Microstructure-informed reduced modes synthesized with Wang tiles and the Generalized Finite Element Method

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Abstract

A recently introduced representation by a set of Wang tiles—a generalization of the traditional Periodic Unit Cell-based approach—serves as a reduced geometrical model for materials with stochastic heterogeneous microstructure, enabling an efficient synthesis of microstructural realizations. To facilitate macroscopic analyses with a fully resolved microstructure generated with Wang tiles, we develop a reduced order modelling scheme utilizing pre-computed characteristic features of the tiles. In the offline phase, inspired by computational homogenization, we extract continuous fluctuation fields from the compressed microstructural representation as responses to generalized loading represented by the first- and second-order macroscopic gradients. In the online phase, using the ansatz of the generalized finite element method, we combine these fields with a coarse finite element discretization to create microstructure-informed reduced modes specific for a given macroscopic problem. Considering a two-dimensional scalar elliptic problem, we demonstrate that our scheme delivers less than 3% error in both the relative $L_2$ and energy norms with only 0.01% of the unknowns when compared to the fully resolved problem. Accuracy can be further improved by locally refining the macroscopic discretization and/or employing more pre-computed fluctuation fields. Finally, unlike standard snapshot-based reduced-order approaches, our scheme handles significant changes in the macroscopic geometry or loading without the need for recalculating the offline phase, because the fluctuation fields are extracted without any prior knowledge of the macroscopic problem.

Keywords Wang tiling · Microstructure-informed modes · Reduced order modelling · Heterogeneous materials

1 Introduction

Reduced Order Modelling (ROM) has become an established way for accelerating numerical analyses by exploiting the information contained in previously obtained solutions (snapshots)—be it time steps/load increments [54] or solutions to other parametrizations [7]—to construct an approximation space better suited to the investigated problem. ROM is thus particularly appealing for problems such as optimization/parameter identification [7], system control [3], and real-time simulations [2,5,26,32,44,52], i.e. scenarios where the increased cost of an offline phase (collecting and processing snapshots) can be amortized in subsequent calculations. Many strategies in multi-scale modelling have a similar multi-query character; ROM thus allows for significant acceleration of FE²-like computational homogenization approaches [36,49,65] and closely related applications in multi-scale topology optimisation [20,62].

1.1 Local reduced models

In general, the projection-based ROM works particularly well for problems with a relatively low-dimensional parametrisation space (e.g. variation in geometric or loading parameters, or prescribed macroscopic strain) and mild non-linearities [30,53]. To avoid a significant increase in dimensions of the reduced approximation spaces for more severe non-linearities, several strategies have been proposed that approximate a solution manifold with multiple reduced approximation subspaces along with procedures allowing for interpolat-
approaches in terms of parametrization partitioning [16] or solution characteristics [1, 50], ROM can be utilized locally in problem’s subdomains; for instance, Kerfriden et al. [30] proposed using reduced modes only in regions without localized damage.

In the FE setting, Oliver et al. [49] split a Representative Volume Element into a linear subdomain and a region of softening cohesive bands, extracting reduced modes for each subdomain separately. Radermacher and Reese [53] introduced an adaptive sub-structuring ROM in forming process simulations, in which only the parts of the domain with mild non-linearity were reduced, while highly non-linear regions remained fully resolved. Similarly, Niroomandi et al. [45] combined global ROM with the Generalized Finite Element Method (GFEM), introduced locally in a patch near a simulated surgical cut, in order to capture localized solution characteristics efficiently. Using Partition of Unity (PU) [43], intrinsic to the previously mentioned GFEM approaches, Ibáñez et al. [28] recently proposed a local variant of Proper Generalized Decomposition.

Still, the parametrization space of problems with fully resolved, stochastic microstructural details is inherently too high-dimensional, see Sect. 5.2.2 for an explicit example, and hence difficult to address within the standard ROM setting. Even though Kerfriden et al. [30] adopted a ROM strategy for fracture modelling in domains with a stochastic microstructure, only the parameters of a damage model varied within the macroscopic domain. Consequently, the regions excluding the damage localization, which were accelerated with ROM, effectively behaved homogeneously in the linear regime. Numerical strategies based solely on PU/GFEM thus seem to be better suited for simulations with stochastic microstructural details.

1.2 Alternatives based on Partition of Unity

Covering linear problems, Strouboulis et al. [59] introduced a dictionary of pre-computed local solutions to selected microstructural features, which were then used as enrichment functions within the Generalized Finite Element Method (GFEM). Fish and Yuan [18] proposed a multiscale enrichment method, combining the Partition of Unity methods with responses of a periodic microstructure representation to unit loading cases from the computational homogenization [22]. Efendiev et al. [15] developed the Generalized Multiscale Finite Element Method that extracts local enrichments in problem’s subdomains from a collection of pre-computed general responses using eigenvalue analyses. In a similar spirit but without pre-calculations, Plews and Duarte [51] generated the microstructure-specific enrichments on-the-fly by subjecting subdomains with finer discretization to boundary values obtained from a coarse global solution, building on the local-global enrichment framework [14]. Outside the GFEM family of approaches, the recently proposed Coarse Mesh Condensation Multiscale method [38], subsequently extended to non-periodic microstructures and non-conforming coarse-scale discretization [39], is conceptually similar to the aforementioned methods as it combines a coarse scale approximation of a strain field with parallel calculations of localization fields within (potentially overlapping) subdomains. In contrast to older works by Zohdi and coworkers, e.g. [69,70], in which a domain-decomposition-like approach with a regularized approximation at the interfaces of subdomains was adopted, the parametrization of the localization fields is linked to the coarse strain field via an $L_2$-norm projection in [38,39].

1.3 Our contribution

In the series of our previous works [11,13,47], we have introduced the framework of Wang tiles as a suitable extension of the (Statistically Equivalent) Periodic Unit Cell methodology for modelling microstructural geometry of random heterogeneous materials. We have shown that replacing the unit cell based representation with a set of domains—Wang tiles—with predefined mutual compatibility enables an efficient generation of (pseudo-)stochastic microstructural realizations that feature suppressed periodicity artefacts [11,13,47]. Even though the spurious periodicity is significantly reduced in the generated microstructural samples, they are still composed of only a handful of tiles. The Wang tile concept thus provides a finite-size discrete parametrization space of all realizations.

Combining both the GFEM and ROM approaches recalled above and benefiting from discrete microstructure parametrization, we develop a reduced order modelling scheme for problems with fully resolved microstructural details generated by the tile-based approach. We first recall the essentials of the Wang tile concept and its use in modelling heterogeneous materials in Sect. 2. Next, inspired by asymptotic homogenization approaches as in [18,42], we propose a method for extracting the characteristic responses of the compressed microstructural representation to parametrized macroscopic loading in Sect. 3. These general, tile-wise defined responses are constructed such that they can be assembled in the same way a microstructural sample is synthesized from the individual Wang tiles, and they serve as an approximation to the fluctuation part of a macroscopic solution. Section 4 then introduces the macroscopic numerical scheme that combines the general pre-computed characteristic responses using the Generalized Finite Element ansatz to generate the microstructure-informed reduced modes, specific for a given macroscopic problems. We illustrate the proposed methodology with two-dimensional, scalar, elliptic examples in Sect. 5, and discuss the obtained results.
in Sect. 6. Finally, we summarize the proposed scheme and outline its possible extensions in Sect. 7.

We adopt the following notation: scalars are written in a normal-weight italic font, e.g. $\theta$; first- and second-order tensors are denoted with bold italics and bold normal font, respectively, e.g. $\mathbf{x}$ and $\mathbf{A}$; operator $\cdot$ stands for a tensor contraction. Column vectors and matrices are written in sans-serif lower-case and capital letters, $\mathbf{u}$ and $\mathbf{A}$.

2 Wang tiles as microstructural ROM

The concept of Wang tiles was originally proposed as an equivalent problem in predicate calculus [61]: instead of proving a logical statement of a certain class directly, it was converted to a question whether a set of square tiles with codes attributed to their edges can tile an infinite plane such that the adjacent tiles have the same code on the corresponding edges. Later, this abstract concept was applied in the Computer Graphics community as a convenient formalism for encoding continuity constraints when assembling pre-generated modules into larger blocks—tilings. Adopting the tile concept has enabled fast synthesis of point patterns with desired blue noise spectrum [27,33] and natural-looking textures [9,57,67]. The latter applications inspired utilisation of the tile concept in modelling materials with random heterogeneous microstructures [47] and, very recently, the design of modular materials and structures [60].

