APPROACHES TO NONCONVEX VARIATIONAL PROBLEMS OF MECHANICS

Laminates, differential schemes, variations, extensions, bounds, and duality

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Abstract. This paper reviews recent developments of mathematical methods for nonconvex variational problems of mechanics, particularly, problems of optimal layouts of material in a heterogeneous medium. These problems are characterized by locally unstable solutions which are interpreted as optimal microstructured media. We discuss variational formulations of these problems, properties of their solutions and several approaches to address them: minimizing sequences and the technique of laminates, laminate closures, and the differential scheme; necessary conditions by structural variations and minimal extension technique; the lower bounds and bounds for the variety of effective tensors of properties. Several examples are presented. Particularly, the bound for the tensor of thermal expansion coefficients is found. Special attention is paid to the use of duality for reformulation of minimax problems as minimal ones.

1. Variational problems with locally unstable solutions

1.1. NONCONVEX VARIATIONAL PROBLEMS

Introduction Nonconvex variational problems in mechanics describe optimal layouts of several materials in a structure. A typical problem is minimization of the energy of a heterogeneous structure by a layout of the phases. This problem is met in many applications. Structural optimization asks for an optimal "mixture" of a solid material and void or for the best structure of a composite. The martensite alloys, polycrystals and similar materials can exist in several forms (phases) and Gibbs principle states that the phase with minimal energy is realized. Biostructures adapt themselves to the environment in a best way. Optimal layouts in man-made structures response to an engineering requirements, minimization of the

energy of natural materials corresponds to the realization of the thermodynamical Gibbs principle, and optimality of biological morphologies reflects evolutionary perfection.

A minimization problem of this type helps to establish bounds of effective properties of a composite. If the mixed materials are linear, a composite is equivalent to a linear material in the sense that if loaded, it stores the same energy as a homogeneous material with stiffness C_*. The problem of G-closure asks about the set of the effective tensors of all microstructures and bounds on that set. In order to find the bound for C_*, we minimize the energy stored in a composite medium, or the sum of the energies corresponding to several linearly independent loadings. The bound for the range of C_* follows from the lower bound of the energy.

Variational problems in elasticity The state of a classical elastic material is defined by the equations of equilibrium of stress tensor σ

$$\nabla \cdot \sigma = 0 \quad \sigma = \sigma^T. \tag{1}$$

The stress is related to the tensor of deformation ϵ and further to the vector of elongation u by the constitutive equation

$$\sigma = F(\epsilon), \quad \epsilon = \epsilon(\nabla u). \tag{2}$$

These relations are the Euler-Lagrange equations for a variational problem

$$J_\epsilon = \min_{\epsilon(u)} \int_\Omega W_\epsilon(\epsilon)\, dx, \quad \epsilon = \epsilon(\nabla u) \tag{3}$$

where $W_\epsilon(\epsilon)$ is the energy of deformation, if the constitutive relation (2) can be written in the form

$$F = \frac{\partial}{\partial \epsilon} W_\epsilon(\epsilon) \tag{4}$$

Boundary conditions are imposed on the displacement u.

Alternatively, the equilibrium can be described by the dual variational problem

$$J_\sigma = \min_{\sigma(\phi)} \int_\Omega W_\sigma(\sigma)\, dx, \quad \sigma = \nabla \times (\nabla \times \phi)^T \tag{5}$$

where $W_\sigma(\sigma)$ is a dual form of energy called the stress energy or the complementary energy, and the potential representation in the right field of (5) accounts for the equilibrium constraints (1).

A linear elastic material corresponds to the constitutive relations

$$\sigma = C : \epsilon \quad \text{or } \sigma_{ij} = \sum_{k,n} C_{ijkn}\epsilon_{nk}, \quad \epsilon = \frac{1}{2}(\nabla u + \nabla u^T) \tag{6}$$

and Lagrangian

$$W\epsilon = \frac{1}{2}\epsilon^T : C : \epsilon \tag{7}$$

where ϵ is the strain, C is the fourth-rank stiffness tensor, and (:) is the convolution by two indices. The stress energy corresponds to the Lagrangian

$$W_\sigma = \frac{1}{2}\sigma^T : S : \sigma, \quad \sigma = \nabla \times (\nabla \times \phi)^T$$

where S is the tensor of compliance that is inverse to C, $S : C = 1$.

Both problems (3) and (5) describe the same elastic equilibrium and deal with fields that are partials of some vector potentials and therefore satisfy the integrability conditions. The sum of the functionals in (3) and (5) is equal to the work of external forces on the displacements of the points of medium, or

$$W_\epsilon + W_\sigma = \epsilon : \sigma$$

Minimization of the energy J_ϵ with prescribed nonzero displacements on the boundary corresponds to minimization of the integral stiffness of the loaded elastic domain. Similarly, minimization of the energy J_σ with prescribed nonzero forces on the boundary corresponds to minimization of the integral compliance of the domain or maximization of its stiffness.

Notations Below, in Section 1.2, we discuss general properties of nonconvex variational problems; the analysis is applicable to both forms of elastic energy. We will write the variational problem in the form

$$J = \min_u \int_\Omega W(\nabla u)\, dx \tag{8}$$

stressing the dependence of the Lagrangian W on the gradient of a vector potential.

For quadratic energies, we will often use the form $W = \frac{1}{2}v^T Dv$ where v is a field; for example $v = \nabla u$ or $v = \sigma$, or $v = \epsilon$, or v is a combination of these fields. Accordingly, D is a tensor of properties, that can be either stiffness or compliance tensor.

Stability to perturbations The energy of a classical material is stable in the following sense: If an unbounded domain filled with the material is subject to an affine external elongation at infinity (that corresponds to the constant strain), the strain is constant everywhere. The minimum of the energy (8) is achieved at an affine function $u(x) = Ax + B$ satisfying the boundary conditions. The energy of such materials is called quasiconvex (see the Section 1.2 for the definition) and the constitutive relations are

elliptic. The ellipticity implies that the solution $u(x)$ in a finite domain Ω is smooth if both the domain Ω and boundary conditions are smooth.

The problems of optimal design, composites, natural polymorphic materials (martensites), polycrystals, smart materials, biomaterials, etc. yield to variational problems with locally unstable solutions. In such problems, the minimizer is not affine even if the external loading is homogeneous. These variational problems are called nonquasiconvex; they were studied in recent books by Dagorogna [26], Cherkaev [20], Milton [63], Allaire [1], Bendsøe and Sigmund [11] from different viewpoints; extensive references can be found there. The problems of nonlinear elasticity are also generally nonquasiconvex, see [27]. The unstable solutions may correspond to the minimization of an objective different from the energy, see for example [20].

Multiwell Lagrangians A transparent example of a nonquasiconvex problem is given by the following problem of structural design: Find a layout of N elastic materials that minimizes the total energy of a domain Ω. It is assumed that Ω is filled with several materials with the energy functions $W_i(\nabla u)$, $i = 1, \dots N$ where N is the number of phases. The energy W of the body is equal to

$$W(\nabla u) = \sum_{i=1}^{N} \chi_i(x) W_i(\nabla u) \tag{9}$$

where χ_i is the characteristic function of the subdomain Ω_i occupied with ith material,

$$\chi_i(x) = \begin{cases} 1 & \text{if } x \in \Omega_i \\ 0 & \text{if } x \notin \Omega_i \end{cases} \qquad \Omega = \bigcup_i \Omega_i$$

It is assumed that the boundary displacement $u(s)$ (s is the coordinate at the boundary $\partial\Omega$) is given and the volume fractures m_i of materials are prescribed, as

$$m_i = \langle \chi_i \rangle, \quad \langle \chi \rangle = \frac{1}{\|\Omega\|} \int_\Omega \chi(x)\, dx \tag{10}$$

where $\langle\ \rangle$ is the symbol of averaging.

Using the definition (9) of the energy, we formulate the problem as

$$I_0 = \min_{\chi_i(x)} \min_{u(x)} \left\{ \int_\Omega \left(\sum_{i=1}^{N} \chi_i(x) W_i(\nabla u) \right) dx + \sum_{i=1}^{N} \gamma_i \left(\int_\Omega \chi_i(x)\, dx - m_i \right) \right\} \tag{11}$$

or

$$I_0 = \min_{\chi_i(x)} \min_{u(x)} \left\{ \int_\Omega \left(\sum_{i=1}^{N} \chi_i [W_i(\nabla u) + \gamma_i] \right) dx - \sum_{i=1}^{N} \gamma_i m_i \right\} \tag{12}$$

where γ_i are the Lagrange multipliers by the constraints (10). An optimal layout χ_i of materials minimizes the sum of the energy W_i and the "cost" γ_i of the materials, adapting itself to the applied load.

Following Kohn and Strang [44], this problem is transformed to a nonconvex variational problem for minimizer u if the sequence of minimal operations is interchanged and the minimization over χ_i is performed first with "frozen" values of ∇u. The problem becomes

$$I_0 = \min_{u(x)} \int_\Omega F(\nabla u, \gamma_i) dx - \sum_{i=1}^{N} \gamma_i m_i \tag{13}$$

where

$$F(\nabla u, \gamma_i) = \min_{i=1,\dots,N} \{W_i(\nabla u) + \gamma_i\}.$$

is a nonconvex function of ∇u.

The second term in (13) is independent of u and defines the amounts of materials in the mixture linking them to the costs of materials. We can assume that the costs γ_i are somehow specified and analyze the problem

$$I = \min_{u(x)} \int_\Omega F(\nabla u, \gamma_i) dx \tag{14}$$

and then define the costs to arrive at the correct volume fractions m_i.

Lagrangian F is equal to the minimum of several functions $W_i + \gamma_i$. It is called multi-well Lagrangian and the components W_i are called wells. The costs γ_i must be chosen so that no well dominates: Minimum corresponds to different wells $W_i(\nabla u) + \gamma_i$ for different values of ∇u. Formally, the range of γ_i is restricted by the requirements that optimal volume fractions are nonnegative, $m_i \geq 0$.

The nonconvexity (more exactly, nonquasiconvexity, see below) of F poses several specific problems. The Euler equation for this problem is not elliptic in certain domains $\mathcal{V}_{\text{frb}}$ of the range of ∇u. These domains must be avoided; the optimal solution ∇u jumps over the forbidden region $\mathcal{V}_{\text{frb}}$.

1.2. UNSTABLE SOLUTIONS

Nonconvex energy leads to nonmonotonic constitutive relations and therefore to nonunique constitutive relations: If W is nonconvex, equations (2), (4) for ∇u have more than one solution. At equilibrium, one stress σ corresponds to several strains. The nonuniqueness is the source of instability of a solution. The variational principle (8) selects the solution with the least energy from the stationary solutions of (4). This optimal solution ∇u typically oscillates between several values that correspond to different wells W_i of the multiwell energy W, and the spatial scale of oscillation can be infinitesimal.

