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# ON HASHIN-SHTRIKMAN-WILLIS VARIATIONAL PRINCIPLES FOR RANDOM HETEROGENEOUS LATTICES

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**Summary:** *The purpose of this paper is to establish variational principles for the mechanical behavior of two-phase random elastic lattices. By restricting the attention to the systems characterized by second-order statistics, the variational bounds on the stored energy of the Hashin-Shtrikman-Willis type are established using basic tools of structural statics and linear algebra. Accuracy of the improved bounds is verified against elementary estimates as well as detailed Monte-Carlo simulations. Finally, selected numerical results related to the accuracy of the bounds are presented.*

## 1. Introduction

Discrete material models, representing a material as a network of particles interacting via inter-particle potentials, have received a steadily increasing attention in the fields of theoretical, computational and applied materials science in the last decade, see, e.g., reviews by Alava et al. (2006); Blanc et al. (2007) and references therein. From the engineering point of view, the interest has been nourished by the possibility to address, in a conceptually simple framework, the interplay among the intrinsic material heterogeneity, discreteness and randomness on different levels of resolution.

In the present paper, we address in detail a specific problem related to mechanics of random discrete media, namely the stored energy estimates for finite two-component lattices with a fixed geometry and the heterogeneity distribution characterized in the sense of the second-order spatial statistics. Variational bounds and estimates are established following recent extensions of the classical Hashin-Shtrikman-Willis (HSW) variational principles (Hashin and Shtrikman, 1962; Willis, 1977) to finite-sized random composite bodies due to Luciano and Willis (2005, 2006). Apart from the theoretical interest in application of HSW principles to discrete systems, the major reason for focusing on the global energy instead of local stress- or strain-related quantities is the fact that, when combined with recent advances in variational models of complete damage (Bouchitté et al., 2008; Mielke et al., 2007), it provides an essential ingredient to the

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development of rational *non-local* damage mechanics of discrete lattices to be reported separately. Moreover, the insights obtained when analyzing the discrete case can provide additional impulse to further advances in damage mechanics of continuous media and interfaces.

The rest of the paper is organized as follows. In Section 2., the relevant steps of the problem definition are specified for both deterministic and randomized settings. The energetic bounds and estimates are derived in Section 3. closely following the procedure proposed recently by Luciano and Willis (2005, 2006) for the Finite Element (FE)-discretized HSW principles. In Section 4., results of a pilot numerical study are presented to assess the accuracy and limitation of the bounds. Finally, Section 5. collects concluding remarks and future extensions of the method.

## 2. Problem setup

The current Section is devoted to the problem statement, starting with a brief summary of structural statics followed by specification of the stochastic framework and quantities of interest. The standard notation and results of linear algebra are employed (Horn and Johnson, 1990), with $a$ and $\boldsymbol{a}$ and $\boldsymbol{A}$ denoting a scalar quantity, a vector (colum matrix) and a generic matrix, respectively. Moreover, the matrix formalism developed in Jirásek and Bažant (2001) for general discrete structures is systematically adopted.

### 2.1. Overview of discrete media mechanics

Consider a discrete structure consisting of $N_n$ nodes with coordinates $\boldsymbol{x}_i \in \mathbb{R}^d$, $i = \{1, 2, \ldots, N_n\}$ and $d \in \{2, 3\}$ connected with $N_e$ discrete elements. On the level of a single element $e \in \{1, 2, \ldots, N_e\}$, the generalized kinematic equations assume the form

$$\boldsymbol{e}_e = \boldsymbol{B}_e \boldsymbol{d}_e, \tag{1}$$

where $\boldsymbol{e}_e \in \mathbb{R}^{N_s}$ is the vector of generalized strains, vector $\boldsymbol{d}_e \in \mathbb{R}^{2N_d}$ stores the $N_d$ generalized displacements at both element nodes and $\boldsymbol{B}_e \in \mathbb{R}^{N_s \times 2N_d}$ denotes the element kinematic matrix. The corresponding generalized element stresses $\boldsymbol{s}_e \in \mathbb{R}^{N_s}$ then follow from

$$\boldsymbol{s}_e = \boldsymbol{D}_e \boldsymbol{e}_e \tag{2}$$

with $\boldsymbol{D}_e \in \mathbb{R}^{N_s \times N_s}$ denoting a positive definite matrix of generalized material stiffness. On the structural level, the relations (1) and (2) attain the form

$$\boldsymbol{e} = \boldsymbol{B}\boldsymbol{d}, \qquad \boldsymbol{s} = \boldsymbol{D}\boldsymbol{e},$$

where, e.g., $\boldsymbol{B} \in \mathbb{R}^{N_e N_s \times N_n N_d}$ and $\boldsymbol{d} \in \mathbb{R}^{N_n N_d}$ stand for the global kinematic matrix and displacement vector defined as

$$\boldsymbol{B} = \mathop{\mathsf{A}}_{e=1}^{N_e} \boldsymbol{B}_e, \qquad \boldsymbol{d} = \mathop{\mathsf{A}}_{e=1}^{N_e} \boldsymbol{d}_e, \tag{3}$$

with the symbol $\mathsf{A}$ representing the assembly operation, cf. (Jirásek and Bažant, 2001).

