On the generation of periodic discrete structures with identical two-point correlation

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Strategies for the generation of periodic discrete structures with identical two-point correlation—called 2PC-equivalent—are developed. It is shown that starting from a set of 2PC-equivalent root structures, 2PC-equivalent child structures of arbitrary resolution and number of phases (e.g. material phases) can be generated based on phase extension through trivial embeddings, kernel-based extension and phase coalescence. Proofs are provided by means of discrete Fourier transform theory. A Python 3 implementation is offered for reproduction of examples and future applications.

1. Introduction

In several fields of science, discrete structures in one, two, three and higher space dimension are essential for the systematic investigation of physical phenomena. Two-dimensional structures are represented by matrices or images. Each discrete colour in the image represents one phase, and a structure can contain an arbitrary number of phases. In materials science, for instance, images are used to characterize microstructured materials with respect to their evolution or physical properties, e.g. [1] or [2]. Furthermore, they are used to train modern machine learning approaches in face-recognition, autonomous driving and many other fields, e.g. [3] or [4]. Via computed tomography, voxelized three-dimensional information of bodies can be gathered in
order to represent three-dimensional structures in a non-destructive fashion. They can improve diagnostics in medicine, e.g. [5] or [6], and they can enable \textit{in situ} examinations of the evolution of mechanical structures, e.g. [7] or [8].

In terms of data analysis of \(n\)-phase multi-dimensional structures, the simplest statistical descriptor is the volume fraction of each phase, which is referred to as the one-point correlation. Higher-order correlations of the phases offer (i) better insight into the structure and (ii) better predictions of physical quantities of the structure.

In materials science, the effective behaviour of heterogeneous materials is dominated by the material arrangement at the microscopic level, e.g. [9]. Therefore, models approximating the effective material law and statistical bounds thereof are usually built at least on the one-point correlation, e.g. [10,11]. More accurate models and bounds take into consideration the two-point correlation (2PC) and even multiple-point correlations of the assumed periodic microstructure, e.g. [12], [13] or [14]. But a central question arises: What if different structures possess the exact same 2PC? This question has not only problematic implications for the deterministic prediction of models relying on the 2PC, e.g. [15], but also it will hinder structure-reconstruction algorithms based on the 2PC alone, e.g. [16,17].

For non-periodic structures of arbitrary dimensions, Chubb & Yellott [18] have shown that the dipole histogram, which corresponds to the 2PC, is a unique representation of any discrete structure. This implies that if two structures differ, then so do their dipole histograms, i.e. no group of structures with identical dipole histograms exists. For periodic structures, the situation is different: in [19,20], it has been proven that structures with identical 2PC exist and examples are provided. This implies that the claim of [17], that the 2PC uniquely determines a periodic structure is not unconditionally valid, as discussed in [20].

The present work aims, compared to [19,20], at a constructive generation of periodic structures with \textit{identical} 2PCs. The approach is based on root structures with identical 2PCs. The comparison of 2PCs is used to state 2PC-equivalence. Formal limitations of [21] are discussed, where it is claimed that the knowledge of specific sets of \((n-1)\) 2PCs generally suffices to uniquely determine all remaining 2PCs. The results of the present work comprise counterexamples to this statement. The results of [21] are nevertheless applicable to a wide range of microstructures in many important applications for materials science, but, as shown here, not to all microstructures. Although this result could be deemed academic, this finding can be relevant for works relying on [21], e.g. [22] or [23]. For the generation of 2PC-equivalent structures, three main operations are investigated in the present work: phase extension, kernel-based extension and phase coalescence. It is proven that these three basic operations conserve the 2PC-equivalence of the given structures, such that an infinite number of 2PC-equivalent structures can be generated starting from a single family of 2PC-equivalent root structures, as graphically summarized in figure 1. Thereby, based on appropriate kernels, structures can be purposely designed for specific applications, such as fibre-reinforced, particle-reinforced and polycrystalline materials with arbitrary number of phases; see figure 1 (left). Furthermore, the present work shows that, additionally, low-dimensional 2PC-equivalent structures can immediately be used in order to generate 2PC-equivalent structures of arbitrary dimensions and shapes; see figure 1 (right). The basic operations can be combined and repeated as needed in order to generate 2PC structures of arbitrary number of phases, dimensions and shapes. In order to make the results of the present work as transparent and useful as possible, an open-source Python 3 implementation with examples in Jupyter notebooks is offered [24]. Furthermore, the present work explores the influence of 2PC-equivalent structures on the effective thermal (or electric) conductivity of periodic materials. 2PC-equivalent structures are found, which show a deviation of 16\% in the effective conductivity matrix. This implies that for specific structures homogenization schemes relying exclusively on the 2PC may not be sufficiently accurate. The provided root structures and derived ones may be used as benchmark problems for new homogenization schemes.

The paper is organized as follows. In §2, \(n\)-phase discrete periodic structures are defined through multi-dimensional arrays, the 2PC and the notion of 2PC-equivalence are specified, and the basic operations preserving 2PC-equivalence are proven based on discrete Fourier transform
Figure 1. Graphical summary of the generation of 2PC-equivalent structures based on phase extension and kernel application using root 2PC-equivalent structures: (left) two-dimensional examples; (right) one-dimensional → three-dimensional example. (Online version in colour.)

(DFT) theory. Examples for the generation of 2PC-equivalent structures and the investigation of the deviation in the effective conductivity are demonstrated in §3. The paper ends with conclusions in §4.

Notation. The sets of natural, integer, real and complex numbers are denoted as $\mathbb{N}$, $\mathbb{Z}$, $\mathbb{R}$ and $\mathbb{C}$, respectively. The set of natural numbers including the 0 is addressed as $\mathbb{N}_0$. The symbol $i$ is reserved for the complex unit, i.e. $i^2 = -1$. Vectors $\mathbf{a} \in \mathbb{C}^P$ of dimension $P$ are addressed through their explicit comma-separated components as $\mathbf{a} = (a_0, a_1, \ldots, a_{P-1})$. Matrices are denoted by double-underlined characters, e.g. $\underline{\mathbf{A}}$. We address the array dimensionality $D \geq 2$ of a number set through a vector of corresponding length in the superscript, e.g. for $D = 3$, $P = (2, 3, 4) \in \mathbb{N}^3$, $\mathbb{C}^P = \mathbb{C}^{2 \times 3 \times 4}$ holds. Arrays of dimensionality $D \geq 3$ are addressed as $\underline{\mathbf{A}}$. Element-wise multiplication is denoted by the Hadamard product $\mathbf{a} \circ \mathbf{b}$, $\mathbf{A} \circ \mathbf{B}$ and $\underline{\mathbf{A}} \circ \underline{\mathbf{B}}$. Complex conjugation is denoted as $\mathbf{A}^\dagger$, where this is carried out element-wise in the array. We define the set $\mathbb{I} = \{0, 1\}$ and its corresponding extensions $\mathbb{I}^P$, $\mathbb{I}^{(P_1, P_2)}$ and $\mathbb{I}^L$ with $P \in \mathbb{N}^D$ for vectors, matrices and $D$-dimensional arrays having components being 0 or 1. Indicator arrays are simply addressed as indicators $\mathbf{I}_\alpha \in \mathbb{I}^P$. Hereby, the symbol $\alpha$ in the subscript is reserved for phase indices in an $n$-phase structure, i.e. $\alpha \in \{1, \ldots, n\}$. The symbols $p$ and $q$ are reserved for 0-based components/position indices, i.e. $I_{\alpha,p}$ denotes the component at position $p = (p_1, \ldots, p_D) \in \mathbb{N}_0^D$ of the indicator $\mathbf{I}_\alpha \in \mathbb{I}^P$ of phase $\alpha$ with $P \in \mathbb{N}^D$, $p_d \in \{0, \ldots, P_d - 1\}$ and $d \in \{1, \ldots, D\}$.