Currently, characterization of a microstructural geometry in a compressed form is mostly based on a Periodic Unit Cell (PUC) representation (under different names such as Repeating Unit Cell [63], Statistically Similar Representative Volume Element [4], Statistically Optimal Representative Unit Cell [40], and Statistically Equivalent Periodic Unit Cell [66]). Although such compression is lossless only for a narrow range of materials with a periodic arrangement of constituents, the modelling error caused by the periodicity and limited variability is negligible in standard concurrent multiscale schemes such as FE$^2$ [17]. On the other hand, the PUC-based compression is unsuitable for generating microstructural geometry for macroscale analyses with a fully resolved microstructure for two reasons: (i) it only produces a single, hence deterministic, sample and (ii) the produced microstructural sample exhibits artificial periodicity. The Wang tile concept addresses both drawbacks, and allows for avoiding computationally intensive optimization algorithms traditionally used to generate an ensemble of stochastic microstructural samples [66].

In the Wang tile (cube) concept, a material microstructure is represented with a set of square (or cubical) domains with codes attributed to their edges (or faces); see the illustration in Fig. 1. The interior of each tile is designed such that (i) the contained microstructural geometry remains continuous across the parts of tile boundary with the same code and (ii) when assembled following the compatibility constraints posed by the codes, the resulting tile assembly resembles the original microstructure in terms of microstructural features, assessed typically via spatial statistics.

So far, three design strategies have been proposed: an optimization approach to minimize a discrepancy between spatial statistics of the reference specimen and generated assemblies [47], a sample-based strategy [11], and a level-set
based framework for particulate and foam-like microstructures [13]. However, most of the methods developed for generating PUC can be modified to adopt the generalized periodicity constraints of Wang tiles.

Unlike mathematicians that focus mainly on tile sets for strictly aperiodic tiling, see the overview in [24, Chapter 11], we prefer the stochastic tile sets introduced by Cohen et al. [9] because these sets perform better in terms of suppressing periodic artefacts [11,13] and are less constrained in their construction. Using the assembly algorithm described next, a sufficient condition for a tile set is that it contains at least one tile for each admissible code combination on the left and top tile edges. Except for this requirement, the number of tiles and code distribution within the set can be chosen arbitrarily, e.g., to control the distribution of individual tile types in the assembled tilings. Individual microstructural samples are generated with a stochastic assembly algorithm that sequentially fills a grid of a predefined size with tile instances from the set. For each position in the grid, the algorithm identifies potential candidate tiles from the set based on the codes of previously placed neighbouring tiles, randomly selects one tile from the candidates, places it, and proceeds to the next grid position. A step of the assembly algorithm is shown in Fig. 1.

From the perspective of Liu and Shapiro [41], who define a model of a material microstructure as a process capable of generating microstructural samples with similar spatial statistics, the Wang tile concept can be seen as a reduced model with spatially local modes (with PUC being a trivial instance with only one mode). Characteristic microstructural features are compressed into the set of tiles in the offline phase, while the geometries of individual microstructural samples are generated almost instantly when required using the stochastic tiling algorithm. Note that, due to random selection during the tiling, repeated runs of the algorithm yield different microstructural realizations. The tile-based representation can thus be advantageously used in, e.g., analyses of the Representative Volume Element (RVE) size [10,12]. The concept can also serve as a microstructural generator for Monte-Carlo-based simulations investigating the influence of microstructural variability on a macroscopic response.

### 3 Extracting characteristic fluctuation fields

The idea of approximating fluctuation fields—see Fig. 2 for an illustration—in microstructural samples generated by means of Wang tiles was first outlined in Novák et al. [48]. Aiming at stress enrichments for Hybrid-Trefftz finite element formulation such as [46], Novák and coworkers proposed extracting tile-wise defined fields from the response of a selected tiling to a prescribed macroscopic strain under periodic boundary conditions. The continuity of traction forces across the corresponding tile edges was incorporated in the objective function during the optimisation-based tile design, resulting in a trade-off between randomness in the system and traction jumps [48].

Here, we present a method for extracting the characteristic fluctuation response of a compressed system in primal variables. Unlike [48], these characteristics follow from an auxiliary problem formulated for the whole tile set. Consequently, they are continuous across the corresponding edges by construction. Moreover, the method is non-intrusively applicable to all existing microstructural compressions. Its only requirement is that the finite element discretizations of individual tile domains $\Omega^T$ are geometrically compatible across the edges with the same code.

We illustrate the method with a scalar, elliptic problem represented by heat conduction governed by

$$- \nabla \cdot (K(x) \cdot \nabla \theta(x)) = 0, \quad \text{(1)}$$

which stems from the Fourier law

$$q(x) = -K(x) \cdot \nabla \theta(x), \quad \forall x \in \Omega, \quad \text{(2)}$$
linking temperature $\theta$ and heat flux $q$ fields in a given domain $\Omega$ via a conductivity tensor $K$, and the conservation of the heat flux (neglecting any heat sources and sinks)

$$\nabla \cdot q(x) = 0. \quad (3)$$

First, we formulate energy functional $\Pi$ for a temperature field $\theta$ defined for the whole tile set $S$ as

$$\Pi(\theta) = \sum_{T \in S} \int_{\Omega_T} \frac{1}{2} \nabla \theta(x) \cdot K(x) \cdot \nabla \theta(x) \, dx. \quad (4)$$

Next, similarly to the ansatz traditionally used in computational homogenization, we assume that a temperature field for each tile $T$ in tile set $S$ can be decomposed, using a Taylor expansion, into a part controlled by the prescribed macroscopic (potentially higher-order) gradients and a fluctuation part caused by the presence of heterogeneities in the microstructure. Restricting ourselves to the second-order Taylor polynomial, we assume the temperature field $\theta(x)$ in the form

$$\theta(x) = G^1 \cdot x + \frac{1}{2} x \cdot G^2 \cdot x + \tilde{\theta}(x), \quad \forall x \in \Omega_T, \forall T \in S, \quad (5)$$

where $G^1 \in \mathbb{R}^2$ and $G^2 \in \mathbb{R}^{2 \times 2}$ are the first- and second-order gradients playing the role of generalized loading and $\tilde{\theta}(x)$ is the fluctuation complement. Consequently, plugging Eq. (5) into Eq. (4) results in the energy functional $\tilde{\Pi}(G^1, G^2, \tilde{\theta})$.

The sought-for characteristic fluctuations, which will be later used as building blocks for microstructure-informed modes $\psi$ in Sect. 4, are obtained as minimizers of the functional $\tilde{\Pi}$ for prescribed $G^1$ and/or $G^2$ over space $\mathcal{U}$ of admissible temperature fields,

$$\tilde{\theta}^{\mathcal{U}}(G^1, G^2) = \arg \min_{\tilde{\theta} \in \mathcal{U}} \tilde{\Pi}(G^1, G^2, \tilde{\theta}). \quad (6)$$

Set $\mathcal{U}$ contains temperature fields that (i) are continuous across the edges with the same code, i.e. the restriction of individual tile-wise fields to an edge of a chosen colour code must be the same for all tiles, and (ii) have zero averaged first- and/or second-order gradients. While the continuity requirement is ensured directly by the construction of the fields, as described in Sect. 3.1 below, the zero averaged gradients are imposed via Lagrange multipliers related to the constraints as discussed in Sect. 3.2.

### 3.1 Enforcing continuity

We solve the auxiliary problem (6) using the Finite Element method. Omitting the explicit dependence on the admissible set $\mathcal{U}$ and the macroscopic gradients $G^1$ and $G^2$ for the sake of brevity, we approximate the unknown fluctuation temperature field $\tilde{\theta}(x)$ within each tile with $n^T_n$ piecewise polynomials $N^T_j(x)$ arising from a finite element discretization such that

$$\tilde{\theta}(x) \approx \sum_{j=1}^{n^T_n} N^T_j(x) u^T_j, \quad \forall x \in \Omega_T, \forall T \in S, \quad (7)$$

where $u^T_j$ denotes the value of $\tilde{\theta}$ at the $j$th node of the discretization of tile $T$.