In order to specify kinematical constraints on the structure, we partition the problem degrees of freedom (DOFs) into two sets

$$\boldsymbol{c} \cup \boldsymbol{u} = \{1, 2, \ldots, N_n N_d\}, \quad \boldsymbol{c} \cap \boldsymbol{u} = \emptyset, \quad \ker({}^{:\boldsymbol{u}}\boldsymbol{B}) = \{\boldsymbol{0}\}, \tag{4}$$

where $\boldsymbol{c}$ and $\boldsymbol{u}$ collects the known (constrained) and unknown DOFs, respectively, and the last condition in Eq. (4) enforces the elimination of rigid-body modes. When subjecting the structure to an additional nodal load ${}^{\boldsymbol{u}}\boldsymbol{f} \in \mathbb{R}^{|\boldsymbol{u}|}$ acting on free DOFs, the unknown displacements ${}^{\boldsymbol{u}}\boldsymbol{d}$ can be found by solving an unconstrained quadratic optimization problem

$$ {}^{\boldsymbol{u}}\boldsymbol{d} = \arg \min_{\widehat{\boldsymbol{d}} \in \mathbb{R}^{|\boldsymbol{u}|}} E(\widehat{\boldsymbol{d}}), \tag{5} $$

where the globally stored energy function $E : \mathbb{R}^{|\boldsymbol{u}|} \rightarrow \mathbb{R}$ is provided by

$$ E(\widehat{\boldsymbol{d}}) = \tfrac{1}{2} \begin{bmatrix} \widehat{\boldsymbol{d}}^{\mathsf{T}} & {}^{\boldsymbol{c}}\boldsymbol{d}^{\mathsf{T}} \end{bmatrix} \begin{bmatrix} {}^{\boldsymbol{u}\boldsymbol{u}}\boldsymbol{K} & {}^{\boldsymbol{u}\boldsymbol{c}}\boldsymbol{K} \\ {}^{\boldsymbol{c}\boldsymbol{u}}\boldsymbol{K} & {}^{\boldsymbol{c}\boldsymbol{c}}\boldsymbol{K} \end{bmatrix} \begin{bmatrix} \widehat{\boldsymbol{d}} \\ {}^{\boldsymbol{c}}\boldsymbol{d} \end{bmatrix} - \widehat{\boldsymbol{d}}^{\mathsf{T}\,\boldsymbol{u}}\boldsymbol{f}, \tag{6} $$

with, for example, ${}^{\boldsymbol{u}\boldsymbol{c}}\boldsymbol{K} = {}^{\boldsymbol{u}:}\boldsymbol{B}^{\mathsf{T}}\boldsymbol{D}^{:\boldsymbol{c}}\boldsymbol{B} \in \mathbb{R}^{|\boldsymbol{u}|\times|\boldsymbol{c}|}$ being a corresponding sub-matrix of the global stiffness matrix $\boldsymbol{K} = \boldsymbol{B}^{\mathsf{T}}\boldsymbol{D}\boldsymbol{B}$. The symbol $\arg\min$ appearing in Eq. (5) denotes the minimizer of the objective function verifying

$$ E({}^{\boldsymbol{u}}\boldsymbol{d}) \leq E(\widehat{\boldsymbol{d}}) \quad \forall \widehat{\boldsymbol{d}} \in \mathbb{R}^{|\boldsymbol{u}|}, \tag{7} $$

where the equality is attained only for the test displacement $\widehat{\boldsymbol{d}}$ coinciding with the true solution due to positive definiteness of ${}^{\boldsymbol{u}\boldsymbol{u}}\boldsymbol{K}$. The optimality conditions for ${}^{\boldsymbol{u}}\boldsymbol{d}$ then yield the global equilibrium equations in the form

$$ {}^{\boldsymbol{u}\boldsymbol{u}}\boldsymbol{K}\,{}^{\boldsymbol{u}}\boldsymbol{d} = {}^{\boldsymbol{u}}\boldsymbol{f} - {}^{\boldsymbol{u}\boldsymbol{c}}\boldsymbol{K}\,{}^{\boldsymbol{c}}\boldsymbol{d}. \tag{8} $$

### 2.2. Stochastic setting

We now proceed with introduction of a suitable framework for binary random discrete media, i.e. structures in which every element can be found in two distinct states $r \in \{1, 2\}$. Due to the discrete nature of the problem at hand, the ensemble space $\mathbb{S}$ collecting all structural configurations is finite-dimensional and as such can be enumerated using an index $\alpha$,

$$ \alpha \in \mathbb{S} = \left\{1, 2, \ldots, 2^{N_e}\right\}. \tag{9} $$

The complete statistical characterization of the discrete stochastic system is then simply provided by attaching probabilities $\mu(\alpha)$ to individual configurations $\alpha$ stored in the probability distribution vector

$$ \boldsymbol{\mu} \in \Delta = \left\{ \widehat{\boldsymbol{\mu}} \in \mathbb{R}^{|\mathbb{S}|}, \widehat{\mu}(\alpha) \geq 0 \; \forall \alpha \in \mathbb{S}, \sum_{\alpha=1}^{|\mathbb{S}|} \widehat{\mu}(\alpha) = 1 \right\}. \tag{10} $$

