part of this group, with an average constituent distribution that closely approximates a periodic lattice. This creates an opportunity to use powerful methods such as the Asymptotic Expansion Homogenisation (AEH) and closely related optimisation methods, making the numerical study and development of these materials free from restrictive micromechanics models which depend on specific types of constituent distributions. This provides the capability of accurately predicting properties for any phase distribution within a cellular material. Moreover, AEH allows for the use of an inverse method, called localisation, which brings macroscale homogenised results back to the detailed heterogeneous material microstructure. This is, in fact, the step that gives in turn way to the optimisation approach called inverse homogenisation. This paper describes the basis of the application of these methods to cellular materials. It focuses on the topology

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optimisation of microstructures for given typical mechanical and thermal requirements. Some numerical strategies are also discussed, as well as a close look at the effective properties of the achieved microstructures. The authors use an in-house developed code to solve all the problems presented along this work [1].

2. Material processing framework

2.1. Asymptotic expansion homogenisation

The asymptotic expansion homogenisation provides an efficient tool to determine global thermomechanical properties based on a Representative Unit-Cell (RUC) of the local material distribution. Moreover, it provides localisation tools and sensitivity information useful for optimisation methodologies. Mathematical formulation and implementation details can be studied in detail in several references [1-5]. Within the scope of this document, the most important part of the AEH methodology is related to the homogenised constitutive matrices of the materials.

Within the topology optimisation approach of this work, the constituent microscale properties are controlled by the base material, with an elasticity constitutive matrix D_0, and the Solid Isotropic Material with Penalisation (SIMP) method [6, 7]. In this, the local material densities, μ, vary between 0 (void) and 1 (base material). Moreover, the densities are penalised, using a penalty value p. Thus, the constitutive matrix D_k for an element k of a material microscale domain Y can be defined as

$$\mathbf{D}_k = \mathbf{D}(\mu_k) = \mu_k^p \mathbf{D}_0 \,. \tag{1}$$

In this sense, the homogenised matrix can be written, based on a finite element discretisation and using a quadratic form (variational) [8], as

$$\mathbf{D}^{\mathrm{h}} = \sum_{k=1}^{n_e} \frac{Y^k}{Y} (\mathbf{I} - \mathbf{B}^k \boldsymbol{\chi}^k)^{\mathrm{T}} \mu_k^p \mathbf{D}^0 (\mathbf{I} - \mathbf{B}^k \boldsymbol{\chi}^k) \,, \tag{2}$$

where Y^k, Y and n_e are the volume of the generic finite element k, the total volume for the RUC and the total number of finite elements, respectively. I is the identity matrix and B is the matrix of the derivatives of the finite element shape functions. χ is the matrix of displacement correctors, which contains the eigendeformations of the representative periodic geometry. These changes to local properties, with the influence of the density interpolation, must also be used for the equations that define the local homogenisation problems [4].

Following the same approach, the homogenised thermal conductivity matrix k^h can be defined as

$$\mathbf{k}^{\mathrm{h}} = \sum_{k=1}^{n_e} \frac{Y^k}{Y} \left(\mathbf{I} - \tilde{\mathbf{M}}^k \boldsymbol{\Upsilon}^k\right)^{\mathrm{T}} \mu_k^p \mathbf{k}^0 \left(\mathbf{I} - \tilde{\mathbf{M}}^k \boldsymbol{\Upsilon}^k\right) . \tag{3}$$

k_0 is the matrix of thermal conductivity coefficients for the base material and M the matrix of shape elements. Υ is the matrix of thermal conductivity correctors and contains the temperature eigendeformations of the representative periodic geometry. Uncoupled thermoelastic behaviour may also be studied with the AEH, defining the homogenised vector of thermal expansion by

$$\boldsymbol{\beta}^{\mathrm{h}} = \sum_{k=1}^{n_e} \frac{Y^k}{Y} \left(\mu_k^{2p} \boldsymbol{\beta}^0 - \mu_k^p \mathbf{D}^0 \mathbf{B}^k \boldsymbol{\Psi}^k\right) . \tag{4}$$

