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Towards a versatile polynomial failure criterion for architected materials

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Résumé :

Les matériaux architecturés, comparés aux matériaux standards, constituent une classe de matériaux où des propriétés intéressantes peuvent être exploitées, comme un rapport rigidité/masse élevé. Avec le développement rapide de la fabrication additive et des outils d'optimisation de la topologie, ces matériaux ont désormais un grand potentiel. Cependant, d'un point de vue mécanique, le fait que les matériaux architecturés aient un comportement particulier peut rendre les choses difficiles. Nous souhaitons optimiser les matériaux treillis (une sous-classe de matériaux architecturés) en considérant la résistance mécanique comme une contrainte de conception. Pour ce faire, nous devons d'abord établir une fonction de seuil qui puisse décrire avec précision leur résistance mécanique. Une fonction de seuil polynomiale de degré élevé est proposée dans cet article.

Abstract:

Architected materials, compared to standard materials, are a class of materials where interesting properties can be exploited, such as a high stiffness to mass ratio. With the rapid development of additive manufacturing and topology optimisation tools, these materials now have great potential. However, from a mechanical point of view, the fact that architected materials have a particular behaviour can make things difficult. We want to optimise lattice materials (a subclass of architected materials) by considering mechanical strength as a design constraint. To do this, we first need to establish a threshold function that can accurately describe their mechanical strength. A generalised polynomial threshold function is proposed in this paper.

Key words: Threshold functions, anisotropy, tensors, harmonic decomposition, architected materials.

1 Context and introduction

Architected materials are materials that present a mesostructure between their macrostructure and their microstructure [1]. They are known to have many interesting properties such as a good stiffness/weight ratio, wave guide, energy absorption [2]. It is important to use all these properties in an optimal way and this can be done with the help of topology optimisation tools [3]. Ensuring mechanical strength while having optimal properties remains, until now, a problem. Architected materials are known to have a particular mechanical behaviour where two modes of failure can be found: (1) plasticity (or brittleness) in traction and (2) buckling (or plasticity) in compression. They are therefore highly anisotropic and exhibit asymmetries (in traction and in compression).

It is necessary to define a failure criterion capable of accurately describing this behaviour in order to ensure the mechanical strength of the optimised structure. In the literature, multiple approaches are available when it comes to to define a criterion that takes into account the anisotropy. We find (i) the group representation theory [4], (ii) linear transformations [5] and (iii) the use of a higher degree polynomials [6]. From all these approaches, we are interested on the (iii). Polynomial criteria have been shown to be efficient and accurate in modelling high-order anisotropy and in modelling asymmetries in traction/compression [7].

Our study will be limited to 2D for a static linear elastic behaviour. A criterion is most often expressed in the stress space and is defined by the function $F(\underline{\sigma})$ which we call *threshold function*, $\underline{\sigma}$ is the Cauchy stress tensor. The presentation is organised as follows: in section 2, we start by briefly recalling some basics of the geometry of the stress space (in 2D only). We introduce in this section the *harmonic basis* with respect to which all threshold functions will be expressed. In section 3, we introduce the proposed threshold function and in a very brief manner, we explain the harmonic decomposition. Finally, we try to identify with our model some existing threshold functions that can be found in the literature for standard and architected materials.

2 Geometry of the stress space

Threshold surfaces are mostly expressed in stress space. The stress tensor is therefore an important variable in our study. In order to get a better insight, we will talk about some geometric basics concerning the stress tensor. We will present some properties that can certainly help us to look for interpretations when it comes to describing the anisotropy.

