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Artificial boundary conditions on polyhedral truncation surfaces for three-dimensional elasticity systems

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Abstract

For a three-dimensional exterior problem in the framework of anisotropic elasticity, artificial boundary conditions are constructed on a polyhedral truncation surface. These conditions do not need an explicit formula for the fundamental matrix. An approach to adapt the shape of truncation surfaces to the shape of the enclosed cavity is discussed. ***To cite this article: S. Langer et al., C. R. Mecanique 332 (2004).***

Résumé

Conditions aux limites artificielles sur des surfaces polyhédrales de troncature pour des systèmes d'élasticité tridimensionalle. Pour un problème extérieur en trois dimensions dans le cadre de l'élasticité anisitrope, on construit des conditions au bord artificielles sur une surface de troncature polyhédrale. Ces conditions ne nécessitent pas une formule explicite pour la matrice fondamentale. On étudie ensuite une méthode permettant d'adapter la forme de la surface de troncature à la forme de cavité. ***Pour citer cet article : S. Langer et al., C. R. Mecanique 332 (2004).***

Keywords: Computational solid mechanics; Elasticity; Polyhedral truncation surfaces; Artificial boundary conditions

Mots-clés : Mécanique des solides numérique ; Élasticité ; Surfaces polyhédrales de troncature ; Conditions aux limites artificielles

1. Statement of the problem

Let $\Omega = \mathbb{R}^3 \setminus \overline{G}$ be a homogeneous anisotropic elastic space with the cavity G bounded by a piecewise smooth closed surface. Introducing the matrices

$$d(x)^\top = \begin{pmatrix} 1 & 0 & 0 & 0 & \alpha x_3 & -\alpha x_2 \\ 0 & 1 & 0 & -\alpha x_3 & 0 & \alpha x_1 \\ 0 & 0 & 1 & \alpha x_2 & -\alpha x_1 & 0 \end{pmatrix}, \qquad D(x)^\top = \begin{pmatrix} x_1 & 0 & 0 & 0 & \alpha x_3 & \alpha x_2 \\ 0 & x_2 & 0 & \alpha x_3 & 0 & \alpha x_1 \\ 0 & 0 & x_3 & \alpha x_2 & \alpha x_1 & 0 \end{pmatrix} \tag{1}$$

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where $\alpha = 2^{-1/2}$ and $\top$ stands for transposition, we formulate an exterior elasticity problem in Ω as follows

$$\begin{aligned} &L(\nabla_x)u(x) := D(-\nabla_x)^\top A D(\nabla_x)u(x) = 0, && x \in \Omega \\ &N(x,\nabla_x)u(x) := D\big(n(x)\big)^\top A D(\nabla_x)u(x) = g(x), && x \in \partial\Omega = \partial G \end{aligned} \tag{2}$$

Here $u = (u_1, u_2, u_3)^\top$ is the displacement vector, n the outward unit normal (all vectors are treated as columns in $\mathbb{R}^3$), the 6×6-matrix A is symmetric and positive definite, and contains the elastic moduli. Note that the column vectors $D(\nabla_x)u$ and $AD(\nabla_x)u$ (of height 6) can be understood as the representatives of strains and stresses while the factors α in (1) force the norms of the columns in $\mathbb{R}^6$ to coincide with the natural norms of the corresponding tensors. It is known that, for any surface loading $g = (g_1, g_2, g_3)^\top \in H^{l-1/2}(\partial G)^3$ (the Sobolev–Slobodetskii space) with $l \in \mathbb{N} = \{1, 2, \ldots\}$, there exists the unique solution $u \in H^{l+1}_{\mathrm{loc}}(\overline{\Omega})^3$ which decays as $|x|$ tends to infinity. This solution has the asymptotic form

$$u(x) = \big(d(-\nabla_x)F(x)\big)^\top b + \big(D(-\nabla_x)F(x)\big)^\top a + \tilde{u}(x) \tag{3}$$

where $a,\ b$ are columns in $\mathbb{R}^6$, F denotes the fundamental (3×3)-matrix for the operator $L(\nabla_x)$ in $\mathbb{R}^3$ (the Kelvin tensor in the isotropic case) and the remainder $\tilde{u}$ fulfils the estimates