2. Periodic structures and two-point correlation

(a) Preliminaries

For an array $\underline{\mathbf{A}} \in \mathbb{C}^L$, we define the trivial embedding $\underline{\mathbf{A}}_{(\mathbf{z})} \in \mathbb{C}^L$ with $\mathbf{z} \in \mathbb{N}^N$ through its components as

$$
N \leq D : \quad A_{(\mathbf{z})} \in \mathbb{C}^L, \quad P' = (z_1 P_1, \ldots, z_N P_N, P_{N+1}, \ldots, P_D)
$$

$$
A_{p_1 \ldots p_N p_{N+1} \ldots p_D}^{(\mathbf{z})} = \begin{cases} 
A_{q_1 \ldots q_N P_{N+1} \ldots P_D} p_r = z_r q_r, r \in \{1, \ldots, N\} \\
0 & \text{else}
\end{cases}
$$

(2.1)
\[ a^{(3)} = \begin{pmatrix} a_0 \\ 0 \\ 0 \\ a_1 \\ 0 \\ 0 \\ a_2 \\ 0 \\ 0 \end{pmatrix} \]

\[ a = \begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix} \]

\[ a^{(2, 3)} = \begin{pmatrix} a_0 \\ 0 \\ 0 \\ 0 \\ a_1 \\ 0 \\ 0 \\ 0 \\ a_2 \\ 0 \\ 0 \\ 0 \end{pmatrix} \]

**Figure 2.** Example for the trivial embedding for a vector \( a \in \mathbb{C}^3 \) (centre): \( a^{(3)} \in \mathbb{C}^9 \) (left); \( a^{(2,3)} \in \mathbb{C}^{(6,3)} \) (right).

\[ A = \begin{pmatrix} A_{00} & A_{01} & A_{02} \\ A_{10} & A_{11} & A_{12} \end{pmatrix} \]

\[ A^{(3,2)} = \begin{pmatrix} A_{00} & 0 & 0 & A_{01} & 0 & 0 & A_{02} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ A_{10} & 0 & 0 & A_{11} & 0 & A_{12} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \]

**Figure 3.** Example for the trivial embedding for a matrix \( A \in \mathbb{C}^{(2,3)} \) (left); \( A^{(3,2)} \in \mathbb{C}^{(6,6)} \) (right).

and

\[ N > D : A^{[z]} \in \mathbb{C}^P', \quad P' = (z_1P_1, \ldots, z_DP_D, z_{D+1}, \ldots, z_N) \]

\[ A_{p_1 \ldots p_D}^{[z]} \equiv \begin{cases} A_{q_1 \ldots q_D} & p_r = z_rq_r, r \in \{1, \ldots, D\}, \\ 0 & \text{else.} \end{cases} \quad (2.2) \]

It should be noted that depending on \( z \in \mathbb{N}^N \), an array may be trivially embedded component-wise \((N \leq D)\) or even extended dimension-wise \((N > D)\). For clarification, consider the examples illustrated in figure 2 for a vector \( a \in \mathbb{C}^3 \) and in figure 3 for a matrix \( A \in \mathbb{C}^{(2,3)} \).

In the following, we further consider the modulo operator \( p | P \) for \( P \in \mathbb{N} \), which returns the positive remainder on division of \( p \) by \( P \), e.g. \(-2|5 = 3, -1|5 = 4, 0|5 = 0, 3|5 = 3 \) and \(7|5 = 2\). We define the repetition operation \( A^{[z]} \in \mathbb{C}^P \) with \( z \in \mathbb{N}^N \) through its components as (see also figure 4)

\[ N \leq D : A^{[z]} \in \mathbb{C}^P', \quad P' = (z_1P_1, \ldots, z_NP_N, P_{N+1}, \ldots, P_D) \]

\[ A_{p_1 \ldots p_N}^{[z]} \equiv A_{(p_1|P_1) \ldots (p_N|P_N)p_{N+1} \ldots p_D} \quad (2.3) \]

and

\[ N > D : A^{[z]} \in \mathbb{C}^P', \quad P' = (z_1P_1, \ldots, z_DP_D, z_{D+1}, \ldots, z_N) \]

\[ A_{p_1 \ldots p_D}^{[z]} \equiv A_{(p_1|P_1) \ldots (p_D|P_D)}. \quad (2.4) \]

From this point on, we consider any array \( A \in \mathbb{C}^P \) with \( P = (P_1, \ldots, P_D) \) as the unit cell of a corresponding \((P_1, \ldots, P_D)\)-periodic array, i.e. we extend the index values to all integers with \( A_{p_1 \ldots p_D} = A_{(p_1|P_1) \ldots (p_D|P_D)} \). For \( A, B \in \mathbb{C}^P \) with \( P \in \mathbb{N}^D \), we consider the circular convolution...
For future purposes, (2.12) is reformulated for $A ∈ C^D$, $A^{(2,3)} ∈ C^6$ (left); $A^{(2,3)} ∈ C^6$ (right).

The following identities for the DFT can be shown for $A, B ∈ C^P$ with $P ∈ N^D, z ∈ N^N$:

\[
\mathcal{F}(A * B) = \mathcal{F}(A) ⊗ \mathcal{F}(B),
\]

(2.9)

\[
\mathcal{F}(A ⊕ B) = \mathcal{F}(A) ⊗ \mathcal{F}(B),
\]

(2.10)

\[
\mathcal{F}(A[z]) = (\mathcal{F}(A))[z]
\]

(2.11)

and

\[
\mathcal{F}(A[z] ⊕ B[z]) = (\mathcal{F}(A ⊕ B))[z].
\]

(2.12)

The identity (2.9) is the well-known convolution theorem for periodic arrays, while (2.10) is an immediate implication of it. Identity (2.11) connects the DFT of a trivially embedded array with the repetition of the DFT of the array. An explicit proof of (2.11) is provided in appendix 4. The identity (2.12) is a simple implication of (2.10) and (2.11), its proof is provided in appendix 4. For future purposes, (2.12) is reformulated for $A, B ∈ R^P$ with $P ∈ N^D, z ∈ N^N$ and $D ≥ 1$ as

\[
A^{[z]} ⊕ B^{[z]} = (A ⊕ B)^{[z]}.
\]

(2.13)

Hence, correlations of trivially embedded arrays correspond to trivially embedded correlations.

**Figure 4.** Example for the repetition operation of a vector $a ∈ C^3$ (centre); $a^{[2]} ∈ C^6$ (left); $a^{(2,3)} ∈ C^6$ (right).

\[
A * B ∈ C^P,
\]

defined through its components as

\[
(A * B)_{p1...pD} = \sum_{q1=0}^{P1-1} \ldots \sum_{qD=0}^{P_D-1} A_{q1...qD} B_{(p1-q1)...(pD-qD)},
\]

(2.5)

and the correlation $A ⊕ B ∈ C^P$

\[
(A ⊕ B)_{p1...pD} = \sum_{q1=0}^{P1-1} \ldots \sum_{qD=0}^{P_D-1} A_{q1...qD} B_{(q1+p1)...(qD+pD)}.
\]

(2.6)

The DFT of an array $A$ and the inverse DFT are defined as

\[
\hat{A} = \mathcal{F}(A), \quad \hat{A}_{p1...pD} = \sum_{q1=0}^{P1-1} \ldots \sum_{qD=0}^{P_D-1} \exp \left( -i2\pi \sum_{d=1}^{D} \frac{p_d q_d}{P_d} \right) A_{q1...qD},
\]

(2.7)

and

\[
A = \mathcal{F}^{-1}(\hat{A}), \quad A_{p1...pD} = \sum_{q1=0}^{P1-1} \ldots \sum_{qD=0}^{P_D-1} \frac{1}{P_1 \ldots P_D} \exp \left( i2\pi \sum_{d=1}^{D} \frac{p_d q_d}{P_d} \right) \hat{A}_{q1...qD}.
\]

(2.8)

The identity (2.9) is the well-known convolution theorem for periodic arrays, while (2.10) is an immediate implication of it. Identity (2.11) connects the DFT of a trivially embedded array with the repetition of the DFT of the array. An explicit proof of (2.11) is provided in appendix 4. The identity (2.12) is a simple implication of (2.10) and (2.11), its proof is provided in appendix 4. For future purposes, (2.12) is reformulated for $A, B ∈ R^P$ with $P ∈ N^D, z ∈ N^N$ and $D ≥ 1$ as

\[
A^{[z]} ⊕ B^{[z]} = (A ⊕ B)^{[z]}.
\]

(2.13)

Hence, correlations of trivially embedded arrays correspond to trivially embedded correlations.