The ensemble average of a configuration-dependent quantity $f(\alpha)$ for a given probability distribution $\boldsymbol{\mu} \in \Delta$ is defined as

$$ \langle f \rangle_{\boldsymbol{\mu}} = \sum_{\alpha=1}^{|\mathbb{S}|} f(\alpha)\mu(\alpha). \tag{11} $$

Of a particular importance is a state characteristic vector $\boldsymbol{\chi}^{(r)}(\alpha)$ defined via

$$ \chi_e^{(r)}(\alpha) = \begin{cases} 1 & \text{if element } e \text{ is in state } r \text{ for configuration } \alpha, \\ 0 & \text{otherwise,} \end{cases} \tag{12} $$

quantifying the local distribution of individual states in a given configuration $\alpha$. For the current case, $\boldsymbol{\chi}^{(r)}(\alpha)$ can be explicitly related to $\alpha$ by employing the identities

$$\boldsymbol{\chi}^{(1)}(\alpha) = (\alpha - 1)_{\mathbb{B}}, \qquad \boldsymbol{\chi}^{(1)}(\alpha) + \boldsymbol{\chi}^{(2)}(\alpha) = \mathbf{1}, \tag{13}$$

where $n_{\mathbb{B}}$ provides the value of a natural number $n$ in the binary notation using $N_e$ digits, see Figure 1 for an illustration.

Following the analogy with quantification of spatial statistics of random heterogeneous media, e.g. (Torquato, 2002), we introduce a $N_e \times N_e$ two-unit probability matrix related to a given probability distribution $\boldsymbol{\mu}$ in the form

$$\boldsymbol{P}^{(rs)} = \sum_{\alpha=1}^{N_e} \boldsymbol{\chi}^{(r)}(\alpha)\boldsymbol{\chi}^{(s)}(\alpha)^{\mathsf{T}}\mu(\alpha) = \left\langle \boldsymbol{\chi}^{(r)}\boldsymbol{\chi}^{(s)\mathsf{T}} \right\rangle_{\boldsymbol{\mu}}, \tag{14}$$

with an individual entry $P_{ij}^{(rs)}$ storing the probability of states $r$ and $s$ being assigned to elements $i$ and $j$ (note that the explicit dependence on $\boldsymbol{\mu}$ is suppressed for the sake of brevity). Note that due to binary character of the problem, it is sufficient to concentrate on the statistics $\boldsymbol{P}^{(11)}$ only.

### 2.3. Statics of two-phase random lattices

When assigning a specific material properties to each state $r$, the previously introduced framework can be readily adopted to two-phase elastic heterogeneous lattices. In particular, the configuration-dependent material stiffness matrix on the element level, $\boldsymbol{D}_e(\alpha)$, yields

$$\boldsymbol{D}_e(\alpha) = \sum_{r=1}^{2} \chi_e^{(r)}(\alpha)\boldsymbol{D}_e^{(r)}, \tag{15}$$

where $\boldsymbol{D}_e^{(r)}$ denote positive-definite material stiffness matrices of individual states. On the global level, the stiffness distribution is characterized by

$$\boldsymbol{D}(\alpha) = \mathop{\mathsf{A}}_{e=1}^{N_e} \boldsymbol{D}_e(\alpha) = \sum_{r=1}^{2} \left( \mathop{\mathsf{A}}_{e=1}^{N_e} \chi_e^{(r)}(\alpha)\boldsymbol{D}_e^{(r)} \right) = \sum_{r=1}^{2} \boldsymbol{\chi}^{(r)} \bullet \boldsymbol{D}^{(r)}, \tag{16}$$

where $\boldsymbol{a} \bullet \boldsymbol{A}$ denotes a block Hadamard-like product implementing the assembly operation.

Consider now a response of a discrete structure with a *stochastic* configuration-dependent material stiffness matrix $\boldsymbol{D}(\alpha)$ subject to *deterministic* loading specified in terms of prescribed

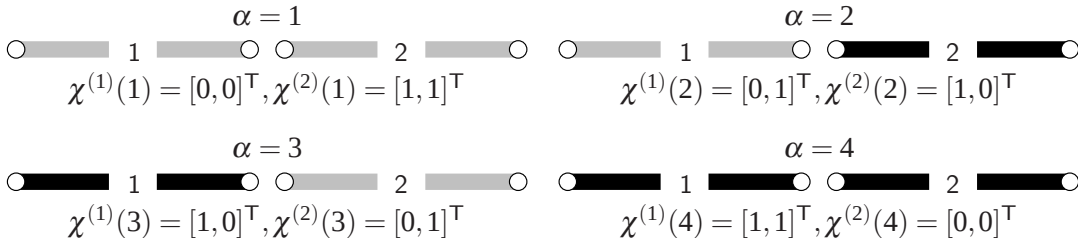


Figure 1: Ensemble space and state characteristic vectors for a two-element structure; state $r = 1$ corresponds to black element, $r = 2$ is indicated by gray color.