$$\big|\nabla_x^k \tilde{u}(x)\big| \leqslant c_k\big(1 + |x|\big)^{-k-3}, \quad k \in \mathbb{N}_0 = \mathbb{N} \cup \{0\} \tag{4}$$

outside a neighborhood of $\overline{G}$. We focus on computation of the polarization matrix P, which is an intrinsic integral attribute of a defect in a solid (see, e.g., [1,2]). The columns $P^1, \ldots, P^6$ of P appear as coefficients in the representation (3) for special right-hand sides in problem (2). Namely, let Z^j denote the unique decaying solution to problem (2) with the right-hand side

$$g^j(x) = D\big(n(x)\big)^\top A\mathrm{e}_j, \quad j = 1, \ldots, 6,\ \mathrm{e}_j \text{ is the } j\text{-th unit vector in } \mathbb{R}^6. \tag{5}$$

We emphasize that the equalities

$$\int_{\partial G} d(x) g^j(x)\,\mathrm{d}s_x = 0 \in \mathbb{R}^6, \quad j = 1, \ldots, 6 \tag{6}$$

are valid, which lead to $b = 0$ in representation (3) of Z^j (see, e.g., [2]). Thus, we obtain the relations:

$$Z^j(x) = \big(D(-\nabla_x)F(x)\big)^\top P^j + \widetilde{Z}^j(x) \tag{7}$$

Since $D(\nabla_x)D(x)^\top$ equals the 6×6 unit-matrix, the difference $D(x)^\top \mathrm{e}_j - Z^j(x)$ satisfies the homogeneous problem (2) but has a linear growth as $|x| \to \infty$ (see (1)).

The polarization matrix is always symmetric and positive definite in the case $\mathrm{mes}_3\, G > 0$ (see, e.g., [2]); it enjoys the 4-rank tensor properties after being rewritten in a proper form. Similarly to the classical harmonic capacity and the virtual mass tensor, P appears as a key object in miscellaneous asymptotic formulae, as increments of potential energy and eigenfrequences due to formation of a void, damage tensors and topological derivatives of shape functionals (cf. [3–6]), to mention a few. At the same time, the polarization matrix has been computed only for an isotropic space and canonical shapes of G such as a ball and a penny-shape crack. By virtue of the integral representation

$$P = -A\,\mathrm{mes}_3\, G - \big(A, D(n)Z\big)_{\partial G} \tag{8}$$

where $Z = (Z^1, \ldots, Z^6)$ (see [6], p. 178), it is a fair approach to calculate P by changing Z^j in (8) for an approximate solution $Z^{j,R}$ in a truncated domain Ω_R with appropriate artificial boundary conditions (ABC), here R is a truncation parameter which will be specified later on. However, ABC are usually constructed via an explicit formula for the fundamental matrix F while, as shown in [7], such formulae are still available only for a transverse isotropic elastic space.

In this Note we modify the approach [8], used to construct ABC on truncation spheres, for *a wide class of polyhedral surfaces* and in Section 2 we derive second order differential ABC without *any specification of the fundamental matrix*. Moreover, since the shape of the truncation surface Γ_R is no longer fixed, we discuss in Section 3 an adaptation of Γ_R to the shape of the cavity G in order to simplify the preparation of data for numerical schemes.

2. Derivation and justification of ABC

Let T be a polyhedron with the sides $\Sigma^1, \dots, \Sigma^J$ which are *tangent to the unit sphere* $\mathbb{S}^2$. We denote $\Gamma = \partial T$ and for $R \geqslant R_0$, we put

$$T_R = \{x\colon\ R^{-1}x \in T\}, \qquad \Gamma_R = \{x\colon\ R^{-1}x \in \Gamma\}$$

while the bound R_0 is chosen such that $\overline{G} \subset T_{R_0}$. For each side Σ^j, we introduce the Cartesian coordinates

$$(y^j, z^j) = \Theta^j x \tag{9}$$

where the axis z^j is perpendicular to Σ^j, $y^j = (y_1^j, y_2^j)$ are coordinates on the plane Π^j parallel to Σ^j, and Θ^j is an orthogonal 3×3-matrix. In coordinates (9) the operator $L(\nabla_x)$ takes the form $D(-\nabla_{(y^j,z^j)})^\top A^j D(\nabla_{(y^j,z^j)})$ (see remark below for an exact expression of the matrix A^j). The inclusion $v \in H^1(\Gamma_R)$ means that $v \in H^1(\Sigma_R^j)$ for $j = 1, \dots, J$, moreover, the traces of v on Σ_R^i and Σ_R^k coincide on the edges $\Sigma_R^i \cap \Sigma_R^k$ of the polyhedral surface Γ_R.