Questions about unstable solutions In dealing with nonconvex variational problems, we cannot define the solution ∇u in every point; instead, we are trying to answer several indirect questions about the solution, which we formulate here repeating them twice in mathematical and mechanical terms.

(1) What are the regions of $v = \nabla u$ that correspond to oscillatory and smooth solutions, respectively? (1a) For what stresses and strains does the composite correspond to less energy than any pure phase?

(2) What are the optimal values of $v = \nabla u$ in each well that alternate in an optimal solution? (2a) What are the strains and stresses inside the materials that form an optimal composite?

(3) What are minimizing sequences $\chi_i^{(k)}$ of partitions for an optimal solution? (3a) What is the microstructure of an optimal composite?

Oscillatory solutions can be described in terms of some averages, by passing to a "relaxed" variational problem with a "relaxed" Lagrangian. The relaxed Lagrangian $W_{\text{relax}}(\nabla u)$ is equal to the average over a small volume Lagrangian $\langle W\rangle(\nabla w)$ of an optimal fast scale oscillatory solution $w(x)$ with a fixed mean value, $\langle w(x)\rangle = u$,

$$W_{\text{relax}}(\nabla u) = \inf_{w(x):\ \langle w\rangle = u} \langle W(\nabla w)\rangle$$

and it is assumed that $w(x)$ is either quasiperiodic or stochastically homogeneous. This Lagrangian is called the *quasiconvex envelope* of the original multiwell Lagrangian, and it corresponds to a unique solution of the stationarity equation. Mechanically, the relaxed relation correspond to the relations that link together locally averaged stresses and strains in a heterogeneous material with optimal microstructures. This averaged description poses several problems as well:

(4) How to compute or bound the quasiconvex envelope that describes the relaxed problem? (4a) What is the constitutive relation (or its estimate) between the averaged stresses and strains in an optimal composite?

(5) How to define and obtain suboptimal solutions? (5a) What finite-scale composites approximate the optimal infinitesimal microstructure? The problem of suboptimality is not easy because of complicated microgeometry. We need to simplify (coarse) this geometry by sacrificing not more than a certain portion of the objective.

Answers: One-dimensional problem The unstable one-dimensional variational problem has the form

$$\min_{u(x)} \int_a^b F(x, u, u')dx \tag{15}$$

where $x \in [a,b]$ is an independent variable. We assume that $F(x,u,v)$ is a nonconvex function of $v(x) = u'(x)$ at least for some values of x and u. Here u and v are n-dimensional vector functions of a real argument x.

The one-dimensional nonconvex problem (15) is relaxed by replacing the Lagrangian F by its convex envelope $\mathcal{C}_v F(x,u,v)$. The convex envelope $\mathcal{C}_v F(v)$ of a scalar function F of a n-dimensional vector $v \in R^n$ is solution to the following problem (see [75])

$$\mathcal{C}_v F(v) = \min_{m_1,\dots m_{n+1},\xi_1,\dots,\xi_{n+1}} \sum_{i=1}^{n} m_i F(v+\xi_i) \tag{16}$$

where m_k are nonnegative parameters, $m_k \geq 0$ such that $m_1 + \ldots + m_{n+1} = 1$, and ξ_i are n-dimensional vectors such that

$$\sum_{i=1}^{n+1} m_i \xi_i = 0.$$

The convex envelope $\mathcal{C}_v F(x,u,v)$ of the Lagrangian $F(x,u,v)$ is computed with respect to the variable v while u and x are treated as parameters.

Consideration of the relaxed problem helps to answer the above questions as follows:

(1) The minimizer $u(x)$ is oscillatory and its derivative $v = u'$ alternates its values infinitely fast if the value of the convex envelope is smaller than the value of the function, $\mathcal{C}_v F(x,u,v) < F(x,u,v)$. If these two coincide, $\mathcal{C}_v F(x,u,v) = F(x,u,v)$, the Lagrangian is convex, and the minimizer is smooth. The derivative v of an optimal solution never takes the values in the *forbidden region*,$v \notin \mathcal{V}_{frb}$ where

$$\mathcal{V}_{frb} = \{v : \ \mathcal{C}_v L(x,u,v) < L(x,u,v)\}.$$

(1a) An oscillatory solution indicates that a composite is optimal, a smooth solution means that a pure phase is optimal.

(2) An oscillatory optimal solution takes at most $n+1$ values $v+\xi_i$ in a proximity of each point (Caratheodory theorem, see [75]); these values correspond to different convex wells and are called supporting points of the envelope. Each well supports not more than one point of $v+\xi_i$. (2a) The values $v+\xi_i$ can be interpreted as strains (stresses) inside the pure material of the optimal composite. Each material is characterized by a pair of stress and strain.

(3) The details of the partition of the interval are of no importance, only the measure m_i of the subintervals where $v = u'$ takes specific values $v+\xi_i$ is important. The fractions m_i vary according to the values of u and x, adapting the composite to the varying conditions.

(4) The computation of the convex envelope is an algebraic problem (16). The constitutive relation between the average stresses and strains is monotone in the sense that the Weierstrass $\mathcal{E}$-function is nonnegative.

$$\mathcal{E}_{\mathcal{C}_v F}(v,\hat{v}) = (v-\hat{v})^T \frac{d}{dv}\mathcal{C}_v F(v) + \mathcal{C}_v F(v) - \mathcal{C}_v F(\hat{v}) \geq 0 \quad \forall v,\hat{v}.$$

(4a) Since the convex envelope is linear at least in one direction, the dual variable (stress or strain) $\frac{\partial}{\partial v}\mathcal{C}_v F$ stays constant when v varies. This constancy is interpreted as the optimality condition for the layout.

(5) Suboptimal solutions may correspond to a finite size of partition of the interval $[a,b]$ or to continuous solutions that oscillate with a finite frequency.

Quasiconvex envelope The multivariable case is more complex because the third argument v of the Lagrangian $F(x,u,v)$ – the matrix $v=\nabla u$ – is subject to linear differential constraints. In contrast with the one-dimensional case where $v=u'$ is an arbitrary integrable function, the partial derivatives $v=\nabla u$ are subject to integrability conditions $\nabla \times v = \nabla \times \nabla u = 0$. These conditions restrict the neighboring values of $v=\nabla u$ of a continuous vector potential u.

Generally, multivariable variational problems deal with divergencefree, curlfree, or otherwise linearly constrained fields that are subject to corresponding integrability conditions. Following Murat [71] and Dacorogna [26], it is convenient to consider the general form of such constraints

$$A\nabla u = \sum_{j=1}^{n}\sum_{k=1}^{d} a_{ijk}\frac{\partial v_j}{\partial x_k} = 0, \quad i=1,\dots,r \tag{17}$$

where $A=\{a_{ijk}\}$ is a constant $r\times n\times d$ third-rank tensor of constraints. We will assume the form $L=L(v)$ of the Lagrangian, where v is subject to (17).

Remark 1.1 *The differential constraints on strain*

$$\nabla \times (\nabla \times \epsilon) = 0,$$

called compatibility conditions, deal with a linear form of second derivatives. Here, for the sake of simplicity, we will deal mostly with the constraints in the form (17); most results can be adjusted to a more general case of constraints that involve the second derivatives.

The integrability conditions (17) introduce the dependence on a partition since they depend on the normal n and tangent t to the dividers of

Ω_i as well as on the properties of the neighbors. The tangent (t) components $t \cdot \epsilon \cdot t$ of strain and the normal (n) components of vector $\sigma \cdot n$ are continuous. These continuity conditions bond the neighboring fields in a structure. Particularly, the supporting points $v+\xi_i$ of convex envelope (16) are interconnected because some of them must neighbor in the microstructure. Therefore the construction of the envelope must be modified to the quasiconvex envelope, see [7, 20, 29, 44].

Consider an infinitely small cubic neighborhood ω of an inner point $x \in \Omega$. Assume that the mean field v is given and that the pointwise fields are (almost) ω-periodic and subject to (17).

Quasiconvex envelope $\mathcal{Q}L(v)$ is the minimum over all admissible perturbations with zero mean of the integral over ω of the Lagrangian $L(v)$,

$$\mathcal{Q}L(v) = \min_{\xi(x)\in\Xi} \frac{1}{\|\omega\|} \int_\omega L(v+\xi)dx \tag{18}$$

where ω is an infinitesimal cube, and the set Ξ is defined as

$$\Xi = \left\{\xi : \quad \int_\omega \xi(x)dx = 0, \quad A\nabla\xi = 0, \quad \xi \in L_\infty(\Omega)\right\}. \tag{19}$$

A Lagrangian $L(v)$ is quasiconvex, if $L(v) = \mathcal{Q}L(v)$. The quasiconvexity of a Lagrangian means stability of the affine solution to all localized zero-mean finite perturbations ξ that are consistent with the differential constraints. The solution is stable to the local perturbations if $\mathcal{Q}L(v) = L(v)$ and is unstable otherwise, when $\mathcal{Q}L(v) < L(v)$. In the construction of the quasiconvex envelope, one treats x as a constant and assumes the periodicity of the perturbations ξ, which corresponds to the assumption that ω is a infinitesimal neighborhood in Ω. In the one-dimensional case, the integrability conditions disappear and the quasiconvex envelope becomes the convex envelope.

In contrast with the convex envelope, the quasiconvex envelope is a solution to a variational not an algebraic problem. Correspondingly, the solution depends on the geometry of the partition of a cube into subdomains occupied with different materials (the microgeometry). The above questions cannot be answered as simply as in the one-dimensional case; in the rest of the paper we discuss the progress in understanding of them.

Methods of investigation of nonconvex variational problems The diversity of the above questions corresponds to a number of methods. Below, we outline recent developments of several explicit approaches to optimal mixtures, methods that specify the problem reducing it to computable algorithms. We assume that a physical problem is formulated as a minimal

variational problem (8). Independently we discuss methods to reformulate a minimax problem as a minimal one, see Section 4

(i). The lamination technique (Section 2) deals with an *a priori* constrained class of microstructures (laminates) and uses various optimization schemes to search for optimal structures. The differential scheme (Section 2.3) allows for treatment of the problem of the best microstructure as a regular control problem.

(ii). The classical variational conditions (Section 3) are based on classical Weierstrass-type structural variations. They are used to analyze fields in optimal structures and describe or approximate regions of stable and oscillatory solutions. One obtains the range of stresses and strains in each of the mixed material and evaluates suboptimal solutions. The minimal extension based on these conditions provides a Lagrangian that is stable against a special class of perturbations, an upper bound for the quasiconvex envelope.

(iii). The technique of bounds (Section 4) replaces the variational problem with a rough finite-dimensional optimization problem that constrains the quasiconvex envelope from below. The bound takes into account differential constraints replacing them with special integral inequalities on admissible fields. In order to obtain the bound, duality is often used.