displacements ${}^{c}\boldsymbol{d}$ and generalized nodal forces ${}^{u}\boldsymbol{f}$. For each configuration $\alpha \in \mathbb{S}$, the energy minimizer is defined as

$$ {}^{u}\boldsymbol{d}(\alpha) = \arg\min_{\widehat{\boldsymbol{d}} \in \mathbb{R}^{|{}^{u}\boldsymbol{d}|}} E(\widehat{\boldsymbol{d}}; \alpha), \tag{17} $$

with the stored energy function introduced analogously to (6):

$$ E(\widehat{\boldsymbol{d}}; \alpha) = \tfrac{1}{2} \begin{bmatrix} \widehat{\boldsymbol{d}}^{\mathsf{T}} & {}^{c}\boldsymbol{d}^{\mathsf{T}} \end{bmatrix} \begin{bmatrix} {}^{uu}\boldsymbol{K}(\alpha) & {}^{uc}\boldsymbol{K}(\alpha) \\ {}^{cu}\boldsymbol{K}(\alpha) & {}^{cc}\boldsymbol{K}(\alpha) \end{bmatrix} \begin{bmatrix} \widehat{\boldsymbol{d}} \\ {}^{c}\boldsymbol{d} \end{bmatrix} - \widehat{\boldsymbol{d}}^{\mathsf{T}} {}^{u}\boldsymbol{f}. \tag{18} $$

The ensemble average of the optimal energy for a given probability distribution $\boldsymbol{\mu}$ is a weighted sum

$$ \langle E({}^{u}\boldsymbol{d}) \rangle_{\boldsymbol{\mu}} = \sum_{\alpha=1}^{|\mathbb{S}|} E\left({}^{u}\boldsymbol{d}(\alpha)\right) \mu(\alpha). \tag{19} $$

The full specification of probability distribution is, however, rarely available. Therefore, we rely on a partial statistical characterization in terms of two-element probabilities and attempt to establish energetic bounds in the form

$$ \mathcal{H}_{-}(\boldsymbol{P}^{(11)}) \leq \langle E({}^{u}\boldsymbol{d}) \rangle_{\widehat{\boldsymbol{\mu}}} \leq \mathcal{H}_{+}(\boldsymbol{P}^{(11)}) \quad \forall \widehat{\boldsymbol{\mu}} \in \mathbb{C}(\boldsymbol{P}^{(11)}), \tag{20} $$

reflecting the limited probabilistic characterization.

## 3. Hashin-Shtrikman-Willis estimates

Following the conceptual lead of Hashin and Shtrikman (1962), we introduce a reference deterministic structure characterized by a positive-definite generalized material stiffness matrix $\boldsymbol{D}^{(0)}$ and consider a realization-dependent quadratic form

$$ \tfrac{1}{2} \begin{bmatrix} \widehat{\boldsymbol{\tau}}^{\mathsf{T}} & \widehat{\boldsymbol{e}}^{\mathsf{T}} \end{bmatrix} \begin{bmatrix} \left(\boldsymbol{D}^{(0)} - \boldsymbol{D}(\alpha)\right)^{-1} & \boldsymbol{I} \\ \boldsymbol{I} & \left(\boldsymbol{D}^{(0)} - \boldsymbol{D}(\alpha)\right) \end{bmatrix} \begin{bmatrix} \widehat{\boldsymbol{\tau}} \\ \widehat{\boldsymbol{e}} \end{bmatrix}, \tag{21} $$

where $\widehat{\boldsymbol{e}} \in \mathbb{R}^{N_e N_s}$ stores an arbitrary strain vector and auxiliary variable $\widehat{\boldsymbol{\tau}} \in \mathbb{R}^{N_e N_s}$ will be commented on later. By virtue of the Schur complement lemma, cf. (Horn and Johnson, 1990, Section 7.7.6), the form (21) is positive-semidefinite as long as $(\boldsymbol{D}^{(0)} - \boldsymbol{D}(\alpha))$ is positive definite, leading to a bound

$$ \tfrac{1}{2} \widehat{\boldsymbol{e}}^{\mathsf{T}} \boldsymbol{D}(\alpha) \widehat{\boldsymbol{e}} \leq \widehat{\boldsymbol{\tau}}^{\mathsf{T}} \widehat{\boldsymbol{e}} - \tfrac{1}{2} \widehat{\boldsymbol{\tau}}^{\mathsf{T}} (\boldsymbol{D}(\alpha) - \boldsymbol{D}^{(0)})^{-1} \widehat{\boldsymbol{\tau}} + \tfrac{1}{2} \widehat{\boldsymbol{e}}^{\mathsf{T}} \boldsymbol{D}^{(0)} \widehat{\boldsymbol{e}}, \tag{22} $$

with the equality reserved for the value

$$ \tilde{\boldsymbol{\tau}}(\alpha) = \left(\boldsymbol{D}(\alpha) - \boldsymbol{D}^{(0)}\right) \widehat{\boldsymbol{e}} = \widehat{\boldsymbol{s}}(\alpha) - \boldsymbol{D}^{(0)} \widehat{\boldsymbol{e}} \tag{23} $$