Lemma 2.1. *For the derivatives $F^{ki} = \partial F^k / \partial x_i$ of fundamental matrix columns, there holds the identity*

$$-\big(NF^{ki}, V\big)_{\Gamma_R} = \mathbf{b}\big(F^{ki}, V; \Gamma_R\big) := \frac{1}{R}\sum_{j=1}^{J}\big(A^j \mathbf{D}_R^j \Theta^j F^{ki}, \mathbf{D}_R^j \Theta^j V\big)_{\Sigma_R^j} \quad \forall V \in H^1(\Gamma_R)^3 \tag{10}$$

where Θ^j is taken from (9)*, and*

$$\mathbf{D}_R^j\big(y^j, \nabla_{y^j}\big) = D\big(R\nabla_{y^j}, -2 - \big(y^j\big)^\top \nabla_{y^j}\big) \tag{11}$$

is a differential operator on the plane Π^j.

We return to the general problem (2), but with boundary data g fulfilling condition (6); recall that this implies $b = 0$ in (3). We look for an optimal approximation of the solution u by a solution u^R to problem (2) restricted to the truncated domain $\Omega_R = \Omega \cap T_R$. Identity (10) becomes a key tool for creating ABC. Indeed, in the Green's formula

$$\big(Lu^R, v\big)_{\Omega_R} + \big(Nu^R, v\big)_{\partial G} = \mathbf{a}\big(u^R, v; \Omega_R\big) - \big(Nu^R, v\big)_{\Gamma_R} \tag{12}$$

we replace the term $(Nu^R, v)_{\Gamma_R}$ by $-\mathbf{b}(u^R, v; \Gamma_R)$ and obtain the variational formulation of the approximation problem

$$\mathbf{a}\big(u^R, v; \Omega_R\big) + \mathbf{b}\big(u^R, v; \Gamma_R\big) = (g, v)_{\partial G} \quad \forall v \in \mathcal{H}^1(\Omega_R)^3 \tag{13}$$

The function space $\mathcal{H}^1(\Omega_R)^3$ consists of vector functions $v \in H^1(\Omega_R)^3$ such that $v|_{\Gamma_R} \in H^1(\Gamma_R)$ and $2^{-1}\mathbf{a}(u^R, u^R; \Omega_R)$ expresses the elastic energy stored by the body Ω_R, i.e.,

$$\mathbf{a}(u, v; \Omega) = \big(AD(\nabla_x)u, D(\nabla_x)v\big)_\Omega \tag{14}$$

Since the above-mentioned change in (12), owing to (10), does not touch the detached asymptotic term in (7), a discrepancy left in (13) by $u|_{\Omega_R}$ is only generated by the remainder $\tilde{u}$, the decay (4) of which makes the discrepancy small. Thus, a technique developed in [8] leads to the following assertion.

Theorem 2.2. *For any $g \in L_2(\partial G)^3$, there exists a unique solution $u^R \in \mathcal{H}^1(\Omega_R)^3$ of problem* (13) *where the quadratic forms* **a** *and* **b** *are taken from* (14) *and* (10). *If g has zero mean value along ∂G, the solution u^R and the solution* (3) *of problem* (2) *are related by*

$$\left\| \left(1+|x|\right)^{-\varepsilon} \nabla_x \left(u-u^R\right); L_2(\Omega_R)\right\| + \left\| \left(1+|x|\right)^{-1-\varepsilon}\left(u-u^R\right); L_2(\Omega_R)\right\| \leqslant C_\varepsilon R^{-\varepsilon-5/2} \left\| g; L_2(\partial G)\right\| \tag{15}$$

where the constant C_ε is independent of g and $R \geqslant R_0$, provided $|\varepsilon| < 1/2$.

