



GROWTH OF SOLID BODIES IN THE FRAMEWORK OF SHAPE AND TOPOLOGY OPTIMIZATION

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Abstract

In the present paper, a model for growth of elastic bodies is proposed for purposes of shape and topology optimization. Growth of solid bodies is herewith considered in the framework of topology and shape optimization, with the goal of mimicking the natural generation of both stiff and light biological structures, consisting of a solid skeleton immersed into a softer phase. The growth process is modeled as the nucleation and subsequent growth of islands of a hard elastic phase within a softer elastic matrix, which plays the role of a reservoir of nutrients for the supply of the newly generated material. Islands of the generated solid skeleton are modeled as balls of small radius, and the position of their center is determined in such a way that the effective compliance, the product of the compliance by the relative density of the hard phase, is minimal for each new generation event. A growth model is set up from the mass balance with a source term involving the growth rate of mass, taken as a constant. The modeling of the growth process relies on the evaluation of the topological derivative of the effective compliance, which allows finding the optimal position of the center of new inclusions of the generated hard phase. This nucleation process is then followed by the shape optimization of the growing solid bodies. A proper mathematical formulation of the topology and shape optimization of growing elastic solid body is provided, relying on a domain decomposition technique allowing to replace the singularly perturbed geometrical domain by a regularly perturbation of Steklov-Poincaré operator. As an enrichment of this model, surface energy is lastly considered in the framework of a linear elastic constitutive model with surface stress.

Key words: continuum growth; solid bodies; topology optimization; topological derivative; effective compliance

1. INTRODUCTION

Growth of biological tissues has attracted the attention of several researchers in continuum mechanics the last two decades (Rodriguez et al., 1994; Epstein & Maugin, 2000; Ambrosi & Mollica, 2002; Lubarda & Hoger, 2002; Taber & Humphrey, 2001; Garikipati et al., 2003; Rajagopal, 1995; Rajagopal & Srinivasa, 1998; Humphrey & Rajagopal, 2002). The most advanced works treat the interactions between the mechanical equilibrium and the transport phenomena leading to growth, see (Ganghoffer &

Haussy, 2005) and (Ateshian, 2007) using the theory of mixtures, or Narayanan et al. (2009) highlighting the coupling between reaction-transport of solutes and mechanics.

Growth of biological structures is often modeled in the literature in terms of a set of differential equations accounting for the sources responsible for growth. Since the early 1990, topology optimization has been applied with good success to the situation of bone remodeling; this process redistributes the material in the domain occupied by the bone to determine an optimal arrangement (Bensoe & Kikuchi,

1989; Bendsoe, 1989; Xie et al., 1993; Hollister et al., 1994; Fernandes & Rodriguez, 1999; Bagge, 2000; Huiskes, 2000). Simulations have shown that the local bone remodeling equations and the structural topology optimization both lead to similar results, which tend to indicate that bone remodeling may be considered as a structural optimization problem. However, while the design of optimization rules for man-made structures is relatively straightforward (optimal stiffness or bending, resistance to impact, indentation, failure, minimum mass,...) due to the fact that the optimal criterion (the cost function in mathematical language) is known a priori, the design principles of biological structures require a deep understanding of their growth mechanisms, generally depending upon genetic factors in addition to epigenetic ones (like mechanical strains and stresses). Mattheck (1990) introduced twenty years ago the Biological Growth Method, which bases its observations in Nature; its major hypothesis is that the process of optimization in natural structures is carried out through the swelling or shrinking of the soft outermost layer of material, which yields the leveling of local stresses. This resembles a lot the way topology optimization proceeds to reach optimal shapes.

While most of the efforts have been spent on the modeling of volumetric growth, fewer works deal with surface growth, which from a conceptual point of view introduces the additional difficulty of a changing number of particles, hence a change of the body topology, in contrast to volumetric growth (an assumption of constant particle numbers is made there, considering that either the density or/and the local volume do change instead). A unifying framework for the treatment of both bulk and surface growth phenomena has been proposed in Di Carlo (2005), relying on the introduction of configurational forces *à la Gurtin* as the internal driving forces for growth. Configurational forces for surface growth have been identified in Ganghoffer (2010a, b), with application to bone remodeling, see Ganghoffer (2012).

Topology optimization is conceived in this contribution as a continuous process that mimics the nucleation of a new phase in growing biological structures; hence it aims at describing the generation of new particles within a solid body, with subsequent growth accompanied by shape and volume changes. Those biological structures usually consist of a solid skeleton, coined the hard phase in the sequel, immersed within a soft phase representing the

nutrients (it may be plasma, an interstitial fluid, or a material with weak elastic properties). A typical problem addressed in this contribution is the growth of the hard phase inside an initial soft phase, both occupying a fixed domain in space.

The main originality advocated in the present work is the setting up of a proper mathematical formulation of the shape and topology optimization of growing solid bodies, in the context of continuum mechanics. Especially, the difficult issue of a varying number of particles shall be addressed in this contribution, for the first time from the authors' knowledge. This contribution is organized as follows: the growth model and the underlying shape functional to be optimized as a result of the growth process are exposed in section 2. The mathematical formulation of the model problem and the domain decomposition technique for the determination of the topological derivative of the considered shape functional is the object of section 3. An extension of the model with consideration of surface stresses acting on the boundary between the hard phase inclusions as a resistance to growth is presented in section 4. Finally, conclusions are given in section 5.

Regarding notations, vectors and second order tensors are denoted with boldface symbols.

2. GROWTH MODEL IN THE CONTEXT OF TOPOLOGY OPTIMIZATION

We consider a fixed domain Ω consisting of a matrix of nutrients with a solid skeleton consisting of solid elastic inclusions denoted $\Omega_h = \{\Omega_h^I / I \in \Lambda\}$, with I an integer in the finite set Λ , denoting the individual domains Ω_h^I . Since the inclusions are endowed with higher mechanical properties compared to the matrix, it will also be coined the hard phase in the sequel.

New inclusions may be generated due to available surrounding nutrients, which further grow by changing their shape: those two separate processes correspond to nucleation of a new phase followed by its growth. As underlined in the introduction, no mechanical models for growth has yet addressed the issue of germination of the growing material, due mostly to the difficulty of describing from a mathematical and mechanical point of view the associated change of topology.