maximizing the right hand side of (22) for a given realization $\alpha$ and test strain field $\widehat{\boldsymbol{e}}$. The variable $\widehat{\boldsymbol{\tau}}$ therefore corresponds to a *generalized polarization* stress associated with the reference stiffness matrix $\boldsymbol{D}^{(0)}$ and generalized strain $\widehat{\boldsymbol{e}}$ (Hashin and Shtrikman, 1962). Note that when the optimization with respect to $\widehat{\boldsymbol{\tau}}$ is performed exactly, attainment of equality in (23) is independent of the reference media. In the opposite case the $\boldsymbol{D}^{(0)}$ should be chosen as close to $\boldsymbol{D}^{(r)}$ while maintaining the positive semi-definiteness of $(\boldsymbol{D}^{(r)} - \boldsymbol{D}^{(0)})$.

Introducing the inequality (22) into the original energy function (18) yields a variational characterization of the true displacement-polarization pair in the form

$$({}^{u}\boldsymbol{d}(\alpha), \boldsymbol{\tau}(\alpha)) = \arg \min_{\widehat{\boldsymbol{d}} \in \mathbb{R}^{|u|}} \max_{\widehat{\boldsymbol{\tau}} \in \mathbb{R}^{N_e N_s}} U(\widehat{\boldsymbol{d}}, \widehat{\boldsymbol{\tau}}; \alpha), \tag{24}$$

where the Hashin-Shtrikman energy function is defined as

$$U(\widehat{\boldsymbol{d}}, \widehat{\boldsymbol{\tau}}; \alpha) = E^{(0)}(\widehat{\boldsymbol{d}}) + \widehat{\boldsymbol{\tau}}^{\mathsf{T}} \widehat{\boldsymbol{e}} + \tfrac{1}{2} \widehat{\boldsymbol{\tau}}^{\mathsf{T}} (\boldsymbol{D}^{(0)} - \boldsymbol{D}(\alpha))^{-1} \widehat{\boldsymbol{\tau}}, \tag{25}$$

with $E^{(0)}$ denoting the energy stored in the reference structure (obtained from Eq. (6) with $\boldsymbol{D} = \boldsymbol{D}^{(0)}$) and the kinematically admissible strain obtained from

$$\widehat{\boldsymbol{e}} = \begin{bmatrix} {}^{:u}\boldsymbol{B} & {}^{:c}\boldsymbol{B} \end{bmatrix} \begin{bmatrix} \widehat{\boldsymbol{d}} \\ {}^{c}\boldsymbol{d} \end{bmatrix}. \tag{26}$$

A completely analogous procedure can be executed when selecting the reference media such that $(\boldsymbol{D}(\alpha) - \boldsymbol{D}^{(0)})$ becomes negative-definite, leading to a lower estimate of the stored energy. For an indefinite $(\boldsymbol{D}(\alpha) - \boldsymbol{D}^{(0)})$, a variational estimate of the stored energy is obtained; see e.g. Luciano and Willis (2006) for additional discussion. Therefore, considering a generic reference media and upon exchanging the order of optimization, the problem (24) is generalized to

$$({}^{u}\boldsymbol{d}(\alpha), \boldsymbol{\tau}(\alpha)) = \arg \operatorname*{stat}_{\widehat{\boldsymbol{\tau}} \in \mathbb{R}^{N_e N_s}} \left( \min_{\widehat{\boldsymbol{d}} \in \mathbb{R}^{|u|}} U(\widehat{\boldsymbol{d}}, \widehat{\boldsymbol{\tau}}; \alpha) \right). \tag{27}$$

Similarly to Willis (1977), we start from the minimization with respect to kinematical variables to obtain the optimal displacement vector $\tilde{\boldsymbol{d}}$ for an arbitrary test polarization stress $\widehat{\boldsymbol{\tau}}$. Due to linearity of the problem, the actual value is expressed as a superposition of two auxiliary problems

$$\begin{bmatrix} {}^{u}\tilde{\boldsymbol{d}} \\ {}^{c}\boldsymbol{d} \end{bmatrix} = \begin{bmatrix} {}^{u}\boldsymbol{d}_{(0)} \\ {}^{c}\boldsymbol{d} \end{bmatrix} + \begin{bmatrix} {}^{u}\tilde{\boldsymbol{d}}_{(1)} \\ \boldsymbol{0} \end{bmatrix}, \tag{28}$$

where ${}^{u}\boldsymbol{d}_{(0)}$ denotes the polarization-independent displacement of a reference structure subject to prescribed displacements ${}^{c}\boldsymbol{d}$ and nodal forces ${}^{u}\boldsymbol{f}$, while ${}^{u}\tilde{\boldsymbol{d}}_{(1)}$ is the displacements due to a polarization stress $\widehat{\boldsymbol{\tau}}$ with ${}^{c}\boldsymbol{d} = \boldsymbol{0}$ and ${}^{u}\boldsymbol{f} = \boldsymbol{0}$. The values of both components follow from equilibrium equations (8):

$$\begin{aligned} {}^{uu}\boldsymbol{K}^{(0)} {}^{u}\boldsymbol{d}_{(0)} &= {}^{u}\boldsymbol{f} - {}^{uc}\boldsymbol{K}^{(0)} {}^{c}\boldsymbol{d}, & (29) \\ {}^{uu}\boldsymbol{K}^{(0)} {}^{u}\tilde{\boldsymbol{d}}_{(1)} &= -{}^{u:}\boldsymbol{B}^{\mathsf{T}} \widehat{\boldsymbol{\tau}}. & (30) \end{aligned}$$