**b) Description of structures**

We consider the array representation of a $D$-dimensional discrete periodic structure comprised of $n$ phases. The indicator $I_α ∈ P^D$ of phase $α$ denotes the unit cell of the periodic structure with
periods \( P = (P_1, \ldots, P_D) \in \mathbb{N}^D \). The last \((n)th\) indicator is uniquely defined by

\[ I_{\tilde{n}} = 1 - \sum_{\alpha = 1}^{n-1} I_{\tilde{\alpha}}, \quad (2.14) \]

where \( \mathbb{1} \) is a \( P \)-array with all components equal to 1. Furthermore, we define the structure as

\[ \mathcal{S} = \sum_{\alpha = 1}^{n} \alpha I_{\tilde{\alpha}}, \quad (2.15) \]

assigning a unique phase to each pixel. An example for \( D = 1, P = 6, n = 3 \) is given by

\[ \mathcal{S} = (1,2,2,3,1,3), \quad I_1 = (1,0,0,0,1,0), \quad I_2 = (0,1,1,0,0,0) \quad \text{and} \quad I_3 = (0,0,0,1,0,1). \quad (2.16) \]

Structures will be visualized in this document through array plots. Hereby, for an \( n \)-phase structure, the \((n-1)\) first phases will be illustrated through colours and the dependent \( n \)th phase will be depicted by a white/translucent background. As an example, the structure \( \mathcal{S} \) given in (2.16) is illustrated in figure 5.

(c) Two-point correlation

The 2PC of phases \( \alpha_1 \) and \( \alpha_2 \) is defined as

\[ C_{\tilde{\alpha}_1 \tilde{\alpha}_2} = \mathcal{L}_{\tilde{\alpha}_1} \otimes \mathcal{L}_{\tilde{\alpha}_2} \in \mathbb{N}_P^D. \quad (2.17) \]

In DFT space, the 2PC can be conveniently computed based on (2.10) as

\[ F(\mathcal{C}_{\tilde{\alpha}_1 \tilde{\alpha}_2}) = F(\mathcal{L}_{\tilde{\alpha}_1}) \odot F(\mathcal{L}_{\tilde{\alpha}_2}). \quad (2.18) \]

The array \( \mathcal{C}_{\tilde{\alpha}_1 \tilde{\alpha}_2} \) inherits \( P \)-periodicity from the indicators. The 2PC considered in this work is not normalized by the total number of points, yielding integer components.

In an \( n \)-phase structure, \( n^2 \) 2PC can be computed. The general relation

\[ C_{\tilde{\alpha}_1 \alpha_2, p_1 \ldots p_D} = C_{\alpha_2, \alpha_1, (-p_1) \ldots (-p_D)} \quad \forall p \in \mathbb{Z}_D^D \quad (2.19) \]

holds, meaning that, for example, \( C_{12} \) is fully determined by \( C_{21} \). Based on (2.14), the 2PC of phase \( n \) can be expressed depending on the correlations of the \((n-1)\) phases. For instance, for any \( \alpha_1 \)

\[ C_{\tilde{\alpha}_1 n} = \mathcal{L}_{\tilde{\alpha}_1} \odot \mathcal{L}_n = \mathcal{L}_{\tilde{\alpha}_1} \odot \left( 1 - \sum_{\alpha_2 = 1}^{n-1} \mathcal{L}_{\tilde{\alpha}_2} \right) = (C_{\alpha_1 \alpha_1, 0 \ldots 0}) \mathbb{1} - \sum_{\alpha_2 = 1}^{n-1} C_{\alpha_1 \alpha_2} \quad (2.20) \]

holds. We define the 2PC sufficiency set (2PCSS) containing the \( n(n-1)/2 \) correlations \( C_{\alpha_1 \alpha_2} \) for \( \alpha_1 \in \{1, \ldots, n-1 \} \) and \( \alpha_2 \in \{\alpha_1, \ldots, n-1 \} \). The 2PCSS suffices for the complete determination of all remaining 2PC. It is shortly remarked that in [21] it is claimed that knowledge of only \((n-1)\) correlations suffices for the unique determination of all 2PC based on the DFT of the 2PC. However, situations exist where the claimed uniqueness is not achieved to the best knowledge of the authors of the present work (see appendix 4 for a detailed discussion and counterexamples). The present work does not intent to adjudicate the achievements of [21] but to make the community aware that their results cannot be applied to all microstructures. Hence, the determination of the minimal set of independent 2PCs still requires more investigation. In the following, the 2PCSS is used in order to assure unambiguous results.
Consider two structures \( S(1) \) and \( S(2) \) with correponding indicator \( L_\alpha(s) \) for \( s \in \{1, 2\} \). Two structures \( S(1) \) and \( S(2) \) are referred to as 2PC-equivalent, shortly denoted as
\[
\sim \quad (2.21)
\]
if all 2PC \( C_{\alpha_1\alpha_2}(1) \) corresponding to \( S(1) \) and its indicators \( L_\alpha(1) \) and all \( C_{\alpha_1\alpha_2}(2) \) corresponding to \( S(2) \) are identical, i.e. \( C_{\alpha_1\alpha_2}(1) = C_{\alpha_1\alpha_2}(2) \) \( \forall \alpha_1, \alpha_2 \in \{1, \ldots, n\} \).

(d) Higher-order correlations

The general \( M \)-point correlation \( C_{\alpha(M)} \) (MPC) for \( M \geq 2 \) for a \( D \)-dimensional structure \( S \) with periods vector \( P = (P_1, \ldots, P_D) \in \mathbb{N}^D \), phase vector \( \alpha = (\alpha_1, \ldots, \alpha_M) \in \mathbb{N}^M \) and indicators \( L_\alpha, \alpha_1 \in \alpha \), is defined as
\[
(C_{\alpha(M)})_{0_1 \ldots 0_{D-1}} = \sum_{q_1=0}^{P_1-1} \ldots \sum_{q_{D-1}=0}^{P_{D-1}-1} (L_{\alpha_1} q_1 L_{\alpha_2} q_2 + P_1 \ldots L_{\alpha_1} q_1 + P_{D-1}).
\]
(2.22)
The definition (2.22) is in accordance with the 2PC in (2.17), i.e. \( C_{\alpha(2)} = \alpha_{\alpha_1 \alpha_2} \). In this work, the focus is on the 2PC, and evaluation of the MPC is limited to specific examples.

(e) Inheritance of two-point correlation-equivalence

(i) Starting point

Let two bi-phasic 2PC-equivalent structures \( S(1) \sim S(2) \) be given, i.e.
\[
C_{11}(1) = C_{11}(2), \quad C_{12}(1) = C_{12}(2), \quad C_{21}(1) = C_{21}(2) \quad \text{and} \quad C_{22}(1) = C_{22}(2)
\]
(2.23)
hold. The indicators \( L_\alpha \) define \( S(s) \) \( (s = 1, 2) \) and \( C_{11}(1) = C_{11}(2) \) states the 2PC-equivalence.

(ii) Phase extension through trivial embedding

Consider a structure \( S \in \{ S(1), S(2) \} \) and related indicators \( L_\alpha \) and \( L_\beta \). We define new indicators \( L'_\alpha \) through trivial embedding (2.1) and (2.2)
\[
L'_\alpha = L'_{\alpha}, \quad \alpha \in \{1, 2\}.
\]
(2.24)
Next, we define the additional new phase indicator \( L'_3 \) and the three-phasic structure \( S' \) as follows:
\[
L'_3 = 1 - \sum_{\alpha=1}^{2} \alpha L'_\alpha \quad \text{and} \quad S' = \sum_{\alpha=1}^{3} \alpha L'_\alpha.
\]
(2.25)
The 2PCs of the new structure \( S' \) are related to the old ones due to the property (2.13) as follows:
\[
C'_{\alpha_1 \alpha_2} = L'_w \otimes L'_z = L'_{\alpha_1} \otimes L'_{\alpha_2} = (C_{\alpha_1 \alpha_2})^{(2)} \quad \forall \alpha_1, \alpha_2 \in \{1, 2\}.
\]
(2.26)
The relation (2.26) makes then clear that if \( S(1) \) is phase-extended and denoted as \( S'(1) \), and \( S(2) \) is phase-extended and denoted as \( S'(2) \), then all corresponding 2PC for \( \alpha_1, \alpha_2 \in \{1, 2\} \) fulfill \( C'_{\alpha_1 \alpha_2}(1) = C'_{\alpha_1 \alpha_2}(2) \). More explicitly, for \( n = 3 \) in the new structures \( S'(1) \) and \( S'(2) \), we have
\[
C'_{11}(1) = C'_{11}(2), \quad C'_{12}(1) = C'_{12}(2), \quad C'_{22}(1) = C'_{22}(2)
\]
(2.27)
for the 2PCSS, implying the 2PC-equivalence \( S'(1) \sim S'(2) \); cf. (2.21).

