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Algorithm of solving the problem of small elastoplastic deformation of fiber composites by FEM

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Abstract. In this paper is presented the solution method for three-dimensional problem of transversely isotropic body's elastoplastic deformation by the finite element method (FEM). The process of problem solution consists of: determining the effective parameters of a transversely isotropic medium; construction of the finite element mesh of the body configuration, including the determination of the local minimum value of the tape width of non-zero coefficients of equation systems by using of front method; constructing of the stiffness matrix coefficients and load vector node components of the equation for an individual finite element's state according to the theory of small elastoplastic deformations for a transversely isotropic medium; the formation of a resolving symmetric-tape system of equations by summing of all state equations coefficients summing of all finite elements; solution of the system of symmetric-tape equations systems by means of the square root method; calculation of the body's elastoplastic stress-strain state by performing the iterative process of the initial stress method. For each problem solution stage, effective computational algorithms have been developed that reduce computational operations number by modifying existing solution methods and taking into account the matrix coefficients structure. As an example it is given, the problem solution of fibrous composite straining in the form of a rectangle with a system of circular holes.

Keywords: modeling; algorithm; grid; front; FEM; transversal isotropy; fiber; composite; hole; elastoplastic; strain, stress

1. Introduction

The development of modern technologies allows us to create mathematical models that really reflect the picture of the stress state distribution of spatial structures. Special attention is paid to the study of structural features influence of materials and configuration on fibrous structures' stress state. The mathematical modeling development and solution of physically nonlinear deformation of transversely isotropic bodies with stress concentrators problems are considered to be the subject of research by many authors, a review of which is presented in (Pobedrya and Gorbachev 1984). In Khaldjigitov and Adambaev (2004), sets out the basic provisions (postulates) of continuum

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mechanics. Along with the classical models, relatively new models of composite are being considered, that take into account the connectedness of mechanical fields. In (Tomashevsky 2011), an algorithm and mathematical modeling of problem solution taking into account the physical nonlinearity of bodies based on the theory of small elastoplastic deformations are considered. It is noted that the process of solving the problem is significantly accelerated when using the deformation theory, compared to the flow theory.

In paper (Tandon and Weng 1988) a simple, albeit approximate, theory is developed to determine the elastoplastic behavior of particle-reinforced materials. The elastic, spherical particles are uniformly dispersed in the ductile, work-hardening matrix. The method proposed combines Mori-Tanaka's concept of average stress inelasticity and Hill's discovery of a decreasing constraint power of the matrix in polycrystal plasticity. Under a monotonic, proportional loading the latter was characterized, approximately, by the secant moduli of the matrix. The theory is established for both traction and displacement-prescribed boundary conditions, under which, the average stress and strain of the constituents and the effective secant moduli of the composite are explicitly given in terms of the secant moduli of the matrix and the volume fraction of particles. In paper (Meleshko and Rutman 2017) application of the flexibility method developed on the bases of generalized Mohr formula (generalized flexibility method) allows to create numerical algorithms for elastoplastic calculation of framed structures and to obtain adequate results with no significant processor and time consumption. In paper (Rutman *et al.* 2018) several computational methods for providing elastoplastic analysis of structural systems and developing its capacity curve is reviewed. These methods vary according to the accuracy level of analysis results. Through the using different of them; inelastic deformation zones distribution is obtained with desirable accuracy level. Consequently; the damage state can be characterized by larger or smaller points on the curve.

In paper (Palizvan *et al.*) a computational homogenization methodology, developed to determine effective linear elastic properties of composite materials, is extended to predict the effective nonlinear elastoplastic response of long fiber reinforced composite. Finite element simulations of volumes of different sizes and fiber volume fractures are performed for calculation of the overall response representative volume element. The dependencies of the overall stress-strain curves on the number of fibers inside the representative volume element are studied in the 2D cases. Volume averaged stress-strain responses are generated from representative volume elements and compared with the finite element calculations available in the literature at moderate and high fiber volume fractions.

The description of the anisotropy of transversely isotropic bodies' mechanical properties is carried out on the basis of a structural-phenomenological model, which allows the source material to be presented as a complex of two jointly working isotropic materials: the base material considered from the standpoint of continuum mechanics, and the fiber material that are oriented along the anisotropy direction of the original material. It is assumed that the fibers perceive only the axial forces of tension-compression and are deformed together with the main material. The elastoplastic medium, which is a heterogeneous solid material, is considered. The medium consists of two components: reinforcing elements and a matrix (or binder), which ensures the joint operation of reinforcing elements. In fibrous materials, the deformation of the elastoplastic matrix provides for the loading of high-strength fibers.