After resolving the "inner" problem in Eq. (27), we proceed with determination of the optimal polarization. Introducing the solutions of (29) and (30) into the two-variable function (27) and exploiting the optimality conditions (8) yields, after some manipulations discussed in detail in, e.g. in Willis (1977) and Luciano and Willis (2005), the characterization of the optimal polarization stresses in the form:

$$\boldsymbol{\tau}(\alpha) = \arg \operatorname*{stat}_{\widehat{\boldsymbol{\tau}} \in \mathbb{R}^{N_e N_s}} H(\widehat{\boldsymbol{\tau}}; \alpha), \tag{31}$$

with the condensed energy function expressed as

$$H(\widehat{\boldsymbol{\tau}}; \alpha) = H_{(0)} + \widehat{\boldsymbol{\tau}}^{\mathsf{T}} \boldsymbol{e}_{(0)} - \tfrac{1}{2} \widehat{\boldsymbol{\tau}}^{\mathsf{T}} (\boldsymbol{D}^{(0)} - \boldsymbol{D}(\alpha))^{-1} \widehat{\boldsymbol{\tau}} - \tfrac{1}{2} \widehat{\boldsymbol{\tau}}^{\mathsf{T}} \boldsymbol{\Gamma}_{(0)} \widehat{\boldsymbol{\tau}}, \tag{32}$$

where $H_{(0)} = E^{(0)}({}^{u}\boldsymbol{d}_{(0)})$ corresponds to a stationary value of the energy stored in the reference structure, $\boldsymbol{e}_{(0)}$ is the associated generalized strain and $\boldsymbol{\Gamma}_{(0)}$ is a discrete counterpart of the Green-function related quantity introduced by Willis (1977) and Luciano and Willis (2005), linking the kinematical quantities to the polarization stress via

$$\tilde{\boldsymbol{e}}_{(1)} = {}^{:u}\boldsymbol{B}\,{}^{u}\tilde{\boldsymbol{d}}_{(1)} = -\left({}^{:u}\boldsymbol{B}\right)\left({}^{uu}\boldsymbol{K}(\boldsymbol{u},\boldsymbol{u})\right)^{-1}\left({}^{:u}\boldsymbol{B}\right)^{\mathsf{T}}\widehat{\boldsymbol{\tau}} = -\boldsymbol{\Gamma}_{(0)}\widehat{\boldsymbol{\tau}}. \tag{33}$$

Since no approximation has been introduced so far, the following equality

$$\left\langle E({}^{u}\boldsymbol{d}(\alpha))\right\rangle_{\boldsymbol{\mu}} = \left\langle H(\boldsymbol{\tau}(\alpha)\right\rangle_{\boldsymbol{\mu}} \tag{34}$$

is still valid for an arbitrary probability density vector $\boldsymbol{\mu} \in \Delta$. With the partial description of the stochastic system at hand, a specific ansatz for the generalized polarization stresses

$$\boldsymbol{\tau}(\alpha) \approx \sum_{r=1}^{2} \boldsymbol{\chi}^{(r)}(\alpha) \bullet \boldsymbol{\tau}^{(r)}, \qquad \widehat{\boldsymbol{\tau}}(\alpha) \approx \sum_{r=1}^{2} \boldsymbol{\chi}^{(r)}(\alpha) \bullet \widehat{\boldsymbol{\tau}}^{(r)}, \tag{35}$$

is employed to utilize the available second order statistics (14) optimally, cf. (Willis, 1977). The $\widehat{\boldsymbol{\tau}}^{(r)}$ and $\boldsymbol{\tau}^{(r)}$ terms in Eq. (35) are *realization-independent* trial and "true" polarization stresses related for the $r$-th phase. The approximations (35) together with the expression for material stiffness matrix (15) yield a variational statement in the form

$$\begin{aligned}
\left\langle E({}^{u}\boldsymbol{d}(\alpha)\right\rangle_{\boldsymbol{\mu}} \;\leqslant\; & H_{(0)} + \sum_{r=1}^{2} \boldsymbol{e}_{(0)} \left( \left\langle \boldsymbol{\chi}^{(r)} \right\rangle_{\boldsymbol{\mu}} \bullet \widehat{\boldsymbol{\tau}}^{(r)} \right)^{\mathsf{T}} \boldsymbol{e}_{(0)} \\
& - \tfrac{1}{2} \sum_{r=1}^{2} \widehat{\boldsymbol{\tau}}^{(r)\mathsf{T}} \left( \left\langle \boldsymbol{\chi}^{(r)} \boldsymbol{\chi}^{(r)\mathsf{T}} \right\rangle_{\boldsymbol{\mu}} \bullet \left( \boldsymbol{D}^{(0)} - \boldsymbol{D}^{(r)} \right)^{-1} \right) \widehat{\boldsymbol{\tau}}^{(r)} \\
& - \tfrac{1}{2} \sum_{r=1}^{2} \sum_{s=1}^{2} \widehat{\boldsymbol{\tau}}^{(r)} \left( \left\langle \boldsymbol{\chi}^{(r)} \boldsymbol{\chi}^{(s)\mathsf{T}} \right\rangle_{\boldsymbol{\mu}} \bullet \boldsymbol{\Gamma}_{(0)} \right) \widehat{\boldsymbol{\tau}}^{(s)},
\end{aligned} \tag{36}$$

where the actual status of the right hand side depends again on the choice of reference material stiffness matrix $\boldsymbol{D}^{(0)}$.