The total mass of the hard phase is evaluated in a small strains framework as the following functional of the displacement field $\mathbf{u} = \mathbf{u}(\mathbf{x})$, function of the



position vector \mathbf{x} , adopting here and in the sequel a Cartesian basis

$$M[\Omega_h] = \int_{\Omega} \chi_h(\mathbf{x}) \rho(\mathbf{x}) d\mathbf{x} = \int_{\Omega} \chi_h(\mathbf{x}) \rho_0(\mathbf{x}) (1 - \operatorname{div} \mathbf{u} + o(\|\nabla \mathbf{u}\|)) d\mathbf{x} \quad (1)$$

wherein the linearized version of the mass balance equation $\frac{\rho_0}{\rho} = J = 1 + \operatorname{div} \mathbf{u}$ has been inserted, considering here as an approximation a situation of fixed mass. The quantities ρ_0, ρ denote respectively the initial and actual densities, with their ratio equal to the relative volume change J , expressed versus the displacement in (1) within the small strains framework (this is reasonable due to the high mechanical properties of the hard phase which prevent large strains). Due to the presence of the characteristic function of the hard phase, noted $\chi_h(\mathbf{x})$, the integral expressed in (1) represents the total mass of the hard phase.

Both domains are supposed to obey a linear elastic behavior, with higher moduli for the hard phase compared to the soft phase. We have thereby considered an approximate behavior of the soft phase, for which a more elaborate viscous model may be adopted in future contributions.

We presently model the growth within the framework of optimization, assuming that nature proceeds in such a way as to produce biological structures which are both light and stiff; this is formalized in terms of a suitable shape functional elaborated as follows. The equivalent density is defined as the ratio of the overall mass of the hard phase $M_{\Omega_h}[\mathbf{u}]$ to the total mass, noted m_{tot} , viz the quantity $M_{\Omega_h}[\mathbf{u}]/m_{\text{tot}}$. The shape functional to be minimized is then elaborated as the product of the compliance with the equivalent density (the constant factor m_{tot} is dropped out of the cost functional).

$$\begin{aligned} \operatorname{Min}_{\Omega_{h_0}} H[\mathbf{u}] &:= \left\{ \int_{\Omega} \chi_h(\mathbf{x}) \rho_0(\mathbf{x}) \operatorname{div} \mathbf{u} d\mathbf{x} \right\} \left\{ \int_{\Gamma_N} \mathbf{t}^d \cdot \mathbf{u} ds + \int_{\Omega} \mathbf{f} \cdot \mathbf{u} d\mathbf{x} \right\} \\ &\equiv M_{\Omega_h}[\mathbf{u}] \cdot C[\mathbf{u}] \end{aligned} \quad (2)$$

with the minimization performed here with respect to the topology of the hard phase in the initial domain; $H[\mathbf{u}]$ has been decomposed into the product of the total mass of the hard phase, quantity $M_{\Omega_h}[\mathbf{u}]$ in (2), by the compliance $C[\mathbf{u}]$. Minimization of the compliance means the achievement of a stiff structure; whereas minimization of mass means that the

final stiff structure has to be as light as possible. Since both conditions are clearly antagonist, an optimum topology of the considered domain may exist, according to possible additional constraints on the volume of the hard phase. The topology of the domains at both initial and final times, respectively t_0, T , is pictured on figure 1 in a space-time diagram. The mathematical formulation of the model will be given in the next section; we first describe the growth model.

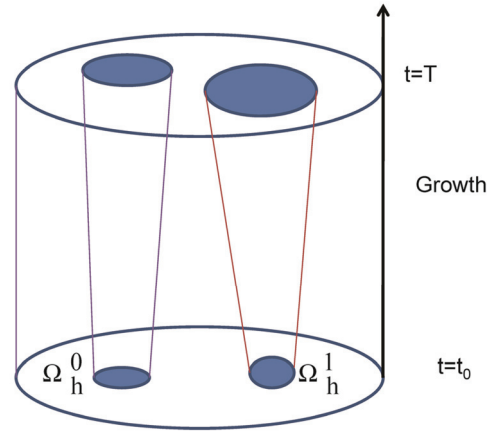


Fig. 1. Topology of the initial and final domains in a time scale diagram showing the growing inclusions of hard phase.

The growth velocity is determined from the mass balance equation for the hard phase:

$$\frac{d}{dt} \int_{\Omega} \chi_h(\mathbf{x}) \rho(\mathbf{x}) d\mathbf{x} = \int_{\Omega} \chi_h(\mathbf{x}) \Gamma(\mathbf{x}) \rho(\mathbf{x}) d\mathbf{x} \quad (3)$$

with $\Gamma(\mathbf{x})$ the mass growth rate; more elaborate growth models would involve a relation between the surface velocity field and a suitable interfacial driving force, as exposed in recent contributions (Ganghoffer, 2010a, 2010b, 2011), especially in the context of configurational mechanics applied to surface growth.

For an assumed constant mass growth rate Γ_0 and constant density of the hard phase, previous equality leads after straightforward calculations to

$$\begin{aligned} \mathbf{x} \in \Omega_h : \Gamma(\mathbf{x}) = \Gamma_0; \rho(\mathbf{x}) = \rho_h \Rightarrow \forall I \in \Lambda, \\ \mathbf{V}_N^I := \mathbf{V}^I \cdot \mathbf{n} = \Gamma_0 V[\Omega_h^I] / P(\Omega_h^I) \end{aligned} \quad (4)$$

introducing therein $V[\Omega_h^I]$ and $P(\Omega_h^I)$ the volume and perimeter of the inclusion respectively.

Assuming a constant density of the hard phase, the mass growth rate is further given by

$$\Gamma_0 = \frac{dM[\Omega_h]}{dt} / M[\Omega_h] \equiv \frac{d\operatorname{Vol}[\Omega_h]}{dt} / \operatorname{Vol}[\Omega_h] \quad (5)$$



denoting therein $\text{Vol}[\Omega_h]$ the actual volume of the hard phase. This last quantity is further related to the surface integral $\int_{\partial\Omega^h} \mathbf{u} \cdot \mathbf{n} dS$ arising from the effective density of the hard phase in the cost functional $H[\mathbf{u}]$, viz

$$\left\{ \int_{\Omega} \chi_h(\mathbf{x}) \rho_0(\mathbf{x}) (1 - \text{div} \mathbf{u}) d\mathbf{x} \right\} \equiv \rho_0 \left(V[\Omega_h] - \int_{\Omega^h} \text{div} \mathbf{u} d\mathbf{x} \right) = \rho_0 \left(V[\Omega_h] - \int_{\partial\Omega^h} \mathbf{u} \cdot \mathbf{n} dS \right) \quad (6)$$

