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ON APPROXIMATE SOLUTION OF THREE DIMENSIONAL MIXED BOUNDARY VALUE PROBLEM OF ELASTICITY THEORY AND SOME OF ITS APPLICATIONS TO NANOSTRUCTURES

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Abstract. In the paper the 3D mixed boundary value problem of elasticity theory for the orthotropic beam with a rectangular cross-section is studied. By means of the Vekua theory the problem is reduced to two dimensional problem. The numerical solution is obtained by means of the finite difference schemes. The initial problem is reduced to the system of algebraic equations. The convergence of the iteration process is proved, the error is estimated. The results could be applied to big size beams as well as to nanostructures whose size is more than 10 nm [4,5].

Keywords and phrases: Elasticity theory, finite difference schemes, orthotropic beam.

AMS subject classification (2000): 34B05; 30E25; 74E30; 65M06; 65D25.

Statement of the problem.

In the paper 3D mixed boundary problem is considered for the parallelepiped type isotropic beam with a constant width 2h. We admit that static forces act to the upper and law boundary of the beam. At these boundaries the displacement vector is given. At the lateral surface the components of external tension tensor are given (Fig.1).

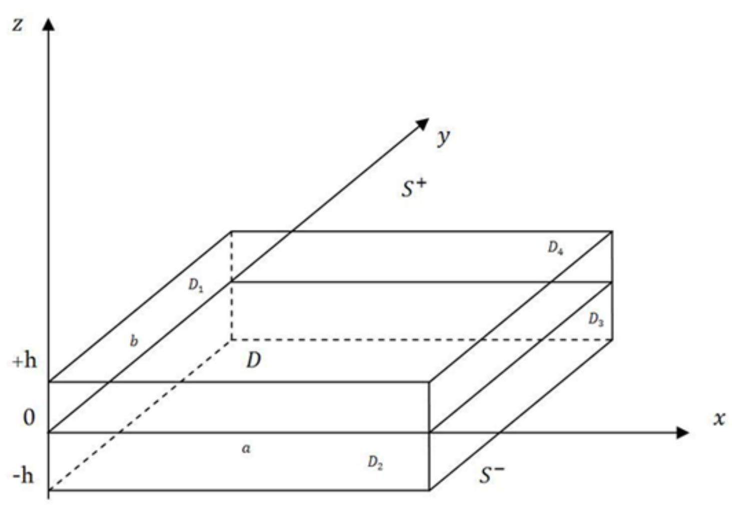

Fig.1.

Let us consider the system of elasticity theory for the displacement:

$$
\begin{aligned}
&c_{11}\frac{\partial^2 u_1}{\partial x^2}+c_{66}\frac{\partial^2 u_1}{\partial y^2}+c_{55}\frac{\partial^2 u_1}{\partial z^2}+(c_{12}+c_{66})\frac{\partial^2 u_2}{\partial x\partial y}+(c_{13}+c_{55})\frac{\partial^2 u_3}{\partial x\partial z}+f_1=0,\\
&c_{66}\frac{\partial^2 u_2}{\partial x^2}+c_{22}\frac{\partial^2 u_2}{\partial y^2}+c_{44}\frac{\partial^2 u_2}{\partial z^2}+(c_{12}+c_{66})\frac{\partial^2 u_1}{\partial x\partial y}+(c_{23}+c_{44})\frac{\partial^2 u_3}{\partial y\partial z}+f_2=0,\\
&c_{55}\frac{\partial^2 u_3}{\partial x^2}+c_{44}\frac{\partial^2 u_3}{\partial y^2}+c_{33}\frac{\partial^2 u_3}{\partial z^2}+(c_{13}+c_{55})\frac{\partial^2 u_1}{\partial x\partial z}+(c_{23}+c_{44})\frac{\partial^2 u_2}{\partial y\partial z}+f_3=0,
\end{aligned}
\tag{1}
$$

where $u_i(x,y,z), (i=1,2,3)$ are the displacement components, $f_i(x,y,z)$, $(i=1,2,3)$ are components of the mass forces, $c_{11}, c_{22}, c_{33}, c_{12}, c_{13}, c_{23}$, c_{44}, c_{55}, c_{66} are the elasticity constants for the orthotropic body.

