Towards the efficient computation of effective properties of microstructured materials

Vers le calcul efficace des propriétés effectives de materiaux microstructurés

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Abstract

An algorithm for partially relaxing multiwell energy densities, such as for marterials undergoing martensitic phase transitions, is presented here. The detection of the rank-one convex hull, which describes effective properties of such materials, is carried out for the most prominent nontrivial case, namely the so-called T_k-configurations. Despite the fact that the computation of relaxed energies (and with it effective properties) is inherently unstable, we show that the detection of these hulls (T_4-configurations) can be carried out exactly and with high efficiency. This allows in practise for their computation up to arbitrary precision. In particular, our approach for detection of these hulls is not based on any approximation or grid-like discretization. This makes the approach very different from previous (unstable and computationally expensive) algorithms for the computation of rank-one convex hulls or sequential-lamination algorithms for the simulation of martensitic microstructure. It can be used to improve these algorithms. In cases where there is a strict separation of length scales, these ideas can be integrated at a sub-grid level to macroscopic finite-element computations. The algorithm presented here enables, for the first time, large numbers of tests for T_4-configurations. Stochastic experiments in several space dimensions are reported here. *To cite this article: C.-F. Kreiner, J. Zimmer, I.V. Chenchiah, C. R. Mecanique 331 (2003).*

Résumé

Nous présentons dans cette Note un algorithme de relaxation partielle de densités d'énergie à plusieurs puits, comme pour la modélisation de matériaux subissant des transitions de phase "martensitiques". La détection de l'enveloppe rang-un convexe, qui décrit les propriétés effectives de tels matériaux, est menée à bien pour le cas non trivial le plus connu, c'est-à-dire les configurations T_k. Bien que le calcul d'énergies relaxées (et donc de propriétés effectives) soit naturellement instable, nous montrons que la détection de ces enveloppes (configurations T_4) peut être effectuée de façon exacte très efficacement. En pratique, cela permet leur calcul à une précision arbitraire. En particulier, notre approche pour la détection de ces enveloppes n'est basée sur aucune approximation ou discrétisation. Ceci la démarque des autres algorithmes (instables et coûteux) de calcul d'enveloppes rang-un convexes ou de lamination séquentielle pour la simulation de microstructures martensitiques. Notre méthode peut être utilisée pour améliorer ces derniers. Dans les cas où il y a une stricte séparation des échelles, ces idées peuvent être utilisées à un niveau inférieur dans des calculs macroscopiques de type éléments finis. La méthode présentée ici permet pour la première fois un grand nombre de tests pour la configuration T_4. Nous rendons compte également d'expériences stochastiques en plusieurs dimensions. *Pour citer cet article : C.-F. Kreiner, J. Zimmer, I.V. Chenchiah, C. R. Mecanique 331 (2003).*

Key words: Continuum mechanics ; rank-one convex hull, T_k-configuration

Mots-clés : Milieux continus ; enveloppe convexe de rang 1 ; configuration de type T_k

1. Introduction

This paper addresses the efficient algebraic detection of so-called T_k-configurations (see Definition 2.1 below), which are the most prominent examples of non-trivial rank-one convex hulls. Rank-one convex hulls of sets and rank-one convex envelopes of functions are important notions in the calculus of variations [10]. Further, the rank-one convex envelope of a nonconvex microscopic energy function of a material serves as a model for its macroscopic energy, which explains the relevance of rank-one convexity to engineering and the importance of a reliable method for the computation of these hulls and envelopes.

Previous algorithms for the computation of the rank-one convex hull of a set $\mathcal{M} \subset \mathbb{R}^{m\times n}$ have been based on a discretization of the space and the rank-one convexification of the distance function $d(x) := \min_{y\in\mathcal{M}} \|x - y\|$ along finitely many rank-one directions [1,2,3]. The complexity of these algorithms is high. The results depend very sensitively on the chosen discretization and especially on the choice of rank-one directions. Moreover, satisfactory results typically require a high degree of precision. It is easy to see that such a discretization-based algorithm will fail completely if essential rank-one lines are missed. An example of a numerical instability is given in [9].