Following the standard finite element procedures for minimizing the quadratic functional $\tilde{\Pi}$ with respect to fluctuations field $\tilde{\theta}$, we construct a stiffness matrix for each tile independently, and we reorder and split vector $u^T$ containing the unknowns $u^T_j$ into the interior, $u^T_i$, and boundary, $u^T_b$, part, resulting in a set of linear equations for each tile $T$ in the form:

$$\begin{bmatrix} K_{bb}^T & K_{bi}^T \\ K_{ib}^T & K_{ii}^T \end{bmatrix} \begin{bmatrix} u^T_b \\ u^T_i \end{bmatrix} = \begin{bmatrix} f^T_b (G^1, G^2) \\ f^T_i (G^1, G^2) \end{bmatrix}. \quad (8)$$

Note that the force term follows from the gradient of $\tilde{\Pi}$ with vanishing $\tilde{\theta}$. The expressions for the stiffness matrix $K$ and the right-hand side vector $f$ are provided in Appendix A. The interior DOFs are then condensed out for each tile, leaving us with

$$\hat{K}^T u^T_b = \hat{f}^T, \quad (9)$$

where the load vector $\hat{f}^T$ (with dependence on $G^1$ and $G^2$ omitted for brevity) and the effective stiffness matrix $\hat{K}^T$ arise from the Schur complement of $K_{ii}^T$ from the original problem (8) as

$$\begin{align*}
\hat{K}^T &= K_{bb}^T - K_{bi}^T K_{ii}^{-1} K_{ib}^T, \\
\hat{f}^T &= f^T_b - K_{bi}^T K_{ii}^{-1} f^T_i.
\end{align*} \quad (10, 11)$$

To enforce the desired continuity of the solution across individual tiles, the remaining boundary DOFs of each tile $u^T_b$ are renumbered such that the corresponding DOFs at tile edges with the same code share the same number throughout the tile set. Consequently, the boundary DOFs of each tile can be expressed through a Boolean mapping from the vector $u^T$ containing the unique unknowns of the whole tile set,

$$u^T_b = L^T u^T, \quad (12)$$

where $L^T$ with $L^T_{ij} \in \{0,1\}$ is a localization matrix stemming from the unique renumbering.

While uniquely enumerating DOFs that belong exclusively to a tile edge is straightforward, enumerating vertex
DOFs requires an auxiliary analysis of the tile set to identify how many unique DOFs are needed for the vertices. A brief description of this analysis is provided in Appendix B.

Finally, following the mapping from \( u^p \) to \( \tilde{u}^p \), effective stiffness matrices \( \hat{K}^T \) and load vectors \( \hat{f}^T \) of individual tiles are assembled into their set-related counterparts

\[
\hat{K}^S = \sum_{T \in S} L^T \hat{K}^T L^T
\]

and

\[
f^S = \sum_{T \in S} L^T \hat{f}^T ,
\]

forming a system that encodes a collective response of all tiles in the set to a prescribed loading,

\[
\hat{K}^S \tilde{u}^S = f^S .
\]

Note that, without loss of generality, we assume all tile domains as spatially centred, making them virtually stacked one atop another. However, their interaction is facilitated only through the shared DOFs.

### 3.2 Constraints on gradient averages

As already mentioned, continuity of \( \tilde{\theta} \) across the corresponding tile edges is only one condition defining \( \mathcal{U} \); the assembled set problem, Eq. (15), must be further equipped with additional constraints. First, the problem is ill-posed because it contains a zero-energy mode. This can be fixed either by prescribing a value for one DOF or by imposing the average value constraint. For simplicity, we pose these constraints exclusively on the boundary DOFs,

\[
\int_{\partial \Omega^S} \tilde{\theta} \, ds = 0 ,
\]

where \( \partial \Omega^S = \bigcup_{T \in S} \partial \Omega^T \).

Second, additional constraints are needed to prevent the fluctuation field from compensating for the prescribed loading. This corresponds to prescribing suitable boundary conditions for the microscale problem in the computational homogenization, e.g. [22].

In standard first-order computational homogenization, the fluctuation field \( \tilde{\theta} \) is required to satisfy

\[
\int_{\Omega} \nabla \tilde{\theta} \, dx = \int_{\partial \Omega} \tilde{\theta} n \, ds = 0 ,
\]

where \( n \) denotes the outer normal to the RVE domain boundary \( \partial \Omega \). This is typically ensured either with the uniform Dirichlet, periodic, or uniform Neumann type of boundary conditions. Albeit the particular selection is a modelling choice, periodic boundary conditions are the most frequently chosen since their effective properties converge the most quickly with respect to the RVE size, e.g. [29].

Loosely inspired, we implement the following three options in which we

(i) set all fluctuation DOFs to zero at the tile boundaries,

\[
\tilde{\theta}|_{\partial \Omega^T} = 0 , \quad \forall T \in S ;
\]

(ii) enforce vanishing gradient of the fluctuation field tile-wise,

\[
\int_{\partial \Omega^T} \tilde{\theta} n \, ds = 0 , \quad \forall T \in S ;
\]

(iii) require zero gradient of \( \tilde{\theta} \) within the tile set on average,

\[
\int_{\partial \Omega^S} \tilde{\theta} n \, ds = 0 .
\]

Treating second-order fluctuations is a more involved process. Since we assume the classical first-order constitutive and conservation equations and we want to pose the extraction of characteristic modes as a boundary value problem, we cannot straightforwardly enforce a direct analogue of Eq. (17) for the second-order gradient. Addressing this limitation in the finite strain setting, Kouznetsova et al. [34,35] derived a constraint on the fluctuation part of the solution that ensures the equality between the prescribed second-order gradient and its average over a Periodic Unit Cell, see [34, Appendix A]. Adapted to the illustrative problem of heat conduction, Kouznetsova et al.’s condition reads

\[
\int_{\partial \Omega} \tilde{\theta} (x \otimes n + n \otimes x) \, ds = 0 ,
\]

where \( \otimes \) denotes the vector outer product defined in the index notation as \( (n \otimes x)_{ij} = n_i x_j \).

Similarly to the previous paragraph, constraint (21) can be ensured

(i) point-wise (leading to the same constraints as in Eq. (18)),

(ii) tile-wise

\[
\int_{\partial \Omega^T} \tilde{\theta} (x \otimes n + n \otimes x) \, ds = 0 , \quad \forall T \in S ,
\]

(iii) set-wise

\[
\int_{\partial \Omega^S} \tilde{\theta} (x \otimes n + n \otimes x) \, ds = 0 .
\]
Note that, unlike the finite strain problem in [34, Appendix A], the second order gradient for the scalar problem is by definition symmetric. Hence, conditions (22) and (23) constitute only three constraints for a two-dimensional scalar problem.

All constraints introduced above are linear in the fluctuation field \( \vec{\theta} \) and depend only on the values of \( \vec{\theta} \) at the tile boundaries. Therefore, within the finite-element implementation, they can be recast to the form

\[
\mathbf{C} \mathbf{u}^S = 0, \quad \text{with} \quad \mathbf{C} = \begin{bmatrix} \mathbf{C}_0 \\ \mathbf{C}_I \\ \mathbf{C}_II \end{bmatrix},
\]

where \( \mathbf{C}_0, \mathbf{C}_I, \) and \( \mathbf{C}_II \) are related to the elimination of the zero-energy mode, and enforcing first- and second-order gradients, respectively. Details are provided in Appendix C.

However, depending on the particular constraint choice and the distribution of edge codes with the tile set, matrix \( \mathbf{C} \) can be rank-deficient. This deficiency arises in several situations. For instance, a tile with periodic codes (i.e. the same codes on the opposite edges) automatically satisfies Eq. (19). In a similar manner, a tile set with an equal occurrence of individual codes on opposite edges yields trivial \( \mathbf{C}_I \) for Eq. (20).

In principle, it is possible to list all such situations and handle them during the assembly of matrix \( \mathbf{C} \). Yet, to avoid an involved analysis of codes in a tile set and complicated assembly, we perform the singular value decomposition of the rank-deficient matrix \( \mathbf{C} \) and replace it with \( \hat{\mathbf{C}} \) containing the right-singular vectors related to non-zero singular values as its rows.