The material derivative of the flux $\int_{\partial\Omega^h} \mathbf{u} \cdot \mathbf{n} dS \equiv \int_{\Omega^h} \text{div} \mathbf{u} d\mathbf{x}$ in (6) is further evaluated from Reynold's transport theorem as

$$\frac{d}{dt} \left(\int_{\Omega^h} \text{div} \mathbf{u} d\mathbf{x} \right) = \int_{\Omega^h} \text{div} \mathbf{v} d\mathbf{x} + \int_{\partial\Omega^h} \mathbf{V} \cdot \mathbf{n} dS \quad (7)$$

with \mathbf{V} defined as the surface growth velocity of the inclusions (figure 2); the notation d/dt is used here and in the sequel for the material derivative. Note that this resembles a surface growth model, since one describes the evolution of the surface of the hard phase; nevertheless, one shall point out that the distinction between surface and volumetric growth is not so clear (Epstein, 2010; Ganghoffer, 2011a), and maybe rather a matter of viewpoint.

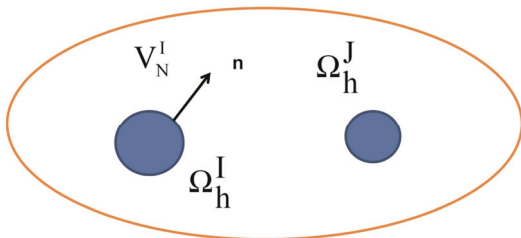


Fig. 2. Domains of hard phase growing inside a softer matrix of nutrients.

Due to the high rigidity of the hard phase, it is further reasonable to further neglect the local variation of the velocity vector field $\mathbf{v} := \frac{d\mathbf{u}}{dt}$ in comparison to the growth velocity in (7), hence

$$\Gamma_0 = \frac{1}{V[\Omega_h]} \int_{\partial\Omega_h} \mathbf{V} \cdot \mathbf{n} dS \cong \frac{1}{V[\Omega_h]} \frac{d}{dt} \int_{\partial\Omega_h} \mathbf{u} \cdot \mathbf{n} dS \quad (8)$$

This intermediate result will prove useful later on when evaluating the topological derivative of the effective compliance. Note that since Γ_0 is assumed not to be time dependent, the equality (8) relates in

fact quantities evaluated in the initial configuration over a fixed domain.

The effective compliance is minimized with respect to the initial topology of the hard phase, the domain Ω_{h0} , viz one has to solve the shape and topology optimization problem

$$\text{Min}_{\Omega_{h0}} H[\Omega(T)]$$

wherein one has slightly modified the notations (compare with (2)) in order to highlight the dependency of $H[\mathbf{u}]$ from the initial topology of the hard phase.

This means that one optimizes the final value of the cost function (effective compliance), by modifying the topology of the domain at initial time. Volume constraints are further introduced to limit the amount of hard phase in both the initial and final configurations, as

$$\begin{aligned} \Omega_h(t_0) &:= \sum_I |\Omega_h^I(t_0)| \leq V_{\max}(t_0); \\ \Omega_h(T) &:= \sum_I |\Omega_h^I(T)| \leq V_{\max}(T) \end{aligned} \quad (9)$$

Those constraints are physically reasonable, since the amount of available nutrients will limit the growth (hence the density of the hard phase at final time), and the initial configuration is such that it corresponds to a non growth situation. Note that the situation of resorption is also included in the model, by adjusting the sign of the mass growth rate Γ_0 .

3. DOMAIN DECOMPOSITION AND TOPOLOGICAL DERIVATIVE

We consider a fixed domain Ω_R in which a first inclusion $B_\epsilon = \Omega_h^0$ of the hard phase appears due to growth (figure 3); the inclusion is represented as a sphere in 3D (a disk in 2D) with radius $\epsilon > 0$, a small parameter, the center of which occupies the spatial position $\hat{\mathbf{x}}$ (figure 3).

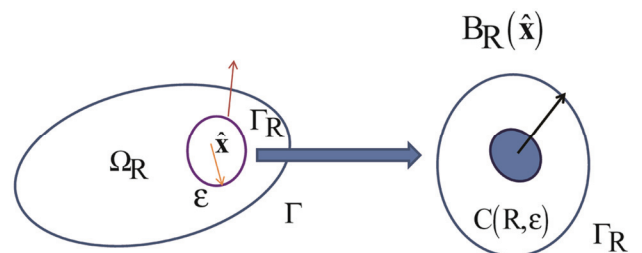


Fig. 3. Singular perturbation of the original domain when an inclusion of hard phase is created.



3.1. Mathematical formulation

Regarding the mathematical foundations of this contribution, we essentially rely on the notion of topological derivative introduced in Sokolowski and Zochowski (1999, 2001, 2005, 2008), which quantifies the sensitivity of a given shape functional with respect to the introduction of a nonsmooth perturbation (here inclusions). The reader is also referred to Nazarov and Sokolowski (2003) for a clear mathematical exposition of the same concept.

It is convenient to perform the domain decomposition of for $\Omega(t)$ into two complementary subsets $\Omega_h(t)$ and $\Omega_s(t)$, the hard and soft phase respectively, such that $\Omega(t) = \Omega_h(t) \cup \Omega_s(t)$, and associated interfaces. From a mathematical viewpoint, it is a transmission problem in a time variable domain. The resulting domain at final time $\Omega(T)$, is considered with respect to the initial topology $\Omega_h(0)$ and the associated interfaces $\partial\Omega_h(0)$. In the model, given the initial topology, its growth is known, so the final domain $\Omega(T) = \Omega_h(T) \cup \partial\Omega_h(T)$ is uniquely determined upon the initial domain $\Omega_h(0) \cup \partial\Omega_h(0)$.

The family of admissible domain is next defined as follows: a finite number of components is considered for $\Omega_h(0) = \bigcup_{I \in \Lambda} \Omega_h^I(0)$. The homogenization phenomena are excluded from our settings, hence $\#\Lambda$ is finite. Given an initial guess for the topology of the domain $\Omega_h(0) = \bigcup_{I \in \Lambda} \Omega_h^I(0)$, we want to

change its interfaces $\partial\Omega_h^I(0)$, $I \in \Lambda$, and possibly define the location of an additional inclusion. This is the objective of the shape optimization applied to the growth model; this also means we decouple the nucleation of the hard phase which occurs at initial time from the growth and motion processes, which occur with ongoing time.