These techniques attack the problem from different directions but none of them gives the complete solution. The lamination technique is based on assumptions about the type of optimal geometry and the found structures are generally not unique. The variational technique is a more direct approach but it assumes a special type of local perturbations. Generally, the bounds are not expected to be exact, either. None of the above questions is fully answered so far: There is a lot of uncharted territory ahead. However, several nonquasiconvex problems are fully understood, particularly we know what are optimal composites for optimal two-phase conducting and elastic composites, see examples in [20, 63].

2. Constrained minimizing sequences and control problems

2.1. THE LEGO OF LAMINATES

Generally, the fields in a microstructure are given by solutions of elasticity problem with periodic boundary conditions and a layout χ_i of the materials. The effective properties of a composite are computed through the integrals of this solution. For a general type of geometry, the solution can be found only numerically. However, there is an exceptional class of laminate microgeometries for which the elastic fields can be explicitly computed at each point. Correspondingly, the effective properties can be explicitly computed as well. Laminates are easily generalized to the structures called *laminates*

of a rank – a multi-scale structure of laminates from laminates, from laminates. The flexibility and richness of this class and relative simplicity of calculation of the fields and effective properties made it subject to detailed investigation by many authors such as Bruggeman, Hashin, Milton, Lurie, Gibiansky, Norris, Avellaneda, Murat, Tartar, Francfort, Bendsøe, Lipton, Kikuchi, Sigmund, and others.

Problems in which laminates are optimal The main feature of laminate structures is constancy of the fields in layers. The fields also satisfy the compatibility conditions (17) that link together the field in the neighboring layers and the normal to layers. For piece-wise constant fields, these conditions take the form

$$B \cdot n = 0 \tag{20}$$

where n is the normal to the layers in the laminate, B is the $r \times d$ tensor of discontinuities:

$$B = \{B_{ik}\}, \quad B_{ik} = \sum_{j=1}^{n} a_{ijk}[v_j]^+_-, \tag{21}$$

$\mathcal{A} = \{a_{ijk}\}$ is the tensor of differential constraints (17), and $[Z]^+_-$ is the jump of the value of Z at the boundary of the layers.

The compatibility conditions depend on the normal n. We show now that if the number r of linearly independent constraints is less than the dimension d, the compatibility conditions can be satisfied for any fields in the layers, if the structure is properly chosen. In this case, the quasiconvex envelope coincides with convex envelope, $\mathcal{Q}F = \mathcal{C}F$ which is supported by the fields $v + \xi_i$ that are constant within each well (material).

Let us show the compatibility of the N-well problem in the case when $r < d$

$$\mathcal{Q}F = \mathcal{C}F \quad \text{if } r < d. \tag{22}$$

We show that any N arbitrary fields are compatible in spite of constraints (20). Consider a hierarchical structure of a laminate of $(N-1)$st rank that is the $(N-1)$ times repeated sequential laminate.

First we observe that any two fields v_1 and v_2 are compatible in a simple laminate with specially chosen normal n_1. Indeed, since the number r of linearly independent constraints is less than the dimension d, rank of the matrix B is equal to r. Therefore, the linear homogeneous system (20) always has a solution – a d-dimensional normal n_1 – because the rank of B is smaller than d. Next, we replace the two fields with an average field v_{12} treating them as a homogeneous field in a new composite material. Then we make the field v_{12} in this laminate compatible with the third field v_3 using

the second-rank laminate structure and choosing its normal n_2. This can be done asymptotically if the width of the new layers is much larger than the width of the layers in the first two materials. Continuing the process, we build a laminate of $(N-1)$st rank that contains N arbitrary fields and the conditions (21) are satisfied. Finally, the convex envelope of N-well potential is supported by at most N fields. Since these fields are compatible in the constructed laminate structure, they also represent a minimizer of the constrained problem – the quasiconvex envelope.

The structure of the described laminate is nonnunique if more than two phases are mixed together. Indeed, one can combine the fields in a different sequence; correspondingly, the normals will be different. Similarly to a simple laminate which is the simplest structure for two-well potentials, the nonunique $(N-1)$th rank laminate is a basic element for problems with the multi-well potentials. Particularly, the relaxation of any nonconvex Lagrangian $L(\nabla u)$ that depends on a gradient of a scalar u (curl-free minimizer) or on one or two divergence-free fields $L(j_1, j_2)$, $\nabla \cdot j_1 = \nabla \cdot j_2 = 0$ is done by constructing a convex envelope of the Lagrangian which coincides with the quasiconvex envelope because (22) holds.

Laminates and minimizing sequences If the number of constraints is larger than dimension, $r \geq d$ (as it is in elastic fields), arbitrary constant fields $v + \xi_i$ cannot be compatible. In this case, the quasiconvex envelope is not smaller than the convex envelope, $\mathcal{Q}F(v) \geq \mathcal{C}F(v)$ but is still not larger than the function itself, $\mathcal{Q}F(v) \leq F(v)$. In order to compute an upper bound of the quasiconvex envelope, we still can minimize the energy over parameters of k-rank-laminate structures. The minimizers are the explicit geometrical parameters of the laminate. Fields inside the layers are constant and the explicit calculations of them is possible. This alone makes the laminates an attractive tool. The minimum of the Lagrangian over all laminates is called the laminate closure (see below, Section 2.2). It is not known yet for what Lagrangians the laminate closure coincides with the quasiconvex envelope. There are numerous examples of such coincidence starting from [52, 78]; however, there are counterexamples, see Sverak [80] and Milton [63] (where the elasticity problem is addressed). The laminate technique is even used for complicated models of materials with time-dependent properties, as in recent paper [50] by Lurie.

Laminates from linear materials The laminate technique is well developed for piece-wise quadratic energies that correspond to piece-wise linear constitutive equations. In this case, effective properties of laminates are explicit tensor-functions of constituent materials, their fractions m_i, and the normal n to the layers; they are independent of the fields in the structures.

Consider a laminate from two phases with the energies

$$W_1(v) = \frac{1}{2} v^T D_1 v + \gamma_1 \text{ and } W_2(v) = \frac{1}{2} v^T D_2 v + \gamma_2$$

where D_1 and D_2 are the matrices of properties, γ_1 and γ_2 are the costs of materials, and v is a vector of the fields. Introduce the subspace q on the discontinuous components of v in a laminate with the normal $n = (n_1, \dots, n_d)$. The subspace q of discontinuous components of v is spanned by all vectors q_i orthogonal to the continuous components of v

$$q^T p = 0, \quad \text{where } p = \{p_{ij}\} : \quad \left\{ p_{ij} = \sum_{k=1}^{d} a_{ijk} n_k \right\}. \tag{23}$$

The vector qv is discontinuous on the boundary with the normal n while vector pv stay continuous.

One can show [20] that the laminate corresponds to the Lagrangian

$$W_0(v) = \min_{m_1 \in [0,1]} \left[\frac{1}{2} v^T D_{\text{lam}}(n, m_1, D_1, D_2) v + m_1 \gamma_1 + (1 - m_1)\gamma_2 \right]$$

where D_{lam} is the effective tensor of the laminate that depends on the mass fractions m_1 and $m_2 = 1 - m_1$ of materials in it, normal n to laminates, and properties D_1 and D_2 of the mixed materials as following

$$\begin{aligned} D_{\text{lam}}(n, m_1, D_1, D_2) &= m_1 D_1 + m_2 D_2 \\ &\quad - m_1 m_2 \left(D_1 - D_2\right) H \left(D_1 - D_2\right) \qquad (24) \\ H(m, q, D_1, D_2) &= q \left(q^T (m_2 D_1 + m_1 D_2) q \right)^{-1} q^T, \qquad (25) \end{aligned}$$

The dependence on normal enters the formula through the dependence (23) of $q = q(n)$.

In order to obtain tensor D^k_{lm} of effective properties of laminates of the kth rank, the iterative operation is used,

$$D^{(k)}_{\text{lm}}(n_k, m_1) = D_{\text{lam}} \left(n_k, m_k, D^{(k-1)}_{\text{lm}\,(1)}, D^{(k-1)}_{\text{lm}\,(2)} \right), \tag{26}$$

where $D^{(k-1)}_{\text{lm}\,(1)}$ and $D^{(k-1)}_{\text{lm}\,(2)}$ are two laminates obtained at the previous $(k-1)$st iteration and function D_{lam} is defined in (24). The two laminates $D^{(k-1)}_{\text{lm}\,(1)}$ and $D^{(k-1)}_{\text{lm}\,(2)}$ correspond to two different sets of structural parameters: normals and volumer fractions of phases. The resulting structures with explicitly known properties are the laminates of kth rank. Optimization of the properties of these structures over the volume fractions and normals on each iteration leads to an upper bound of the quasiconvex envelope, or to the laminate closure.

Special structures: Matrix laminates Formula (26) is especially simple when the obtained on each step composite is laminated k times with the pure phase D_1. In this case, a matrix of layers of D_1 is enveloping the kernel D_2; the structure is called *matrix laminate* of k-rank [20], its effective properties tensor D_{ml} is

$$D_{ml} = D_1 + m_2 \left((D_2 - D_1)^{-1} + m_1 P_k \right)^{-1} \tag{27}$$

where

$$P_k = \sum_{i=1}^{k} \alpha_i q_i \left(q_i^T D_1 q_i \right)^{-1} q_i^T \tag{28}$$

and α_i are nonnegative parameters such that

$$\alpha_i \geq 0, \quad \sum_{i=1}^{k} \alpha_i = 1. \tag{29}$$

The energy of these or otherwise specialized laminates provides a computable upper bound of the quasiconvex energy. Moreover, it was shown that this bound is exact for several problems, such as G-closure of two conducting phases, [51–53], the optimal elastic composite of maximal and minimal stiffness, suggested in [35, 36], and developed in [1, 2, 9, 10] the optimal composite that minimizes a sum of energies of several loadings [5, 28, 31]. The iteration of the scheme leads to nesting sequence of multiply coated structures that are optimal in a problem of coupled bounds, [21, 25]. In these problems, the upper bound coincides with an independently obtained lower bound (see below, Section 4)

2.2. LAMINATION CLOSURE

The lamination closure consists of all tensors that can be obtained by sequential laminates of an arbitrary order. The boundary of the closure can be described as a minimal set of tensors that includes the stiffness tensors of the original materials and stays convex under a class of transformations. It was studied in many papers starting from Francfort and Milton [30], Milton [61], see also a recent development in [20, 63].