This is related to the homogenised vector of thermal expansion coefficients, obtained as

$$\boldsymbol{\alpha}^{\mathrm{h}} = \left(\mathbf{D}^{\mathrm{h}}\right)^{-1} \boldsymbol{\beta}^{\mathrm{h}} . \tag{5}$$

The material properties for each finite element are obtained from the base material properties,

$$\boldsymbol{\beta}_0 = \mathbf{D}_0 \boldsymbol{\alpha}_0 \tag{6}$$

according to its density value, as

$$\boldsymbol{\beta}_k = \mu_k^p \mathbf{D}_0 \mu_k^p \boldsymbol{\alpha}_0 * \mu_k^{2p} \boldsymbol{\beta}_0 \tag{7}$$

$\boldsymbol{\Upsilon}$ is the matrix of thermal expansion correctors and contains the expansion eigendeformations of the representative periodic geometry. Note that if the corrector gradients are zero, the homogenised quantities become the volume average of the properties of the microscale constituents.

2.2. Local optimisation

In structural mechanics, there are alternative methods to determine the optimal material distribution for a given application. This is also valid when approaching specifically the material distribution within a representative volume. One possibility is to approach the microstructural problem with the topology optimisation method commonly used for macrostructural problems. In this case, the objective function can be the work of external loads, defining a compliance measure to be minimised. For the

mechanical case this can be solved using a common FEM based practical approach [9], as

$$\min_{\substack{0\le\mu\le 1 \\ \int_Y \mu(\mathbf{y})\mathrm{d}Y=\bar{\rho} \\ \mathbf{Ku}=\mathbf{f}}} \int_\Omega \mathbf{u}^{\mathrm{T}}\mathbf{K}\mathbf{u}\,\mathrm{d}\Omega\,, \tag{8}$$

u and K define the displacement vector and the global stiffness matrix, respectively. r defines a macrostructural density value for the RUC, equivalent to the imposed volume fraction. For a thermal conductivity problem, the same can be done with [10]

$$\min_{\substack{0\le\mu\le 1 \\ \int_Y \mu(\mathbf{y})\mathrm{d}Y=\bar{\rho} \\ \mathbf{K}_{\mathrm{T}}\mathbf{T}=\mathbf{q}}} \int_\Omega \mathbf{T}^{\mathrm{T}}\mathbf{K}_{\mathrm{T}}\mathbf{T}\mathrm{d}\Omega. \tag{9}$$

T and K_T define the nodal temperature vector and the global thermal conductivity matrix, respectively. In practice, the main difference to the usual macrostructural approach resides on the boundary conditions. First of all, a far-field approach is used [11], where the stress and strain fields are imposed over the periodic RUC. These are converted and treated as antiperiodic Neumann or periodic Dirichlet boundary conditions imposed on the finite microscale element problem. The RUC behaviour must provide a periodic response, for which periodicity boundary conditions are imposed over the RUC using multifreedom constraints [12]. While on the AEH problem these periodic boundary conditions are homogeneous, since the material oscillations over an average state lead to the correctors (eigenvectors), this approach requires heterogeneous boundary conditions. These allow a global deformation of the cell, in response to the imposed far-field state, while guaranteeing deformed periodicity [1,13].

2.3. Inverse homogenisation

Inverse homogenisation makes use of the AEH to define not only effective material properties but also sensitivities for the optimisation of the topology. As for the case of the local approach, far-field strains can be imposed over the microstructure. The objective function is defined as a strain energy density function that leads to a local optimisation problem. This relates to a hierarchical optimisation approach, which can be written in linear elasticity as [14]

$$\min_{\mathbf{u}\in U}\left|\frac{1}{2}\int_\Omega \Phi(\mathbf{u})\mathrm{d}\Omega-\left(\int_\Omega \mathbf{b}\cdot\mathbf{u}\mathrm{d}\Omega+\int_{\Gamma_{N_u}}\bar{\mathbf{t}}\cdot\mathbf{u}\mathrm{d}\Gamma\right)\right|, \tag{10}$$