We can therefore propose the following algorithm:

- Solve the model for the initial domain $\Omega_h(0)$;
- Compute the shape derivatives of the cost functional with respect to perturbations of the interface $\partial\Omega_h(0)$;
- Compute the topological derivative of the cost functional with respect to perturbations of the interface $\partial\Omega_h(0)$;

If the topological derivative indicates the new position of the new inclusion $\Omega_h^I(0)$, change the

topology and perform shape optimization with respect to $\partial\Omega_h^I(0)$.

The family of admissible domains is defined as

$$U_{ad} = \left\{ \Omega_h(0) \mid |\Omega_h(0)| \leq V_{max} \right\}, \quad \#\Lambda \leq N$$

$$\text{with } V_{max} \propto |\Omega_h(0)|.$$

The optimization problem then writes as

$$\text{Sup}_{\Omega_h(0) \in U_{ad}} J(\Omega(T))$$

The cost functional $J(\Omega(T))$ depends on the state variables, which are computed from the model defined in the cylinder $\bigcup_{0 \leq t \leq T} \Omega(t) \times \{t\}$. The model is

linear elasticity combined with growth; it is accordingly a growth model defined in the time-dependent domain $\Omega(t)$, $t \in [0, T]$. From mathematical viewpoint, the model is quasi static; so, we have the initial domain $\Omega(0) = \Omega_h(0) \cup \Omega_s(0)$ and consider some functions $u(x, t)$, $t \in [0, T]$, $x \in \Omega(t)$, called the state variables, with $\Omega(t) = F(\Omega(0))$, and evaluate the functional $J(\Omega(T)) := \int_{\Omega(T)} G(u(T, x), \nabla u(T, x)) dx$,

considering the shape mapping $\Omega_h(0) \rightarrow J(\Omega(T))$.

Material properties of the inclusions $\Omega_h(0)$ determine the solution of the model in $\Omega(t) = \Omega_h(t) \cup \Omega_s(t)$. Therefore, we are interested in how to change the initial distribution of the inclusions $\Omega_h(0)$ within the set of admissible domains in order to maximize the cost $J(\Omega(T))$.

We assume that the shape optimization procedure does not influence the growth model, hence the same model holds for all admissible distributions of the hard phase $\Omega_h(0)$ in the admissible class.

The questions from mathematical point of view for our shape optimization problem are:

1. The existence of an optimal domain in the class of admissible domains.
2. The first optimality conditions of this shape and topology optimization problem.
3. The numerical results which ensure an efficient way of computing an optimal domain.

3.2. Domain decomposition and Steklov-Poincaré operator

We set up a linear elasticity problem on this singularly perturbed domain that writes in strong form



$$(S_1): \begin{cases} \operatorname{div} \boldsymbol{\sigma}(\mathbf{u}_\varepsilon) = \mathbf{0} & \text{in } \Omega \\ \boldsymbol{\sigma}_\varepsilon(\mathbf{u}_\varepsilon) = \mathbf{C}_\gamma : (\nabla \mathbf{u}_\varepsilon)^S & \text{in } \Omega \\ \mathbf{u}_\varepsilon = \bar{\mathbf{u}} & \text{on } \Gamma_D \\ \boldsymbol{\sigma}(\mathbf{u}_\varepsilon) \cdot \mathbf{n} = \bar{\mathbf{t}} & \text{on } \Gamma_N \\ [\mathbf{u}_\varepsilon] = \mathbf{0} & \text{on } \partial B_\varepsilon \\ [\boldsymbol{\sigma}(\mathbf{u}_\varepsilon)] \cdot \mathbf{n} = \mathbf{0} & \text{on } \partial B_\varepsilon \end{cases}$$

with the jump of any quantity over the inclusion interface defined as the quantity $[\boldsymbol{\varphi}] := \boldsymbol{\varphi}|_{\Omega \setminus B_\varepsilon} - \boldsymbol{\varphi}|_{B_\varepsilon}$,

$$\mathbf{C}_\gamma = \begin{cases} \mathbf{C} & \text{in } \Omega \setminus B_\varepsilon \\ \gamma^{-1} \mathbf{C} & \text{in } B_\varepsilon \end{cases} \text{ the elasticity tensor involving}$$

a contrast parameter γ , and $\mathbf{C} = 2\mu \mathbf{I}_4 + \lambda \mathbf{I} \otimes \mathbf{I}$ the tensor of rigidities of the matrix phase in an isotropic situation (\mathbf{I} and \mathbf{I}_4 denote the second and fourth order identity tensors respectively), which is adopted for simplicity reasons here and in the sequel.

The displacement field \mathbf{u}_ε solution of this BVP is further characterized as the unique minimizer of the functional $J_\Omega[\mathbf{u}_\varepsilon] = \int_\Omega W(\mathbf{u}_\varepsilon) dx - \int_{\Gamma_N} \bar{\mathbf{t}} \cdot \mathbf{u}_\varepsilon ds$ over

the functional space

$$\mathbf{u}_\varepsilon \in U_\varepsilon = \{ \boldsymbol{\varphi} \in U : [\boldsymbol{\varphi}] = 0 \text{ on } \partial B_\varepsilon \}.$$

The singular perturbation of the geometrical domain is replaced the original variational problem of a boundary nonlocal operator (Steklov-Poincaré) living on the interface Γ_R of a disk of radius R enclosing the inclusion (figure 3).

The main idea of the analysis is to replace the original variational problem in Ω_ε by a variational problem in the truncated domain Ω_R . Hence, we shall determine the topological asymptotic expansion of the considered cost functional from its expansion in the truncated domain.

We next decompose the previous elliptic BVP into two complementary parts, defined in two disjoint domains, the matrix domain Ω_R and the ring

$$C(R, \varepsilon) := B_R(\hat{\mathbf{x}}) \setminus \Omega_\varepsilon^I(\hat{\mathbf{x}}).$$

We first formulate a linear elasticity problem in the ring $C(R, \varepsilon) := B_R(\hat{\mathbf{x}}) \setminus \Omega_\varepsilon^I(\hat{\mathbf{x}})$, with $R > \varepsilon > 0$, to which we accordingly restrict the asymptotic analysis:

Find \mathbf{w}_ε s.t.