In this paper, we study a simpler, but closely related and important question rigorously. Specifically, we answer a question posed in [7, Section 8] by presenting an efficient algorithm for the detection of T_k-configurations as an important example of nontrivial rank-one convex hulls. The guiding idea is to exploit the algebraic structure of rank-one convexity.

2. T_k-configurations and their algorithmic detection

We start with the definition of T_k-configurations.

Definition 2.1 *A finite set $\mathcal{M} = \{M^{(1)}, M^{(2)}, \dots M^{(k)}\} \subset \mathbb{R}^{m\times n}$ of $k \geq 4$ matrices is called a T_k-*configuration *if there exist a permutation σ of $\{1,\dots,k\}$, rank-one matrices $C^{(1)}, C^{(2)}, \dots, C^{(k)} \in \mathbb{R}^{m\times n}$, positive scalars $\kappa_1, \kappa_2, \dots, \kappa_k$, and matrices $X^{(1)}, X^{(2)}, \dots, X^{(k)} \in \mathbb{R}^{m\times n}$ such that the relations*

$$X^{(j+1)} - X^{(j)} = C^{(j)}, \qquad M^{(\sigma(j))} - X^{(j+1)} = \kappa_j C^{(j)} \tag{1}$$

hold, where the index j is counted modulo k (see Fig. 1). □

This differs only slightly from the definition in [7, Definition 7] where $\mathcal{M}$ is considered as a tupel rather than as a set (i.e., $\sigma = \mathrm{id}$).

A *degenerated T_k-configuration* arises as limit of T_k-configurations where the inner polygon formed by the $X^{(j)}$ reduces to a single point. More precisely, there exists an $X \in \mathcal{M}^{co}$ (the usual convex hull of $\mathcal{M}$) with $\mathrm{rank}(X - M^{(j)}) = 1$ for all $M^{(j)} \in \mathcal{M}$.

We state some connections between T_k-configurations and rank-one convex hulls. For a set $\mathcal{M} \subset \mathbb{R}^{m\times n}$, the rank-one convex hull will be denoted by $\mathcal{M}^{rc}$ (see, e.g., [10] for the precise definition).

It is easy to verify that the rank-one convex hull of a T_k-configuration $\mathcal{M}$ (indexed such that $\sigma = \mathrm{id}$) contains at least $\bigcup_{j=1}^{k}[M^{(j)}, X^{(j)}]$, where $[A, B]$ is the line segment between A and B. For a degenerated

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T_k-configuration, one has $\bigcup_{j=1}^{k}[M^{(j)}, X]$, see [6, Corollary 4.19]. Note that, unlike in the classical example given by Tartar [14], $\mathcal{M}$ need not lie in a plane, even for $k = 4$.

The question asked in [7, Section 8] and addressed here can be phrased as follows. *Let $k \geq 4$ matrices $M^{(1)}, \ldots, M^{(k)} \in \mathbb{R}^{m\times n}$ without rank-one connections (i.e., $\operatorname{rank}(M^{(i)} - M^{(j)}) \geq 2$ for $i \neq j$) be given. Do they form a T_k-configuration?*

We will study only the interesting case $k \geq 4$, since T_3-configurations lie necessarily in a plane consisting of rank-one lines. The stochastic experiments in Section 3 will concentrate on T_4-configurations. In the special case of $\mathbb{R}^{2\times 2}$, the T_4-configurations are in some sense the universal example for finite sets with nontrivial rank-one convex hull. This is due to the following theorem [13, Theorem 2].

Theorem 2.2 (Székelyhidi, '03) *Let $\mathcal{M} \subset \mathbb{R}^{2\times 2}$ be a compact set without rank-one connections but $\mathcal{M}^{rc} \neq \mathcal{M}$. Then $\mathcal{M}$ contains a (possibly degenerated) T_4-configuration.* $\square$

For $k = 4$, an attempt was made to solve the system (1) of $4\binom{m}{2}\binom{n}{2} + 8mn$ quadratic and linear equations directly (for some permutation σ of $\{1, 2, 3, 4\}$). But even Gröbner basis methods implemented in *Macaulay 2* failed to solve the system even for simple test cases.