By performing optimization with respect to deterministic phase polarization fields and imposing the constraint $\boldsymbol{\mu} \in \mathbb{C}(\boldsymbol{P}^{(11)})$ finally delivers the searched energetic bounds and estimates:

$$\mathcal{H}_{\pm}(\boldsymbol{P}^{(11)}) = H_{(0)} + \frac{1}{2} \sum_{r=1}^{2} \boldsymbol{e}_{(0)}{}^{\mathsf{T}} \left( \boldsymbol{p}^{(r)} \bullet \boldsymbol{\tau}_{\pm}^{(r)} \right), \tag{37}$$

where the optimal phase polarization stresses follows from the system of linear equations:

$$\left( \boldsymbol{P}^{(rr)} \bullet \left( \boldsymbol{D}^{(0)} - \boldsymbol{D}^{(r)} \right)^{-1} \right) \boldsymbol{\tau}_{\pm}^{(r)} + \sum_{s=1}^{2} \left( \boldsymbol{P}^{(rs)} \bullet \boldsymbol{\Gamma}_{(0)} \right) \boldsymbol{\tau}_{\pm}^{(s)} = \boldsymbol{p}^{(r)} \bullet \boldsymbol{e}_{(0)}. \tag{38}$$

## 4. Illustrative examples

Although the theory presented in previous sections is applicable to generic 2D or 3D discrete structures, basic features of the method are illustrated for a planar truss system in the small-strain regime. Within this framework, the generalized displacement vector and can be found in (Jirásek and Bažant, 2001, Appendix A).

A regular lattice structure appearing in Figure 2 is employed as a benchmark problem. The prescribed boundary conditions include uniform loading and bending scenarios, imposed either using nodal forces (force control (FC) case) or by prescribed nodal displacements (displacement control (DC) programme). In addition, a dimensionless parameter in the form

$$\zeta(\boldsymbol{P}^{(11)}) = \frac{\mathcal{H}(\boldsymbol{P}^{(11)}) - \mathcal{H}(\boldsymbol{0})}{\mathcal{H}(\boldsymbol{1}) - \mathcal{H}(\boldsymbol{0})} \tag{39}$$

is introduced to aid visualization of the results.

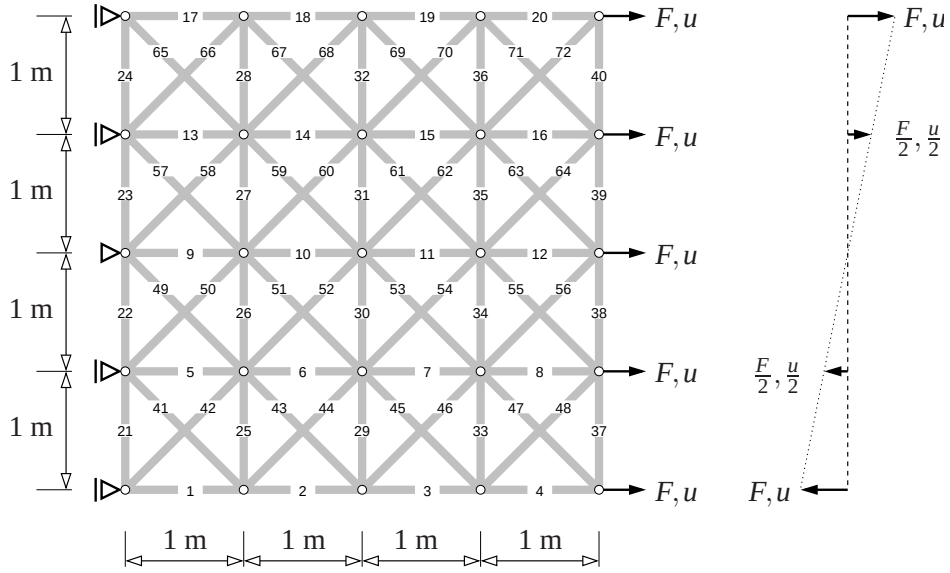


Figure 2: Scheme of the lattice structure

The results for the second-order bounds presented hereafter are accompanied with the elementary counterparts of the Voigt and Reuss type, determined for a deterministic problem with spatially variable Young moduli in the form

$$E_e^{\mathrm{V}}(p_e^{(1)}) = p_e^{(1)}E_e^{(1)} + (1-p_e^{(1)})E_e^{(2)}, \qquad E_e^{\mathrm{R}}(p_e^{(1)}) = \left(\frac{p_e^{(1)}}{E_e^{(1)}} + \frac{1-p_e^{(1)}}{E_e^{(2)}}\right)^{-1}. \tag{40}$$

Finally, data obtained by direct Monte-Carlo (MC) simulations with $N = 10,000$ realizations are included as a reference value.