with

$$\Phi(\mathbf{u})=\max_{\substack{\mu(\mathbf{y}) \\ 0\le\mu(\mathbf{y})\le 1 \\ \int_Y \mu(\mathbf{y})\mathrm{d}Y=V}}\left|\langle D^{\mathrm{h}}_{ijkl}(\mu)\rangle\varepsilon_{kl}(\mathbf{u})\varepsilon_{kl}(\mathbf{u})\right| \tag{11}$$

while using only the local anisotropy problem defined in equation 11. This is due to the clear separation between the two scales, making the local problem available for a standalone approach. This leads to the definition of the inverse homogenisation or local anisotropy problem as

$$\Phi(\mu,\bar{\varepsilon})=\max_{\substack{\mu(\mathbf{y}) \\ 0\le\mu(\mathbf{y})\le 1 \\ \int_Y \mu(\mathbf{y})\mathrm{d}Y=V}}\left|D^{\mathrm{h}}_{ijkl}(\mu)\bar{\varepsilon}_{ij}\bar{\varepsilon}_{kl}\right|, \tag{12}$$

for the elasticity case, or, in the same sense,

$$\Theta(\mu,\bar{\mathbf{T}}')=\max_{\substack{\mu(\mathbf{y}) \\ 0\le\mu(\mathbf{y})\le 1 \\ \int_Y \mu(\mathbf{y})\mathrm{d}Y=V}}\left|k^{\mathrm{h}}_{ij}(\mu)\bar{T}'_i\bar{T}'_j\right|, \tag{13}$$

for the thermal conductivity problem. e and T' are imposed (far-field) strain and temperature variation fields, respectively. The objectives are the maximisation of stiffness and thermal conductivity. Note that these problems can also be solved in multiload and multiobjective approaches, with weight control for each objective [1].

2.4. Numerical procedures

Along each of the strategies introduced over the previous sections, the AEH procedures are always an integrated part of this work. Requiring the use of periodicity conditions using homogeneous multifreedom constraints, the AEH problem solves several systems of equations to obtain the correctors. For linear elasticity the number of systems to solve is either three or six, for two or three dimensions, respectively. The expansion effect of thermoelasticity adds a further one and the thermal conductivity evaluation adds another system for each problem dimension. This adds up to six for 2-D and nine for 3-D. In what concerns the optimisation procedures, the AEH calculations are used in different ways. After convergence and in both cases, the final material evaluations are done with these procedures. This results on the effective homogenised material properties of the optimal microstructure topology. However, while at this point the local optimisation approach only uses homogenisation, the inverse homogenisation uses AEH

on all iterations, even for the first evaluation. The objective function is calculated using the homogenised material property matrices, as well as the calculation of sensitivities. As a consequence, for the same number of iterations, this is a more time consuming process, with several times more systems of equations to be solved. However, the potential and overall stability is higher, making the focus of this paper much more oriented towards the inverse homogenisation procedure.

3. Material topology optimisation

3.1. Local approach

The following problems are solved with a material volume fraction f_v=0.5 and the SIMP method is used with a penalisation of p=4. Each effective property is normalised with the respective base material property. The Method of Moving Asymptotes (MMA) [15] is used to update the optimisation variables and the problem is stabilised with a sensitivity filter. The 2-D example that follows is a multiobjective application [13]. A structured mesh of 80×80 linear quadrilaterals is subjected to normalised homogeneous far-fields of strain, $\mathbf{e}=\{1.0; 0.0; 0.0\}^T$, and of surface heat transfer, $\mathbf{q}=\{0.0; 1.0\}^T$. Each one of these fields tends to generate a dominant material phase aligned with the field orientation, orthogonal to each other. A weight w_t is used to control this multiobjective approach, with the objective-function weighted as $f=(1-w_t)f_m+w_tf_t$ between the mechanical (m) and thermal (t) objectives. Note that the end results can lead to singularities for the complementary objective problem, due to the lack of material connectivity. This is controlled to a given point with the use of a lower density limit that is higher than zero ($\mathbb{m}_{min}$=0.001).