The constitutive equations for laminates with a fixed normal can be solved (see [6]) for the discontinuous components of stresses and strains,

$$\begin{pmatrix} t \cdot \sigma \cdot t \\ n \cdot \sigma \cdot t \\ n \cdot \epsilon \cdot n \end{pmatrix} = \mathcal{T}_n(C) \begin{pmatrix} n \cdot \sigma \cdot n \\ t \cdot \sigma \cdot n \\ t \cdot \epsilon \cdot t \end{pmatrix} \tag{30}$$

After this transform, the effective coefficients of laminates $\mathcal{T}_n(C_{\text{lam}})$ with a fixed normal n can be described as a convex envelope stretched on the matrices $\mathcal{T}_n(C_i)$ of the coefficients of the original materials C_i,

$$\mathcal{T}_n(C_{\text{lam}}) = \sum_i m_i \mathcal{T}_n(C_i)$$

because the vector in the right-hand side of (30) is constant in the laminate structure. The lamination closure $\mathcal{L}C$ of the set of stiffness tensors C_i of the original materials is the minimal set of tensors C that (i) results in convex set of transforms $\mathcal{T}_n(C)$ for any normal n and (ii) includes the tensors C_i,

$$\mathcal{T}_n(C)|_{C\in\mathcal{L}c} \text{ is convex } \forall n, \quad C_i \in \mathcal{L}C$$

The procedure of explicit calculation of lamination closure is complicated unless the additional restrictions on the geometry are imposed, see for example [30], [60] [61], [46] or the asymptotics are considered, as in [65].

2.3. DIFFERENTIAL SCHEMES AND CONTROL PROBLEM

Differential scheme The rank of laminates can be infinite. In this case, effective properties are found using the so-called differential scheme. Differential scheme further restricts the class of laminates but allows for formulation of a regular control problem. It was used starting from Bruggeman [14, 15], developed by Norris [74], Lurie and Cherkaev [55], Avellaneda [3], Hashin [40], and other authors.

Assume that an infinitesimal amount of a material is added to a composite in a laminate and consider the variation of effective properties. One can show [20] that the evolution of the effective tensor is described by the tensor-valued differential equation

$$\mu \frac{d}{d\mu}\Delta(\mu) = \Psi(\Delta(\mu), D, n). \tag{31}$$

where $\mu \in (0, 1]$ is the current amount of the materials in the mixture, $\Delta(\mu)$ is the current value of the effective tensor of the material under construction, and $D = D(\mu)$ is the tensor properties of the material added at the "instance" μ. The formula for Ψ can be easily derived from (24) in the form

$$\Psi(\Delta(\mu), D, n) = [(\Delta(\mu) - D) - (\Delta(\mu) - D)H(\Delta(\mu) - D)], \tag{32}$$

where

$$H = q[q^T D q]^{-1} q^T \quad \text{and } q = q(n(\mu)).$$

Functions $n(\mu)$ and $D = D(\mu)$ can be treated as controls. The optimization objective is to minimize the energy $\sigma : D(1) : \sigma$ of the final mixture.

Generalizations The scheme can be easily generalized if we allow to add to the mixture not only pure materials $D(\mu)$ but also a known structures of them, such as the laminates in a smaller scale. In this case, the added material $D(\mu)$ becomes an effective tensor of these structures which is assumed to be a known function of the properties D_i of initially given materials, their volume fractions $c_i = c_i(\mu)$ and the orientation $n_a = n_a(\mu)$. If two-materials laminates are added, the tensor $D(\mu)$ is given by (24), (23) where $m_1 = c_1(\mu)$, $m_2 = 1 - c_1(\mu)$, and $n = n(\mu)$. The formula is naturally generalized if N-phase-laminate is added,

$$D(\mu) = D_{\rm lam}(c_1(\mu), \dots, c_{N-1}(\mu), n_a(\mu)). \tag{33}$$

Remark 2.1 *The differential scheme assumes infinitely many scales of averaging and leads to "physically unrealistic" structures. However, this and similar schemes are used to show the attainability of a homogenized constitutive relations or to find the limiting constitutive relations. From this viewpoint, we should not worry about the realistic character of the microstructures more than about manufacturing Serpinsky gasket.*

The structures obtained by the differential scheme form a subset of lamination closure. The herring-bone-type structures, random laminates, etc. are not included in the scheme, unless it is modified. An obvious modification would allow us to add use more complex structures than simple laminates. At the other hand, the described structures are obtained by a regular differential equation and their variety is easy to describe and optimize.

Optimal control problem Using the differential scheme, one can formulate a regular control problem as in [55]. The problem is: Minimize $\phi(D(1))$ subject to differential constraint (32), the representation (33), and the integral constraints

$$m_i = \int_0^1 c_i d\mu, \quad i = 1, \dots k-1$$

that express the constraints on available amounts of materials.

The controls are: the normal $n(\mu)$ of the laminate at the instance μ, and the characteristics of the added laminate: Its relative volume fractions $c_{ik}(\mu)$ and the normal $\upsilon(\mu)$. Evidently, the added laminate can be replaced by some other known microstructure, including those obtained by the differential scheme itself.

Remark 2.2 *A distinguished feature of this problem is the irreversibility of the mixing. One can show that the constructed optimal structure belongs to the boundary of the G-closure all the time; if it does not, the trajectory can be improved. What is changing is the amounts of the already used materials.*

The solution to this control problem exists and it can be found from either Pontryagin maximum principle or Bellman's dynamic programming. The set of extremal properties obtained by differential scheme is yet another narrowing of the laminate closure that can be called the *sequential-lamination envelope*.

3. Variations and analysis of fields

3.1. STRUCTURAL VARIATION

Structural variations method focuses on evaluation of the fields in optimal structures. This method investigates stability of solutions to a special class of variations. An optimal layout may form either a finite or infinitesimally fine structure, but it still consists of the patterns from initially given materials. Variational method characterizes the stress in the materials (phases) within an optimal structure. Basic technique of calculus of variations is used. No assumptions are made about the geometry of microstructures in optimal layouts. To the contrary, the very appearance of microstructures in an optimal design is deducted from analysis of the necessary conditions. The earlier development of structural variations was done by Lurie [48] (see also related approach by Murat [69]); the technique was developed in [59] and in the recent works [16, 17, 20, 43, 45].

Structural variations – Weierstrass-type test Consider again the problem (11) of optimal layout of several materials in the domain Ω that minimizes the energy of the elastic equilibrium. The finite number of given materials requires special variational technique because the variation of the properties caused by interchanging of the materials are finite, not infinitesimal. The only small parameter is the measure of the support of the variation.

Consider the following local variation. Place an infinitesimal inclusion of one of the admissible materials $C_{\rm incl}$ into an arbitrary interior point of the domain Ω_H of the host material $C_{\rm host}$. Alternatively, place a dilute matrix-laminate composite (27) made of the material $C_{\rm host}$ (the matrix) and an infinitesimal fraction of the material $C_{\rm incl}$ (the inclusions). Then, perform the following calculations:

(i) Compute the perturbation of the fields and the increment of the objective functional – energy. To compute the increment we may either use modified Eshelby-type formulas [68] or simply compute effective properties of a dilute matrix-laminate structure (27) when the volume fraction of the inclusions becomes infinitesimal. The corresponding formula for the variation δD of average properties follows from (23) when $m_2 = \delta m \ll 1$

$$\delta D = \Big((D_{\rm host} - D_{\rm incl})^{-1} + P_k(D_{\rm incl}, n, \alpha) \Big)^{-1} \delta m.$$

Here δm is the infinitesimal volume of the inclusion, and the term $P_k(D_{\rm incl}, n, \alpha)$ is defined in (28) where one puts $D_1 = D_{\rm incl}$.

Applied to the stress energy W_σ, The increment δW_σ of the energy becomes

$$\delta W_\sigma = \frac{1}{2}\sigma : (\delta S) : \sigma\, \delta m + o(\delta m). \tag{34}$$

The increment δJ of the objective is equal to

$$\delta J = \delta W_\sigma + (\gamma_{\rm incl} - \gamma_{\rm host})\delta m + o(\delta m)$$

where the second term accounts for the difference in costs of the materials.

(ii) Next, the increment δW_σ in (34) is maximized by choosing the "most dangerous" variations, that is by choosing structural parameters $\alpha_1, \dots, \alpha_k$ and $n_1, \dots, n_k$. (Here we follow the method suggested by Lurie in [48]). These parameters enter the problem through term $P_k(D_{\rm incl}, n, \alpha)$ (see (28)) that represents the shape and orientation of the inclusions. The resulting *most dangerous* variation

$$\Delta(\sigma, D_{\rm host}) = \max_{n,\alpha}\ \delta J, \quad \alpha = \{\alpha_1, \dots, \alpha_k\}, \quad n = \{n_1, \dots, n_k\} \tag{35}$$

depends only on the field σ at the point of the subdomain $\Omega_{\rm host}$ where the inclusion is inserted.

Remark 3.1 *If the number of available materials is greater than two, we generalize the variation scheme by allowing more complex inclusion such as a laminate composite of several materials and maximize the increment by the composition of $D_{\rm incl}$; in this case, the cost $\gamma_{\rm incl}$ of the inclusion becomes*

$$\gamma_{\rm incl} = \sum_m \beta_m \gamma_m$$

where γ_m is the cost of mth material in the composition, and β_m is its volume fraction in the inclusion. If the composite inclusions are used, $\Delta(\sigma, D_{\rm host})$ is the result of maximization of the increment over the structural parameters and the composition of the inclusion.

Remark 3.2 *One can argue that an optimal structure could be a never-ended sequence of embedded laminates, or similar fractal structure, see [4], [13] and there is no solid neighborhood of a material to put the inclusion in. However, this sequence is a result of an asymptotic process and the inclusion can be smaller that the domain of a pure phase; its size should go to zero faster than the size of the domain. The fields in materials are defined almost everywhere except of the points of accumulation; correspondingly, the conditions could be applied almost everywhere.*

3.2. ANALYSIS OF OPTIMALITY CONDITIONS

Increment $\Delta(\sigma, D_{\text{host}})$ of an optimal configuration is nonnegative for all trial inclusions, therefore the uniform in x inequality holds

$$\Delta(\sigma, D_{\text{host}}) \geq 0 \quad \forall x \in \Omega_{\text{host}}.$$

Indeed, if the increment can be made negative by inserting an inclusion to the design, the layout is not optimal and the variation improves it.

Solving the optimality conditions $\Delta(\sigma, D_{\text{host}}) \geq 0$ for σ, we obtain inequalities for the region $\mathcal{V}_{\text{host}}$ of optimality of the tested material in the form

$$\sigma_{\text{host}} \in \mathcal{V}_{\text{host}} \quad \text{if } D = D_{\text{host}}.$$

The procedure is repeated for all given materials. This way, we construct the sets $\mathcal{V}_1, \ldots, \mathcal{V}_n$ where field σ in the corresponding materials satisfies the optimality conditions. If the materials are isotropic, these sets depend only on invariants of the fields σ. Notice that the optimality conditions assume the form of inequalities. This feature is expected because the set $D_1, \ldots, D_N$ of values of the controls consists of several isolated points.