In the isotropic case

$$
c_{11}=c_{22}=c_{33}=\lambda+2\mu=\frac{E(1-\nu)}{(1+\nu)(1-2\nu)},\ c_{44}=c_{55}=c_{66}=\mu=\frac{E}{2(1+\nu)},
$$

$$
c_{12}=c_{13}=c_{23}=\lambda=\frac{E\nu}{(1+\nu)(1-2\nu)},
$$

where λ and μ are the Lame constants, E is Young's modulus, ν is Poisson's coefficient.

The boundary conditions are given for the external forces at the lateral surface:

$$
\begin{aligned}
&\sigma_x=F_k^1(x,y,z),\ \tau_{xy}=F_k^2(x,y,z),\ \tau_{xz}=F_k^2(x,y,z): D_k\ (k=1,3);\\
&\sigma_y=F_k^1(x,y,z), \tau_{xy}=F_k^2(x,y,z),\ \tau_{yz}=F_k^2(x,y,z): D_k\ (k=2,4);
\end{aligned}
\tag{2}
$$

and the beam bases $S^{\pm}$, $(i=1,2,3)$ are fixed

$$
u_i(x,y,z)=0. \tag{3}
$$

The algorithm for the approximate solution

Here we consider the stress-strain 3D problem and reduce this problem to 2D by means of Vekua method [1,2]. We represent the solutions by Legendre polynomials with respect to the width of the beam. We represent the components of displacement vector as Fourier-Legendre series with respect to the Legendre polynomials differences:

$$
\begin{aligned}
u_j(x,y,z)&=\sum_{i=1,3\ldots}^{N}\overset{i}{u}_j(x,y)(P_{i+1}(z/h)-P_{i-1}(z/h)),\quad (j=1,2);\\
u_3(x,y,z)&=\sum_{i=1,3\ldots}^{N}\overset{i+1}{u}_3(x,y)(P_{i+2}(z/h)-P_{i}(z/h)),
\end{aligned}
\tag{4}
$$

where $P_i(z/h)$ are the Legendre polynomials.

By the operation of projection on 2D area for the definition of the coefficients from (1) we obtain the recurrent system of the elliptic type differential equations:

$$
\begin{aligned}
&-h\alpha_{i-1}\left[\left(c_{11}\frac{\partial^2}{\partial x^2}+c_{66}\frac{\partial^2}{\partial y^2}\right)\overset{i-2}{u}_1+(c_{12}+c_{66})\frac{\partial^2\overset{i-2}{u}_2}{\partial x\partial y}\right]\\
&+h\beta_i\left[\left(c_{11}\frac{\partial^2}{\partial x^2}+c_{66}\frac{\partial^2}{\partial y^2}\right)\overset{i}{u}_1+(c_{12}+c_{66})\frac{\partial^2\overset{i}{u}_2}{\partial x\partial y}\right]\\
&-h\alpha_{i+1}\left[\left(c_{11}\frac{\partial^2}{\partial x^2}+c_{66}\frac{\partial^2}{\partial y^2}\right)\overset{i+2}{u}_1+(c_{12}+c_{66})\frac{\partial^2\overset{i+2}{u}_2}{\partial x\partial y}\right]\\
&+2(c_{13}+c_{55})\frac{\partial}{\partial x}\left(\overset{i+1}{u}_3-\overset{i-1}{u}_3\right)-c_{55}\frac{4\overset{i}{u}_1}{h\alpha_i}=\overset{i+1}{f}_1-\overset{i-1}{f}_1,\\
&-h\alpha_{i-1}\left[(c_{12}+c_{66})\frac{\partial^2\overset{i-2}{u}_1}{\partial x\partial y}+\left(c_{66}\frac{\partial^2}{\partial x^2}+c_{22}\frac{\partial^2}{\partial y^2}\right)\overset{i-2}{u}_2\right]\\
&+h\beta_i\left[(c_{12}+c_{66})\frac{\partial^2\overset{i}{u}_1}{\partial x\partial y}+\left(c_{66}\frac{\partial^2}{\partial x^2}+c_{22}\frac{\partial^2}{\partial y^2}\right)\overset{i}{u}_2\right]\\
&-h\alpha_{i+1}\left[(c_{12}+c_{66})\frac{\partial^2\overset{i+2}{u}_1}{\partial x\partial y}+\left(c_{66}\frac{\partial^2}{\partial x^2}+c_{22}\frac{\partial^2}{\partial y^2}\right)\overset{i+2}{u}_2\right]\\
&+2(c_{23}+c_{44})\frac{\partial}{\partial y}\left(\overset{i+1}{u}_3-\overset{i-1}{u}_3\right)-c_{44}\frac{4\overset{i}{u}_2}{h\alpha_i}=\overset{i+1}{f}_2-\overset{i-1}{f}_2,\\
&-h\alpha_i\left(c_{55}\frac{\partial^2}{\partial x^2}+c_{44}\frac{\partial^2}{\partial y^2}\right)\overset{i-1}{u}_3+h\beta_{i+1}\left(c_{55}\frac{\partial^2}{\partial x^2}+c_{44}\frac{\partial^2}{\partial y^2}\right)\overset{i+1}{u}_3\\
&-h\alpha_{i+2}\left(c_{55}\frac{\partial^2}{\partial x^2}+c_{44}\frac{\partial^2}{\partial y^2}\right)\overset{i+3}{u}_3+2(c_{13}+c_{55})\frac{\partial}{\partial x}(\overset{i+2}{u}_1-\overset{i}{u}_1)\\
&+2(c_{23}+c_{44})\frac{\partial}{\partial y}\left(\overset{i+2}{u}_2-\overset{i}{u}_2\right)-c_{33}\frac{4\overset{i+1}{u}_2}{h\alpha_{i+1}}=\overset{i+2}{f}_3-\overset{i}{f}_3,\quad (i=1,3,5,\cdots,N).\quad (5)
\end{aligned}
$$