In terms of graph theory, the structures \( S(1) \sim S(2) \) are regarded as parent structures, while the derived ones \( S'(1) \sim S'(2) \) are denoted as child structures inheriting the 2PC-equivalence. It should be noted that the described reasoning for the extension from 2 \( \rightarrow \) 3 phases can be repeated for 3 \( \rightarrow \) 4 and so on. This means that

(i) a phase-extension of 2PC-equivalent \( n \)-phase structures through trivial embedding yields 2PC-equivalent \( (n+1) \)-phase structures,
(ii) 2PC-equivalent structures with arbitrary number of phases can always be generated starting from two-phase 2PC-equivalent structures, and
(iii) the described phase extension goes along with an increase of the size of the structure, possibly with increasing spatial dimension $D$.

For example, $I_1 \in \mathbb{I}^{12}$, $I_1^{(2,4,5)} \in \mathbb{I}^{(24,4,5)}$, and corresponding one-dimensional 2PC-equivalent structures would then generate three-dimensional 2PC-equivalent structures (e.g. figure 1).

(iii) Kernel-based extension

For an $n$-phase structure $S$ with corresponding indicators $I_\alpha$, we assume that a kernel list $K = \{K_1, \ldots, K_n\}$ with $K_\alpha \in \mathbb{I}$ $\forall \alpha \in \{1, \ldots, n\}$ is given. Based on the dimensions $z \in \mathbb{N}^N$ of the given kernels, we extend the structure through trivial embedding of the indicators $I_\alpha^{(1)} \in \mathbb{I}^P$ and extend the kernels through appended trivial embedding $K_\alpha^0 \in \mathbb{I}^P$ to match the new structure dimensions as follows:

For $N \leq D$: $P' = (z_1P_1, \ldots, z_NP_N, P_{N+1}, \ldots, P_D)$,

\[
K_{\alpha, p_1' \ldots p_N'}^0 = \begin{cases} 
K_{\alpha, p_1' \ldots p_N'} \quad & p_r' \in \{0, \ldots, z_r - 1\} \forall r \in \{1, \ldots, N\} \quad \text{and} \quad p_r' = 0 \quad \forall t \in \{N + 1, \ldots, D\} \\
0 & \text{else}
\end{cases}
\] (2.28)

For $N > D$: $P' = (z_1P_1, \ldots, z_PD, z_{D+1}, \ldots, z_N)$,

\[
K_{\alpha, p_1' \ldots p_N'}^0 = \begin{cases} 
K_{\alpha, p_1' \ldots p_N'} \quad & p_r' \in \{0, \ldots, z_r - 1\} \forall r \in \{1, \ldots, N\} \\
0 & \text{else}
\end{cases}
\] (2.29)

Based on the dimension $z$ of the kernels and correspondingly $K_\alpha^0$, the $(n+1)$ indicators

\[
I_{\alpha}^{(n+1)} = K_\alpha^0 * I_\alpha^{(1)} \in \mathbb{I}^P, \quad \alpha \in \{1, \ldots, n\}, \quad I_{n+1}^{(n+1)} = 1 - \sum_{\alpha=1}^{n} I_{\alpha}^{(n+1)}
\] (2.30)

describe the kernel-based extended $(n+1)$-phase structure $S' \in \mathbb{N}^P$. The corresponding 2PC of the new structure $S'$ are related to the original ones due to (2.18), (2.29) and (2.11) as follows:

\[
\mathcal{F}(C_{\alpha_1, \alpha_2}) \approx \mathcal{F}\left(\tilde{I}_{\alpha_1}^{(1)} \circ \tilde{I}_{\alpha_2}^{(1)}\right) = \mathcal{F}\left(K_{\alpha_1, \alpha_2}^0 \circ I_{\alpha_1}^{(1)} \circ I_{\alpha_2}^{(1)}\right) = \mathcal{F}(K_{\alpha_1}^0) \circ \mathcal{F}(I_{\alpha_1}) \circ \mathcal{F}(I_{\alpha_2})
\] (2.31)

Starting from the $n$-phase parent structures $S(1) \sim S(2)$ with $C_{\alpha_1, \alpha_2}(1) = C_{\alpha_1, \alpha_2}(2) \forall \alpha_1, \alpha_2 \in \{1, \ldots, n\}$, the 2PC of the structures $S'(1), S'(2)$ fulfill

\[
C_{\alpha_1, \alpha_2}(1) = C_{\alpha_1, \alpha_2}(2) \quad \forall \alpha_1, \alpha_2 \in \{1, \ldots, n\}
\] (2.32)

due to (2.31). This implies that the 2PCSS of $S'(1)$ and the one of $S'(2)$ are identical, i.e. $S'(1) \sim S'(2)$ holds. Arbitrarily sized kernels with components $K_{\alpha, p_1' \ldots p_N'} = 1$ simply return the original structure in a higher resolution with possible rescaling, i.e. a change of aspect ratio of the pixels.

In summary:

(i) 2PC-equivalence is invariant under appropriate application of kernels (i.e. through kernel extensions (2.28)–(2.29) and application to trivially embedded indicators in (2.30)), and
(ii) 2PC-equivalence is invariant under arbitrary discrete rescaling.
(iv) Phase coalescence

It is remarked that any subset of the phases within 2PC-equivalent structures can be coalesced to a single phase without affecting 2PC-equivalence. For instance, consider a given four-phase structure $\mathcal{S}$ with phase indicators $I_\alpha$, $\alpha \in \{1, 2, 3, 4\}$. One option would be to coalesce the three first phases and generate a new two-phase structure with indicators $I'_1 = \sum_{\alpha=1}^{3} I_\alpha$ and $I'_2 = I_4$. The 2PC of phases $(\alpha_1, \alpha_2) = (1, 2)$ of the new two-phase structure is $C'_12 = I'_1 \ast I'_2 = (I_1 + I_2 + I_3) \ast I_4$.

$\sum_{\alpha=1}^{3} I_\alpha + I_4 = C'_14 + C'_24 + C'_34$. \hspace{1cm} (2.33)

For 2PC-equivalent structures, (2.33) makes clear that not only the 2PC for $(\alpha_1, \alpha_2) = (1, 2)$ of the new two-phase structures are equal, but all of the 2PC: the phase-coalesced structures preserve 2PC-equivalence. This statement holds independent of the dimension $D$, the number of phases $n$ and the resolution vector $P$.

3. Examples and application

(a) Root structures

The generation of 2PC-equivalent structures based on the inheritance properties proven in §2e (phase extension, kernel-based extension and phase coalescence) requires given 2PC-equivalent structures. Small 2PC-equivalent structures with a low number of phases can easily be searched for by brute force. These small structures can be used to generate 2PC-equivalent child structures. For given dimension vector $P \in \mathbb{N}^D$ for $D \in \{1, 2, 3\}$ and number of phases $n \leq 3$, we search for 2PC-equivalent structures using the following procedure:

(S.1) Based on $P$ and $n$ generate all possible $n_S$ structures $\mathcal{S} = \{\mathcal{S}(1), \ldots, \mathcal{S}(n_S)\}$.

(S.2) Compute the 2PCSS $\mathcal{C}(s)$ of the structure $\mathcal{S}(s)$ for all $1 \leq s \leq n_S$.

(S.3) Set $s_{\text{ref}} = 1$, i.e. select the first structure as start reference.

(S.4) Extract labels $\Sigma \subset \mathbb{N}$ of structures matching 2PC $\mathcal{C}(s_{\text{ref}})$: $\forall s \in \Sigma : \mathcal{C}(s) = \mathcal{C}(s_{\text{ref}})$.

(S.5) Remove all structures from $\Sigma$ that are related to $\mathcal{S}(s)$ by periodic shift, axis reflection, phase interchange or combination of these operations $\rightarrow \Sigma^* \subset \Sigma$.

(S.6) If $\Sigma^*$ is non-empty, then remove all related structures within $\Sigma^*$ and obtain the index set $\Sigma^{**} \subset \Sigma^*$. Return 2PC-equivalent structures $\mathcal{S}^{**} = (\mathcal{S}(s_{\text{ref}})) \cup \{\mathcal{S}(s), s \in \Sigma^{**}\}$. If $\Sigma^* = \emptyset$, move to next structure: $s_{\text{ref}} \leftarrow s_{\text{ref}} + 1$ and go to (S.4) or terminate if $s_{\text{ref}} = n_S$ (no 2PC-equivalent structure found).

Structures found by this procedure will be referred to as root structures. Routines for their generation and examples in Jupyter notebooks are available at [24].