The detailed analysis of the optimal fields in optimal conducting [20] and elastic [16, 17] designs reveals the following properties of two-material mixtures (two-well Lagrangian) from linear elastic materials: Strong and expensive material C_1 is never understressed. A norm $\mathcal{N}_s(\sigma)$ of the stress in the strong and expensive material in an optimal structure is bounded from below:

$$\mathcal{N}_s(\sigma) \geq \eta_s(C_2, C_1, \gamma_2 - \gamma_1), \quad \text{if } \sigma \in \mathcal{V}_1 \tag{36}$$

Similarly, weak and cheap material C_1 is never overstressed: In an optimal structure, a norm $\mathcal{N}_w(\sigma)$ of the stress tensor in that material is bounded from above

$$\mathcal{N}_w(\sigma) \leq \eta_w(C_1, C_2, \gamma_1 - \gamma_2), \quad \text{if } \sigma \in \mathcal{V}_2 \tag{37}$$

Satisfaction of these necessary conditions is equivalent to the requirement that a norm of the field is each material is uniformly bounded everywhere in the optimal design.

We show the expressions for $\mathcal{N}_w$ and $\mathcal{N}_s$ assuming for simplicity in formulas that the Poisson ratios in the materials equal zero. These conditions are as follows: The eigenvalues σ_1, σ_2 of the stress field in the weak material belong to the intersection of two elliptic neighborhoods of zero,

$$\mathcal{N}_w(\sigma) = \min\{\alpha\sigma_1^2 + \beta\sigma_2^2,\ \alpha\sigma_2^2 + \beta\sigma_1^2\}$$

where $\alpha_1 > 0$, $\alpha_2 > 0$, and $\eta_w > 0$ are the constants that depend only on the material's properties of the inserted and the host materials, see [16].

The eigenvalues of the stress tensor in the strong material lie outside of the convex envelope of the ellipses,

$$\mathcal{N}_s(\sigma) = \mathcal{C}\left\{\frac{\sigma_1^2}{\alpha} + \frac{\sigma_2^2}{\beta},\ \frac{\sigma_2^2}{\alpha} + \frac{\sigma_1^2}{\beta}\right\}$$

where η_s depends on the material's properties. Sets $\mathcal{V}_1$ and $\mathcal{V}_2$ are dual.
Forbidden region There is a nonempty supplement $\mathcal{V}_{\rm frb}$ to sets $\mathcal{V}_1$ and $\mathcal{V}_2$ where none of the materials is optimal. This is the region where the quasiconvex envelope of the Lagrangian is strictly less than the Lagrangian itself. If the applied average field $\langle\sigma\rangle$ belongs to this region, the pointwise field splits into several pieces σ_i, each in an allowed region $\mathcal{V}_i$,

$$\langle\sigma\rangle = \sum_i c_i\sigma_i, \quad \sigma_i \in \mathcal{V}_i, \quad \langle\sigma\rangle \in \mathcal{V}_{\rm frb}. \quad c_i \geq 0, \quad c_1 + \ldots c_N = 1$$

and the optimality conditions are satisfied in every point. Because of this split, the structure appears that sends the point-wise fields in the materials away from the forbidden region $\mathcal{V}_{\rm frb}$. This phenomenon explains appearance of composites in optimal structures. In the optimal composite zone, the stresses inside the materials belong to the boundaries of the $\mathcal{V}_i$ sets everywhere, while the mean stress belongs to the forbidden region. An optimal structure adjusts itself to the stress conditions by varying volume fractions of the phases and the normals to the boundaries.

Necessary conditions and optimal microstructures The optimality conditions (36) and (37) also explain the infinitesimal scale of alternations. Indeed, we expect that the stress in each material remains on the boundary of its permitted regions in some subdomains Ω_w^+ and Ω_s^+ of the design domain Ω. In these subdomains, the stress field satisfies the elasticity equations and, in addition, the conditions

$$\begin{array}{ll} \mathcal{N}_s(\sigma) = \eta_s & \text{if } x \in \Omega_s^+, \\ \mathcal{N}_w(\sigma) = \eta_w & \text{if } x \in \Omega_w^+. \end{array} \tag{38}$$

The last conditions overdetermine the system for the stress and cannot be satisfied in the domains Ω_w^+ and Ω_s^+ with nonzero interiors. Indeed, the stress of any fixed layout is uniquely determined from the elasticity equations; varying the division line between phases, one can enforce the equalities (38) along some lines but not everywhere in a domain with nonzero interiors. To solve this contradiction we suggest that the domains Ω_w^+ and Ω_s^+ of finite measures are divided by a dense (fractal-type) boundary that passes infinitely close to each point in these domains. This means the appearance of a microstructure in an optimal design.

The fields in different materials within the structure belong to the disconnected sets $\mathcal{V}_i$ that surround the forbidden region; in the same time, they are competitive with each other, which means that the equations

$$n \cdot [\sigma_a - \sigma_b] \cdot n = t \cdot [\sigma_a - \sigma_b] \cdot n = t \cdot [S_a\sigma_a - S_a\sigma_b] \cdot t = 0, \quad \sigma_a \in \mathcal{V}_a,\ \sigma_b \in \mathcal{V}_b$$

hold on the dividing line. Here the indices a and b denote the neighboring materials. The jump over forbidden region $\mathcal{V}_{\text{frb}}$ is only possible if the normal n to the dividing surface is specially chosen or composite has a special microstructure. Particularly, one can check that the norms of the fields in the first and the second materials in laminates and in second-rank orthogonal laminates belong to the boundaries of their sets $\mathcal{V}_1$ and $\mathcal{V}_2$ if structural parameters are optimally adjusted to the applied field σ. The structural parameters are: the orientation of the layers and their fraction(s). When the applied field varies, the norms $\mathcal{N}_1$ and $\mathcal{N}_2$ stay constant. The same is true (see [20]) for the Hashin-Shtrikman coated spheres structures [41] that are optimal if the external stress is isotropic.

Three-dimensional optimal structures The analysis can be extended to a three-dimensional case, see [17]. The permitted regions are similar: The eigenvalues of the optimal stress in the weak material correspond to the intersection of three oblate spheroids, $\mathcal{N}_w \le \eta_w$ where

$$\mathcal{N}_w(\sigma) = \min\left\{\alpha(\sigma_1^2 + \sigma_2^2) + \beta\sigma_3^2,\ \alpha(\sigma_2^2 + \sigma_3^2) + \beta\sigma_1^2,\ \alpha(\sigma_3^2 + \sigma_1^2) + \beta\sigma_2^2\right\}.$$

In each point, stress belongs either to surface of a spheroid, or to the line of intersection of two spheroids, or to a point of intersection of all three of them.

The permitted region for the eigenvalues of the stress in the strong material corresponds to the convex envelope stretched on the three larger prolate spheroids dual to the first ones, $\mathcal{N}_s \ge \eta_s$

$$\mathcal{N}_s(\sigma) = \mathcal{C}\left\{\frac{\sigma_1^2 + \sigma_2^2}{\alpha} + \frac{\sigma_3^2}{\beta},\ \frac{\sigma_2^2 + \sigma_3^2}{\alpha} + \frac{\sigma_1^2}{\beta},\ \frac{\sigma_3^2 + \sigma_1^2}{\alpha} + \frac{\sigma_2^2}{\beta}\right\}.$$

This envelope consists of the parts of original spheroids, the cylindrical surfaces between pairs of them, and a plane triangle supported by three symmetric points of the three ellipsoids. The two norms are dual.

The constraints on the optimal three-dimensional stress field matches the variety of optimal structures independently found in [33], [1] in which the necessary conditions are satisfied as equality pointwise. It is shown that the optimal structures are the matrix laminates of third rank, that can degenerate into second-rank laminates and further into simple laminates. Optimal simple laminates correspond to the fields in both phases

that belong to the boundaries of spheroids of the permitted fields. Optimal second-rank cylindrical matrix laminates correspond to a field in the weak material that belongs to the intersection of two spheroids, and to a field in the strong material that belongs to the cylindrical part of complex envelope stretched on two spheroids. Optimal third-rank matrix laminates correspond to an isotropic constant field in the weak material that belongs to the intersection of all three spheroids, and a field in the strong material that belongs to the flat part of the complex envelope stretched on three spheroids. This analysis again shows the duality of the structures and fields in optimal micro-geometries.

Types of optimal micro-geometry in three-material composites Three-material mixtures can be optimal only if the cost of the intermediate material is accurately chosen, see [20]. The too expensive intermediate material never enters the optimal composition, and the too cheap material will be used together with the worst and the best materials, but not with these two together.

The region of permitted fields in the intermediate material lies between the permitted regions of outside materials; therefore the norm of the intermediate material in an optimal mixture is distanced from both zero and infinity. This implies that the three materials in an optimal structure cannot meet in an isolated point because then the norm of fields in all material would go either to zero or to infinity in the proximity of this point. We conclude that either the three materials never meet in an optimal microstructure because two of them are inclusions in the third one, or they meet in a dense set of points as in laminate of the second rank.

Suboptimal projects The necessary conditions technique allows to evaluate suboptimal designs, see [16]. The optimality is naturally expressed through the fields in materials, not through the microstructure which can be nonunique and which parameters are hard to quantify. Checking the fields in a design, we can find out how close these fields are to the boundaries of the permitted regions $\mathcal{V}_i$ and conclude about suboptimality of the design. In a suboptimal structure, the fields in phases do not always belong to the regions $\mathcal{V}_i$ but one can measure the norm of the distance between the actual field and its region of optimality $\mathcal{V}_i$ and judge about the closeness of a design to the optimal one. The ability to quantify suboptimal projects is specific for this method and cannot be extended to the laminate technique.

3.3. MINIMAL EXTENSION

The structural variation methods allows us to construct an upper bound of the quasiconvex envelope of the Lagrangian obtained by the *minimal extension* procedure, [20]. The minimal extension provides a Lagrangian that is stable to a specified class of variations. As other variational methods, the extension is based on an *a priori* assumptions about the class of used variations, therefore it does not result in a "final" or universal extension.

Minimal extension $\mathcal{S}F(\sigma)$ is the maximal function that is smaller than the original Lagrangian $F(\sigma)$,

$$\mathcal{S}F(\sigma) \leq F(\sigma) \quad \forall \sigma$$

and cannot be improved by any local variations,

$$\min_{variation} \delta_{\text{local}} \left(\int_\Omega F(\sigma) dx \right) = 0$$

In other words, the extended Lagrangian $\mathcal{S}W(\epsilon)$ has the following properties:
(i) It preserves the cost of the variational problem (3);
(ii) It leads to a stationary solution defined for all fields (including those in the forbidden region), which cannot be improved by the class of considered variations.