With the final form \( \hat{\mathbf{C}} \mathbf{u}^S = 0 \), the constrained minimization (6) over \( \mathcal{U} \) is ultimately reformulated as an unconstrained saddle-point problem using the standard approach of Lagrange multipliers; see e.g. [64, Section 3.5] for their application in the computational homogenization context. As a result of this procedure, Eq. (15) transforms into

\[
\begin{bmatrix} \mathbf{K}^S & \hat{\mathbf{C}}^T_i \\ \hat{\mathbf{C}}_i & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u}^S \\ \hat{\mathbf{C}}^T \end{bmatrix} = \begin{bmatrix} \mathbf{f}^S \\ 0 \end{bmatrix}.
\]

Once the solution \( \mathbf{u}^S \) is found, the remaining interior DOFs in each tile \( T \) follow from back substitution\(^1\) in Eq. (8),

\[
\mathbf{u}_i^T = \mathbf{K}_ii^{-1} \left( \mathbf{f}_i^T - \hat{\mathbf{C}}_i^T \mathbf{u}^T_b \right).
\]

Notice that the added Lagrange multipliers do not directly appear in the expression above because the related constraints concern only the boundary DOFs.

\(^1\) In the case of zero fluctuations prescribed at tile boundaries, i.e. Eq. (18), the above described treatment is only formal. In practice, solving Eq. (25) is skipped, and only the interior DOFs are sought for because no information is effectively communicated across individual tiles.

### 3.3 Field options

In the illustrative linear two-dimensional problem, five basic macroscopic loading cases suffice, consecutively prescribing a unit value to the individual components of the first-, \( \mathbf{G}^1 \), and second-order, \( \mathbf{G}^2 \), macroscopic gradients, respectively. Each load case is further complemented with one of the constraint options mentioned above. Unlike computational homogenization, where a particular type of boundary conditions is assumed a priori, we combine the characteristic responses of the compressed system extracted for different constraint options to enrich the basis of the fluctuation approximation space. While this approach allows for a range of combinations regarding which gradients are prescribed and restricted, we consider only three choices for the rest of the paper, labelled 1st, 1st \( \lor \) 2nd, and 1st \( \land \) 2nd, respectively.

The first choice, labelled 1st, denotes the fluctuation fields extracted by prescribing and constraining only the first-order macroscopic gradient, i.e. \( \mathbf{G}^2 = \mathbf{0} \) and only the constraints (18)–(20) are considered (\( \mathbf{C}_{II} \) is not present in Eq. (24)). An example of the resulting fluctuation field obtained for \( \mathbf{G}^1 \) prescribed in the form \( \mathbf{G}^1 = [1.0 \ 0.0]^T \) while enforcing the zero average gradient per each tile, i.e. Eq. (19), is shown in Fig. 3. Note the same profile of the fluctuation field at the edges of the same colour and orientation stemming from the by-construction enforced continuity.

The second choice, labelled 1st \( \lor \) 2nd, stands for the case where the first and second-order macroscopic gradients were prescribed independently, i.e. extending the set of fields from the previous choice with additional ones obtained similarly by setting \( \mathbf{G}^1 = \mathbf{0} \) and prescribing only the second-order gradient along with constraints (18), (22), or (23), i.e. omitting \( \mathbf{C}_I \) in Eq. (24) for the additional fields.

Finally, the last choice, labelled 1st \( \land \) 2nd, corresponds to the setup in which both gradients are prescribed simultaneously and constraints of the same type related to the first- and second-order gradients are imposed, i.e. the first constraint option is rendered by Eq. (18) (which ensures both Eqs. (17) and (21) at the same time), the second includes Eqs. (19) and (22), and finally the last uses Eqs. (20) and (23).

The first choice thus results in six fluctuation fields (arising from two unit loading cases with non-zero entries \( G_{11}^1 = 1 \) and \( G_{22}^1 = 1 \), respectively, combined with three constraint options), while the latter two yield 15 fluctuation fields each (the previous two unit loading cases for the first-order gradient and three unit load cases with non-zero entries \( G_{11}^2 = 1, \ G_{22}^2 = 1, \) and \( G_{12}^2 = G_{21}^2 = 1 \), respectively, for the symmetric second-order macroscopic gradient combined again with three constraint options).
Fig. 3 An example of a tile-wise defined fluctuation field $\tilde{\theta}(G^1, G^2)$ obtained for $G^1 = \begin{bmatrix} 1.0 & 0.0 \end{bmatrix}^T$ and $G^2 = 0$ and $U$ corresponding to boundary conditions (19).

Fig. 4 Illustration of a global approximation $\psi(x)$ assembled from the tile-wise defined fluctuation field, b a standard macroscopic shape function $N(x)$ used as a Partition of Unity function in the Generalized Finite Element Method, and c the final microstructure-informed reduced mode $N(x)\psi(x)$.

4 Macroscopic numerical scheme

From the procedure outlined in the previous section, the tile set carries a collection of tile-wise defined fields $\tilde{\theta}$ with the a priori enforced continuity. Using the same assembly procedure that is used to generate a stochastic microstructural geometry of a macroscopic domain from the Wang tiles, the characteristics fluctuation fields $\tilde{\theta}$ can be assembled into continuous approximation basis functions $\psi_i$ spanning the macroscopic domain $\Omega$, using the same procedure as in generating microstructural geometry in order to define a set of continuous approximation basis functions $\psi_i$ in the macroscopic domain $\Omega$; see Fig. 4a. Note that the precomputed characteristic fields are universal in the sense that they are not extracted with respect to a particular macroscopic geometry, arrangement of tiles in $\Omega$, or loading; hence, the assembled $\psi_i$ approximates the microstructural response to a constant or linear macroscopic gradient. However, the general macroscopic problem (with arbitrary geometry and loading) usually does not yield a uniform macroscopic gradient in the domain.

Thus, the macroscopic numerical scheme must be able to locally interpolate between individual $\psi_i$ basis functions.

To facilitate such an interpolation, we resort to the Generalized Finite Element Method (GFEM) strategy [6,19,58]. We assume two levels of finite element discretization for the macroscopic problem. The first level comprises the fine discretization that comes directly from the tile-wise discretization already used to pre-compute the tile characteristic fluctuation fields. Recall that the individual tile discretizations must be geometrically and topologically compatible for the strategy outlined in Sect. 3 to work. Hence, these discretizations can be assembled along with the microstructural geometry, yielding $n^f$ shape functions $N_i^f$ defining a finite element approximation space $\mathcal{U}^f = \text{span}\{N_i^f\}$, in which $\psi_i$’s are defined, i.e. $\text{span}\{\psi_i\} \subset \mathcal{U}^f$.

The second level contains a coarse discretization of the macroscopic domain $\Omega$ that does not resolve microstructural features. With $n^c$ shape functions $N_i^c(x)$, it serves two purposes: (i) the related approximation space $\mathcal{U}^c$, $\mathcal{U}^c = \text{span}\{N_i^c\}$, captures the homogeneous part of the solution.
(recall that \( \psi_i \) approximate only fluctuations caused by material heterogeneity), and (ii) the shape functions form a Partition of Unity basis for interpolating between individual \( \psi_i \)'s.

Following the GFEM ansatz, we seek a solution to a macroscopic problem in the form

\[
\theta(x) = \sum_{i=1}^{n_f} N_{i}^f(x) a_i^0 + \sum_{i=1}^{n_f} \sum_{j=1}^{n'} N_{i}^f(x) \psi_j(x) a_j^f = \sum_{i=1}^{n_f} \sum_{j=0}^{n'} N_{i}^f(x) \psi_j(x) a_j^f, \quad x \in \Omega ,
\]

where \( n' \) denotes the number of provided fluctuation fields and \( \psi_0 \) is artificially defined as a constant unit function. Fig. 4 shows an illustration of a particular \( \psi_i \) field and a \( N_j^i \) shape function along with their final product serving as a basis function in our numerical scheme.

While we use the GFEM ansatz to construct the basis functions, we build the final numerical scheme upon the reduced order modelling ideas. We benefit from the availability of the fine discretization of the macroscopic domain; plugging the fine discretization in the form

\[
\theta(x) = \sum_{i=1}^{n_f} N_{i}^f(x) u_i^f, \quad x \in \Omega ,
\]

into the weak form of Eq. (1) yields the standard, fine-scale system of linear equations

\[
\mathbf{K}^f \mathbf{u}^f = \mathbf{f}^f.
\]

However, instead of solving Eq. (29), we project the basis functions from Eq. (27) on the space \( \mathcal{U}^f \) and approximate \( \mathbf{u}^f \) as

\[
\mathbf{u}^f \approx \mathbf{\Phi} \mathbf{a} ,
\]

where the matrix \( \mathbf{\Phi} \in \mathbb{R}^{n_f \times n_f (n_f + 1)} \) collects as its columns the individual products \( N_{i}^f(x) \psi_j(x) \) projected onto \( \mathcal{U}^f \), and vector \( \mathbf{a} \) contains the related \( a_j^f \) DOFs. The final reduced system to solve thus follows from the Galerkin projection common in Reduced Order Modelling,

\[
\mathbf{\Phi}^T \mathbf{K}^f \mathbf{\Phi} \mathbf{a} = \mathbf{\Phi}^T \mathbf{f}^f .
\]

Note that the projection and adoption of the ROM approach bypasses the need for a special quadrature rule that would have be otherwise needed in GFEM to accurately integrate functions that vary rapidly over elements of the coarse discretization.