(b) Two-phase and $n$-phase structures

(i) One-dimensional example

For the period $P = 12$ and number of phases $n = 2$, consider the given 2PC-equivalent root structures

$\mathcal{S}(1) = (1, 1, 1, 2, 1, 2, 2, 1, 2, 2, 2) \in \mathbb{N}^{12}$ and $\mathcal{S}(2) = (1, 1, 2, 1, 2, 1, 2, 2, 2, 2) \in \mathbb{N}^{12}$, \hspace{1cm} (3.1)

displayed in figure 6. Phase extension through trivial embedding with $z = 3$, see (2.24) and (2.25), yields the three-phase structures $\mathcal{S}'(1) \sim \mathcal{S}'(2) \in \mathbb{N}^{36}$, shown in figure 6.
(ii) Two-dimensional example

Consider the 2PC-equivalent root structures for \( P = (4, 3), n = 2 \)

\[
S(1) = \begin{pmatrix} 1 & 2 & 2 \\ 2 & 2 & 1 \\ 2 & 1 & 1 \\ 2 & 2 & 1 \end{pmatrix} \quad \text{and} \quad S(2) = \begin{pmatrix} 1 & 2 & 2 \\ 2 & 1 & 1 \\ 1 & 2 & 2 \\ 1 & 2 & 2 \end{pmatrix}.
\] (3.2)

The two-phase root structures \( S(1) \sim S(2) \in \mathbb{N}^{(4,3)} \) given by (3.2) are illustrated in figure 7. A phase extension of the two-phase structures to three phases based on a trivial embedding with \( z = (2, 3) \), see (2.24) and (2.25), is shown in figure 7 by \( S'(1) \sim S'(2) \in \mathbb{N}^{(6,9)} \). It should be noted that the axis ratio is changed from 4 : 3 to 8 : 9. The property (2.13) and its implication (2.26) can be seen in the 2PC \( C_{11} \) and \( C'_{11} \) of the root and phase extended structures at the bottom of the corresponding columns in figure 7. Application of the kernels

\[
K_1 = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad \text{and} \quad K_2 = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \end{pmatrix},
\] (3.3)

with \( z = (2, 3) \) as described through (2.28)–(2.30) on the embedded phases 1 and 2, respectively, yields the 2PC-equivalent structures \( S''(1) \sim S''(2) \) shown in figure 7. It should be noted that in the case of \( K_{1,p_1,p_2} = 1 \) and \( K_{2,p_1,p_2} = 1 \), the root two-phase structures \( S(1) \sim S(2) \) would have been returned, only in a higher resolution and with some relative stretching along the second dimension. This emphasizes that from given 2PC-equivalent structures, derived child structures with arbitrary resolution and size changes are also 2PC-equivalent. Finally, \( S'''(1) \sim S'''(2) \) in figure 7 show a phase coalescence of phases 1 and 2 of the structures \( S''(1) \sim S''(2) \), which naturally drastically changes the phase volume fractions and topology of the structures, but the 2PC-equivalence is still preserved.

Finally, it should be noted that the results of the present work may be used in order to generate 2PC-equivalent structures for practical applications, e.g. for fibre- and particle-reinforced materials. Again, starting from the root structures \( \mathbb{G}_1 \sim \mathbb{G}_2 \), inclusion-reinforced 2PC-equivalent structures can be generated. The composition shown in figure 8 shows how bimodal 2PC-equivalent fibre structure with two different fibre orientations and, strictly speaking, different fibre lengths can be generated. Alternatively, instead of the two-phase structures \( \mathbb{G}_1 \sim \mathbb{G}_2 \) one could begin, for example, with the generated three-phase structures \( \mathbb{G}''(1) \sim \mathbb{G}''(2) \) displayed in figure 7 as parent structures and construct 2PC-equivalent child structures with three different orientations and lengths. Naturally, this strategy can also be used for arbitrary particle structures. Jupyter notebooks reproducing the illustrated examples are available at [24].

As a further option, kernels or binary structures with coherent edges can be used in order to form structures with inter-phase coherent transitions. As an example consider figure 9, where edge-coherent kernels have been applied. Postponed phase coalescence yields new phase distributions with more complex statistics. The structures displayed in figure 9 can be interpreted in the field of materials science as the cross section of a three-dimensional fibre-reinforced structure with four main fibre bundles (illustrated in black, blue, red and orange in figure 9). In order to generate complex and realistic microstructures with identical 2PC, the use of a set of

---

**Figure 6.** Root structures \( S(1) \sim S(2) \) and corresponding phase extended structures \( S'(1) \sim S'(2) \) for \( z = 3 \). (Online version in colour.)
Figure 7. Root structures $S_1 \sim S_2$, trivial embedding extended structures $S_1' \sim S_2'$, kernel-based extended structures $S_1'' \sim S_2''$ and phase coalesced structures $S_1''' \sim S_2'''$ by phase coalescence $\{1 \leftarrow \{1, 2\}\}$. The 2PC for $(\alpha_1, \alpha_2) = (1, 1)$ of the corresponding structures is shown at the bottom of each column. (Online version in colour.)

Finally, it should be remarked that applications needing a high number of phases can generate 2PC-equivalent structures by applying the phase extension operation repeatedly. As an example from materials science, polycrystals can be considered as structures with a high number of phases, where each phase corresponds to a single grain. The root structures $S_1 \sim S_2$, for example, can be used to generate 2PC-equivalent polycrystals with arbitrary number of grains/phases.

(iii) Three-dimensional example

Consider again the root one-dimensional structures $S_1 \sim S_2$ given by (3.1) and illustrated in figure 6. We now extend these structures based on the kernels $K_1, K_2 \in \mathbb{E}$ for $\mathbf{z} = (2, 2, 3)$

$$K_{1,p_1,p_2,p_3} = \begin{cases} 1 & (p_1, p_2, p_3) \in \{(0, 0, 0), (0, 0, 1), (0, 0, 2), (0, 1, 0), (1, 0, 0), (1, 1, 0)\} \\ 0 & \text{else} \end{cases}$$  \hspace{1cm} (3.4)

and

$$K_{2,p_1,p_2,p_3} = \begin{cases} 0 & (p_1, p_2, p_3) \in \{(0, 0, 2), (0, 1, 1), (1, 1, 0), (1, 1, 1)\} \\ 1 & \text{else}. \end{cases}$$  \hspace{1cm} (3.5)

The root one-dimensional structures are again displayed at the top of figure 10, while the corresponding kernel-based extended structures are illustrated at the bottom of figure 10.
It should be stressed that this example illustrates not only a three-dimensional example but also the possibility to dimension-extend any given set of 2PC-equivalent structures to arbitrary dimensions, sizes and aspect ratios.

(c) Effective linear properties in homogenization theory of periodic media

In the following, the structure is interpreted as a microscopic unit cell of a periodic medium. We consider the two-dimensional periodic conductivity problem on \( S \subset \mathbb{R}^2 \) with phase-wise constant conductivity \( K(x) \in \mathbb{R}^{2 \times 2} \)

\[
\text{div}(K(x) \text{grad}(u(x))) = 0 \quad x \in S, \quad u(x) = \hat{g}^T x + v(x) \quad x \in \partial S. \quad (3.6)
\]

For given \( \hat{g} \), the solution \( u(x) \) is a superposition of the linear field \( \hat{g}^T x \) and a fluctuation \( v(x) \), which is periodic over the structure. The flux in the structure

\[
f(x) = K(x) \text{grad}(u(x)) \quad (3.7)
\]
Figure 10. Kernel-based extension: root one-dimensional structures $S(1) \sim S(2)$, kernels $K_1$ and $K_2$ for the extension of phases 1 and 2, and extended structures $S'(1) \sim S'(2)$. (Online version in colour.)

is of interest. The periodicity implies that the effective gradient of the solution equals the prescribed $\bar{g}$

$$\frac{1}{|S|} \int_S \text{grad}(u(x)) \, dS = \bar{g}.$$ (3.8)

The effective (volume averaged) flux $\bar{f}$ is linear in the effective gradient $\bar{g}$. Therefore, the relation holds. The constant $\bar{K}$ is referred to as the effective conductivity of the structure. It characterizes the macroscopic constitutive behaviour of the periodic material inherited from the microscopic one (3.7). If the solution $u(x)$ is considered as the temperature field, then $\bar{K}$ corresponds to the negative of the effective heat conductivity, while for $u(x)$ being the electric potential $\bar{K}$ reflects the effective electric conductivity.

Many homogenization schemes target an approximation or bounds of the effective material properties, here in terms of $\bar{K}$. These are often built upon the material properties of the constituents and statistical properties of the structure. The vast majority of such schemes rely on one-point statistical information, i.e. volume fractions of the constituent materials. The 2PC of the present work corresponds to the two-point statistics of the microstructure. Homogenization schemes based on the 2PC are expected to be vastly superior to ones based on volume fractions. But what if the 2PC is not enough information? The investigations of the present work motivate the question: can two or more 2PC-equivalent microstructures have large deviations in the respective $\bar{K}$? This would then imply that corresponding homogenization schemes based on the 2PC have from the very beginning no chance to accurately approximate $\bar{K}$ for all of these 2PC-equivalent structures.