2.1 The Cauchy stress tensor (2D)

In an orthonormal basis \mathcal{B} , the stress tensor is represented by a the given matrix $[\underline{\sigma}]$:

$$[\underline{\sigma}] = \begin{bmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{12} & \sigma_{22} \end{bmatrix}_{\mathcal{B}}.$$

Noticing the index symmetry, we write $\underline{\sigma} \in S^2(\mathbb{R}^2)$ where $S^2(\mathbb{R}^2)$ is the space of totally symmetric 2nd-order tensors on \mathbb{R}^2 . We have the decomposition of $\underline{\sigma}$ into a deviatoric part and a spheric part:

$$\underline{\sigma} = \underline{\sigma}^{(d)} + \underline{\sigma}^{(s)}, \quad \text{where } \underline{\sigma}^{(s)} = \frac{1}{2} \text{Tr}(\underline{\sigma}) \mathbf{I} \text{ and } \underline{\sigma}^{(d)} = \underline{\sigma} - \underline{\sigma}^{(s)}.$$

We introduce the *polar parameterisation*:

$$\begin{cases} \sigma_{11} = t + r \cos(2\theta), \\ \sigma_{22} = t - r \cos(2\theta), \\ \sigma_{12} = r \sin(2\theta), \end{cases} \quad \text{where } t = \frac{\text{Tr}(\underline{\sigma})}{2}, \text{ and } r = \sqrt{\frac{\underline{\sigma}^{(d)} : \underline{\sigma}^{(d)}}{2}},$$

θ is related to the orientation of $\underline{\sigma}$ with respect to the principal basis (diagonal form). The polar parameterisation is a parameterisation of the $O(2)$ -orbit of a given stress tensor.

Harmonic basis:

The *harmonic basis* \mathcal{H} is an interesting basis that separates the deviatoric and spherical parts of the stress tensor. From the polar parameterisation, the expression of the stress tensor in \mathcal{H} is given by:

$$\underbrace{\{\tilde{\sigma}\} = \begin{pmatrix} \sigma_{d_1} \\ \sigma_{d_2} \\ \sigma_h \end{pmatrix}_{\mathcal{H}} = \begin{pmatrix} r \cos(2\theta) \\ r \sin(2\theta) \\ \sqrt{2}t \end{pmatrix}_{\mathcal{H}}}_{\text{Harmonic basis}} .$$

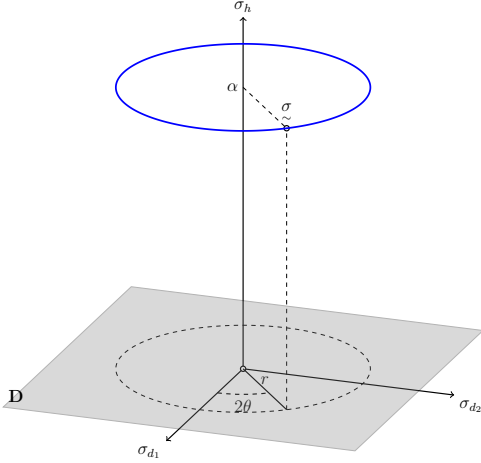


Figure 1: Harmonic basis (Cylindrical coordinates).

- The polar parameters $(r, 2\theta, \sqrt{2}t)$ in harmonic basis can be interpreted as cylindrical coordinates.
- The blue circle represents the orbit of the stress tensor (which is the set of all tensors coming from all $O(2)$ actions on $\tilde{\sigma}$).
- In \mathcal{H} , an orthogonal transformation on $\tilde{\sigma}$ is represented by a rotation around the hydrostatic axis σ_h .

3 Threshold functions

The transition of the behaviour of a material from elasticity to anelasticity occurs when the stress tensor reaches a critical state in the stress space. Mathematically, the critical state is usually defined by a relationship between the components of the stress tensor defined by the application F as follows:

$$\begin{aligned} F : S^2(\mathbb{R}^2) &\longrightarrow \mathbb{R}^+, \\ \tilde{\sigma} &\longrightarrow F(\tilde{\sigma}), \end{aligned}$$

F is called the *threshold function*. The level set $F^{-1}(\sigma_{eq})$ is a surface \mathcal{S} in the stress space defined as follows:

$$\mathcal{S} = \left\{ \tilde{\sigma} \in S^2(\mathbb{R}^2), F(\tilde{\sigma}) - \sigma_{eq} = 0 \right\}.$$

The surface \mathcal{S} is the *threshold surface* and $\sigma_{eq} \in \mathbb{R}^{*+}$ is the *threshold stress*.

3.1 The proposed threshold function

We are interested in using the high-degree polynomial function approach. Polynomial threshold functions has proven to be very effective when it comes to modelling higher order anisotropy and showing the asymmetric aspects in traction/compression stress state [7, 8, 9].