To exploit the algebraic structure, let us define for a matrix $M \in \mathbb{R}^{m\times n}$ its *rank-one cone* $\mathcal{R}_1(M)$ as

$$\begin{aligned}\mathcal{R}_1(M) &:= \{X \in \mathbb{R}^{m\times n} \mid \operatorname{rank}(X - M) \leq 1\} \\ &= \left\{ X \;\middle|\; \det\begin{pmatrix} X_{rs} - M_{rs} & X_{ru} - M_{ru} \\ X_{ts} - M_{ts} & X_{tu} - M_{tu}\end{pmatrix} = 0, \quad \begin{matrix} 1 \leq r < t \leq m \\ 1 \leq s < u \leq n \end{matrix} \right\},\end{aligned} \tag{2}$$

i.e., $\mathcal{R}_1(M)$ is the set of all matrices that are rank-one connected to M.

In order to describe $\mathcal{R}_1(M)$ algebraically, the following notation is used. Let $X = (X_{rs})$ be an $m \times n$-matrix of the indeterminates $X_{11}, X_{12}, \ldots, X_{1n}, X_{21}, \ldots, X_{mn}$. The real polynomials in these indeterminates will be denoted by $\mathbb{R}[X]$ (considered as a ring, i.e., addition and multiplication are well defined). Whenever necessary, we will silently identify $\mathbb{R}^{mn}$ and $\mathbb{R}^{m\times n}$. For simplicity, the ideas leading to Algorithm 2.3 will be explained for $\sigma = \mathrm{id}$.

If the matrices $M^{(1)}, \ldots, M^{(k)}$ form a T_k-configuration then the corners of the inner polygon lie necessarily in the intersections of rank-one cones, i.e.,

$$X^{(j)} \in \mathcal{J}_j := \mathcal{R}_1(M^{(j)}) \cap \mathcal{R}_1(M^{(j-1)}),$$

where the index j is counted modulo k. It can be shown that if $m, n \geq 3$ then $\mathcal{J}_j$ is generically empty.

The intersections $\mathcal{J}_j$ ($j = 1, \ldots, k$) are the zero set of the 2×2-minors of $(X^{(j)} - M^{(j)})$ and $(X^{(j)} - M^{(j-1)})$,

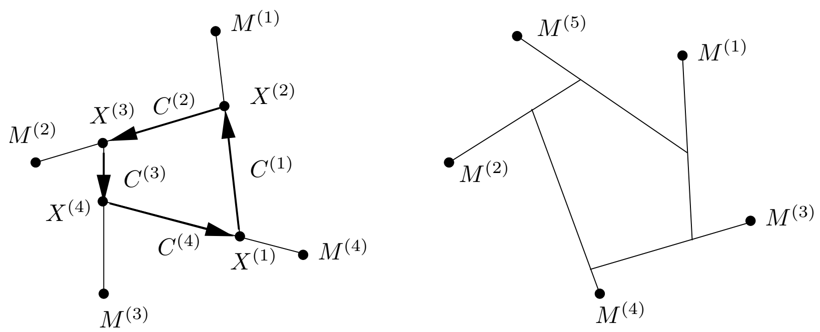

Figure 1. A T_4-configuration and a T_5-configuration, both projected to $\mathbb{R}^2$.

$$\det\begin{pmatrix} X_{rs}^{(j)} - M_{rs}^{(j)} & X_{ru}^{(j)} - M_{ru}^{(j)} \\ X_{ts}^{(j)} - M_{ts}^{(j)} & X_{tu}^{(j)} - M_{tu}^{(j)} \end{pmatrix}, \quad \det\begin{pmatrix} X_{rs}^{(j)} - M_{rs}^{(j-1)} & X_{ru}^{(j)} - M_{ru}^{(j-i)} \\ X_{ts}^{(j)} - M_{ts}^{(j-1)} & X_{tu}^{(j)} - M_{tu}^{(j-1)} \end{pmatrix} \in \mathbb{R}[X^{(j)}],$$

$$1 \le r < t \le m, \quad 1 \le s < u \le n, \qquad j = 1, \dots, k \text{ (counted modulo } k). \tag{3}$$