$$\begin{cases} -\operatorname{div} \boldsymbol{\sigma}(\mathbf{w}_\varepsilon) = \mathbf{0} & \text{in } C(R, \varepsilon) \\ \boldsymbol{\sigma}_\varepsilon(\mathbf{w}_\varepsilon) = \mathbf{C}_\gamma : (\nabla \mathbf{w}_\varepsilon)^S & \text{in } C(R, \varepsilon) \\ \mathbf{w}_\varepsilon = \mathbf{v} & \text{on } \Gamma_R \\ [\boldsymbol{\sigma}(\mathbf{w}_\varepsilon) \cdot \mathbf{n}] = \mathbf{0} & \text{on } \partial B_\varepsilon \end{cases}$$

We next introduce Steklov-Poincaré nonlocal boundary operator for the elliptic problem in $C(R, \varepsilon)$, as the family of mappings (indexed by ε)

$$A_\varepsilon : \mathbf{v} \in H^{1/2}(\Gamma_R) \rightarrow \boldsymbol{\sigma}(\mathbf{w}_\varepsilon) \cdot \mathbf{n} \in H^{-1/2}(\Gamma_R)$$

which accordingly sends the boundary displacement (a datum in previous BVP) \mathbf{v} on Γ_R to the traction $\boldsymbol{\sigma}(\mathbf{w}_\varepsilon) \cdot \mathbf{n}$. The interest of Steklov-Poincaré operator is to express the expansion of the energy functional with respect to the small parameter ε with surface integrals well defined for functions in $L^1(\Gamma_R)$. We shall then have according to previous definition

$$\boldsymbol{\sigma}(\mathbf{u}_\varepsilon^R) \cdot \mathbf{n} = A_\varepsilon(\mathbf{u}_\varepsilon^R) \text{ on } \Gamma_R.$$

The restriction of the solution \mathbf{u}_ε to the domain Ω_R , quantity $\mathbf{u}_\varepsilon^R := \mathbf{u}_\varepsilon|_{\Omega_R}$, solves the following variational problem:

$$\begin{aligned} \int_{\Omega_R} \boldsymbol{\sigma}(\mathbf{u}_\varepsilon^R) : \nabla(\boldsymbol{\eta} - \mathbf{u}_\varepsilon^R) + \int_{\Gamma_R} A_\varepsilon(\mathbf{u}_\varepsilon^R) : (\boldsymbol{\eta} - \mathbf{u}_\varepsilon^R) = \\ \int_{\Omega_R} \mathbf{b} \cdot (\boldsymbol{\eta} - \mathbf{u}_\varepsilon^R), \quad \forall \boldsymbol{\eta} \end{aligned} \quad (10)$$

In the ring itself, the following equilibrium equation holds

$$\int_{C(R, \varepsilon)} \boldsymbol{\sigma}(\mathbf{w}_\varepsilon) : (\nabla \mathbf{w}_\varepsilon)^S = \int_{\Gamma_R} A_\varepsilon(\mathbf{w}_\varepsilon) \cdot \mathbf{w}_\varepsilon \quad (11)$$

wherein \mathbf{w}_ε is the solution of previous BVP. One can next prove that the energy in $C(R, \varepsilon)$ admits the following topological expansion

$$\begin{aligned} \int_{C(R, \varepsilon)} \boldsymbol{\sigma}(\mathbf{w}_\varepsilon) : (\nabla \mathbf{w}_\varepsilon)^S = \\ \int_{B_R} \left\{ \boldsymbol{\sigma}(\mathbf{w}) : (\nabla \mathbf{w}(\hat{\mathbf{x}}))^S - 2\pi\varepsilon^2 \mathbf{P} \cdot \boldsymbol{\sigma}(\mathbf{w}) : (\nabla \mathbf{w}(\hat{\mathbf{x}}))^S + o(\varepsilon) \right\} \end{aligned} \quad (12)$$

with \mathbf{w} the solution of previous BVP with $\varepsilon = 0$. Hence, from the two previous equalities, the Steklov-Poincaré operator admits the asymptotic expansion for small $\varepsilon > 0$:



$$A_\varepsilon = A - f(\varepsilon)B + o(\varepsilon^2) \quad (13)$$

with the function $f(\varepsilon) \equiv \pi\varepsilon^2$ depending upon the boundary conditions on the inclusion. The topological asymptotic expansion of the energy functional $J_{\Omega_\varepsilon}[\mathbf{u}_\varepsilon]$ proves then to be identical to that of Steklov-Poincaré operator:

$$J_{\Omega_\varepsilon}[\mathbf{u}_\varepsilon] = J_{\Omega}[\mathbf{u}] - f(\varepsilon)\langle B(\mathbf{u}), \mathbf{u} \rangle_{\Gamma_R} + o(\varepsilon^2) =$$

$$J_{\Omega}[\mathbf{u}] - \pi\varepsilon^2 \mathbf{P} \cdot \boldsymbol{\sigma}(\mathbf{u}(\hat{\mathbf{x}})) \cdot (\nabla \mathbf{u}(\hat{\mathbf{x}}))^S + o(\varepsilon^2) \quad (14)$$

involving the nonlocal operator defined as the following duality product

$$\langle B(\mathbf{w}), \mathbf{w} \rangle_{\Gamma_R} = \pi \mathbf{P} \boldsymbol{\sigma}(\mathbf{w}(\hat{\mathbf{x}})) \cdot (\nabla \mathbf{w}(\hat{\mathbf{x}}))^S \quad (15)$$

with $B \in \mathbf{L}(L^2(\Gamma_R); L^2(\Gamma_R))$ a bounded linear operator. The previous expansion of the energy functional is possible when the strong convergence of the solution occurs $\mathbf{u}_{\varepsilon|\Omega_R} \xrightarrow{\varepsilon \rightarrow 0} \mathbf{u}_R$ in the norm of $H^1(\Omega_R)$. The previous expansion of the total potential energy $J_{\Omega_\varepsilon}[\mathbf{u}_\varepsilon]$ then allows to identify its topological derivative

$$T_J(\hat{\mathbf{x}}) = \mathbf{P} \cdot \boldsymbol{\sigma}(\mathbf{u}(\hat{\mathbf{x}})) \cdot (\nabla \mathbf{u}(\hat{\mathbf{x}}))^S \quad (16_1)$$

which is a function of the point $\hat{\mathbf{x}}$, center of the inclusion of hard phase. For the considered three dimensional isotropic linear elasticity problem, the polarization operator is given by the following fourth order isotropic tensor (Khludnev et al., 2009)

$$\mathbf{P} = \frac{1-\nu}{7-5\nu} \left(10\mathbf{I}_4 + \frac{1-5\nu}{1-2\nu} \mathbf{I} \otimes \mathbf{I} \right) \quad (16_2)$$

with the parameters α , β given versus Poisson's ratio as

$$\alpha = \frac{1+\nu}{1-\nu}; \quad \beta = \frac{3-\nu}{1+\nu} \quad (16_3)$$

In a first step of the optimization problem, one has then to determine the position of the first inclusion (figure 4) such that the topological derivative is maximal (hence the cost functional will be minimized as required).