Remark 3.3 *The last property distinguishes the minimal extension from quasiconvex envelope. The quasiconvex envelope is the maximal Lagrangian that is smaller then the original Lagrangian and corresponds to a solution that cannot be improved by any local variations. The definition of minimal extension softens the last requirement by specifying the class of trial local variations, thus making the extension computable by a regular procedure. In other words, the quasiconvex envelope is a limit of the minimal extension when the class of variations includes "everything".*

Let us illustrate the approach on the same problem of optimal mixture of two linearly elastic materials. It is convenient to represent *extended Lagrangian* $\mathcal{S}W(\sigma)$ in the form

$$\mathcal{S}W(\sigma) = \frac{1}{2}\sigma : S_{\text{extd}} : \sigma + \gamma_{\text{extd}}, \quad S_{\text{extd}} = S_{\text{extd}}(\sigma). \tag{39}$$

Here $S_{\text{extd}}(\sigma)$ is a tensor of properties that depends on σ. The tensor S_{extd} can be interpreted as an anisotropic compliance tensor of composite, made of initially given materials. The structure of the optimal composite and its effective tensor S_{extd} varies together with the external field σ. The compliance S_{extd} and the cost γ_{extd} must be chosen so that no structural variation

can improve the cost of the variational problem and that the most dangerous variation leaves the cost unchanged. The cost term of the extension accounts for composition of the mixture

$$\gamma_{\text{extd}} = \sum_{i=1}^{N} m_i \gamma_i. \tag{40}$$

When the mean field σ belongs to one of the permitted regions $\mathcal{V}_i$, the extended Lagrangian $\mathcal{S}W(\sigma)$ coincides with the original Lagrangian:

$$\mathcal{S}W(\sigma) = W(\sigma) \quad \forall \sigma \in \mathcal{V}_i,\ i = 1, \dots, P.$$

or

$$S_{\text{extd}} = S_i, \quad \gamma_{\text{extd}} = \gamma_i \quad \forall \sigma \in \mathcal{V}_i,\ i = 1, \dots, P.$$

When the mean field σ belongs to the forbidden region $\mathcal{V}_{\text{frb}}$ we define the extended Lagrangian (the tensor S_{extd}) from the requirement that no structural variation improve the objective and the most "dangerous" variation keeps the objective unchanged.

The scheme is as follows: A trial inclusion from the given materials or their composition is inserted in the unknown optimal material $S_{\text{extd}}(\sigma)$ that corresponds to the field $\sigma \in \mathcal{V}_{\text{frb}}$. We call the extension neutral with respect to the variation if

$$\Delta_{\text{extd}}(\sigma, S_{\text{extd}}) = 0 \quad \forall \sigma \in \mathcal{V}_{\text{frb}} \tag{41}$$

where Δ is the maximal increment computed as in (35). The *condition of neutrality* (41) implicitly determines the optimal tensor $S_{\text{extd}}(\sigma)$ and the extended Lagrangian.

Thus, the minimal extension $\mathcal{S}W$ of the Lagrangian W is defined by a variational inequality:

$$\begin{array}{lll} \mathcal{S}W(\sigma, S_{\text{extd}}) = W_i(\sigma), & \Delta_{\text{extd}}(\sigma, S_{\text{extd}}) \geq 0, & \forall \sigma \in \mathcal{V}_i, \\ \mathcal{S}W(\sigma, S_{\text{extd}}) \leq W_i(\sigma), & \Delta_{\text{extd}}(\sigma, S_{\text{extd}}) = 0, & \forall \sigma \notin \cup \mathcal{V}_i \end{array}$$

Remark 3.4 *Applied to one-dimensional variational problems, a similar scheme of minimal extension results in an extension equal to the convex envelope of the Lagrangian. Assuming that the extension is based on Weierstrass variation instead of the structural variation, it is easy to check that the extension is equal to the convex envelope $\mathcal{C}_v L(x, u, v)$ of the Lagrangian $L(x, u, u')$.*

In the multivariable case, the described extension gives an upper boundary of the "final" extension (the quasiconvex envelope of the Lagrangian) which may or may not coincide with it. An example of exact extension given

in [20]. At the other hand, one could think of a wider class of variations that could lead to another extension with larger $\Delta(\sigma)$.

4. Bounds and duality

4.1. VARIATIONAL PROBLEMS AND BOUNDS FOR EFFECTIVE PROPERTIES

The sets of the effective properties of all possible structures from given materials is called the G-closure of the set of these materials. To obtain the bounds for effective properties, we consider variational problems of energy minimization by a periodic layout.

Bound related to the energy minimization The first problem is minimization of the energy of an affine external field is applied to the structure. Assume for definiteness that the strain energy $W_\epsilon(C(\chi), \epsilon)$ is minimized. The energy $W_\epsilon(C(\chi), \epsilon)$ of a periodic layout equals to the energy of the equivalent homogeneous material (composite),

$$\langle W_\epsilon(C(\chi), \epsilon)\rangle = W_\epsilon(C_*, \langle\epsilon\rangle) \tag{42}$$

and defines the effective properties tensor C_* as the coefficients in the right-hand side of (42).

In order to constrain the set of tensors C_*, we find a lower bound for the energy of the type

$$W_\epsilon(C(\chi), \epsilon) \geq \mathcal{B}_\epsilon(C_B, \langle\chi_i\rangle, \langle\epsilon\rangle), \quad \forall\epsilon \quad \forall\chi$$

where $\mathcal{B}$ is an explicit function of the mean field $\langle\epsilon\rangle$ and volume fractions $m_i = \langle\chi_i\rangle$. One can show that $\mathcal{B}$ is a second-degree homogeneous function of $\langle\epsilon\rangle$,

$$\mathcal{B} = \langle\epsilon\rangle : C_B\left(\langle\chi_i\rangle, \frac{\langle\epsilon_i\rangle}{\|\langle\epsilon_i\rangle\|}\right) : \langle\epsilon\rangle. \tag{43}$$

In this procedure, the energy of an optimal composite is defined by the quasiconvex envelope of the multiwell Lagrangian and the lower bound should restrict this envelope from below.

Then, we pass from the bounds for an optimal energy to constraints on the range of optimal effective properties tensor and conclude that $C_* \geq C_B$. Tensor C_B depends on invariants of the applied field, see (43). We eliminate this dependence and obtain the G-closure.

Duality and bounds The energy and its estimate are defined up to additive constants. To deal with this uncertainty, we take into account the dual form

of the energy – the Legendre transform of it. The dual energy has the form

$$W_\sigma(\sigma) = \max_\epsilon \{\epsilon : \sigma - W_\epsilon(\epsilon)\} \tag{44}$$

and it is an involution

$$W_\epsilon(\epsilon) = \max_\sigma \{\epsilon : \sigma - W_\sigma(\sigma)\} \tag{45}$$

the differential constrains (1) on σ and the constraint in (3) on ϵ are also mutually dual. The sum of the energy W_σ and its dual form W_ϵ is equal to the work of applied forces

$$W_\epsilon(\epsilon) + W_\sigma(\sigma) = \epsilon : \sigma$$

and is completely defined. On the other hand, the sum of the quadratic energy and its dual is still a quadratic form of the vector (σ, ϵ) of double dimensionality and can be estimated by the same procedure as a single energy.

Physically, the estimation of two forms of the energy correspond to estimation of the reaction of a structure to two ways of loading. A structure can be loaded by either external tension forces or external elongation, or both: Forces in one direction and elongation in the other. Hence, either the average stress $\langle\sigma\rangle$ or the average strain $\langle\epsilon\rangle$ in a structure are prescribed. The estimate of the strain energy $W\epsilon(\epsilon)$ is expressed thorough the prescribed average strain $\langle\epsilon\rangle$, and the estimate of the dual stress energy $W^*(\sigma)$ – through the prescribed average stress $\langle\sigma\rangle$.

Several loadings To tighten the bounds, we can minimize the sum of energies caused by several mutually orthogonal homogeneous external loadings applied to the periodic structure, which is expressed by the Lagrangian of the type

$$\Pi_\epsilon(\chi, \epsilon_1, \dots, \epsilon_n) = \sum_{i=1}^{n} W_\epsilon(\chi, \epsilon_i))$$

The layout χ remains the same for all loadings; in particular, the jumps of the fields caused by different independent external fields occur at the same dividing surfaces; therefore the pointwise fields in the structures are related. This relation is taken into account by the translation method (described in the next section) that tightens the lower bound for the sum of energies.

A more general minimized quantity $\Pi^{(k)}_{\epsilon\sigma}$ is the sum of the energy of the periodicity cell and its dual form; it has the form

$$\Pi^{(k)}_{\epsilon\sigma} = \Pi_\epsilon(\chi, \epsilon_1, \dots, \epsilon_k) + \Pi_\sigma(\chi, \sigma_{k+1}, \dots, \sigma_n)$$

One must consider several problems of this type for different $k = 0, \ldots, n$ to completely characterize the set of effective coefficients. When the loading varies, the optimal structure varies too; the procedure must be applied for all possible combination of the loadings. The resulting set of coefficients describes the set of effective tensors of the structure that optimally respond to any given loading combination; they form the boundary of the G-closure.

4.2. TRANSLATION METHOD AND DEVELOPMENTS

We show the technique for derivation of lower bounds working on the example of bounding the quadratic strain energy W_ϵ.

Convex envelope and harmonic-mean (Wiener) bound The simplest lower bound for the nonconvex Lagrangian can be obtained by neglecting the differential constraints on the strain field ϵ. Lifting the constraints, we enlarge the set of minimizers and achieve a deeper minimum. If these constraints are lifted, the field becomes constant within each material and the calculation of the minimum of a multiwell Lagrangian becomes elementary algebraic problem; its solution is given by the convex envelope $\mathcal{C}L$ of the Lagrangian L. Because the wells are convex, the convex envelope is supported by at most one point in a well. Therefore the convex envelope $\mathcal{C}W_\epsilon(\epsilon)$ at the point ϵ has the form

$$\mathcal{C}W(\epsilon) = \min_{\epsilon_i, m_i} \sum_i^n m_i W_\epsilon(\epsilon_i) \tag{46}$$

where

$$\sum_i^n m_i = 1, \quad m_i \geq 0, \quad \epsilon = \sum_i^n m_i \epsilon_i$$

and the bound is given by the inequality

$$W_\epsilon(C_*, \epsilon) \geq \mathcal{C}W(\epsilon) \quad \forall C_*. \tag{47}$$

As we mentioned above, this bound is achievable at a laminate structure, if the rank of $a_{ijk}u_j$ is less than d.

For quadratic energies of the type $W(\epsilon) = \frac{1}{2}\epsilon^T D_i \epsilon + c_\epsilon$ where c_ϵ is an undefined constant, the bound is computed to be

$$\mathcal{C}W(\epsilon) = \frac{1}{2}\epsilon^T C_H \epsilon + c_B, \quad C_H = \left(\sum_i m_i C_i^{-1} \right)^{-1} = \langle C_i^{-1} \rangle^{-1} \tag{48}$$

where C_H is a harmonic mean and c_B is an additive constant. Because of arbitrariness of the field ϵ, the above bound implies the inequality

$$C_* \geq C_H$$

known in elasticity as one of the Hill bounds.