The proposed threshold function is the contribution of all terms from 1st degree to 4th polynomial in $\tilde{\sigma}$:

$$F(\tilde{\sigma}) = \underset{\cong}{\mathbb{A}} \cdot (\tilde{\sigma} \otimes \tilde{\sigma} \otimes \tilde{\sigma} \otimes \tilde{\sigma}) + \underset{\cong}{\mathbb{B}} \cdot (\tilde{\sigma} \otimes \tilde{\sigma} \otimes \tilde{\sigma}) + \underset{\cong}{\mathbb{C}} :: (\tilde{\sigma} \otimes \tilde{\sigma}) + \underset{\cong}{\mathbb{D}} : \tilde{\sigma},$$

where $\underset{\cong}{\mathbb{A}}$, $\underset{\cong}{\mathbb{B}}$, $\underset{\cong}{\mathbb{C}}$ and $\underset{\cong}{\mathbb{D}}$ are respectively 8th, 6th, 4th and 2nd order tensor which contain all material parameters.

With polynomial terms of even degree, we can only generate symmetric surfaces [7] verifying $F(-\tilde{\sigma}) = F(\tilde{\sigma})$. On the other hand, with odd terms, we can generate asymmetric surfaces.

3.2 Harmonic decomposition

We recall that the expression of our threshold function is in a general form and can be simplified according to the anisotropy of the described material. To do it in the spatial basis is complicated specially for high order tensors. In order to do so, we use what we call the *harmonic decomposition*. In a nutshell, it is a generalisation of deviatoric and spheric decomposition of the stress tensor to higher order tensors. In the *harmonic basis*, we can distinguish some physical aspects e.g. isotropic and anisotropic materials. Technically, the harmonic decomposition is the decomposition of \mathbb{T}^n , n th-order tensor space, into a direct sum of $O(2)$ -irreducible subspaces \mathbb{K}^n :

$$\mathbb{T}^n \simeq \bigoplus_k \alpha_k \mathbb{K}^k, \quad (1)$$

in which \mathbb{K}^n denotes the space of n th-order *harmonic tensors* (i.e. totally symmetric and traceless tensors, for $n=0$, we have scalars). The equation (1) gives us the harmonic structure of a given tensor space and can be established using *Clebch-Gordan* formulas [10]. The harmonic structure of our 4 given tensors are as follows:

$$\begin{array}{l} \mathbb{A} \in \mathbb{A} \simeq \mathbb{K}^8 \oplus \mathbb{K}^6 \oplus 2\mathbb{K}^4 \oplus 2\mathbb{K}^2 \oplus 3\mathbb{K}^0, \\ \mathbb{B} \in \mathbb{B} \simeq \mathbb{K}^6 \oplus \mathbb{K}^4 \oplus 2\mathbb{K}^2 \oplus 2\mathbb{K}^0, \\ \mathbb{C} \in \mathbb{C} \simeq \mathbb{K}^4 \oplus \mathbb{K}^2 \oplus 2\mathbb{K}^0, \\ \mathbb{D} \in \mathbb{D} \simeq \mathbb{K}^2 \oplus \mathbb{K}^0, \end{array} \quad \left. \begin{array}{l} \dim(\mathbb{A}) = 15, \\ \dim(\mathbb{B}) = 10, \\ \dim(\mathbb{C}) = 6, \\ \dim(\mathbb{D}) = 3. \end{array} \right\}$$

where \mathbb{A} , \mathbb{B} , \mathbb{C} and \mathbb{D} are tensor spaces to which \mathbb{A} , \mathbb{B} , \mathbb{C} and \mathbb{D} respectively belong. In total we have 34 harmonic parameters. Knowing the harmonic structure of each tensor, an algorithm [11] is used in order to obtain the explicit decomposition. At the end, the function can be written as follows:

$$F(\sigma, \mathbb{A}, \mathbb{B}, \mathbb{C}, \mathbb{D}) = \varphi(\sigma, \mathbb{E}^{8,4}, \mathbb{S}^{8,3}, \mathbb{S}^{6,3}, \mathbb{H}^{8,4}, \mathbb{H}^{8,2}, \mathbb{H}^{6,2}, \mathbb{H}^{4,2}, \mathbb{h}^{8,3}, \mathbb{h}^{8,1}, \mathbb{h}^{6,3}, \mathbb{h}^{6,1}, \mathbb{h}^{4,1}, \mathbb{h}^{2,1}, \alpha^{8,4}, \alpha^{8,2}, \alpha^{8,0}, \alpha^{6,2}, \alpha^{6,0}, \alpha^{4,2}, \alpha^{4,0}, \alpha^{2,0}),$$

where

Terms degree	\mathbb{K}^8	\mathbb{K}^6	\mathbb{K}^4	\mathbb{K}^2	\mathbb{K}^0
4	$\mathbb{E}^{8,4}$	$\mathbb{S}^{8,3}$	$\mathbb{H}^{8,4}, \mathbb{H}^{8,2}$	$\mathbb{h}^{8,3}, \mathbb{h}^{8,2}$	$\alpha^{8,4}, \alpha^{8,2}, \alpha^{8,0}$
3		$\mathbb{S}^{6,3}$	$\mathbb{H}^{6,2}$	$\mathbb{h}^{6,3}, \mathbb{h}^{6,2}$	$\alpha^{6,2}, \alpha^{6,0}$
2			$\mathbb{H}^{4,2}$	$\mathbb{h}^{4,1}$	$\alpha^{4,2}, \alpha^{4,0}$
1				$\mathbb{h}^{2,1}$	$\alpha^{2,0}$

The harmonic parameters have some physical meaning, e.g. the \mathbb{K}^0 parameters are isotropic.

Considering $\mathbb{T}^{q,p} \in \mathbb{K}^n$, the index q means that \mathbb{T} is derived from a tensor of order q . Meanwhile, the index p is related to the related to the process of decomposition (not detailed in the paper).

4 Some identification examples

With the proposed threshold function, we want to find out whether we can identify some existing functions in the literature. We only show here 2 examples. The first one is Cazacau threshold function [12] and the second one is a threshold surface established numerically by V. Jeanneau [13]. The process of identification is simple. The first step consists of generating enough number of points from a given example. For second step, we try to identify all harmonic parameters by using standard fitting tools.

4.1 Cazacu 2004 (3D)

The Cazacu et al. [12] threshold function is given by:

$$F(\underline{\sigma}) = (J_2)^{3/2} - cJ_3,$$

where c is a material parameter and J_2 and J_3 are the second and third invariant of the deviatoric part of the 3D stress tensor. The function is meant to be used for isotropic materials that present a traction/compression asymmetry in tensile yield stress. In planar stress the function is given by:

$$\begin{aligned} F_{2D}(\underline{\sigma}) &= \left[\frac{1}{3} (\sigma_1^2 - \sigma_1\sigma_2 + \sigma_2^2) \right]^{3/2} - \frac{c}{27} [2\sigma_1^3 + 2\sigma_2^3 - 3(\sigma_1 + \sigma_2)\sigma_1\sigma_2], \\ &= \left[\frac{1}{3} (I_1^2 - 3I_2) \right]^{3/2} - \frac{c}{27} (2I_1^3 - 9I_1I_2), \end{aligned} \quad (2)$$

where σ_1 and σ_2 are the principal stresses while I_1 and I_2 are the first and the second invariant of the stress tensor. The expression (2) proves that the function is isotropic. We notice that the function is purely deviatoric in 3D but not in 2D.