Fig. 1 shows the variation of objectives with the multiobjective weighting. Fig. 2 shows a Pareto curve for the same problem, along with the obtained microstructures, where the variation of each dominant problem is noticeable. The equivalent (homogenised) properties are presented in Fig.s 3(a) and 3(b), relative to the base material property. These are obtained, after convergence, with the AEH. The Young's modulus and the thermal conductivity coefficients change abruptly at the limits because at these points the material becomes disconnected and leads to a drastic change of transverse properties. On the other hand, longitudinal properties converge to the expected value, corresponding to the material volume average within a serial constituent association. The behaviour at the multiobjective limits also leads to a second effect, where the thermal expansion coefficients drop from the base value. This is expected, since the thermal expansion behaviour for cellular materials (material and void) is identical to the behaviour of the base material base for as long as there is a connected continuous material phase along the expansion direction [7]. The characteristic fields, in the form of each of the correctors, are presented in Fig. 4, for w_t=0.3.

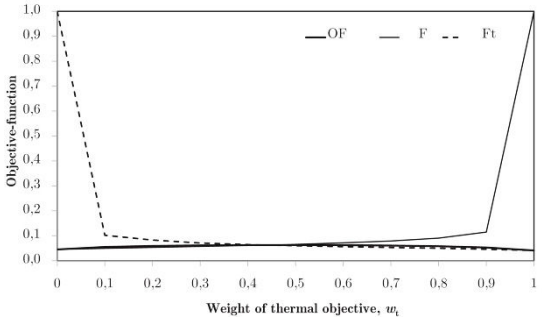

Fig. 1. Evolution of the mechanical, thermal and total objective-functions with the variation of w_t for a multiobjective optimisation problem.

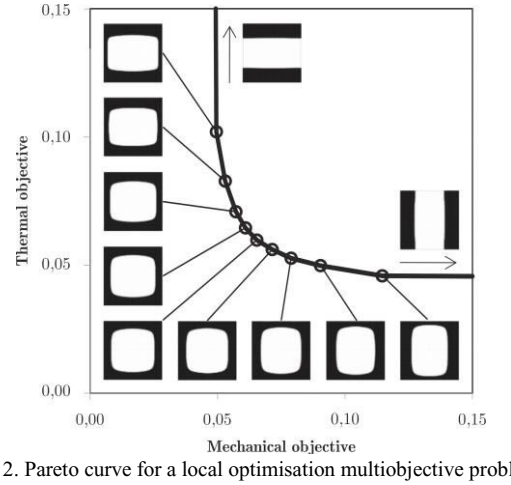

Fig. 2. Pareto curve for a local optimisation multiobjective problem.

The previously described method is perfectly valid for material optimisation, with the added virtue of, setting aside the homogenisation part, needing little change over a typical macrostructural topology optimisation program. On the one hand, this method has some limitations. Namely the fact that it is not naturally included in multiscale procedures, such as hierarchical optimisation, and becomes limited in terms of convergence with increasing complexity of the requirements and in cases where the conditioning of the system of equations is not ideal. On the other hand, inverse homogenisation evolves integrated with the constitutive information of the material topology,

naturally integrating multiscale procedures and providing significantly improved stability [1].

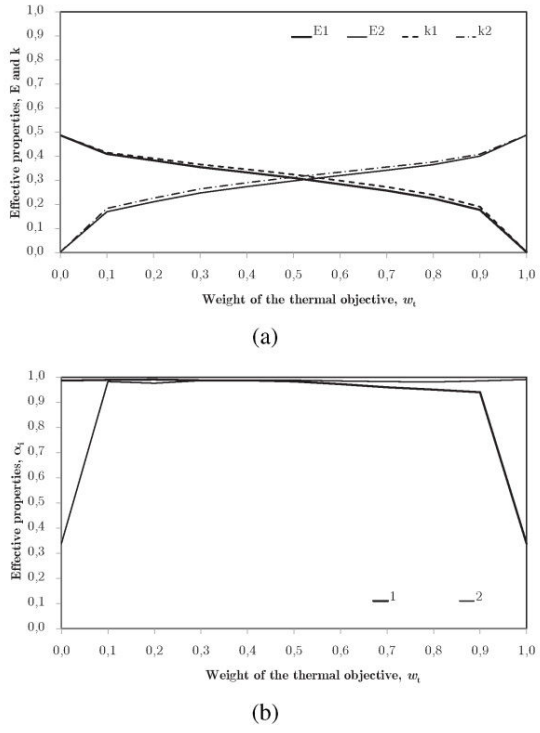

Fig. 3. Variation of (a) the thermal conductivity coefficient, k, and Young's modulus, E, and of (b) the thermal expansion coefficients, α, with the thermal problem weight, w_t