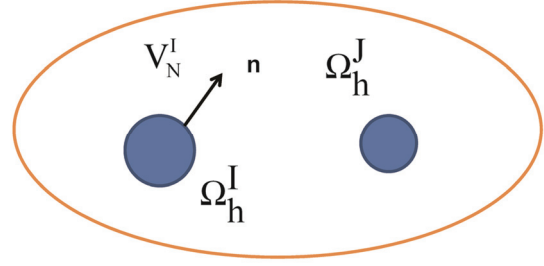


Fig. 4. Growth of the hard phase by generation of new inclusions.

3.3. Topological derivative of the effective compliance

We next proceed to evaluate the topological derivative of the chosen cost function: as the effective compliance is the product of two terms, the evaluation of its topological derivative involves Leibniz rule. The compliance may be rewritten in terms of the total energy using Clapeyron's theorem in linear elasticity

$$\left\{ \int_{\Gamma_N} \mathbf{t}^d \cdot \mathbf{u} + \int_{\Omega} \mathbf{f} \cdot \mathbf{u} \right\} = \int_{\Omega} W(\boldsymbol{\varepsilon}(\mathbf{u})) \Rightarrow$$

$$\left\{ \int_{\Gamma_N} \mathbf{t}^d \cdot \mathbf{u} + \int_{\Omega} \mathbf{f} \cdot \mathbf{u} \right\} = -2J_{\Omega}[\mathbf{u}] \quad (17)$$

in which the inner dot represents the internal product between two vectors. Recall that the cost functional is evaluated at the final time as a choice of the present model. In order to evaluate both topological derivatives, we perform a shape variation of the inclusion domain, letting

$$\partial \Omega_h^p = \partial \Omega_h + \rho \mathbf{n}(\mathbf{V} \cdot \mathbf{n}) \quad (18)$$

with $\mathbf{V} \cdot \mathbf{n}$ the normal velocity of the perturbation on the inclusion surface, and ρ a small parameter. The topological derivative of the effective compliance $H[\Omega_h^p(T)]$ is then calculated as the differential

$$\lim_{\rho \rightarrow 0} \frac{H[\Omega_h^p(T)] - H[\Omega_h(T)]}{\rho} \equiv dH(\Omega_h(T); \mathbf{V} \cdot \mathbf{n}) \quad (19)$$

evaluated in the direction of the normal velocity $\mathbf{V} \cdot \mathbf{n}$.

We next evaluate the asymptotic expansion of the cost functional in (2), rewritten as



$H[\Omega_h^p(T)] = M(\Omega_h(T))C(\Omega_h(T))$. From the decomposition of the total mass of the hard phase in (6), one can express the differential of the effective compliance in the direction of the normal growth velocity as

$$\begin{aligned} dH(\Omega_h(T); \mathbf{V}\cdot\mathbf{n}) &= dM_h(\Omega_h(T); \mathbf{V}\cdot\mathbf{n})C[\Omega_h(T)] + \\ &M_h[\Omega_h(T)]dC(\Omega_h(T); \mathbf{V}\cdot\mathbf{n}) \\ &\quad - dJ(\Omega_h(T); \mathbf{V}\cdot\mathbf{n})C[\Omega_h(T)] \\ &\quad - J[\Omega_h(T)]dC(\Omega_h(T); \mathbf{V}\cdot\mathbf{n}) \end{aligned} \quad (20)$$

using the notation $J[\partial\Omega_h(T)] := \int_{\partial\Omega_h(T)} \mathbf{u}\cdot\mathbf{n}ds$ for the surface integral in (6).

In order to evaluate topological derivatives of the quantities involved in the effective compliance, the domain obtained when a new inclusion is generated is decomposed as $\Omega_h^\varepsilon(T) = \Omega_h(T) \cup \omega^\varepsilon$, with ω^ε the new generated inclusion of size $\varepsilon^3|\omega|$.

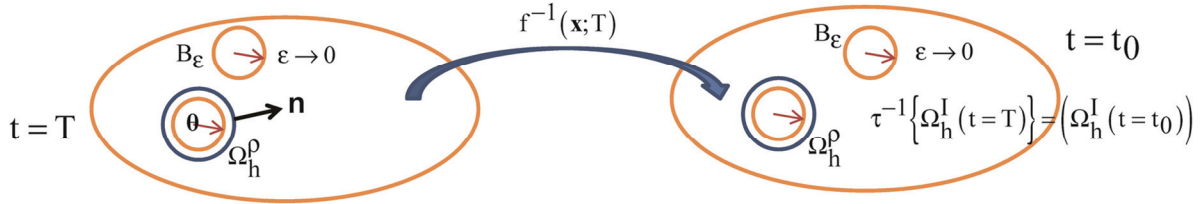


Fig. 5. Pull-back of the topology at final time on the initial domain.

The compliance receives the asymptotic expansion

$$C(\Omega_h^\varepsilon) = C(\Omega_h) + \varepsilon^3 T_C(\boldsymbol{\theta}) + (\varepsilon^3) \quad (21)$$

with $T_C(\boldsymbol{\theta})$ its topological derivative (the vector $\boldsymbol{\theta}$ is the center of the inclusion), given from (16)_{1,2,3} and (17) as

$$T_C(\boldsymbol{\theta}) = -2T_I(\boldsymbol{\theta}) \quad (22)$$

The flux integral $J[\partial\Omega_h^\varepsilon(T)]$ in (6) is then expanded versus ε , starting from an evaluation of the material derivative obtained by pulling-back the integral onto the fixed initial configuration (figure 1) and using (8), as

$$\begin{aligned} \frac{d}{dt} J[\partial\Omega_h^\varepsilon(T)] &= \frac{d}{dt} \left(\int_{\Omega_{h0}} (\text{div} \mathbf{u}^\varepsilon)_{t=0} J dX \right) = \\ &\Gamma_0 \left(|\Omega_h| + \varepsilon^3 |\omega| \right) \end{aligned} \quad (23)$$

Integrating (23), $J[\partial\Omega_h^\varepsilon(T)]$ becomes a linear function of time, which can be developed versus ε as

$$\begin{aligned} J[\partial\Omega_h^\varepsilon] &= \left(J[\partial\Omega_h] + Cte \right) + \varepsilon^3 \Gamma_0 |\omega| t \equiv \\ &\left(J[\partial\Omega_h] + Cte \right) + \varepsilon^3 T_I(\boldsymbol{\theta}) \end{aligned} \quad (24)$$

wherein the topological derivative of $J[\partial\Omega_h(T)]$ is clearly identified to $T_I(\boldsymbol{\theta}) = \Gamma_0 |\omega| t$.