Regarding the imposition of essential boundary conditions at the macroscale, we exclude the prescribed DOFs by removing the corresponding rows from \( \mathbf{\Phi} \). Their presence is then indirectly imposed by the action of relevant elements. Consequently, the unknown \( a_j^f \)'s corresponding to macroscopic elements influenced by the prescribed values are not set to zero by construction.

Note also that the projection strategy enables trivial switching to fully resolved microstructural details in parts of the macroscopic domain when desired, see Sect. 5.2.1.

## 5 Numerical examples

For the numerical examples in this section, we used the two-dimensional set of 16 Wang tiles depicted in Fig. 1. The geometry of each tile was discretized using linear triangular elements. On average, each tile contained approximately 25,500 DOFs and 50,500 elements that were refined along the inclusion boundaries.

Both material phases (depicted in light and dark grey) were considered as linear isotropic with conductivities \( \mathbf{K} = 10\mathbf{I} \) for the matrix phase and \( \mathbf{K} = 100\mathbf{I} \) for the inclusion phase, respectively, where \( \mathbf{I} \) denotes the second-order identity tensor.

Please note that a general discussion of the results is deferred to Sect. 6.

### 5.1 Uniformly loaded square sample

As the first example, we considered a simple square domain composed of five tiles in each direction with the size of the domain scaled to unity. The domain was loaded with a uniform macroscopic gradient \([0.6 \ 0.3]^T\) with boundary conditions similar to the standard first-order computational homogenization: periodic and Dirichlet ones; see Fig. 5 for an example of the resulting field \( \theta \) for the periodic boundary conditions.

#### 5.1.1 Set of a single Periodic Unit Cell

As a sanity check, we first tested the proposed framework with a trivial case of a Wang tile set—a Periodic Unit Cell. The self-compatible tile 16 from the set shown in Fig. 1 was chosen as the PUC and the microstructure-informed modes were recomputed considering only this tile. Note that in the particular case of PUC, the tile-wise and set-wise constraints coincide and thus only one has to be considered in order to avoid ill-posedness of the reduced problem.

As expected, due to the linearity of the problem, the proposed reduced numerical scheme (ROM) yields exactly the same results as the Direct Numerical Simulation (DNS).
even for a very coarse macroscopic discretization containing two elements, when the periodic boundary conditions are assumed; see Fig. 6a for an illustration of the discretization. Moreover, only the fluctuation modes extracted under the periodic constraints and the first order macroscopic gradient, Eq. (19), are sufficient in this case.

However, the same conclusions do not hold when a domain with the same periodically repeating microstructure is subjected to the macroscopic gradient under Dirichlet boundary conditions. In such a case, the numerical scheme only approximates the reference solution. Figure 6a illustrates the discrepancy between DNS and ROM solutions with the coarsest macroscopic discretization (which was sufficient for the previous loading) and only the modes extracted under periodic constraints. Enriching the approximation space with fluctuation fields obtained under the Dirichlet-type constraints reduces the error at the domain boundary, because the precomputed fluctuation fields now also include the situation with zero fluctuations on the boundary, and consequently localizes the solution discrepancy predominantly to the tile edges within the domain; see Fig. 6b. In particular, the largest discrepancies are observed in the first layer along the boundary, because the further from the boundary, the less pronounced the effect of the Dirichlet boundary conditions is and the closer the tiles are to the uniform periodic case. The local difference both in its magnitude and localization can be further improved by refining the macroscopic discretization; note that the local discrepancy dropped by an order of magnitude in Fig. 6c compared to the previous Fig. 6a and b.

In addition to the local discrepancy, we quantify the error of ROM solution using (i) a relative $L_2$-norm of the results difference,

$$
\epsilon_{L_2} = \frac{\|\theta^{\text{DNS}} - \theta^{\text{ROM}}\|_{L_2}}{\|\theta^{\text{DNS}}\|_{L_2}},
$$

where

$$
\|\theta\|_{L_2} = \left(\int_{\Omega} \theta(x)^2 \, dx\right)^{1/2},
$$

and (ii) a relative error in energy,

$$
\epsilon_E = \frac{|E^{\text{DNS}} - E^{\text{ROM}}|}{E^{\text{DNS}}},
$$

with

$$
E^* = \int_{\Omega} \frac{1}{2} \nabla \theta^*(x) \cdot K(x) \cdot \nabla \theta^*(x) \, dx.
$$

Fig. 5 The resulting temperature field $\theta$ from a Direct Numerical Simulation (DNS) of a square domain with a microstructure assembled from $5 \times 5$ tiles and subjected to a macroscopic temperature gradient $\begin{bmatrix} 0.6 & 0.3 \end{bmatrix}$ under periodic boundary conditions.

Fig. 6 The magnitude of discrepancy between the direct numerical simulation and the result of the proposed reduced scheme for a square domain with periodic microstructure: a two-element coarse discretization a with only selected fluctuation fields obtained under the periodic constraint Eq. (19) and b with all fluctuation fields labelled 1st, and c a refined discretization with all fluctuation fields considered. Edges of the macroscopic discretization are plotted in the light grey colour.
Fig. 7 Evolution of the relative $L_2$-norm error ($\epsilon_{L_2}$) and the relative error in energies ($\epsilon_E$) with a uniform refinement of the macroscopic discretization for the simple square domain with a periodically repeating microstructure under Dirichlet boundary conditions and b a microstructure assembled from the set of 16 tiles under both periodic and Dirichlet boundary conditions. The average and the standard deviation of results obtained for 50 different realizations are plotted in (b). Data labels correspond to the different choices of fluctuation fields: 1st denotes the fields extracted by prescribing only the first-order macroscopic gradient; 1st $\lor$ 2nd and 1st $\land$ 2nd stand for the cases in which the first and second-order macroscopic gradients were prescribed independently or simultaneously, respectively. Additionally, a case in which no fluctuation fields are considered (labelled w/o) is plotted for comparison.

Figure 7a illustrates the evolution of these errors with a uniform refinement of the macroscale discretization. The results are shown for three choices of fluctuation fields: 1st, 1st $\lor$ 2nd, and 1st $\land$ 2nd; recall their definition in Sect. 3.3. In addition, the results for a case when no fluctuation fields are assumed is also plotted (labelled as w/o) to highlight the influence of fluctuation fields on the errors.

5.1.2 Set of 16 tiles

Finally, the same analysis is repeated for a domain with a microstructure assembled from the full tile set instead of a single PUC. The global errors shown in Fig. 7b were obtained as an average over 50 stochastic realizations, i.e. 50 different microstructural geometries obtained from the fixed set of Wang tiles shown in Fig. 1 by running 50 times the tiling algorithm introduced in Sect. 2. Results for both the periodic and Dirichlet boundary conditions and different fluctuation field choices are reported. For the sake of brevity, we omit the 1st $\land$ 2nd fluctuation field choice in Fig. 7b because its results were very close to those of 1st $\lor$ 2nd. Similarly to Fig. 7a, the errors improve with refining the coarse discretization (increasing the ratio between the number of unknowns in our reduced scheme compared to DNS).
Fig. 8 Illustration of L-shape domain problem. Values \( \hat{\theta} \) are prescribed at the grey-shaded edges. The red dashed line (with the parametrization coordinate \( p \)) indicates a cross-section along which the local error profile was extracted. The triangulation depicts the initial coarse discretization for the macroscopic problem. Scaling the length of the domain arms for unity, several analyses with varying number of tiles, denoted by \( s \), are considered and inclusion of more types of fluctuation fields (compare solid and dashed lines). The graphs also attest to the importance of the microstructure-informed modes in reducing the errors, because no significant improvement is achieved with progressive refining of the coarse discretization without them (compare the dotted line against the remaining lines).