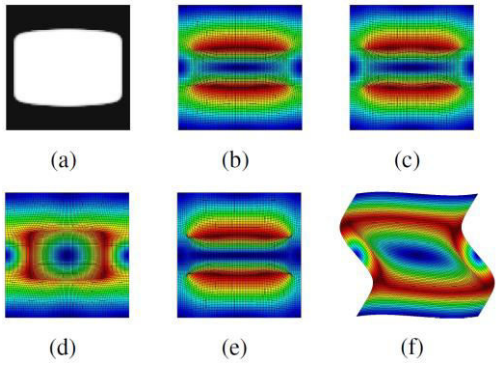

Fig. 4. Local 2-D optimisation problem: (a) optimal material distribution and (b) thermocharacteristic displacements, U, (c) thermal expansion characteristic fields, Y, and (d-f) characteristic displacements, C_{11}, C_{22} and C_{12} (w_t =0.3).

3.2. Inverse homogenisation

Also using a MMA application, the previous problem is once again solved with the inverse homogenisation approach. It is solved without any numerical stability control (Fig. 5) and with a sensitivity filtering technique (Fig. 6).

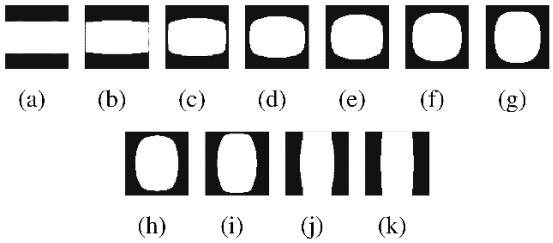

Fig. 5. Multiobjective optimisation topologies for inverse homogenisation, with a thermal problem weight of w_t =0.0; 0.1; 1.0, without stability control.

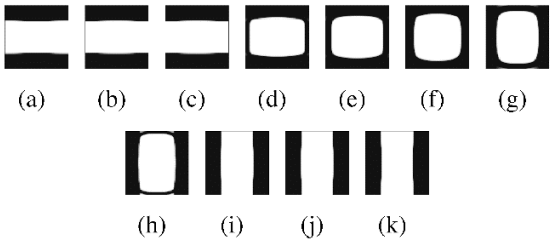

Fig. 6. Multiobjective optimisation topologies for inverse homogenisation, with a thermal problem weight of w_t=0.0; 0.1; 1.0, with sensitivity filtering.

Fig. 7 shows the effect of the multiobjective problem weighting extremes, where there is a premature tendency to generate an unconnected topology. Considering the case of a thermal problem weight of w_t=0.2, it is noted that this is a tendency accentuated by the filtering. For the present mesh refinement (80×80), since the material connection is thin, the initial material is gradually filtered out. This is an effect that can be controlled through mesh refinement, filtering radius adjustment and softening the density update algorithm. Note also that the unfiltered results are less sensitive to this effect, albeit still present. Comparing this with the results for the local approach, this tends to be even less prone to this premature filtering.

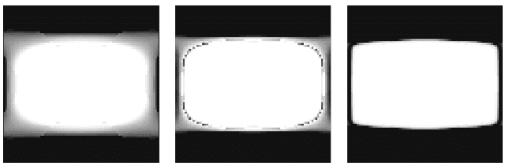

Fig. 7. Intermediate solutions for the evolution of an inverse homogenisation multiobjective problem with w_t =0.2: (a) i=6, (b) i=9 and (c) i=22.

Fig. 8 presents a mechanical anisotropy variation for the obtained topologies. These anisotropy charts denote the variation of the Young's modulus with the material orientation. Note the lack of stiffness on the Pareto thermal objective extreme, similar to the transverse stiffness obtained on the mechanical response optimum. This leads to the singularity issues denoted before for the complementary responses on this multiobjective approach. Even with the minimum value for the density higher than zero, the fact that the conditioning of the systems of equations is aggressively deteriorated by the penalties used for the periodicity boundary conditions leads to a tendency for linear dependence.