Remark 4.1 *The presence of the additive constant c_ϵ in this energy does not poses a problem because the strain fields ϵ can be made arbitrary large and the constant c_ϵ can be neglected. However, in the next problem (Section 4.3) c_B should be eliminated by estimating the sum of energy and its dual form.*

The complementary bound for the effective properties is obtained by the same procedure, estimating the dual energy $W_\sigma = \frac{1}{2}\sigma : S : \sigma + c_\sigma$ where $S = C^{-1}$ is the compliance and c_σ is a constant. It has the form

$$S_* \geq S_H \quad \text{or } C_* \leq \langle C \rangle.$$

Alternatively, one can estimate the sum of these two energies obtaining the above bounds at once and not worrying about the additive constant, because $c_\epsilon + c_\sigma = 0$ due to the duality relations (44), (45).

Improved bounds The bound by a convex envelope can be improved if some relations which follow from the differential constraints (17) are taken into account. Indeed, the vector $\Theta = \{\epsilon_1, \dots, \epsilon_k, \sigma_{k+1}, \sigma_n\}$ combined from components of all fields is not a free vector but relates to the solution of an elasticity problem (2). As such, it is constrained by inequalities of the type

$$\phi\left(\langle\Theta\rangle_1, \dots, \langle\Theta\rangle_n, m_1, \dots, m_n, D_1, \dots, D_n\right) \leq 0 \tag{49}$$

Here, $\langle\ \rangle_i$ is the average field within ith phase, $m_1, \dots, m_n$ are the volume fractions and $D_1, \dots, D_n$ are material properties of the phases.

To obtain the bounds we need to find (prove) inequality that holds for all admissible layouts. This inequality should be nontrivial: It should not hold for arbitrary vectors Θ but for the solutions of the elasticity equations. The inequality (49) must be added to the procedure of estimation of the lower bound (47) with the Lagrange multiplier $t \geq 0$. The bound becomes

$$W\epsilon \geq \max_{t \geq 0} \mathcal{C}(W - \epsilon + t\phi) - t\phi \tag{50}$$

The Hashin-Shtrikman bound [42], the translation bounds [20], and the bound by Nesi [73] are all the examples of such bounds. They all relax pointwise differential constraints by replacing them with integral inequalities.

This technique was implemented to obtain bounds for effective compliance tensor S_* well-studied starting from the classical bounds by Reuss, Voigt, and Hill. The bounds were tighten for isotropic materials by Hashin and Shtrikman [41] and Walpole [83], then these bounds were coupled and further tighten by Berryman and Milton [12] and (for two-dimensional case)

by Cherkaev and Gibiansky in [22]. The coupled bound were obtained exploring the differential constraints on the stress and strain tensors using the translation method [20]. Similar bounds for conducting materials were obtained by by Hashin and Shtrikman, then these bounds were coupled and further tighten by Lurie and Cherkaev [52], [53] and Tartar [81].

The key component of the technique is the inequalities (49). The quadratic in Θ inequalities of the type

$$\langle \Theta^T T \Theta \rangle \le \langle \Theta \rangle^T T \langle \Theta \rangle \tag{51}$$

where T is not nonnegatively defined matrix, can be found either immediately from the divergence theorem, [52] or by using the theory of compensated compactness [26, 62, 70, 71, 81]; numerous examples can be found in [20] and [63]. For example, the quadratic inequalities (51) imposed on the stress and strain tensors in two-dimensional elasticity are

$$\langle \det \sigma \rangle = \det \langle \sigma \rangle, \quad \langle \det \epsilon \rangle \le \det \langle \epsilon \rangle, \tag{52}$$

(the inequality sign in the second relation is due to second-oder differential constraints on ϵ)

Accounting for quadratic inequalities, we get the *translated* bounds of the type

$$W_\epsilon(C_*\epsilon) \ge \frac{1}{2}\epsilon^T C_P \epsilon + c_B, \quad C_P = \left(\sum_{i=1}^{N} m_i (C_i + T)^{-1} \right)^{-1} - T$$

where matrix T satisfy (51) and the inequalities $C_i + T \ge 0$ for all C_i. One can see that the property tensors are translated by matrix T, thereafter comes the name of the method [62]. The known quadratic inequalities (translators) provide the exact bounds that match the lamination closure for a number of two-phase composites. They are too rough to provide exact bounds for multimaterial mixtures but they are sometimes exact even for these problems [66] and and they always improve the harmonic mean bounds.

There is no known technique to regularly derive nonquadratic inequalities for the average fields. The hunt for new translators is a nonregular problem of finding inequalities for the solutions of partial differential equations with periodic piece-wise constant coefficients that are valid independently of the geometry of the structure. A recently found in [73] inequality of such type states that in two-dimensional conductivity problem the determinant of the matrix of gradients of the two solutions does not change its sign anywhere in the periodicity cell. Adding this inequality to the translation bound, Nesi [73] obtained new more restrictive bounds for multimaterial mixtures.

Meanwhile, the technique of the translation bounds is developed in another direction: The bounds for effective properties are applied to various problems. Among these problems are: minimization of the sum of elastic energies in two [5] and three dimensions [31], see also [46], minimization of a functional different from the energy, [19], [67], and compliance minimization in the worst possible scenario of loading [24].

4.3. DUALITY AND BOUNDS FOR EXPANSION COEFFICIENTS

Here, we apply the method to find bounds for the anisotropic effective stiffness and extension tensors of a multiphase composite made of expandable materials, following [18]. These bounds link an anisotropic effective compliance S_* and anisotropic extension tensor α_* of a composite. One meets these problems dealing with composites made of materials that experience phase transition or thermal expansion.

The bounds for expansion coefficients are less developed than bounds for stiffness. The existing bounds [77], [76], [39] deal with the isotropic case, and the bounds by Gibiansky and Torquato [39] are extremely close to the results of numerical optimization by Sigmund and Torquato [79]. The complicated algebraic structure of the isotropic bounds makes their generalization for general anisotropic case not too attractive. In next section, we derive general bounds for the anisotropic thermal expansion tensor which are given by rather elegant tensorial expressions of a clear algebraic structure.

Study of these anisotropic multiphase thermal expansion is important for applications because most composites (for instance, laminates) are anisotropic. The bound for anisotropic expansion coefficients estimates the maximum and minimum of the effective expansion in any direction; they can be used in structural optimization.

Composite from expanding phases An expandable material subject to a transformation impact and an elastic load. The constitutive relation for such a material is described as

$$\epsilon = S : \sigma + \alpha, \quad \nabla \cdot \sigma = 0, \quad \nabla \times (\nabla \times \epsilon)^T = 0 \tag{53}$$

The expansion tensor α is a symmetric second rank tensor of deformation due to the temperature change or the phase transition. In thermal elasticity, α is proportional to the temperature change; equation (53) is normalized with this respect (the temperature change is equal to one). For isotropic thermal-elastic materials, α is a spherical tensor; for materials under austenite-martensite transformation, α is close to a deviator (tracefree) tensor. The form of α_* in a composite is unknown.

We want to bound the range of effective tensors, knowing only properties of the phases and their volume fractions in the mixture. The energy of an expandable material can be presented in two mutually dual forms

$$W_\epsilon(C,\Gamma,\epsilon)=\frac{1}{2}\epsilon:C:\epsilon+\epsilon:\Gamma+c_v,\quad W_\sigma(S,\alpha,\sigma)=\frac{1}{2}\sigma:S:\sigma+\sigma:\alpha-c_p$$

where $\Gamma=-C:\alpha$ is the expansion stress tensor, the constant tensor fully determined by the eigenstrain α and the stiffness tensor C. The difference between the parameters c_v and c_p

$$c_v-c_p=\frac{1}{2}\alpha:C:\alpha$$

can be derived from the duality relations (44). Notice that α enters a lower-order term in the energy which makes the estimation more delicate than the one for the compliance S that determines the main term.

A composite with perfect bonds between phases is characterized by the effective relation between volume averaged stress $\langle\sigma\rangle$ and strain $\langle\sigma\rangle$ that is similar to (53) with tensors S and α being replaced by the tensors of effective moduli S_* and α_*, respectively. The expression for the energy changes accordingly. The effective tensors depend on the moduli and expansion coefficients of the mixed materials and on microstructure, but are independent of the acting fields.

The bounds for the effective moduli are independent of the microstructure; they are represented by the inequalities of the type

$$\mathcal{G}(S_*,\alpha_*,S_{ph},\alpha_{ph},m_{ph})\geq 0$$

where $m_{ph}=\{m_1,\dots m_N\}$ are the volume fractions of the phases in the composite, $S_{ph}=\{S_1,\dots S_N\}$ and $\alpha_{ph}=\{\alpha_1,\dots\alpha_N\}$ are the moduli of the phases. In order to obtain the bound, we deal with the following questions: (i) What functional should be estimated? (ii) What expression bound the functional from below? (iii) How to pass from the bound for the functional to the bounds for the effective coefficients? (iv) What are the bounds when void is present in the mixture?

The method We estimate the sum $W_\sigma+W_\epsilon$ of the energy and its dual form from below by using the translation method. Namely, we neglect the differential constraints in (53) replacing them with inequalities of the type $\langle\sigma:T_\sigma:\sigma\rangle\geq\langle\sigma\rangle:T_\sigma:\langle\sigma\rangle$ which are considered as algebraic constraints. Here, T_σ is the matrix translator (for explicit form of T, see (52)). Matrix T_σ is nonpositive defined and it provides the above inequality due to differential

constraints on the field σ. The minimization problem becomes algebraic, and the standard minimization procedure yields to the inequality

$$W_\sigma(S_*,\alpha_*,\langle\sigma\rangle)+W_\epsilon(C_*,\alpha_*,\langle\epsilon\rangle)\ge\frac{1}{2}\Theta^T P_B\Theta+q_B^T\Theta+r_B,\quad\forall\Theta=(\langle\sigma\rangle,\langle\epsilon\rangle)^T \tag{54}$$

where the tensors $P_B=P_B(m_{ph},C_{ph})$ and $q_B=q_B(m_{ph},C_{ph},\alpha_{ph})$ of the fourth and second rank, respectively, and the constant $r_B=r_B(m_{ph},C_{ph},\alpha_{ph})$ are explicitly calculated. The left-hand side of the (54) is also a quadratic function of averaged fields $\Theta=[\langle\sigma\rangle,\langle\epsilon\rangle]$ which coefficients are effective properties C_*,α_* of the composite. Eliminating the dependence of Θ, we obtain the bounds for the effective properties as it is described below.