Since the special right-hand side (5) of problem (2) for Z^j verifies equality (6), we arrive at the following assertion.

Corollary 2.3. *Let P^R be the matrix calculated according to formula* (6) *with Z^j changed for the solution $Z^{j,R}$ of problem* (13) *where $g = g^j$ is taken from* (5). *Then the inequality*

$$\left\| P - P^R; \mathbb{R}^{6\times 6}\right\| \leqslant c_\varepsilon R^{-\varepsilon-5/2}$$

holds true with $\varepsilon \in (-1/2, 1/2)$ and the constant c_ε depending on A and G.

3. Affine transform for the elasticity system

Employing an approach used in [9] in the framework of two-dimensional elasticity, we consider the affine transform

$$x \mapsto \mathbf{x} = mx \tag{16}$$

where $m = (m_{ij})$ is a (3×3)-matrix with $\det m = 1$.

By a direct calculation, we obtain that problem (2) in the new variables $\mathbf{x}$ keeps the form

$$\begin{aligned} &D(-\nabla_{\mathbf{x}})^\top \mathbf{A} D(\nabla_{\mathbf{x}})\mathbf{u}(\mathbf{x}) = 0, \quad \mathbf{x} \in \mathbb{R}^3 \setminus \overline{\mathbf{G}} \\ &D\big(\mathbf{n}(\mathbf{x})\big)^\top \mathbf{A} D(\nabla_{\mathbf{x}})\mathbf{u}(\mathbf{x}) = \mathbf{g}(\mathbf{x}), \quad \mathbf{x} \in \partial\mathbf{G} \end{aligned} \tag{17}$$

where $\mathbf{G} = \{\mathbf{x} \in \mathbb{R}^3\colon\ x \in G\}$, $\mathbf{u}(\mathbf{x}) = (m^\top)^{-1}u(x)$, $\mathbf{g}(\mathbf{x}) = |(m^\top)^{-1}n(x)|^{-1} m g(x)$, $\mathbf{A} = MAM^\top$ and the matrix M of size (6×6) can be written as follows

$$\begin{pmatrix} m_{11}^2 & m_{12}^2 & m_{13}^2 & \sqrt{2}m_{12}m_{13} & \sqrt{2}m_{11}m_{13} & \sqrt{2}m_{11}m_{12} \\ m_{21}^2 & m_{22}^2 & m_{23}^2 & \sqrt{2}m_{22}m_{23} & \sqrt{2}m_{21}m_{23} & \sqrt{2}m_{21}m_{22} \\ m_{31}^2 & m_{32}^2 & m_{33}^2 & \sqrt{2}m_{32}m_{33} & \sqrt{2}m_{31}m_{33} & \sqrt{2}m_{31}m_{32} \\ \sqrt{2}m_{21}m_{31} & \sqrt{2}m_{22}m_{32} & \sqrt{2}m_{23}m_{33} & m_{23}m_{32}+m_{22}m_{33} & m_{23}m_{31}+m_{21}m_{33} & m_{22}m_{31}+m_{21}m_{32} \\ \sqrt{2}m_{11}m_{31} & \sqrt{2}m_{12}m_{32} & \sqrt{2}m_{13}m_{33} & m_{13}m_{32}+m_{12}m_{33} & m_{13}m_{31}+m_{11}m_{33} & m_{12}m_{31}+m_{11}m_{32} \\ \sqrt{2}m_{11}m_{21} & \sqrt{2}m_{12}m_{22} & \sqrt{2}m_{13}m_{23} & m_{13}m_{22}+m_{12}m_{23} & m_{13}m_{21}+m_{11}m_{23} & m_{12}m_{21}+m_{11}m_{22} \end{pmatrix}$$

Remark 1. If $m^j = \Theta^j$ is an orthogonal matrix as in (9), then M^j is orthogonal as well while the matrix A^j in (10) is equal to $MAM^\top$.