A final set of reference 3-D problems [16] is solved using a linear hexahedral mesh of 30×30×30 elements. Fig. 9 shows an illustration of periodicity (tiles of 8 RUC) and anisotropy for far-field strains $\epsilon=\{0; 0; 0; 1; 1; 1\}^T$, $\epsilon=\{1; -1; 0; 1; 1; 1\}^T$ and $\epsilon=\{1; 1; 1; 0; 0; 0\}^T$ plus $\epsilon=\{1;-1; 0; 0; 0; 0\}^T$ (multiload). The procedures used for 2-D are also valid for 3-D problems. Furthermore, the evaluation of the optimal cellular material thermomechanical properties accurately provided by the AEH. This is also illustrated in Fig. 10, with the optimal topology for the case of $\epsilon=\{1; 1; 1; 0; 0; 0\}^T$. The optimal topology is shown, as well as the AEH correctors: (b-g) mechanical, (h) thermomechanical (thermal expansion) and (i) thermal.

4. Final remarks

A crucial aspect of this work lies on the use of the asymptotic expansion homogenisation. It proves to be a valuable tool for behaviour prediction cellular materials, providing not only effective property evaluation but also complete constitutive definition for thermoelasticity. This is very important for the numerical study of cellular materials, with material characterization capabilities and multiscale integration. At the same time, AEH well is an integral part of the inverse homogenisation procedure. This optimisation

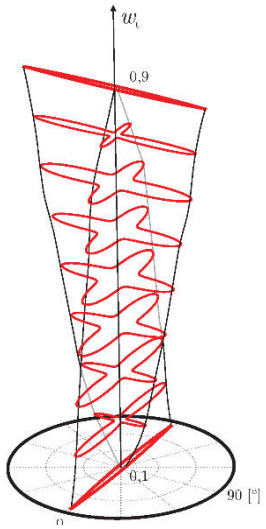

Fig. 8. Variation of elastic modulus with the material orientation and weight of the thermal problem, w_t, for an inverse homogenisation problem.

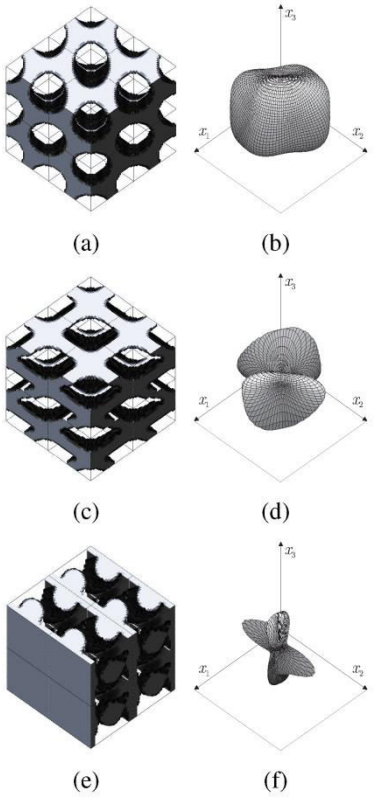

Fig. 9. Periodicity illustration and anisotropy plots (stiffness)for 3-D examples with filtering: (a,b) $\epsilon=\{0; 0; 0; 1; 1; 1\}^T$, (c, d) multiload d+g, $\epsilon=\{1; 1; 1; 0; 0; 0\}^T + \epsilon=\{1; -1; 0; 0; 0; 0\}^T$ and (e, f) $\epsilon=\{2; 1; 5; 1.5; 9; 4\}^T$.

technique allows the optimisation of topology, distributing the material within a representative unit-cell to achieve the optimal response for a given structural requirement. This technique integrates directly the sensitivity information of the material definition, with the constitutive matrices and localised fields. It is more robust and provides a broader reach than the more conventional local approach. The numerical implications of this study are valid for 2-D and 3-D problems, as well as for multiscale procedures.