New bounds The inequality (54) yields to the following inequalities for the effective coefficients. A matrix inequality

$$\begin{pmatrix} S_*+T_\sigma & T_{\epsilon\sigma}\\ T_{\epsilon\sigma} & C_*+T_\epsilon\end{pmatrix}-P_B\ge 0\quad\forall T:\begin{pmatrix} S_i+T_\sigma & T_{\epsilon\sigma}\\ T_{\epsilon\sigma} & C_i+T_\epsilon\end{pmatrix}\ge 0, \tag{55}$$

where $i=1,\dots,N$,

$$P_B=\left\langle\begin{pmatrix} S+T_\sigma & T_{\epsilon\sigma}\\ T_{\epsilon\sigma} & C+T_\epsilon\end{pmatrix}^{-1}\right\rangle^{-1},$$

and $T_{\epsilon\sigma}$ and T_ϵ are the translators similar to T_σ. This inequality is obtained from (54) when $\|\Theta\|\to\infty$. Inequality (55) estimates the leading term in the energy; it does not depend on α_{ph} and coincides with the translation bound for the effective elastic tensor. It contains, as particular cases, the Hill bounds and the Hashin-Shtrikman-Walpole bounds for isotropic S_*. Notice that tensorial inequality (55) for the sum of energy and its dual naturally includes lower bounds for S_* and C_* and coupling between them.

The range of α_* is determined by the scalar inequality

$$(\alpha_*-\alpha_E(T)):P_E(S_*,T):(\alpha_*-\alpha_E(T))\le r_E(T)\quad\forall T\text{ as in (55)} \tag{56}$$

where explicitly calculated coefficients: fourth-rank tensor P_E, the second-order tensor α_E, and the scalar r_E depend on the properties of the phases, volume fractions, effective tensor S_*, and translator $T\sigma$. It is obtained from the requirement that the minimum of the difference $d(\Theta)$ between the left- and right-hand sides of (54) over Θ is nonnegative for all Θ. We compute the minimum of the quadratic $d(\Theta)$ over Θ and exclude Θ. The bounds are independent of the structure of a composite and depend only on the moduli of the phases and their volume fractions. The bounds for S_* are independent of the extension tensors of the phases, but the bounds for α_*

depend on the compliance and expansion coefficients of the phases and on the effective compliance tensor S_* of a composite.

For each admissible tensor T, the coefficients of the effective tensor α_* are bounded by an ellipsoid centered at $\alpha_E(T)$, and the bound (56) states that they belong to the intersection of all such ellipsoids.

Special cases The results for the mixtures with voids are easily obtained. This case poses difficulties for previously suggested bounds, see [79]. In this case, the coefficients in (56) are simplified to

$$P_E = \left(\tilde{S}_* - \langle \tilde{S}^{-1}\rangle^{-1}\right)^{-1}, \quad \alpha_E = -\langle \tilde{S}^{-1}\rangle^{-1} : \langle \Gamma\rangle,$$
$$r_E = \langle \Gamma^T : S : \Gamma\rangle - \langle \Gamma\rangle : \langle \tilde{S}^{-1}\rangle^{-1} : \langle \Gamma\rangle$$

where $\tilde{S} = S + T_\sigma$ and $\Gamma = -S^{-1}\alpha$.

The previously obtained bounds by Schapery [77], Rozen and Hashin [76], and Gibiansky and Torquato [39] follow from our bounds. Particularly, for the two-phase mixtures, the constant r_E vanishes which leads to the explicit relation $\alpha_* = \alpha_E$, which agrees with the result by Rozen and Hashin [76]. If the effective tensor S_* approaches its bound, some eigenvalues of tensor P_E go to infinity and the effective expansion coefficients tends to the coefficients of α_E, which agrees with the result by Gibiansky and Torquato [39].

4.4. DUALITY AND BOUNDS FOR VISCOELASTIC MATERIALS

Reformulation of a saddle problem The duality and the Legendre transform allows to reformulate several minimax variational problems as minimal problems and to establish new minimal variational principles. In turn, these principles permit applying the translation method technique. For example, the translation bounds for a viscoelastic material tensors were established in [23]. When a viscous-elastic material is subject to a harmonic excitation, its state is described by equations of complex elasticity which look exactly as the usual elasticity equations but the fields and properties are complex-valued tensors. The real part and imaginary parts C' and C'' of this tensor represent the stiffness and viscosity of a material.

The approach is based on an observation that the real and imaginary part of complex elasticity equation can be viewed as the Euler equation for a minimax variational problem with a quadratic Lagrangian

$$L(\epsilon', \epsilon'') = \frac{1}{2}\begin{pmatrix}\epsilon' \\ \epsilon''\end{pmatrix}^T \begin{pmatrix} C' & C'' \\ C'' & -C'\end{pmatrix}\begin{pmatrix}\epsilon' \\ \epsilon''\end{pmatrix} \tag{57}$$

where the symbols $'$ and $''$ denote the real and imaginary parts. The variational problem for the real and imaginary parts of the fields is

$$\min_{\epsilon'} \max_{\epsilon''} \int_\omega L(\epsilon', \epsilon'') dx \tag{58}$$

where ϵ' and ϵ'' satisfy inhomogeneous boundary conditions. Problem (58) is of the min-max type which prevents the immediate use of the technique of bounds.

Performing Legendre transform with respect to the real or imaginary part of the complex field, or with respect to both, one transforms the Lagrangian to one of four forms; two of these forms correspond to minimax problems, and two other correspond to minimal problems for the transformed Lagrangian. The dual with respect to ϵ' form of Lagrangian (57) is

$$L_{\sigma'\epsilon''}(\sigma', \epsilon'') = \frac{1}{2} \begin{pmatrix} \sigma' \\ \epsilon'' \end{pmatrix}^T \begin{pmatrix} C'^{-1} & C'^{-1}C'' \\ C'^{-1}C'' & C' + C''(C'^{-1})C'' \end{pmatrix} \begin{pmatrix} \sigma' \\ \epsilon'' \end{pmatrix} \tag{59}$$

and the variational problem becomes a minimization problem

$$\min_{\sigma'} \min_{\epsilon''} \int_\omega L_{\sigma'\epsilon''}(\sigma', \epsilon'') dx$$

Euler equations of this transformed Lagrangian still give the real and imaginary part of complex conductivity equation. The functional is a positive defined quadratic function of the fields and the obtained variational principle expresses minimum of the energy release rate (entropy production) per period of oscillation. The technique of bounds is applicable to the Lagrangian (59), it allows to obtain the coupled bounds for the real and imaginary part of the effective tensor of a viscoelastic material, see [37, 38, 64].

4.5. DUALITY AND STRUCTURAL OPTIMIZATION

Optimal design problems often lead to minimax variational problems, see for example [82] or are formulated as non-self-adjoin extremal problem for a self-adjoin operator see [49] and [20]. Duality is used to relax a poly-linear minimax problem of optimal design that cannot be immediately regularized by the Legendre transform. To illustrate the approach, consider the simplest problem of minimization of a functional related to a solution of conductivity problem. One can choose the layout of several isotropic conductors in a domain Ω to achieve the minimum. This way, a structural problem of minimization of a weakly lower semicontinuous functional of the solution of the boundary value problem is formulated as a control problem:

Minimize

$$I = \int_\Omega \Phi(u)dx + \int_{\partial\Omega} \phi(u)ds \tag{60}$$

where Φ and ϕ are continuous functions, and u solved the boundary value problem

$$\nabla \cdot \frac{\partial}{\partial \nabla u} F(\chi, \nabla u) = 0 \tag{61}$$

that links together control χ and the solution u.

Adding this differential constraint with the Lagrange function v to the functional (60) and integrating by parts, we obtain the following min-max problem

$$\min_\chi \min_u \max_v I(\chi, u, v)$$

where

$$I(\chi, u, v) = \int_\Omega (\Phi(u) + \nabla v \cdot F(\chi, \nabla u))dx + \int_{\partial\Omega} (\phi(u) + vF(\nabla u) \cdot n)ds$$

If the materials are linear, $F(\nabla u) = C(\chi)\nabla u$.

Local problem To find the best structure, we pass to the local problem that describes an optimal microstructure in a neighborhood ω a point $x_0 \in \Omega$. We obtain the min-max problem

$$\mathcal{L} = \min_\chi \min_u \max_v I; \quad I = \int_\omega \nabla v^T C(\chi) \nabla u \, dx$$

where the mean fields $\langle \nabla u \rangle$ and $\langle \nabla v \rangle$ and amounts $m_i = \langle \chi_i \rangle$ of the materials must be prescribed (they are determined later from the solution of the problem in large). The formulated local problem describes the basic element of an optimal structure, while the global problem describes the distribution of these elements and variation of their properties on the large scale.

In order to transform the local minimax problem to the minimal one, a three-step procedure is needed because the Legendre transform with respect to a linear term ∇v is degenerative.

(i) Observe that the objective of the local problem linearly depends on both magnitudes $|\langle \nabla u \rangle|$ and $|\langle \nabla v \rangle|$ which implies that the magnitudes of the fields in the local problem do not affect the distribution of the properties. Therefore, we normalize the fields assuming that $|\langle \nabla u \rangle| = 1$ and $|\langle \nabla v \rangle| = 1$.

(ii) Introduce new potentials

$$a = \frac{1}{\sqrt{2}}(u + v) \quad \text{and } b = \frac{1}{\sqrt{2}}(u - v)$$

and rewrite the local problem as the difference

$$I = \int_\omega \left[\frac{1}{2}\nabla a^T C(\chi)\nabla a - \frac{1}{2}\nabla b^T C(\chi)\nabla b \right] dx \tag{62}$$

One can check that gradients of a and b are orthogonal, $\langle\nabla a\rangle \cdot \langle\nabla b\rangle = 0$.

(iii) Finally, perform the Legendre transform of the quadratic Lagrangian (62) with respect to ∇b, introducing the dual to ∇b divergencefree variable j ($\nabla \cdot j = 0$) and we arrive at the minimization problem

$$J = \min_{a,\chi,j} \int_\omega \left[\frac{1}{2}\nabla a^T C(\chi)\nabla a + \frac{1}{2} j^T C^{-1}(\chi) j - \nabla b^T j \right] dx \tag{63}$$

that requires the minimization of the energy (the first term of the Lagrangian) of the field ∇a and the complementary energy (second term) caused by an orthogonal current field j.

Optimal composite minimizes the sum of the energy of the field ∇a and complimentary energy of the orthogonal field $j = \nabla \times \theta$; the mean values of both fields are given. This requirement implies that an optimal composite must have the minimal resistance in a direction and the minimal conductivity (or the maximal resistance) in an orthogonal direction. The result is evident: the best structure is a laminate oriented so that the normal to the layer is oriented along b. In terms of the original fields, the normal bisects the directions of gradients ∇u and ∇v of the primary and dual potentials.

The technique remains the same for the elasticity operator. An optimal structure minimizes a weighted sum of difference of the stress and strain energy caused by two transversal fields. The structures are not completely described yet but it can be shown that laminates of a rank are optimal in asymptotic cases, see [20, 63, 65].

Conclusion The outlined techniques provide partial answers to the questions about solutions of nonquasiconvex variational problems. Each method is being actively developed in recent years, and still none of them is complete today.

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