Suppose $\overset{-1}{u}_j\equiv 0\quad (j=1,2),\overset{1}{u}_3\equiv 0$, then the system (5) will be closed and the coefficients α_i,β_i,f_j will be given by:

$$\alpha_i=\frac{2}{2i+1},\quad \beta_i=\frac{1}{\alpha_{i+1}}+\frac{1}{\alpha_{i-1}},$$

$$\overset{k}{f}_j(x,y)=\left(k+\frac{1}{2}\right)\int\limits_{-h}^{+h}f_j(x,y,z)P_k\left(\frac{z}{h}\right)dz\quad (j=1,2,3).$$

At the lateral surface of the beam the condition (2) could be represented by means of Legendre polynomials in the form:

$$
\begin{aligned}
F_k^m(x,y,z) &= \sum_{i=1}^{N} \overset{i}{F}{}_k^m(x,y) P_i\left(\tfrac{z}{h}\right), \\
\overset{i}{F}{}_k^m(x,y) &= \left(i+\tfrac{1}{2}\right) \int_{-h}^{+h} F_k^m(x,y,z) P_i\left(\tfrac{z}{h}\right) dz.
\end{aligned} \tag{6}
$$

The system of differential equations (6) could be represented in the form of three-point operator [2,3]

$$
P \overset{i-2}{V} + Q \overset{i}{V} + R \overset{i+2}{V} = \overset{i+1}{G} - \overset{i-1}{G}, \quad i = 1, 3, \ldots, N. \tag{7}
$$

Analogously for the boundary conditions we obtain

$$
p \overset{i-2}{V} + q \overset{i}{V} + r \overset{i+2}{V} = \overset{i}{g}, \tag{8}
$$

where P, p, Q, q, R, r are the (3×3) matrix differential operators

$V^{i-2} = (u_1^{i-2}, u_2^{i-2}, u_3^{i-1})^{-1}; V^i = (u_1^i, u_2^i, u_2^{i+1})^{-1}; V^{i+2} = (u_1^{i+2}, u_2^{i+2}, u_3^{i+3})^{-1}$,

are vector columns for unknown functions, and

$G^{i+1} - G^{i-1} = (f_1^{i+1} - f_1^{i-1}, f_2^{i+1} - f_2^{i-1}, f_2^{i+2} - f_3^i)^{-1}; g^i = (F_1^i, F_2^i, F_3^{i+1})^{-1}$,

are vector columns for given functions.