As a first example, we consider again the two-dimensional structures $S(1) \sim S(2)$ presented in figure 7. We consider the phase-wise constant conductivity field for isotropic constituents

$$\bar{K}(x) = k(x)I, \quad k(x) = \begin{cases} k_1 & x \in \text{phase 1} \\ k_2 & x \in \text{phase 2}. \end{cases}$$ (3.10)
Figure 11. Structures $S(1)$ and $S(2)$ (left plots) displayed in figure 7 with $2 \times$ resolution solution fields $u(\vec{x})$ for $\vec{g} = (1, 0)$ (middle plots) and corresponding solution fields for $32 \times$ resolution (right plots). (Online version in colour.)

For the current case of isotropic two-phase materials, bounds on the effective conductivity are well known in homogenization theory. Based purely on the volume fraction $v_1 \in [0, 1]$ of phase 1, the upper and lower so-called first order bounds can be computed

$$\bar{K}^1_{1+} = [v_1 k_1 + (1 - v_1) k_2] \quad \text{and} \quad \bar{K}^1_{1-} = \left[ v_1 \frac{1}{k_1} + (1 - v_1) \frac{1}{k_2} \right]^{-1} \quad (3.11)$$

where $\bar{K}^1_{1+}$ is referred to in the literature as the Voigt bound, while $\bar{K}^1_{1-}$ is referred to as the Reuss bound, e.g. [10,11] or [13]. The Voigt and Reuss bounds given in (3.11) bound the effective conductivity from below and above via

$$\bar{\bar{\sigma}} \leq \bar{\bar{\sigma}} \leq \bar{\bar{\sigma}} \quad (3.12)$$

More elaborated bounds can be constructed based on higher-order correlation information of the microstructure. The so-called Hashin–Shtrikman bounds, e.g. [13] or [9], are second-order bounds based on the 2PC. These bounds are usually simplified by assuming no long-range order and isotropic 2PC. For two-dimensional conductivity problem, these simplifications yield

$$\bar{K}^{2+/\pm} = \left[ \left( v_1 \frac{1}{k_{1+/\pm} + k_1} + (1 - v_1) \frac{1}{k_{1+/\pm} + k_2} \right)^{-1} - k^+/- \right] L \quad (3.13)$$

with $k^+ = \max\{k_1, k_2\}$, $k^- = \min\{k_1, k_2\}$; see [9]. Strictly speaking, since the structures of the present work do not show isotropic 2PC, the Hashin–Shtrikman bounds are not valid, i.e. analogous relations to (3.12) do not hold already if the 2PC is not isotropic. For some structures, the corresponding 2PC may be considered as approximately isotropic and to show approximately no long-range order, such that the Hashin–Shtrikman bounds (3.13) can be considered as bounds in the corresponding approximate sense.

The two-dimensional homogenization problem for conductivity has been solved numerically for $k_1 = 10$ and $k_2 = 1$ with the Fourier-accelerated nodal solver approach of [27] for $2 \times$ resolution and $32 \times$ resolution of the structures $S(1) \sim S(2)$; see figure 11a,b. The oversampling ratios of 2 and 32 have been considered in order to rule out discretization issues.

For the $2 \times$ resolution of the structures, the corresponding effective conductivities evaluate to

$$\bar{K}^{2\times}(1) = \begin{pmatrix} 3.1455 & 0 \\ 0 & 2.2687 \end{pmatrix} \quad \text{and} \quad \bar{K}^{2\times}(2) = \begin{pmatrix} 3.6099 & 0 \\ 0 & 2.9865 \end{pmatrix}. \quad (3.14)$$
For the $32 \times$ resolution of the structures, the corresponding effective conductivities evaluate to

$$
\bar{K}^{32 \times}_{(1)} = \begin{pmatrix} 2.8305 & 0 \\ 0 & 2.1615 \end{pmatrix} \quad \text{and} \quad \bar{K}^{32 \times}_{(2)} = \begin{pmatrix} 3.1981 & 0 \\ 0 & 2.6198 \end{pmatrix}.
$$

The volume fraction of phase 1 equals $v_1 = 5/12 \approx 42\%$. Based on $k_2 < k_1$ and $v_1 < 1/2$, the structures $S(1) \sim S(2)$ can be interpreted as reinforced structures of a material with conductivity $k_2$. Evaluation of the Voigt, Reuss and Hashin–Shtrikman bounds is illustrated in figure 12. As remarked in the introduction of the bounds, only the Voigt and Reuss bounds are definite bounds for the considered structures; the Hashin–Shtrikman bounds are not strictly valid, since the structures do not possess the corresponding statistical properties.

The relative deviations of the effective conductivities from computational homogenization are

$$
\frac{\| \bar{K}^{2 \times}_{(1)} - \bar{K}^{2 \times}_{(2)} \|}{\| \bar{K}^{2 \times}_{(1)} \|} = 22.05\% \quad \text{and} \quad \frac{\| \bar{K}^{32 \times}_{(1)} - \bar{K}^{32 \times}_{(2)} \|}{\| \bar{K}^{32 \times}_{(1)} \|} = 16.50\%. \quad (3.16)
$$

This example shows that even though some structures may have identical 2PC the effective properties can still strongly deviate from structure to structure. This naturally implies that the accuracy of many homogenization schemes based not only on one- but also on two-point statistics may not be sufficient for the application at hand. The structures provided in this work offer benchmark structures for such homogenization schemes.

It should be remarked that the 2PC-equivalent structures $S(1)$ and $S(2)$ potentially differ with respect to the 3PC, cf. (2.22), which is supported by the computed relative deviations

$$
\frac{\| \bar{\kappa}^{2 \times}_{(3,111)(1)} - \bar{\kappa}^{2 \times}_{(3,111)(2)} \|}{\| \bar{\kappa}^{2 \times}_{(3,111)(1)} \|} = 31.88\% \quad \text{and} \quad \frac{\| \bar{\kappa}^{32 \times}_{(3,111)(1)} - \bar{\kappa}^{32 \times}_{(3,111)(2)} \|}{\| \bar{\kappa}^{32 \times}_{(3,111)(1)} \|} = 24.36\%. \quad (3.17)
$$

The deviation in the 3PC for the structures $S(1) \sim S(2)$ indicates that even for relatively fine discretization (e.g. $32 \times$ resolution) a clear statistical difference can be found between $S(1)$ and $S(2)$. Homogenization schemes aiming for the effective properties of these structures may have to include the 3PC or even higher correlations for linear and, probably, also for nonlinear material behaviour in order to make reliable predictions in the utmost general scenarios.

Of course, the magnitude of the deviation in the effective properties depends on the structure and material behaviour taken into account. Consider as a second example the child structures $S''(1) \sim S''(2)$ of figure 7. These structures are generated from the previous $S(1) \sim S(2)$ by a phase extension, kernel application and phase coalescence. The volume fraction of phase 1 changes to $v_1 = 41/72 \approx 57\%$. For $k_2 < k_1$ and $v_1 > 1/2$, the generated structures $S''(1) \sim S''(2)$ can be interpreted as weakened structures of a material with conductivity $k_1$ for phase 1. Analogous increase in the resolution to $2 \times$ and $32 \times$ yields the results depicted in figure 13.
The corresponding effective conductivities for $k_1 = 10$ and $k_2 = 1$ are

$$\bar{\mathbf{K}}^{2\times(1)} = \begin{pmatrix} 4.5169 & 0.2396 \\ 0.2396 & 3.6756 \end{pmatrix}, \quad \bar{\mathbf{K}}^{2\times(2)} = \begin{pmatrix} 4.4771 & 0.2304 \\ 0.2304 & 3.6825 \end{pmatrix}, \quad (3.18)$$

and

$$\bar{\mathbf{K}}^{32\times(1)} = \begin{pmatrix} 4.3133 & 0.2890 \\ 0.2890 & 3.5431 \end{pmatrix}, \quad \bar{\mathbf{K}}^{32\times(2)} = \begin{pmatrix} 4.2577 & 0.2859 \\ 0.2859 & 3.5518 \end{pmatrix}. \quad (3.19)$$

In figure 14, the Voigt, Reuss and Hashin–Shtrikman bounds are illustrated, together with the effective conductivities of the structures $S'''(1)$ and $S'''(2)$.