(As a zero set of polynomials, $\mathcal{J}_j$ is by definition a *variety.*) The set of polynomials with the zero set $\mathcal{J}_j$ has the structure of an *ideal* and will be denoted I_j. It is generated by the minors in (3), see, e.g., [5]. If $I_j = \mathbb{R}[X^{(j)}]$, then the associated variety $\mathcal{J}_j$ is empty and there is no candidate point for the corner $X^{(j)}$ of the inner polygon of a possible T_k-configuration.

If $\mathcal{M}$ is a T_k-configuration, then for each j, the matrices $M^{(j)}$, $X^{(j+1)}$ and $X^{(j)}$ lie on a line, in this particular order. This yields the equations and inequalities

$$\lambda_j M^{(j)} + (1-\lambda_j)X^{(j)} = X^{(j+1)}, \qquad 0 < \lambda_j < 1, \qquad \text{for } 1 \le j \le k. \tag{4}$$

In order to describe this in terms of varieties we introduce the polynomial ring $\mathcal{P} := \mathbb{R}[X^{(1)}, \dots, X^{(k)}, \lambda_1, \dots, \lambda_k]$ in $kmn + k$ indeterminates. Then we obtain naturally from (4) the polynomials

$$\lambda_j M_{rs}^{(j)} + (1-\lambda_j)X_{rs}^{(j)} - X_{rs}^{(j+1)} \qquad \text{for } 1 \le j \le k,\ 1 \le r \le m,\ 1 \le s \le n. \tag{5}$$

These kmn polynomials and the polynomials in (3), the latter taken for all $1 \le j \le k$, generate an ideal $I \subseteq \mathcal{P}$. For a permutation σ, let I_σ be the ideal generated analogously, with $M^{(j)}$ substituted by $M^{(\sigma^{-1}(j))}$ in (3) and (5). The real variety associated to I_σ will be denoted by $\mathcal{V}_\sigma \subset \mathbb{R}^{kmn+k}$.

With the notation introduced above, $\mathcal{M} = \{M^{(1)}, \dots, M^{(k)}\} \subset \mathbb{R}^{m\times n}$ is a T_k-configuration if and only if there exists a permutation σ of $\{1, \dots, k\}$ such that $\mathcal{V}_\sigma \subset \mathbb{R}^{kmn+k}$ contains a point $(X^{(1)}, \dots, X^{(k)}, \lambda_1, \dots, \lambda_k)$ with $\lambda_j \in (0,1)$ for $1 \le j \le k$.

The preceding arguments immediately show the correctness of the following algorithm.

Algorithm 2.3

Input: $\mathcal{M} = \{M^{(1)}, \dots, M^{(k)}\} \subset \mathbb{R}^{m\times n}$ without rank-one connections.

Procedure: For all permutations σ of $\{1, \dots, k\}$ perform the following test.

1. For $j = 1, \dots, k$ compute a Gröbner basis for the ideal $I_{\sigma,j}$ generated by the polynomials from (3), with $M^{(j)}$ substituted by $M^{(\sigma^{-1}(j))}$. If $I_{\sigma,j} = \mathbb{R}[X^{(j)}]$ for some j then there exists no solution to (1) for this σ. Else:
2. Compute a Gröbner basis for the ideal generated by the polynomials in (5) with $M^{(j)}$ substituted by $M^{(\sigma^{-1}(j))}$.
3. Compute a Gröbner basis for the ideal I_σ generated by the union of the ideals in Steps 1 and 2. If $I_\sigma = \mathcal{P}$ then there exists no solution to (1) for this σ. Else:
4. Check if there is a a point $(X^{(1)}, \dots, X^{(k)}, \lambda_1, \dots, \lambda_k) \in \mathcal{V}_\sigma$ with $\lambda_j \in (0,1)$ for all $1 \le j \le k$. If yes, this is a T_k-configuration; if not, there exists no solution to (1) for this σ.