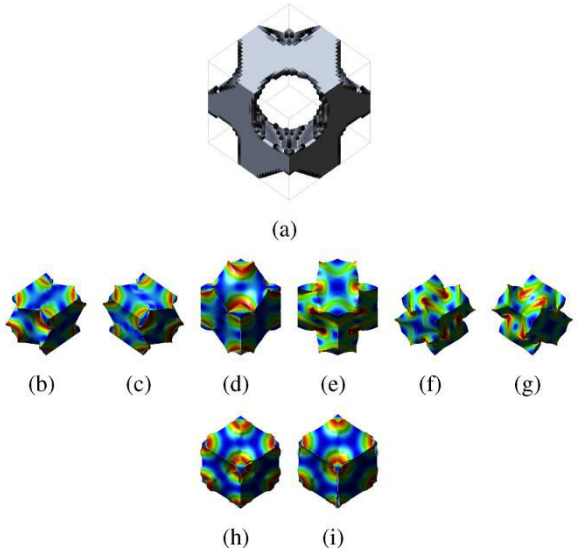

Fig. 10. Inverse homogenisation and asymptotic expansion homogenisation: (a) optimal topology for $\ominus=\{0; 0; 0; 1; 1; 1\}^T$, (b-g) mechanical, (h) thermomechanical and (i) thermal correctors.

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References

[1] J. Dias-de-Oliveira, Topology Optimisation Methodologies for Structural Analysis (in Portuguese), PhD Thesis in Mechanical Engineering, Universidade de Aveiro, Aveiro, Portugal, 2013.
[2] J. Guedes, N. Kikuchi, Comput. Methods in Appl. Mech. Eng. 83 (1990) 143.
[3] J. Pinho-da-Cruz, Thermomechanical Characterisation of Multiphasic Materials Using Homogenisation Procedures (in Portuguese), PhD Thesis in Mechanical Engineering, Universidade de Aveiro, Aveiro, Portugal, 2007.
[4] J. Pinho-da-Cruz, J. Oliveira, F. Teixeira-Dias, Comput. Mater. Sci. 45 (2009) 1073.
[5] J. Oliveira, J. Pinho-da-Cruz, F. Teixeira-Dias, Comput. Mater. Sci. 45 (2009) 1081.
[6] M. Bendsøe, O. Sigmund, Arch. Appl. Mech. 69 (1999) 635.
[7] M. Bendsøe, O. Sigmund, Topology optimization: theory, methods, and applications, Springer Verlag, Berlin, Germany, 2003.
[8] M. Bendsøe, Optimization of structural topology, shape, and material, Springer Verlag, Berlin, Germany, 1995.
[9] O. Sigmund, Struct. Multidiscip. O. 21 (2001) 120.
[10] N. de Kruijf, S. Zhou, Q. Li, Y. Mai, Int. J. Solids Struct. 44 (2007) 7092.
[11] H. Böhm, A short introduction to basic aspects of continuum micromechanics, ILSB Report/ILSB-Arbeitsbericht 206, Institute of Lightweight Design and Structural Biomechanics (ILSB), Vienna University of Technology, Vienna, Austria, 2012.
[12] C. Felippa, Introduction to finite element methods – material assembled from lecture notes for the course Introduction to Finite Elements Methods, Aerospace Engineering Sciences Department of the University of Colorado, Boulder, USA, 2004.
[13] J. Oliveira, J. Pinho-da-Cruz, F. Teixeira-Dias. In: H. Rodrigues, J. Herskovits, C.M. Soares, J.M. Guedes, J. Folgado, A. Araújo, F. Moleiro, J.P. Kuzhichalil, J.A. Madeira, Z. Dimitrovová (Eds.). Proceedings of the 2nd International Conference on Engineering Optimization (EngOpt 2010), Lisboa, Portugal, (2010), pp. 1-10.
[14] H. Rodrigues, J. Guedes, M. Bendsoe, Struct. Multidiscip. O. 24 (2002) 1.
[15] K. Svanberg. Int. J. Numer. Meth. Eng. 24 (1987) 359.
[16] P. Coelho, Modelos hierárquicos para a análise e síntese de estruturas e materiais com aplicações à remodelação óssea (in Portuguese), PhD Thesis in Mechanical Engineering, Resistance of Materials, Universidade Nova de Lisboa, Faculdade de Ciências e Tecnologia, Lisbon, Portugal, 2009.