Evaluation of the analogous relative deviation yields

$$\frac{\|\bar{\mathbf{K}}^{2\times(1)} - \bar{\mathbf{K}}^{2\times(2)}\|}{\|\bar{\mathbf{K}}^{2\times(1)}\|} = 0.72\% \quad \text{and} \quad \frac{\|\bar{\mathbf{K}}^{32\times(1)} - \bar{\mathbf{K}}^{32\times(2)}\|}{\|\bar{\mathbf{K}}^{32\times(1)}\|} = 1.00\%, \quad (3.20)$$

such that this second example demonstrates that for some 2PC-equivalent structures the deviation in the effective conductivities may also be small.
4. Conclusion

It has been shown for discrete periodic structures that when starting from given/root 2PC-equivalent structures, new 2PC-equivalent child structures can be constructed systematically based on the basic operations: phase extension through trivial embedding, kernel-based extension and phase coalescence. These results allow for the immediate generation of an infinite number of 2PC-equivalent structures of arbitrary dimension, size, aspect ratio and number of phases through composition of the basic operations. Open-source software is provided for the generation of root 2PC-structures and construction of 2PC-equivalent child structures. With the provided software interested readers can generate their own root structures and derive 2PC-equivalent child structures for the application of interest, e.g. for fibre- or particle-reinforced materials and polycrystals. Examples of 2PC-equivalent structures have been demonstrated and analysed in the context of homogenization theory of periodic media for the two-dimensional conductivity problem. It has been shown that 2PC-equivalent structures exist, which may show significant or almost negligible deviations in the effective material behaviour. The magnitude of the deviation depends not only on the structures but also on the considered material behaviour. The presented structures may serve as benchmark problems for homogenization schemes using the 2PC and possibly further microstructure information in order to test their accuracy or uncertainty with respect to the predicted effective properties.

Data accessibility. The data and Python 3 source code for the generation of the 2PC-equivalent structures can be found in the GitHub repository [24].

Authors’ contributions. M.F. and F.F. developed the theory and wrote the manuscript together. M.F. implemented the results in Python 3 and created the repository [24]. All authors gave final approval for publication and agree to be held accountable for the work performed therein.

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Appendix A. Auxiliary proofs based on discrete Fourier transform

The property (2.11) \( \mathcal{F}(\mathcal{A}_p) = (\mathcal{F}(\mathcal{A}))_p \) connected to the case-sensitive trivial embedding (2.1)–(2.2), and repetition operation (2.3)–(2.4) can be shown as follows. Consider \( \mathbf{z} \in \mathbb{N}^N \) and \( \mathcal{A} \in \mathbb{C}^{\mathbb{L}} \) with \( P \in \mathbb{N}^D \). For the case \( N \leq D \) (2.11) is shown by eliminating \( \mathbf{z} \) as follows:

\[
(\mathcal{F}(\mathcal{A}_p))_{\mathbf{z}_1 \ldots \mathbf{z}_N \mathbf{p}_{N+1} \ldots \mathbf{p}_D} = \sum_{\mathbf{q}_1 = 0}^{\mathbf{z}_1 - 1} \ldots \sum_{\mathbf{q}_N = 0}^{\mathbf{z}_N - 1} \sum_{\mathbf{q}_{N+1} = 0}^{\mathbf{p}_{N+1} - 1} \ldots \sum_{\mathbf{q}_D = 0}^{\mathbf{p}_D - 1} \mathcal{A}_{\mathbf{q}_1 \ldots \mathbf{q}_N \mathbf{q}_{N+1} \ldots \mathbf{q}_D} 
\times \exp\left( -i2\pi \left( \frac{\mathbf{p}_1 \mathbf{q}_1}{\mathbf{z}_1 \mathbf{p}_1} + \ldots + \frac{\mathbf{p}_N \mathbf{q}_N}{\mathbf{z}_N \mathbf{p}_N} + \frac{\mathbf{p}_{N+1} \mathbf{q}_{N+1}}{\mathbf{p}_{N+1}} + \ldots + \frac{\mathbf{p}_D \mathbf{q}_D}{\mathbf{p}_D} \right) \right) 
\]

\[
= \sum_{\mathbf{q}_1 = 0}^{\mathbf{p}_1 - 1} \ldots \sum_{\mathbf{q}_N = 0}^{\mathbf{p}_N - 1} \sum_{\mathbf{q}_{N+1} = 0}^{\mathbf{p}_{N+1} - 1} \ldots \sum_{\mathbf{q}_D = 0}^{\mathbf{p}_D - 1} \mathcal{A}_{\mathbf{q}_1 \ldots \mathbf{q}_N \mathbf{q}_{N+1} \ldots \mathbf{q}_D} 
\times \exp\left( -i2\pi \left( \frac{\mathbf{p}_1 \mathbf{q}_1}{\mathbf{p}_1} + \ldots + \frac{\mathbf{p}_N \mathbf{q}_N}{\mathbf{p}_N} + \frac{\mathbf{p}_{N+1} \mathbf{q}_{N+1}}{\mathbf{p}_{N+1}} + \ldots + \frac{\mathbf{p}_D \mathbf{q}_D}{\mathbf{p}_D} \right) \right) 
\]

\[
= (\mathcal{F}(\mathcal{A}))_{\mathbf{p}_1 \ldots \mathbf{p}_N \mathbf{p}_{N+1} \ldots \mathbf{p}_D},
\]

(A 1)
For the case \( N > D \)

\[
(F(A^{[\ell]}))_{p_1 \ldots p_D} \approx \sum_{q_0=0}^{z_1} \sum_{q_D=0}^{z_D} A_{q_1 \ldots q_D} \exp \left( -i2\pi \left( \frac{p_1q_1}{z_1} + \cdots + \frac{p_Dq_D}{z_D} + \frac{p_{D+1}q_{D+1}}{z_{D+1}} + \cdots + \frac{p_Nq_N}{z_N} \right) \right)
\]

holds, implying (2.11). The property (2.12) is derived based on (2.10) and (2.11) as follows:

\[
F(A^{[\ell]} \otimes B^{[\ell]}) = \overline{F(A)} \otimes F(B) = F(A^{[\ell]}) \otimes F(B^{[\ell]})
\]

\[
= \left( F(A) \otimes F(B) \right)^{[\ell]} = (F(A \otimes B))^{[\ell]}.
\]  

**Appendix B. Counterexamples regarding [21]**

For a compact notation in this appendix, we denote the corresponding components of the DFT of the 2PC as \( \hat{C}_{\alpha \beta, p} \in \mathbb{C} \). Furthermore, we define the number of events \( I_{\alpha, p} = 1 \) in phase \( \alpha \) as \( \#_\alpha \)

\[
\#_\alpha = \sum_{p_0=0}^{P_1-1} \sum_{p_D=0}^{P_D-1} I_{\alpha, p}, \text{ and } \#_\alpha \leq P_1 \ldots P_D.
\]  

In [21], the following system of equations is presented:

\[
\hat{C}_{\alpha \beta, p} = \overline{\hat{C}_{\alpha \beta, (p_p - p)}}, \quad \hat{C}_{\alpha \beta, p} = \overline{\hat{C}_{\beta \alpha, p}}, \quad \hat{C}_{\alpha \gamma, p} = \overline{\hat{C}_{\gamma \alpha, p}} \hat{C}_{\alpha \beta, p}
\]  

\[
\sum_{p=1}^{n} \hat{C}_{\alpha \beta, p} = \left\{ \begin{array}{ll} (P_1 \ldots P_D) \sqrt{\hat{C}_{\alpha \alpha, 0}} & \text{if } p = 0 \\ 0 & \text{else} \end{array} \right.,
\]  

\[
\sum_{p_1=0}^{P_1-1} \sum_{p_D=0}^{P_D-1} \hat{C}_{\alpha \beta, p} = \left\{ \begin{array}{ll} (P_1 \ldots P_D) \sqrt{\hat{C}_{\alpha \alpha, 0}} & \text{if } \alpha = \beta \\ 0 & \text{else} \end{array} \right.,
\]  

\[
0 \leq \hat{C}_{\alpha \alpha, 0} \leq (P_1 \ldots P_D)^2
\]

and

\[
0 \leq |\hat{C}_{\alpha \beta, p}| \leq (P_1 \ldots P_D)^2.
\]  