Let's rewrite the system (7),(8) in the form:

$$
Q \overset{i}{V} = -P \overset{i-2}{V} - R \overset{i+2}{V} + \overset{i+1}{G} - \overset{i-1}{G}, \tag{9}
$$

$$
q \overset{i}{V} = -p \overset{i-2}{V} - r \overset{i+2}{V} + \overset{i}{g}. \tag{10}
$$

For the system (9), (10) any iteration method is applicable (for example Zeidel's method):

$$
\begin{aligned}
Q \overset{i}{V}_{(s)} &= -P \overset{i-2}{V}_{(s)} - R \overset{i+2}{V}_{(s-1)} + \overset{i+1}{G} - \overset{i-1}{G}, \\
q \overset{i}{V}_{(s)} &= -p \overset{i-2}{V}_{(s)} - r \overset{i+2}{V}_{(s-1)} + \overset{i}{g}, \quad s = 1, 2, \cdots.
\end{aligned}
$$

For the solution of two dimensional problems we use the finite-difference schemes. According to this method we obtain the system of algebraic equations with the matrix of three diagonal blocks. By the inversion of blocks and applying the Zeidel's method (internal iteration) at each step of the iteration process a matrix successive overrelaxation method is used. The accuracy of this method is $\left| \overset{i}{V}_s - \overset{i}{V}_{s-1} \right| < \varepsilon$ (s- is the number of iterations, ε- is the accuracy). As the matrix is symmetrical and positively defined, the process is convergent.

At the middle of the beam (rectangle D) we introduce the net

$$\Omega = \Big\{(x_i, y_j) = (ih_x, jh_y) \in D; i = 1, 2, \ldots, n_1, j = 1, 2, \ldots, n_2;$$

$$h_x = \frac{a}{n_1 - 1}; h_y = \frac{b}{n_2 - 1}\Big\}.$$

Applying the finite-difference scheme to the initial system we obtain:

$$\begin{aligned} -S_1\vec{\xi}_1 + W_1\vec{\xi}_2 &= -\vec{\Psi}_1, \\ V_i\vec{\xi}_{i-1} - S_i\vec{\xi}_i + W_i\vec{\xi}_{i+1} &= -\vec{\Psi}_i, \\ V_{n_1\vec{\xi}_{n_1-1}} - S_{n_1}\vec{\xi}_{n_1} &= -\vec{\Psi}_{n_1}. \end{aligned} \tag{11}$$

The first $i = 1$ and the last $i = n_1$ corresponds to the boundary conditions, also the boundary conditions contain the matrices for $j = 1$ and $j = n_2$, $1 < i < n_1$. At the system (11) V_i, S_i, W_i there are three diagonal matrices of n_2 order, each element of which is a three diagonal matrix, ξ vectors j order components of which are the U vector-function components values at the points (x_i, y_j).

Analogously, are constructed $\vec{\psi}_i$ vectors

$$\vec{\xi}_i = \begin{bmatrix} U_1(x_i, y_1) \\ U_2(x_i, y_1) \\ U_3(x_i, y_1) \\ \cdots\cdots \\ U_1(x_i, y_j) \\ U_2(x_i, y_j) \\ U_3(x_i, y_j) \\ \cdots\cdots \\ U_1(x_i, y_{n_2}) \\ U_2(x_i, y_{n_2}) \\ U_3(x_i, y_{n_2}) \end{bmatrix}, \quad \vec{\psi}_i = \begin{bmatrix} f_1(x_i, y_1) \\ f_2(x_i, y_1) \\ f_3(x_i, y_1) \\ \cdots\cdots \\ f_1(x_i, y_j) \\ f_2(x_i, y_j) \\ f_3(x_i, y_j) \\ \cdots\cdots \\ f_1(x_i, y_{n_2}) \\ f_2(x_i, y_{n_2}) \\ f_3(x_i, y_{n_2}) \end{bmatrix}.$$

The system of finite difference equations can be solved by the method of internal iteration. Series sequentially approximation will be given by

$$\begin{aligned} S_i\vec{\xi}^{(m)}_i &= \omega\{V_i\vec{\xi}^{(m)}_{i-1} + W_i\vec{\xi}^{(m-1)}_{i+1} + \vec{\psi}_i\} \\ &+ (1 - \varpi)S_i\vec{\xi}^{(m-1)}_i, \quad m = 1, 2, \ldots, n_1, \end{aligned}$$

where m is a number of iterations, ϖ is parameter of relaxation. If $\varpi = 0$, we have simple iteration and for $\varpi = 1$ Zeidel's iteration.