A binary system with the first phase assigned to each element independently with a probability $\phi$ is investigated. The associated second-order statistics then becomes

$$P_{ij}^{(11)} = \begin{cases} \phi & \text{if } i = j, \\ \phi^2 & \text{otherwise.} \end{cases} \tag{41}$$

The contrast of phase stiffnesses is set to $E^{(2)} : E^{(1)} = 10 : 1$.

Figure 3 gathers the stored energy plots for all the considered loading scenarios. In all cases, the HSW bounds substantially narrow the domain defined by the first-order bounds while preserving the concave/convex dependence of the mean stored energy on the $\phi$ parameter for the displacement- or force-driven loads, respectively. The increase in accuracy due to considering

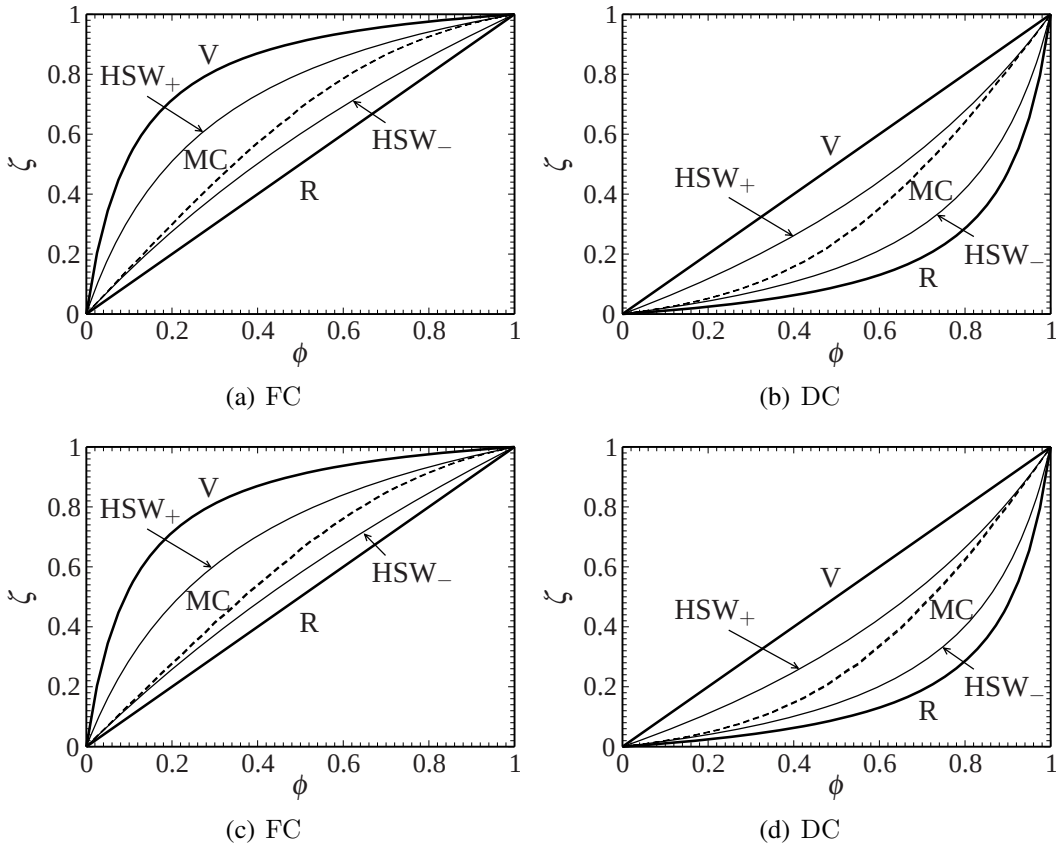


Figure 3: Energetics of random truss model; (a)–(b) uniform loading, (c)–(d) bending.

non-local spatial statistics is especially pronounced for small and large values of $\phi$, for which even the asymptotic behavior seems to be exactly reproduced by the lower bound for the force-controlled conditions or upper bound in case of kinematically constrained case. Note that the match between the HSW predictions and the results of the MC simulations in the whole range of probabilities $\phi$ can be further increased by an appropriate choice of the reference stiffness $\boldsymbol{D}^{(0)}$. Nevertheless, the optimal value is highly problem-specific, which somehow limits applicability of the variational estimates, see (Sharif-Khodaei and Zeman, 2008) for further discussion.

## 5. Conclusions

In this work, the variational bounds and estimates of the HSW-type for two-phase random structures were derived and verified against the results of direct MC simulations. The most important findings can be summarized as follows:

- when applied to discrete structures, the derivation of the HSW principles becomes rather straightforward and requires only elements of matrix structural analysis and linear algebra,
- the variational framework naturally incorporates the general statistically non-uniform systems,
- the second-order bounds provide a computationally feasible alternative to direct MC simulations.

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## 7. References

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