We do not rewrite tensor and vector fields in $\mathbf{x}$-coordinates! Instead of this, we introduce 'nonphysical' displacements $\mathbf{u}$ and stresses $\mathbf{A}D(\nabla_{\mathbf{x}})\mathbf{u}(\mathbf{x})$ so that we immerse our original problem (2) into a 'virtual elastic world'. We emphasize that if problem (17) is solved, real elastic fields can be reconstructed from the solution by simple algebraic calculations. At the same time, using this transformation, one can avoid the assumption on the polyhedron T in Section 2. Indeed, one can choose a convex polyhedron, e.g., with sides tangent to an ellipsoid, and transform by (16) the ellipsoid into unit ball. Then one can either deal with problem (17), or one has to transform back the ABC constructed for problem (17) in accordance to (10). In this way, it is possible to choose any parallelepiped $\{x\colon\ |x_k| < L_k\}$ as the polyhedron T. Then the matrices look as follows:

$$m = \operatorname{diag}\left\{L_1^{-1}, L_2^{-1}, L_3^{-1}\right\}, \qquad M = \operatorname{diag}\left\{L_1^{-2}, L_2^{-2}, L_3^{-2}, L_2^{-1}L_3^{-1}, L_3^{-1}L_1^{-1}, L_1^{-1}L_2^{-1}\right\} \tag{18}$$

The corresponding ABC provide accuracy (15) while position and sizes of the parallelepiped can be adopted to the shape of the cavity G.

Proposition 3.1. *The polarization matrices* P *and* $\mathbf{P}$, *calculated for problems* (2) *and* (17) *respectively, are related by*

$$\mathbf{P} = MPM^{\top} \tag{19}$$

Let m^1, m^2 and $m = m^1 m^2$ be the matrices of the affine transforms (16) while M^1, M^2 and M are found in accordance with the formula before the remark. A direct calculation of the matrix products leads to the equality

$$M = M^1 M^2$$

This homomorphism property shows that the set $\mathfrak{A}$ of symmetric and positive definite (6×6)-matrices A, which can play a role of elastic moduli matrix in the elasticity problem (2), can be divided into classes of *algebraically equivalent matrices*. For the algebraic equivalent matrices A and $\mathbf{A}$, any attribute and characteristics of problem (2) are transformed with the help of elementary algebraic operations into the attribute and characteristics of problem (17) and vice versa. In particular, the fundamental matrix $\mathbf{F}(\mathbf{x})$ of the operator $\mathbf{L}(\nabla_{\mathbf{x}}) = D(-\nabla_{\mathbf{x}})^{\top}\mathbf{A}D(\nabla_{\mathbf{x}}) \in \mathbb{R}^3$ takes the form

$$\mathbf{F}(\mathbf{x}) = \left(m^{\top}\right)^{-1} F\left(m^{-1}\mathbf{x}\right) m^{-1} \tag{20}$$

As it was mentioned, the fundamental matrix $F(x)$ is known for a transverse isotropic elastic space while the corresponding matrix A contains 5 arbitrary constants. Thus, formula (20) gives an exact expression of the fundamental matrix $\mathbf{F}(x)$ for an elastic material with $5 + (9 - 1 - 3) = 10$ constants. Here 9 stands for the number of entries of the matrix m, 1 for the normalization factor causing $\det m = 1$, and 3 corresponds to rotations of the space which, of course, cannot influence elastic properties. Unfortunately, the authors do not know a description of the class $\mathfrak{F}$ of elastic materials which are algebraically equivalent to transverse isotropic materials forming the class $\mathfrak{T}$ and, due to (20), have an explicit formula for the fundamental matrix. In any case, $\mathfrak{F}$ is much wider than $\mathfrak{T}$ (take, e.g., matrices (18)).

In $\mathbb{R}^3$ arbitrary anisotropic material has $21 - 3 = 18$ free constants (3 is used, e.g., to fix the Cartesian coordinates). Based on the fact that the matrix $\mathbf{A} = MAM^{\top}$ gains $5 = 9 - 3 - 1$ constants from m, we formulate

Conjecture 3.2. *Any anisotropic material is algebraically equivalent to an elastic material with a plane of elastic symmetry.*

It is known (see, e.g., [9]) that in the two-dimensional case any material ($5 = 6 - 1$ constants) is algebraically equivalent to an orthotropic material, where two Young moduli coincide ($3 = 5 - (4 - 1 - 1)$ constants).

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