5.2 L-shape domain

As the second example, we chose an L-shaped domain with values \( \hat{\theta}_b = 0 \) and \( \hat{\theta}_r = 5 \) prescribed at the bottom (AB) and right (ED) edge of the domain, respectively; see the illustration in Fig. 8. The domain was scaled such that its both ends had a unit length; however, the number of tiles along each edge—denoted as \( s \)—varied, giving a notion of scale separation of the problem. This time, only the non-periodic microstructures assembled with Wang tilings were investigated. Figure 8 also introduces a relative parametrization coordinate \( p \), which will be later used for a comparison of the local profile of the solution in Fig. 10.

Similarly to the previous section, we ran 10 realizations for \( s \in \{5, 10, 15, 20\} \) with four sequential refinements and different fluctuation field choices, and we recorded the global errors \( \epsilon_{L2} \) and \( \epsilon_E \); see Fig. 9. Similarly to the results in Fig. 7b, only the 1st and 1st \( \lor \) 2nd fluctuation field choices are eventually shown, because the results of 1st \( \lor \) 2nd and 1st \( \land \) 2nd were almost identical. Again, there is a threshold beyond which considering more characteristic fluctuation fields (dashed line) outperforms the refinement of the coarse discretization (solid lines) in terms of the number of DOFs of our reduced scheme. The positive effect of including additional characteristic fields is more pronounced in problems with weak separation of microstructural and problem scale, i.e., problems with lower \( s \), in which each tile experiences a less uniform strain field.

Figure 10 illustrates the point-wise convergence for one microstructure realization for \( s = 5 \) with a solution profile along the cross-section depicted in Fig. 8. While the initial coarse discretization renders a system response that is too stiff, the first refinement already significantly improves the...
local profile of the solution and the discrepancy almost vanishes after the second refinement; see how the colour lines converge to the grey thick one pointwise. The cross-section was chosen such that it cuts through the centres of tiles. However, similar trends were also observed in the cross-section coinciding with the tile edges (not shown for brevity).

5.2.1 Local refinement

As mentioned in the previous section, adopting the viewpoint of Reduced Order Modelling with GFEM as a mean of constructing the final reduced modes allows for straightforward switching to a discretization resolving all microstructural details in selected regions. As an illustration, Fig. 11a depicts a solution to the L-shape problem for one realization with \( s = 3 \). The plot of local differences, Fig. 11b, reveals that the largest local errors are expectedly concentrated around the re-entrant corner, where the microstructure experiences highly non-uniform loading.

Thus, a region containing 3 tiles around the corner was marked for local refinement and the analysis was repeated. Local errors of this refined model are shown in Fig. 11c. Clearly, almost all discrepancies in the refined region vanished, also effecting the adjacent regions. Global errors were consequently reduced from \( 2.654 \times 10^{-3} \) to \( 1.393 \times 10^{-3} \) for \( \epsilon_{L2} \), and from \( 1.055 \times 10^{-2} \) to \( 5.712 \times 10^{-3} \) for \( \epsilon_E \), respectively. Note that, given the small separation of scales (only 27 tile domains were present in the domain altogether), the local refinement leads to a significant increase in unknowns from 0.14\% to 11.16\% of all DOFs present in the domain.

5.2.2 Comparison against snapshot-based ROM

In order to put the number of necessary modes into the perspective of the classical snapshot-based Reduced Order Modelling strategy, we devise the following test: While keeping the same microstructural geometry as the one shown in Fig. 1, we replace the unstructured finite element discretization with a regular, pixel-based mesh, in which two triangular elements with alternating orientation constitute one pixel. Each tile is then represented with \( 100 \times 100 \) nodes and 19,602 finite elements. Consequently, each microstructural realization features the same discretization and hence solutions of the illustrative L-shape domain example can be straightforwardly stored as a snapshot without the need for a remapping/projection onto a fixed mesh.

We generate 10,000 distinct microstructural realizations for the L-shape domain with \( s = 4 \) and solve the temperature field for each. We then perform Singular Value Decomposition for the matrix containing individual snapshots as its columns; Fig. 12a displays the sorted relative eigenvalue magnitudes. Note the significant drop by almost two orders of magnitude to around \( i = 500 \), which indicates the dimensionality of the snapshot-based ROM basis inherent to the given problem. Next, we replace the GFEM-based microstructure-informed modes arising from Eq. (27) with \( n \) eigenmodes corresponding to \( n \) largest eigenvalues and compute the response of the compressed system for \( n \in \{ 50, 100, 250, 400, 500, 550, 1000 \} \), plotting the global errors \( \epsilon_{L2} \) and \( \epsilon_E \) in Figures 12b and c, respectively. The errors of the snapshot-based ROM are also compared with the scheme proposed in this work applied to the above mentioned discretization. Unsurprisingly, the snapshot-based modes specific for the problem outperform our generic modes, even though our generic modes manage to deliver similar energy error when not all needed modes from the snapshot-based ROM are present. Also note that, while the error uniformly decreases in our scheme (red curves), the drop in eigenvalue magnitudes from Fig. 12a also appears in the global errors \( \epsilon_{L2} \) and \( \epsilon_E \) in Figs. 12a and b.

Finally, keeping the same geometrical setup, we also consider modified loading conditions such that zero temperature is fixed at the inner vertical edge (BC) and \( \theta = 5 \) is prescribed at the top edge (FE). To illustrate the universality of our GFEM-based modes when compared to the standard snapshot-based ROM, we test reusing the snapshot-based modes from the previous loading conditions and report the corresponding errors in Fig. 13. Clearly, the standard snapshot-based modes rendered for different loading conditions carry very little information needed for the analysis, and including more modes does not greatly improve performance. On the other hand, the universal modes generated by our scheme feature almost the same performance as in the previous loading case.

![Fig. 10](image-url) The pointwise convergence of a solution profile taken along the cross-section depicted in Fig. 8 with a dashed red line and parametrized with a relative coordinate \( p \in [0, 1] \). All results are shown for \( s = 5 \). Different line colours correspond to consecutive refinements of the initial macroscopic discretization (the legend also states the ratio between the number of ROM and DNS degrees of freedom).
Fig. 11 An example of a DNS solution for $s = 3$ and the local errors of the reduced scheme without b and with c the microstructure fully resolved in the highlighted region.

Fig. 12 Results of the snapshot-based Reduced Order Modelling (labelled as sROM) scheme described in Sect. 5.2.2 for the L-shape domain example with $s = 4$: a sorted eigenvalues (normalized by the largest eigenvalue) from Singular Value Decomposition of 10,000 collected snapshots, and the relative b $L_2$-norm error $\epsilon_{L_2}$ and c error $\epsilon_E$ in energies computed for 50 unique microstructure realizations both contained in the snapshots (in blue) and not used in the training phase (in green), compared to the proposed microstructure-informed reduced scheme (in red).

Fig. 13 Comparison of the standard snapshot-based Reduced Order Modelling strategy (sROM) and the proposed microstructure-informed reduced scheme (in red) in terms of a $L_2$-norm error $\epsilon_{L_2}$ and b error $\epsilon_E$ in energies computed for 50 unique microstructure realizations with the modified loading conditions. The basis for sROM was computed from the snapshots obtained under the original loading conditions. The blue lines correspond to errors related to microstructural realizations considered during snapshot extraction, while the green lines depict results of realizations not contained in the original training phase.
5.2.3 Time comparison

Even though comparing the wall-clock time is always biased by the implementation, chosen solvers, and the hardware configuration, we provide calculation times of our implementation (limited to the setup described below) for the sake of completeness.

Originally, the whole framework was developed and tested using an in-house MATLAB® implementation. However, similarly to other interpreted languages, MATLAB® is inefficient with low-level raw loops, which should be replaced with a suitable vectorization whenever possible. Unfortunately, the construction of the reduced basis $\Phi$ cannot be efficiently vectorized in MATLAB®. In order to provide a fair comparison, solvers for both DNS and ROM were eventually implemented as C/C++ MEX functions, using Eigen [25] as a C++ library for linear algebra. Moreover, the construction of the stiffness matrix $K$ and the reduced basis $\Phi$ was parallelized using OpenMP interface.

Figure 14 shows the average computational time needed for reduced problems relative to the time needed to solve DNS. The refinement levels correspond to the errors given in Figs. 9 and 10. An iterative solver with preconditioning was employed for DNS while a ROM-related linear system of equations was solved using a direct sparse solver based on the Cholesky decomposition with pivoting.