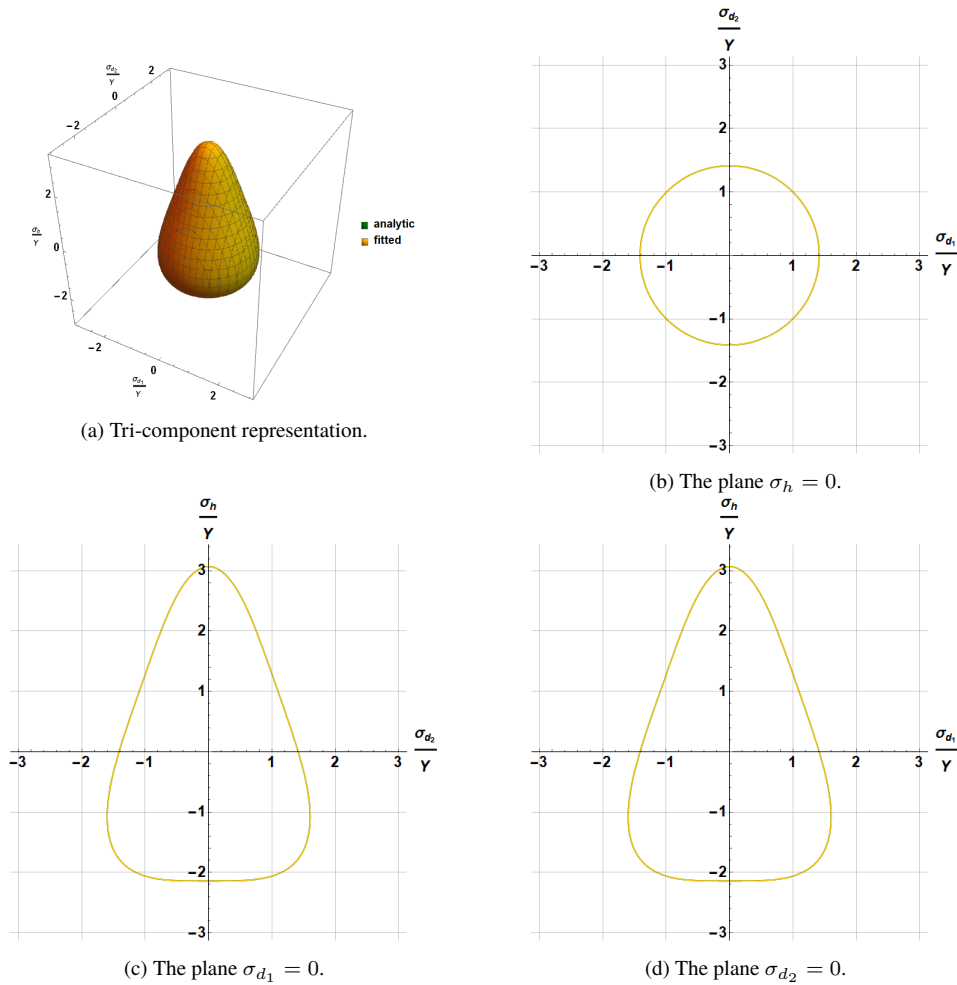


Figure 2: The threshold surface and the fitted of Cazacu's function for $F(\underline{\sigma}) = 1$. The green one is the analytical expression from equation (2). The orange one is the fitted one from the proposed function.

For the proposed function, it means that all harmonic tensors of order $n \geq 1$ are null. Indeed, only pure scalar

harmonic parameters remain in order to be isotropic and they are:

$$\{\alpha^{8,4}, \alpha^{8,2}, \alpha^{8,0}, \alpha^{6,2}, \alpha^{6,0}, \alpha^{4,2}, \alpha^{4,0}, \alpha^{2,0}\}.$$

The identification results are shown in the figure 2. It shows that with the proposed threshold function we are able identify precisely the Cazacu's one. The surface is axi-symmetric with respect to the hydrostatic axis σ_h which means that the creterion is isotropic (i.e. constant over the $O(2)$ -orbit of $\underline{\sigma}$).

4.2 A numerical example

A threshold surface is established numerically by V. Jeanneau [13] for triangular 2D lattice by using buckling instability theories. A semi-analytical technique is used, which combines Bloch wave theory and a finite element model of the 2D lattice unit cell [14]. The resulting threshold surface is shown in figure 3. We can see clearly in figure 3b that the material is completely anisotropic due to traction/compression asymmetry. In the process of identification, we attempted to identify the numerically established threshold surface. In the proposed threshold function we considered only the terms of degree 3 and 4. This means we have the following harmonic parameters:

$$\{\underset{\approx}{E}^{8,4}, \underset{\approx}{S}^{8,3}, \underset{\approx}{S}^{6,3}, \underset{\approx}{H}^{8,4}, \underset{\approx}{H}^{8,2}, \underset{\approx}{H}^{6,2}, \underset{\approx}{h}^{8,3}, \underset{\approx}{h}^{8,1}, \underset{\approx}{h}^{6,3}, \underset{\approx}{h}^{6,1}, \alpha^{8,4}, \alpha^{8,2}, \alpha^{8,0}, \alpha^{6,2}, \alpha^{6,0}\}.$$