The asymptotic expansion of the mass of the hard phase for the domain Ω_h^ε is given by

$$\begin{aligned} M_h[\Omega_h^\varepsilon] &= \rho_0 |\Omega_h^\varepsilon| = M_h[\Omega_h] + \varepsilon^3 \rho_0 |\omega| \equiv \\ &M_h[\Omega_h] + \varepsilon^3 T_M(\boldsymbol{\theta}) \end{aligned} \quad (25)$$

thus identifying $T_M(\boldsymbol{\theta}) := \rho_0 |\omega|$ as the topological derivative of the mass functional.

Combining (20) through (25), the asymptotic expansion of the effective compliance leads after straightforward calculations to the identification of its topological derivative

$$\begin{aligned} H(\Omega_h^\varepsilon) &= H(\Omega_h) + \varepsilon^3 \left(C[\Omega_h] (T_M(\boldsymbol{\theta}) - T_I(\boldsymbol{\theta})) + \right. \\ &\quad \left. T_C(\boldsymbol{\theta}) (M_h[\Omega_h] - J[\partial\Omega_h]) \right) \\ \rightarrow T_H[\Omega_h] &= C[\Omega_h] (T_M(\boldsymbol{\theta}) - T_I(\boldsymbol{\theta})) + \\ &\quad T_C(\boldsymbol{\theta}) (M_h[\Omega_h] - J[\partial\Omega_h]) \end{aligned} \quad (26)$$

The minimization of the effective compliance then amounts to finding the new topology at each time step by inserting an inclusion of hard phase such that $H[\Omega_h(T)]$ is minimum; the obtained topology may then be pulled-back to the initial configuration (at time t_0) to reflect the fact that the optimization is performed with respect to the initial domain. Note that since we consider growth in finite time, the topology remains the same under the pull-back



(a ball with small radius) remains a ball with a radius of the same magnitude).

The optimality problem under the above mentioned volume (or density) constraints is further translated into an algorithm for the growth process as follows (we refer the reader to the figure 11):

1. Search for the position of the center of the first inclusion ($t = t_0$) such that the cost functional is extremum (minimum). This step will be based on the evaluation of the topological derivative of the cost function expressed in (26).
2. Solve the BVP in linear elasticity, S_1 , in order to determine the mechanical fields (displacements, stresses) in the singularly perturbed domain.
3. Search for the position of a new inclusion such that the cost functional $H[\Omega(T)]$ is decreased, relying on the determination of the optimal value of the topological derivative of the effective compliance.
4. Let then impose that each inclusion grows according to the fixed growth rate of mass Γ_0 . The newly added mass during the considered time increment is distributed so as to optimize the shape of inclusions. This step relies on the evaluation of the shape derivative of the effective compliance, which we do not detail as a such derivation is classical. As an option, one may consider the growth model exposed in section 2, which prescribes the evolution of the hard phase as a fixed process, independent of the local stress field.
5. Insert a new inclusion and repeat previous steps considering the volume constraints, inequalities (9).
6. Stop when optimality is reached or when the inequality constraints (9) are saturated.

4. CONSIDERATION OF SURFACE STRESSES

The previous model is next refined accounting for a surface energy of the interface between the hard and soft phase domains, surface stress is especially important for small inclusions, and represents the tensorial generalization of the concept of scalar surface energy. Surface effects become important for small inclusions (in comparison to volume effects), whereby the existing surface energy may act as a resistance to growth.

Models accounting for surface stresses have been developed in the literature in both stable situations (Altenbach et al., 2010) and considering sur-

face growth (Ganghoffer, 2010b, 2012), considering a general framework based on the thermodynamics of surfaces. We shall herewith adopt a simpler model to describe surface effects, relying on the framework elaborated in (Altenbach et al., 2010).

The BVP of linear elasticity with surface stresses writes:

$$\begin{cases} \operatorname{div} \boldsymbol{\sigma} + \rho \mathbf{f} = \mathbf{0} & \text{in } \Omega \\ \boldsymbol{\sigma} = \lambda \operatorname{Tr}(\boldsymbol{\varepsilon}) \mathbf{I} + 2\mu \boldsymbol{\varepsilon} & \text{in } \Omega \\ \boldsymbol{\tau} = \lambda_S \operatorname{Tr}(\boldsymbol{\varepsilon}(\mathbf{v})) \mathbf{I} + 2\mu_S \boldsymbol{\varepsilon}(\mathbf{v}) & \text{surface stress, constitutively prescribed on } S_2 \\ \mathbf{u}|_{S_1} = \mathbf{0} \\ \mathbf{u}|_{S_2} = \mathbf{v} & \text{non separation condition} \\ [\mathbf{u}]_{\partial\Omega_h^i} = \mathbf{0} = [\mathbf{t}]_{\partial\Omega_h^i} & \text{displacement and traction continuity across interfaces} \\ \boldsymbol{\sigma} \cdot \mathbf{n} = \mathbf{t} = \boldsymbol{\varphi} + \mathbf{t}_S \Rightarrow (\boldsymbol{\sigma} \cdot \mathbf{n} - \nabla_S \cdot \boldsymbol{\tau}) = \boldsymbol{\varphi} & \text{given load on } S_2 \end{cases}$$

with $\mathbf{t}_s = \nabla_s \cdot \boldsymbol{\tau}$ the surface divergence of the stress tensor, λ_s, μ_s the Lamé constants of the interface. The surface strain $\boldsymbol{\varepsilon}(\mathbf{v}) := \frac{1}{2}(\nabla_s \mathbf{v} \cdot \mathbf{P} + \mathbf{P} \cdot (\nabla_s \mathbf{v})^T)$ is elaborated as the projection of the volumetric strain onto the tangent plane with unit normal \mathbf{n} , using the projector $\mathbf{P} := \mathbf{I} - \mathbf{n} \otimes \mathbf{n}$. The solution of previous BVP is characterized as the unique minimizer of the functional

$$J_2[\mathbf{u}] = \int_{\Omega} W(\boldsymbol{\varepsilon}(\mathbf{u})) dx + \int_{S_2 \cup \{\partial\Omega_h^i; i \in \Lambda\}} U(\boldsymbol{\varepsilon}) dx - \int_{S_2 \cup \{\partial\Omega_h^i; i \in \Lambda\}} \boldsymbol{\varphi} \cdot \mathbf{u} ds - \int_{\Omega} \mathbf{f} \cdot \mathbf{u} ds \quad (27)$$

involving the volumetric and surface energy densities, respectively the quantities $W(\boldsymbol{\varepsilon}(\mathbf{u}))$ and

$$U(\boldsymbol{\varepsilon}) := \frac{1}{2} \lambda_S (\operatorname{Tr}(\boldsymbol{\varepsilon}))^2 + \mu_S \boldsymbol{\varepsilon} : \boldsymbol{\varepsilon}.$$