These properties are extracted from equations N.(15), N.(8), N.(9), N.(13), N.(14) and N.(11) in [21]. It is remarked that \( \hat{C}_{\alpha \beta, p} \) is related to \( S \times \eta^p F_k \) in [21], but with a different convention of the DFT, and, probably, the relation \( |\eta^p F_k| \leq S^2 \) in equation N.(11) is a typo and \( |\eta^p F_k| \leq S \) was meant. The properties (B2)–(B8) can easily be derived as follows. Property (B2) is the standard DFT symmetry of real signals. Property (B3) is obtained directly from the 2PC definition or based on (2.19). Property (B4) is considered a key result in [21] and can be obtained through simple
rearrangement of the term \( \hat{I}_{\alpha} \odot \hat{J}_{\gamma} \odot \hat{J}_{\gamma} \odot \hat{J}_{\beta} \). Property \((B 5)\) is exactly the determination of the last 2PC based on \((n - 1)\) counterparts, see \((2.20)\), and is derived by taking the DFT of \((2.20)\) and exploiting \( \hat{C}_{a\alpha} = \hat{I}_{\alpha} \odot \hat{J}_{\alpha} \) and \( \hat{C}_{a\alpha} = \#^2_a \). The property \((B 6)\) is a reformulation of \(C_{a\beta, a\beta} \) expressed through the inverse DFT. Finally, the bounds \((B 7)\) and \((B 8)\) can be derived based on \(|\hat{I}_{\alpha, p}| \leq \#_a \), \((B 1)\) and the even tighter relation

\[
|\hat{C}_{a\beta, p}| \leq \#_a \#_\beta = \hat{C}_{a\beta, 0} \leq (P_1 \ldots P_D)^2.
\]

In \([21]\), equation \((B 4)\) is reformulated as

\[
\hat{C}_{a\beta, p} = \frac{\hat{C}_{a\beta, p} \hat{C}_{\gamma, p}}{\hat{C}_{\gamma, p}}.
\]

Although valid in certain situations, more precisely if \( \hat{C}_{\gamma, p} \neq 0 \) for any \( p \), Niezgoda et al. have not considered the case \( \hat{C}_{\gamma, p} = 0 \) for some \( p \) and, to the best of our knowledge, the resulting indefiniteness of \((B 10)\) was not addressed. Still, \((B 10)\) is attractive since for given \( \gamma \) and given 2PCs \( \{C_{\gamma, 1}, \ldots, C_{\gamma, (n-1)}\} \), \( C_{\gamma, n} \) can be determined by \((2.20)\) (or equivalently \((B 5)\)) and \((B 10)\) could be used in combination with \((2.19)\) (or equivalently \((B 3)\)) in order to determine all remaining 2PCs—without any usage of \((B 2)\) or \((B 6)\). In \([21]\) \((B 10)\) is considered as the building block for stating that for an \( n \)-phase structure with known \((n - 1)\) 2PC \( \{C_{\gamma, 1}, \ldots, C_{\gamma, (n-1)}\} \) (or their DFTs) and for arbitrarily chosen \( \gamma \), all remaining 2PCs can be computed. This implies that \((n - 1)\) 2PCs fully can determine all \( n^2 \) 2PCs. This remarkable property is stated without a supporting proof that the system of equations implicitly described through \((B 2)–(B 8)\) is uniquely solvable for given \( \{C_{\gamma, 1}, \ldots, C_{\gamma, (n-1)}\} \) for any \( \gamma \) if \( \hat{C}_{\gamma, p} = 0 \) for some \( p \).

Although a considerable effort was invested, the authors of the present work failed in closing the proof. Eventually, several counterexamples were found for which \( \hat{C}_{\gamma, p} \) vanishes. For instance, consider the following simple one-dimensional structure:

\[
S = (1, 1, 1, 2, 2, 3) \in \mathbb{Z}^6,
\]

with \( n = 3 \) phases and with phase indicators \( I_1, I_2 \) and \( I_3 \). The 2PC of \( S \) are

\[
\begin{align*}
C_{11} &= (3, 2, 1, 0, 1, 2), & C_{12} &= (0, 1, 2, 2, 1, 0), & C_{13} &= (0, 0, 0, 1, 1, 1), \\
C_{21} &= (0, 0, 1, 2, 2, 1), & C_{22} &= (2, 1, 0, 0, 0, 1), & C_{23} &= (0, 1, 1, 0, 0, 0), \\
C_{31} &= (0, 1, 1, 1, 0, 0), & C_{32} &= (0, 0, 0, 0, 1, 1), & C_{33} &= (1, 0, 0, 0, 0, 0).
\end{align*}
\]

The 2PCSS for the current example is given by \( \{C_{111}, C_{112}, C_{222}\} \). The corresponding DFTs of the 2PC \( C_{a\alpha} \) for \( \alpha \in \{1, 2, 3\} \) are computed as

\[
\begin{align*}
\hat{C}_{11} &= (9, 4, 0, 1, 0, 4), & \hat{C}_{22} &= (4, 3, 1, 0, 1, 3) & \text{and} & & \hat{C}_{33} &= (1, 1, 1, 1, 1, 1).
\end{align*}
\]

For the example structure \((B 11)\), the DFTs of the 2PCs evidently contain some zero entries. Hence, \((B 10)\) cannot be computed for arbitrary \( p \). For example, if \( \gamma = 1 \) is chosen and \( \{\hat{C}_{11}, \hat{C}_{12}\} \) are considered as given, then \( \hat{C}_{13} \) can be determined through \((B 5)\). Then, using \((B 3)\), \( \hat{C}_{21} \) and \( \hat{C}_{31} \) can be computed. Subsequently, based on \((B 10)\) most components of \( \hat{C}_{22} \) and \( \hat{C}_{23} \) can be computed. Still, \( \hat{C}_{a\beta, 2} \) and \( \hat{C}_{a\alpha, 4} \) cannot be determined from \((B 10)\) since \( \hat{C}_{11, 2} = \hat{C}_{11, 4} = 0 \) hold. Only the additional consideration of \((B 2)\) and \((B 6)\) allows the determination of all entries of all 2PCs. The situation is the same for \( \gamma = 2 \). Only for \( \gamma = 3 \) can one compute all 2PCs without additional considerations. However, this contradicts the arbitrariness of \( \gamma \).

A two-dimensional counterexample is given by

\[
S = \begin{pmatrix}
2 & 3 & 1 \\
2 & 2 & 1 \\
2 & 3 & 3 \\
2 & 2 & 3
\end{pmatrix} \in \mathbb{N}^{4 \times 3}.
\]

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The DFTs of the three 2PCs \{C_{11}, C_{12}, C_{22}\} are denoted by \{\hat{C}_{11}, \hat{C}_{12}, \hat{C}_{22}\}. The DFTs \hat{C}_{11} and \hat{C}_{22} contain 3 and 6 zero entries, respectively. For the choice of \(\gamma = 1\), i.e. assuming given \{\hat{C}_{11}, \hat{C}_{12}\}, [21] states that the remaining \(\hat{C}_{\alpha\beta}\) are uniquely determined by the system (B 2)–(B 8). However, this system cannot be solved uniquely. The following analytic deviation in DFT space:

\[
\Delta_{\alpha\beta} = \begin{cases} 
0 & (\alpha, \beta) \in \{(2, 2), (3, 3)\} \\
0 & (\alpha, \beta) \in \{(2, 3), (3, 2)\} \\
0 & \text{else}
\end{cases}
\]

has been generated by the authors. Perturbing the true 2PC \(\hat{C}_{\alpha\beta}\) of \(S\) by \(\Delta_{\alpha\beta}\) the arrays \(\hat{C}'_{\alpha\beta} = \hat{C}_{\alpha\beta} + \Delta_{\alpha\beta}\) are generated. Both \(\hat{C}_{\alpha\beta}\) as well as \(\hat{C}'_{\alpha\beta}\) satisfy (B 2)–(B 8). Setting \(\gamma = 1\) hence yields two ambiguous solutions, contradicting the aspired uniqueness. The example is also contained in the provided Python 3 software [24]. It should be remarked that examples with vanishing DFT components in all phases exist. For example, for the structure

\[
S = \begin{pmatrix}
1 & 1 & 3 \\
1 & 2 & 3 \\
1 & 1 & 3 \\
3 & 1 & 2
\end{pmatrix},
\]

with \(n = 3\), in \(\hat{C}_{11}, \hat{C}_{22}\) and \(\hat{C}_{33}\) respectively, 2, 2 and 3 entries vanish. Therefore, unless the available data are free of zeros in \(\hat{C}_{\gamma\gamma}'\), the smallest set of equations for obtaining the full set of 2PCs remains open. Finding the set of independent 2PC requires, from the perspective of the authors of the present work, further investigation.

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