Below two numerical examples are given in the case when the normal forces are applied to the lateral surface of the beam and the other part of the beam surface is free.

Numerical examples

We suppose:

$$\sigma_x = -P, \qquad \tau_{xy} = 0, \qquad \tau_{xz} = 0 \;:\; D_1;$$
$$\sigma_x = 0, \qquad \tau_{xy} = 0, \qquad \tau_{xz} = 0 \;:\; D_3;$$
$$\sigma_y = -P, \qquad \tau_{xy} = 0, \qquad \tau_{yz} = 0 \;:\; D_2;$$
$$\sigma_y = 0, \qquad \tau_{xy} = 0, \qquad \tau_{yz} = 0 \;:\; D_4;$$

and

$$\sigma_x = -P, \qquad \tau_{xy} = 0, \qquad \tau_{xz} = 0 \;:\; D_1;$$
$$\sigma_x = 0, \qquad \tau_{xy} = 0, \qquad \tau_{xz} = 0 \;:\; D_3;$$
$$\sigma_y = 0, \qquad \tau_{xy} = 0, \qquad \tau_{yz} = 0 \;:\; D_2 \cup D_4;$$

also the following non-dimensional quantities are given: the size of the beam, the division number, the number of Legendre polynomials and the elasticity constants.

1. For the coal beam

$$2h = 0.6; 0.8; 1.0; \quad a = b = 1.98; \quad h_x = h_y = 0.09; \quad N_x = N_y = 22; \quad N = 3, 5;$$

$$c_{11} = 1.03 \cdot 10^6; \quad c_{12} = c_{13} = 3.52 \cdot 10^5; \quad c_{22} = c_{33} = 1.53 \cdot 10^6;$$
$$c_{23} = 4.35 \cdot 10^5; \quad c_{44} = 5.5 \cdot 10^5; \quad c_{55} = c_{66} = 3.6 \cdot 10^5;$$
$$\nu = 0.3; \quad E = 5.5 \cdot 9.81 \cdot 10^7.$$

The results of calculations are given in Table 1.

Tensions	Meanings of the tensions at net-points					
net-points	(1,1)	(5,5)	(9,9)	(13,13)	(17,17)	(21,21)
$\frac{\sigma_x}{p} = \frac{\sigma_y}{p}$	-1.140	-0.726	-0.366	-0.157	-0.055	-0.010
$\frac{\tau_z}{p}$	-0.936	-0.282	-0.106	-0.045	-0.016	0.007
$\frac{\tau_{xy}}{p}$	0.006	0.054	0.017	-0.003	-0.007	-0.002

Table 1.

2. These results could be applied to nanomaterials whose size is more than 10 nm [4,5]. In the isotropic, homogeneous and thermodynamically stable materials Poisson's coefficient varies between 1 and 0.5 [7]. For carbon nanomaterials it varies between 0.29 and 0.16 [6,7], Young's modulus is about 1TPa, as of diamond. For the nanomaterials of width about 20 nanometer Poisson's coefficient is about $\nu = 0.3$ [6,7].

The results of calculations are given in Table 2.

Tensions	Meanings of the tensions at net-points					
net-points	(1,1)	(5,5)	(9,9)	(13,13)	(17,17)	(21,21)
$\frac{\sigma_x}{p}$	-1.090	-0.498	-0.165	-0.051	-0.015	-0.002
$\frac{\sigma_y}{p}$	-0.026	-0.074	-0.038	-0.012	-0.003	0.0001
$\frac{\sigma_z}{p}$	-0.390	-0.061	-0.016	-0.005	-0.001	0.0001
$\frac{\tau_{xy}}{p}$	0.027	0.014	0.002	-0.0003	-0.0005	-0.0002

Table 2.

Conclusion. By the algorithm suggested above we can find displacements at any internal point of the beam and then find strain tensor components.

It is clear from numerical examples: a) The stresses field vanishes inside the beam; b) In case of rigid fixation of top and bottom bases, enhancement of beam thickness causes enhancement of normal stresses in the middle plane; c) In the formula of expansion of Legendre Polynomials (4) it is necessary to take many members, in order to describe more precisely distribution of stresses at the part of the boundary, where the outer forces are applied.

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