The shape and topology optimization problem is then formulated as follows: part of the external boundary is allowed to grow in addition to the inclusions of hard phase. Accordingly, the following boundary conditions are prescribed (figure 6):

$$\begin{cases} S_1 \cup S_2 \cup S_g = \partial\Omega; S_1 \cap S_g = \emptyset \\ \boldsymbol{\theta} \cdot \mathbf{n} = 0 & \text{on } S_1 \\ \boldsymbol{\theta} \cdot \mathbf{n} = V_{g_n} & \text{on } S_g \end{cases}$$

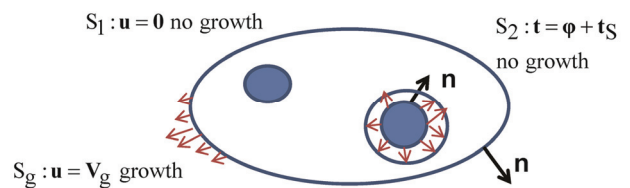


Fig. 6. Growth model in linear elasticity with surface stress.



The calculation of the topological derivative of the effective compliance is based on the same steps as in previous model (section 3), so it can still be evaluated from (26), involving the solution of the present BVP of surface elasticity. The determination of the topological derivative of the surface energy contribution remains however a challenging task, and will be the object of future contributions.

5. CONCLUSION AND PERSPECTIVES

We have presently elaborated a mathematical framework for the topology and shape optimization of solid bodies undergoing an internal evolution due to growth, whereby the growth process is described by a regular change of the topology of the initial configuration (figure 1), and thereby mimicking nucleation of the new phase inside a reservoir a nutrients provided by a softer surrounding phase. New islands of a hard phase representing the solid skeleton of the growing medium are generated within a softer matrix representing the available nutrients for growth. The successive generation of the hard phase domains followed by their growth and shape changes lead to an overall change of mass. The mass balance is written as a differential equation for the density of the hard material, which is ruled by the growth rate of mass, a datum of the model. This entails the growth velocity of the surface of the hard inclusions, and growth proceeds in such a way to minimize the overall compliance (defined in (2)) at a prescribed final time. The successive positions of the newly generated islands of the hard phase are decided basing on the optimal value of the topological derivative of the cost function at each time step, accounting for volume constraints of the domain of hard phase in both initial and final configurations, eqs. (9). A subsequent step of shape optimization is next performed, whereby the increased mass of the hard phase is redistributed in an optimal manner.

The mathematical formulation of the model has been given, and the mathematical setting for the growth model and topology optimization problem has been elaborated. The topological derivative of the effective compliance has been formally evaluated in (26), basing on a domain decomposition technique, whereby the singular perturbation of the geometrical domain is replaced by a regular perturbation of the boundary nonlocal operator.

An improved model shall further account for the surface energy of the islands of hard phase, as exposed in a preliminary manner as a perspective of

this work. Simulations of the growth model are postponed to a forthcoming contribution.

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rów zbudowanych z materiału twardego oraz na powiększaniu się obszaru zajmowanego przez ten materiał. Tą ewolucję opiszemy wzdłuż linii czasu. Zatem podobszar wypełniony słabym materiałem jest źródłem składnika potrzebnego do wzrostu szkieletu. Zakładamy, że obszary wypełnione twardym materiałem pojawiające się w obszarze słabym mają formę kul o małych promieniach i lokalizacja ich zarodkowania wynika z warunku minimalizacji zastępczej sztywności szkieletu. Położenie nowego obszaru zbrojenia materiałem twardym jest wyznaczane przez rozwiązanie zadania minimalizacji pochodnej topologicznej zastępczej sztywności szkieletu. W ten sposób otrzymuje się model wzrostu szkieletu z możliwością generacji nowych składników szkieletu poprzez optymalizację jego topologii jako podobszaru fazy słabej. Wzrost szkieletu przy zadanej topologii odbywa się zgodnie z prawem wzrostu podlegającym zasadzie zachowania masy ze źródłem o stałej wydajności. Otrzymany model matematyczny procesu wzrostu wykorzystuje technikę optymalizacji kształtu i topologii do wyznaczenia kształtu struktury poprzez minimalizację jej sztywności przy zmianie topologii szkieletu. W celu zastąpienia osobliwych zaburzeń obszaru całkowania przy zarodkowaniu nowych składników szkieletu przez zaburzenia nieosobliwe, w optymalizacji topologii ciała można więc stosować znaną technikę dekompozycji obszaru całkowania i operator Steklova-Poincare. Z matematycznego punktu widzenia praca dotyczy modelu quazistatycznego ciała sprężystego o zmiennej geometrii. Zmiany geometrii podlegają optymalizacji kształtu i topologii ze względu na funkcjonal jakości jakim jest sztywność konstrukcji w każdym kroku czasowym rozpatrywanego okresu wzrostu.

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METODY TEORII WZROSTU W ZAGADNIENIACH OPTYMALIZACJI KSZTAŁTU I OPTYMALIZACJI TOPOLOGICZNEJ CIAŁ ODKSZTAŁCALNYCH

Streszczenie

W pracy wprowadza się nowe, quasi-statyczne ujęcie opisu wzrostu ciała stałego w celu opracowania nowych technik optymalizacji kształtu i topologii. Wprowadzono opis wzrostu jaki obserwujemy przy powstawaniu jednocześnie sztywnych i lekkich struktur biologicznych, z wykorzystaniem technik zaczerpniętych z teorii optymalizacji kształtu i topologii. Rozważono struktury szkieletowe z twardego materiału, stanowiące konstrukcję nośną materiału słabego. Proces wzrostu dotyczy szkieletu i polega na pojawianiu się w słabym materiale obsza-