Output: If $\mathcal{M}$ is a T_k-configuration this is detected in Step 4 for some σ. If $\mathcal{M}$ is not a T_k-configuration, then for every σ, either Step 1, 3 or 4 give a negative answer. □

To perform the check in Step 4, we use a combination of the BKR algorithm [11] and the eliminant method [12]. This requires I_σ to be zero-dimensional in $\mathcal{P}$ (i.e., the complex variety $\mathcal{V}_\sigma \subset \mathbb{C}^{kmn+k}$ has to consist of single points). This was true in every one of the more than 200 000 examples we checked. However, a rigorous proof of the zero-dimensionality is lacking.

Similar ideas can be applied for the detection of degenerated T_k-configurations.

3. Stochastic experiments for T_4-configurations

Extensive tests with random integer matrices in $\mathbb{R}^{2\times 2}, \mathbb{R}^{4\times 2}$ and $\mathbb{R}^{3\times 3}$ have been carried out for $k = 4$. Such computations were not possible with previous methods. Algorithm 2.3 allows for the first time the investigation of stochastic questions, such as the distribution of T_4-configurations in the space of quadruples of matrices. We report some results.

Algorithm 2.3 has been implemented in the computer algebra package *Macaulay 2* [4]. For every experiment, we had *Macaulay 2* generate four random matrices $\mathcal{M} = \{M^{(1)}, M^{(2)}, M^{(3)}, M^{(4)}\}$ with integer entries in the interval $[0, R]$ for $R = 20, 30, 50, 150$. If the set $\mathcal{M}$ was found to have a rank-one connection between two of its elements, the experiment was terminated since such a set $\mathcal{M}$ cannot be a T_4-configuration.

Table 1 shows some results. In particular, almost 9%—a remarkably large number—of all random four-element sets in $\mathbb{R}^{2\times 2}$ were found to form a T_4-configuration. This suggests that the set of all T_4-configurations, considered as a subset of $(\mathbb{R}^{2\times 2})^4$, has positive measure.

Somewhat surprisingly, quite a few *sixfold T_4-configurations* were found. By this term, we mean sets $\mathcal{M}$ that satisfy (1) for *every* permutation σ of $\{1, 2, 3, 4\}$. As shown by Székelyhidi [13, Theorem 3], a T_4-configuration admits a real solution for (1) either for only one σ (up to a rotation) or for all permutations σ. Consistent with this, no twofold or threefold T_4-configurations were found.

As expected, a larger range of entries in the matrices leads to fewer configurations with rank-one connections.

In the cases of $\mathbb{R}^{3\times 3}$ and $\mathbb{R}^{4\times 2}$, no random set of matrices was found to be a T_4-configuration. In $\mathbb{R}^{3\times 3}$, no random configuration yielded four nonempty intersections $\mathcal{J}_j$ of the respective rank-one cones. It was already a rare exception (ca. 0.1% of experiments) to find at least one nonempty intersection. Rank-one cones are five-dimensional objects in a nine-dimensional space; thus this is intuitively not surprising. In $\mathbb{R}^{4\times 2}$, however, the $\mathcal{J}_j$ are two-dimensional, but the ideal I_σ equaled the entire ring $\mathcal{P}$ in every experiment. The complexity of the algorithm increases by necessity for larger k. However, the case $k = 4$ we focussed on is the most interesting and important one for theoretical reasons (see Section 2).

	$\mathbb{R}^{2\times 2}$			$\mathbb{R}^{4\times 2}$	$\mathbb{R}^{3\times 3}$
Range R	30	50	150	50	20
Number of experiments	5 000	50 000	50 000	25 000	100 000
with a rank-one connection	748	776	133	0	0
T_4-configurations	368	4 351	4 392	0	0
thereof sixfold T_4-configurations	2	108	80	0	0
thereof degenerated T_4-configurations	0	0	0	0	0
not a T_4-configuration	3 884	44 873	45 475	25 000	100 000
Average time per experiment on a 1GHz Dual Pentium III	n/a	8.79 s	9.70 s	3.66 s	0.41 s

Table 1
Overview of some results of stochastic experiments

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