6 Discussion

Incorporating the pre-computed fluctuation fields as a basis for constructing the microstructure-informed reduced modes enables analyses of models with fully resolved microstructural details with a fraction of degrees of freedom compared to fully detailed models. The comparison against the coarse discretization without enrichments, recall Fig. 7, clearly demonstrates that a similar reduction in unknowns cannot be achieved without modes which efficiently approximate the local character of the solution. Even for the coarsest discretizations with four orders of magnitude fewer DOFs than the fully resolved models, both the relative global errors $\epsilon_{L2}$ and $\epsilon_E$ were already below 3% in all examples.

Higher accuracy can be achieved in two ways: (i) by considering more fluctuation fields when constructing the microstructure-informed reduced modes, recall Eq. (27), or (ii) by refining the coarse discretization of the macroscopic domain. Irrespective of whether a domain is loaded in such a way that it exhibits a constant (Sect. 5.1) or varying (Sect. 5.2) macroscopic gradient, the benefits of refining the discretization while assuming only 1st fluctuation fields prevail only to a certain threshold. With the size of macroscopic elements below the size of a tile, adding the fluctuation fields obtained also for the second-order macroscopic gradient results in fewer errors and a better convergence rate. Interestingly, the convergence rate of $\epsilon_{L2}$ was almost identical for the 1st case in all tested values of $s$, while it exhibited dependence on $s$ in the 1st $\lor$ 2nd case of $\epsilon_{L2}$ and in both cases of $\epsilon_E$.

Except for the simplest example of a uniformly loaded domain with periodic microstructure, we also observed only a minor difference between the fluctuation fields obtained for the first- and second-order macroscopic gradients prescribed separately (1st $\lor$ 2nd) or simultaneously (1st $\land$ 2nd), with the latter option slightly outperforming the former for refined macroscopic discretizations in terms of solution errors.

Local discrepancy between the reduced models and DNS appears in two forms. First, a more uniformly distributed discrepancy arises from an insufficiently coarse macroscopic discretization unable to capture the overall kinematics of the problem, see Fig. 11b. The straightforward remedy here is to refine the discretization. For instance, the local solution profile in Fig. 10 already significantly improves upon the first refinement; the second refinement then yields a solution for the reduced scheme that is almost indistinguishable from DNS.

The second form of discrepancy reflects the underlying microstructure and stems from an inaccurate approximation by the pre-computed fluctuation fields; compare e.g. Figs. 6a and 6b. Taking into account more fluctuation fields improves these local errors. Yet, because the number of fluctuation fields is limited, some errors will always linger (albeit with a

\[ \text{https://www.mathworks.com/help/matlab/call-mex-file-functions.html} \]
diminishing magnitude). These errors localize mainly along tile boundaries, where the effect of the modelling assumptions during the extraction of the fluctuation fields is the most pronounced; see for instance the local discrepancies at tile edges adjacent but parallel to the domain boundary in Fig. 6c.

Finally, the solution of the reduced model can be further enhanced by resorting to the fine, microstructure-resolving discretization in selected parts of the macroscopic domain as demonstrated in Sect. 5.2.1; see also Fig. 11.

Admittedly, the proposed microstructure-informed reduced scheme requires more degrees of freedom than the standard snapshot-based ROM, recall Sect. 5.2.2 and Fig. 12. The reported reduction in degrees of freedom thus may seem unsatisfactory given the fact that we are dealing with a linear, scalar problem. However, as follows from Fig. 13, any significant change in macroscopic loading necessitates recalculation of the basis for the standard ROM. Results from Sect. 5.2.2 show that problems with fully resolved stochastic microstructures are inherently high dimensional, despite the linearity of the considered constitutive material law. Even a very small problem with \( s = 4 \) and a simplified finite element discretization requires \( \approx 500 \) modes for an acceptable accuracy. Thus, even in the most favourable case, at least 500 simulations with fully resolved microstructures must be performed in order to extract a relevant basis for the snapshots-based Reduced Order Modelling scheme. Note that for the vertex-based tile set considered throughout this work, the L-shape problem with \( s = 4 \) allows for \( 2^{65} \approx 3 \times 10^{19} \) unique microstructure realizations; however, the drop threshold in the number of required modes seems to be proportional to the number of tile positions multiplied by tile types, i.e. \( 48 \times 16 = 768 \) in this particular case. By contrast, our fluctuation fields are pre-computed only once at the level of tiles and they can be re-used for different macroscopic analyses when transformed into the microstructure-informed reduced modes using the GFEM ansatz.

Following from our tentative comparison, the computational time of our reduced scheme depends on the macroscopic discretization and the size of the original problem. In general, the reduction in computational cost is not directly proportional to the reduction in the number of unknowns. For the coarsest macroscopic mesh, the reduced scheme takes from one half to one fifth of the time needed to solve DNS, with a more favourable comparison holding for larger problems. Time savings upon refinement follow from the interplay between the assembly of the reduced system, including construction of the reduced modes and the subsequent Galerkin projection, and solution of the reduced system of linear equations, which inherits the sparsity pattern of the coarse discretization. Eventually, there is a threshold at which the time saved by solving a smaller system cannot compensate for the time needed to construct the system. Albeit the time comparison is pertinent to the adopted Galerkin projection at the global matrix level, i.e. following exactly Eq. (31), and other implementations are possible, similar observations are a common problem of all reduced order modelling strategies, and additional accelerations such as Hyper-reduction [55] or Discrete Empirical Interpolation Method [8] should be incorporated to further improve their performance.

7 Summary

Corroborating the potential the Wang tiling concept has in modelling heterogeneous materials with stochastic microstructure, we have introduced a numerical scheme which reduces the number of unknowns in macroscopic analyses with underlying microstructural geometry generated from a set of Wang tiles.

Unlike our previous work [47], which approximates stress fields in heterogeneous materials and hence it must be directly incorporated in creating the compressed microstructural representation, we have developed a procedure that extracts primal-unknown fluctuation fields non-intrusively, and can be therefore used with any existing Wang-tile based representation. Inspired by computational homogenization, we extract the characteristic fluctuation fields as collective responses of individual Wang tiles to a parametrized loading, represented in our case with uniform and linear macroscopic gradients.

Since the extracted fields defined at the tile level are by construction continuous across edges with the same code, they can be assembled within a macroscopic domain in the same manner as the microstructural geometry, creating an approximation for the fluctuation part of the solution providing the macroscopic domain is homogeneously loaded. These approximations are finally transformed into a microstructure-informed reduced modes using the Generalized Finite Element Method’s ansatz in order to locally interpolate between individual approximations and thus to adapt to a non-uniform macroscopic loading.

We have illustrated the proposed approach with two numerical examples. Even with a relatively coarse discretization (containing less than 0.01% of the unknowns in the unreduced problem), we were able to achieve less than 3% error in the relative \( L_2 \)-norm and energy difference. We demonstrated that accuracy is further improved by (i) refining the macroscopic discretization and (ii) considering more pre-computed fluctuation fields. Moreover, the proposed numerical scheme allows for a simple transition to a fully-resolved/high-fidelity model in regions of interest.

Admittedly, compared to the traditional, snapshot-based Reduced Order Modelling scheme, our approach requires more modes for comparable accuracy. This stems from the fact that, unlike the standard applications where the modes are obtained from very similar macroscopic problems, our
modes are pre-computed without any information about the macroscopic geometry or loading. However, we have demonstrated that problems with a fully resolved stochastic microstructure inherently possess a high dimensional solution manifold and, consequently, a high number of training problems must be solved in order to extract an accurate basis when the loading changes significantly. Conversely, our pre-computed fields are universal and can be used in various macroscopic analyses.

Even though the proposed methodology for extracting the characteristic responses and reusing them in macroscopic analyses was illustrated with the simplest case of a two-dimensional, scalar problem, it can be straightforwardly applied to elasticity and/or three-dimensional applications as well. Except for swapping the scalar elliptic governing equation (1) with its mechanical counterpart when appropriate, this only requires replacing the particular form of constraints (Eqs. (18)–(23)) with a form related to a chosen problem and/or considering the corresponding unit load cases.

In principle, the same procedure can be also used for a non-linear material response. In such a case, the extraction of fluctuation fields for the unit load cases is insufficient. Instead, the space of the parametrized macroscopic loading during the extraction must be carefully explored, e.g. [23], and the pre-computed fields stored and post-processed using, for instance, the Proper Orthogonal Decomposition approach [31]. However, the applicability of such an approach depends on the number of resulting fields, since too many fields needed to capture the characteristic fluctuations in microstructural response render the reduced model inefficient. Covering material non-linearities within the proposed framework constitutes the next step in our research.