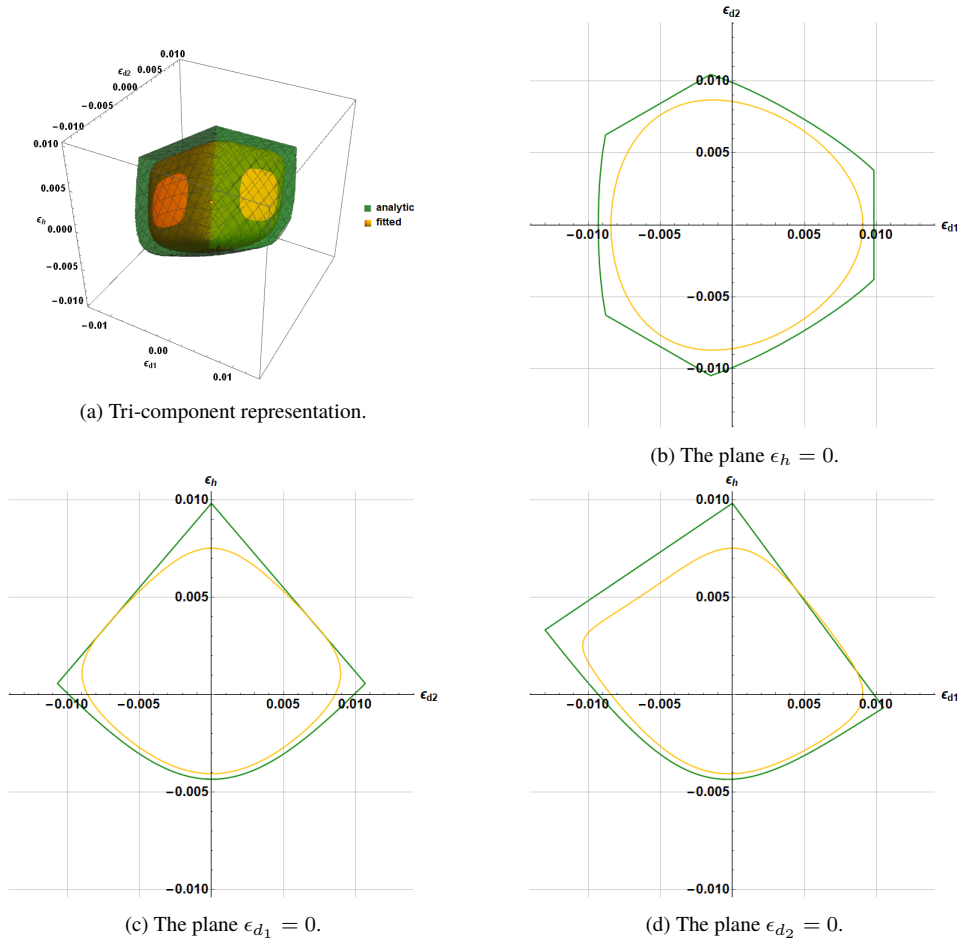


Figure 3: The threshold surface of the a triangular lattice (green) and the fitted surface (orange).

The results are shown in figure 3, we observe that despite that the material is completely anisotropic we are able to approximate the threshold. In order to be more precise, we should add more higher degree terms in the proposed threshold function.

5 Conclusion

We proposed a polynomial threshold function where we considered the contribution of terms from degree 1 to 4 in σ . Thanks to the harmonic decomposition, we were able to use harmonic parameters instead of spatial ones. The harmonic parameters allow us to have some physical interpretation of the higher degree coefficients involved in the model. With the proposed threshold function, we were able to approximate some existing criteria from the literature.

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