Related to the non-linearities is also a question of numerical efficiency. Similarly to other reduced order modelling schemes, reducing the number of unknowns in our strategy does not translate directly to the same reduction in computational times, which is critical in non-linear problems. As a remedy, Hyper-reduction [55], the Discrete Empirical Interpolation Method [8], and many other methods have been developed to approximate the Galerkin projection in Eq. (31) with only a subset of unknowns/quadrature points; see e.g. a brief overview in [21]. Our preliminary tests with Hyper-reduction indicate that modifications of these methods are necessary for our microstructure-informed modes, because these methods have been developed primarily for modes with global support. However, due to the GFEM-based construction, our modes have a local support inherited from the macroscopic discretization. Consequently, the standard strategies for choosing the suitable subset of unknowns do not work in our case. Therefore, open questions to be investigated include efficient implementation and the right choice and modifications of the acceleration methods.

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Declarations

Conflict of interest The authors declare that they have no conflict of interest.

A Expressions for stiffness matrix and load vector

Assuming the standard Finite Element approximation of the solution in the form of a piecewise polynomial, recall Eq. (7), individual entries of the stiffness matrix $K^T$, which corresponds to the Hessian of $\tilde{\Pi} \left( G^1, G^2, \hat{\theta} \right)$ with fixed $G^1$ and $G^2$, follow from the standard expression

$$K^T_{mn} = \int_{\Omega_T} \nabla N^T_m(x) \cdot K(x) \cdot \nabla N^T_n \, dx \, .$$

(36)

Analogously, components of load vector $f^T \left( G^1, G^2 \right)$ from Eq. (8) are obtained by plugging the assumed solution (5) into the stationary conditions of $\tilde{\Pi} \left( G^1, G^2, \hat{\theta} \right)$ with respect to the sought-for coefficients $\mu^T_m$

$$f^T_m \left( G^1, G^2 \right) = -\int_{\Omega_T} \nabla N^T_m(x) \cdot K(x) \cdot (G^1 + G^2 \cdot x) \, dx \, .$$

(37)

The integrals are computed element-wise, using the Gauss numerical quadrature rule and the standard finite element procedures [68].

B Unique vertex numbering

To generate fluctuation fields that are by construction continuous, boundary degrees of freedom (DOFs) must be enumerated consistently, i.e. corresponding nodes at the edges with the same code within different tiles should be assigned the same number. While the enumeration is straightforward for edge-related DOFs, it does not hold for vertex DOFs. Assigning the same number to all vertex DOFs is not always correct because—depending on the code distribution within the set—it may happen that certain vertices will never coincide during the tile assembly, thus there might be sepa-
rate vertex group with distinct DOFs. This typically happens for tile sets derived from the vertex-defined Wang tiles [37].

Inspired by the pragmatic question of where to copy a particle that intersects more than one edge during microstructural generation [13], we devised an algorithm that is capable of identifying the separate vertex groups. First, we construct an undirected graph from the provided tile set definition such that (i) each node of the graph corresponds to one half of each tile and (ii) arcs between the graph nodes are obtained from the individual vertices of each tile.

Next, using the Depth-First Search algorithm [56, Section 18.2], we identify the connected components of the graph. If several sub-graphs are identified, the arcs corresponding to this group yield vertices that belong to a distinct group and only these should be assigned the same number. For more details, including illustrations for several tile sets, readers are referred to [13, Section 2.3].

C Discrete form of constraints

For completeness, implementation details of the individual constraint matrices from Eq. (24) are provided next. We assume the standard isoparametric finite elements [68]. The boundary of each domain is consistently discretized by restricting planar finite element discretization to the tiles’ boundary, e.g. domain discretization by linear triangles yields linear line elements along individual edge elements is constant, which simplifies the following expressions.

First, the average value of \( \bar{\theta} \) along all boundaries of all tiles, appearing in Eq. (16), is obtained through

\[
\int_{\partial\Omega^S} \bar{\theta} \, ds = \sum_{T \in S} \int_{\partial\Omega^T} \bar{\theta} \, ds \\
\approx \sum_{T \in S} \sum_{\tilde{e}} \int_{\Omega^\tilde{e},T} \tilde{\Phi}(x) \bar{\theta}, \tilde{e},T \, dx \\
= \sum_{T \in S} \left( \sum_{\tilde{e}} \int_{\Omega^\tilde{e},T} \tilde{\Phi}(x) \, dx \, L_{\bar{\theta}},T \right) u_{\bar{\theta}}^T \\
= \left\{ \sum_{T \in S} \left( \sum_{\tilde{e}} \left[ \tilde{\Phi}^T, \tilde{e},T \right] L_{\bar{\theta}} \right) u_{\bar{\theta}}^T \right\} \tilde{e}, \tag{38} \]

where \( \tilde{\Phi} \) is a row vector of shape functions pertinent to the vertices of element \( \tilde{e} \), \( \left[ \tilde{\Phi}^T, \tilde{e}, \right] \) denotes its integrated counterpart using a suitable quadrature rule, \( L_{\bar{\theta}}^{\tilde{e},T} \) maps boundary DOFs of tile \( T \) onto nodal unknowns of boundary element \( \tilde{e} \) such that \( u_{\bar{\theta}}^{\tilde{e},T} = L_{\tilde{e},T}^T u_{\bar{\theta}}^T \), and \( L_{\tilde{e}}^T \) is the localization matrix introduced in Sect. 3.1.

Proceeding with Eq. (17), the boundary integral related to the average of the first-order gradient of each tile is approximated as

\[
\int_{\partial\Omega^T} \bar{\theta} \, n \, ds \approx \sum_{\tilde{e}} \int_{\Omega^\tilde{e},T} \left[ n_{x}^{\tilde{e}} \bar{N}_\tilde{e}(x) \right] \theta_{x}^{\tilde{e},T} \, dx \\
= \left( \sum_{\tilde{e}} \int_{\Omega^\tilde{e},T} n_{x}^{\tilde{e}} \bar{N}_\tilde{e}(x) \, dx \right) L_{\bar{\theta}}^{\tilde{e},T} u_{\bar{\theta}}^T \tag{39} \\
= \left( \sum_{\tilde{e}} \int_{\Omega^\tilde{e},T} \left[ n_{x}^{\tilde{e}} \bar{N}_\tilde{e} \right] \tilde{e},T \right) L_{\bar{\theta}}^T u_{\bar{\theta}}^S. \\
\]

Depending whether the average first-order gradient is set to vanish for each tile individually, Eq. (19), or for the whole set only, Eq. (20), the corresponding \( C_1 \) takes either the form

\[
C_1 = \begin{bmatrix} \bar{C}_{1I}^T \\
\vdots \\
\bar{C}_{16}^T \end{bmatrix} \tag{40} \\
\]

or

\[
C_1 = \sum_{T \in S} \bar{C}_1^T. \tag{41} \]

Analogously, a similar approximation is used also for the second-order gradient constraints. Note that the second-order gradient is a symmetric \( 2 \times 2 \) tensor; hence, it constitutes only three independent scalar constraints, which we represent with a vector using Voigt notation. Starting with the constraints (21) posed on an individual tile and with \( x = [x, y]^T \), we obtain

\[
\int_{\partial\Omega^T} \bar{\theta} (x \otimes n + n \otimes x) \, ds \\
\approx \sum_{\tilde{e}} \int_{\Omega^\tilde{e},T} \left[ 2n_{x}^{\tilde{e}} x \bar{N}_\tilde{e}(x) \right] \theta_{x}^{\tilde{e},T} \, dx \\
= \left( \sum_{\tilde{e}} \int_{\Omega^\tilde{e},T} \left[ 2n_{x}^{\tilde{e}} x \bar{N}_\tilde{e} \right] \tilde{e},T \right) \bar{\theta}^{\tilde{e},T} u_{\bar{\theta}}^S. \tag{42} \]

with \( [x\bar{N}]_\tilde{e} \) and \( [y\bar{N}]_\tilde{e} \) denoting the corresponding quantities integrated over element \( \tilde{e} \). Again, depending whether the constraint is posed on individual tiles, Eq. (22), or the set as a whole, Eq. (23), the tile constraint matrices \( C_2^S \) are either
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stacked,
\[ C_{II} = \begin{bmatrix} C_{II}^{T_1} \\ \vdots \\ C_{II}^{T_{16}} \end{bmatrix}, \quad (43) \]
or summed,
\[ C_{II} = \sum_{T \in \mathcal{S}} C_{II}^{T}. \quad (44) \]

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