It is known that a fibrous material has the properties of a transversely isotropic medium. In this regard, to solve the problem of physically nonlinear deformation of fibrous composites, the theory of small elastoplastic deformations is used for a transversely isotropic medium proposed by

Pobedrya (Pobedrya 1994). The paper notes that when considering the reinforced composite, reinforcing elements stiffness of which stiffness of the binder significantly exceeds, it becomes possible to use the simplified deformation theory of plasticity. The simplified theory allows to solve specific applied problems by applying the theory of small elastoplastic deformations. The essence of simplification lies in the assumption that with a simple stretching of the composite in the direction of the transverse isotropy axis and in the direction perpendicular to it, plastic deformations do not occur. As a result, the intensity of stresses and strains is determined separately, by the main axis of transverse isotropy and by the perpendicular plane. The application of the simplified theory is based on the fact that, the rigidity of the reinforcing elements substantially exceeds the rigidity of the binder in the reinforced composite that is under consideration.

This paper is devoted creation numerical method to computational the elastoplastic material stress-strain state of fiber composite based on the theory of small elastoplastic deformations of transversely isotropic media. An innovation of the present work is the research of the elastoplastic state material of fiber composite, what significantly affects strength characteristics of constructions. Further the algorithm was proposed for solving the problem of elastoplastic deformation of transversely isotropic multiply connected bodies. The algorithm for solving the problem includes:

1) determining the effective parameters of the transversely isotropic medium;
2) the construction of a finite element mesh body configuration;
3) calculation of the locally minimum value of the width of the tape of nonzero coefficients of the system of equations;
4) construction of stiffness matrix coefficients and components of the vector of nodal loads of a separate finite element;
5) the formation of a resolving symmetric-tape system of equations;
6) solving the system of a symmetric-tape system of equations using the square root method;
7) calculation of the elastoplastic stress-strain state of a transversally isotropic body.

For each stage of solving the problem, computational algorithms have been developed that allow reducing the number of computational operations by modifying the existing methods of solving and taking into account the structure of the matrix coefficients. As an example, the solution of the problem of deforming a fibrous composite in the form of a rectangle with a system of holes is given.

2. Problem statement and solution method

The elastoplastic medium of inhomogeneous solid material is investigated. The medium consists of two components: fibers and a matrix (binder) material. The matrix material ensures the joint operation of reinforcing elements. To solve the problem, the theory of small elastoplastic deformations is used for a transversely isotropic medium (Pobedrya 1984).

The general formulation of the boundary value problem of the theory of elasticity for anisotropic bodies includes:

- equilibrium equations $\sigma_{ij,j} + X_i = 0, \quad x_i \in V$; (1)

- generalized Hooke's law $\sigma_{ij} = C_{ijkl}\varepsilon_{kl}$; (2)

- Cauchy relations $$\varepsilon_{kl} = \frac{1}{2}\left(\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k}\right); \quad (3)$$

- boundary conditions $$u_i\big|_{\Sigma_1} = u_i^0, \qquad x_i \in \Sigma_1,$$
$$\sum_{j=1}^{3} \sigma_{ij}\, n_j\big|_{\Sigma_2} = S_i^0, \qquad x_i \in \Sigma_2, \quad (4)$$

where u_i - is the component of the displacement vector;

X_i, S_i^0 - bulk and surface forces;

Σ_1, Σ_2 - part of the volume Σ bounding surface V;

n_j - external normal to the surface Σ_2;

C_{ijkl} - tensor of elastic constants.

In the simplified theory of small elastoplastic deformations of a transversely isotropic medium, the generalized Hooke law (2) takes the following form:

$$\tilde{\sigma} = (\lambda_2 + \lambda_4)\tilde{\theta} + \lambda_3\varepsilon_{33}, \qquad \sigma_{33} = \lambda_3\tilde{\theta} + \lambda_1\varepsilon_{33}, \qquad P_{ij} = \frac{P_u}{p_u} p_{ij}, \qquad Q_{ij} = \frac{Q_u}{q_u} q_{ij}, \quad (5)$$

where

$$P_u = 2\lambda_4(1 - \pi(p_u))p_u, \quad Q_u = 2\lambda_5(1 - \chi(q_u))q_u \quad (6)$$

$\pi(p) = \bar{\lambda}_1(1 - p_s/p)$ and $\chi(q) = \bar{\lambda}_2(1 - q_s/q)$ - Ilyushin's plasticity functions, whose values in the elastic zone are equal to zero,

P_u, Q_u and p_u, q_u - stress and strain tensor intensity (respectively plane isotropy and isotropy transversal axis),

$\bar{\lambda}_1$, p_s - hardening coefficients and elastic deformation limits in the isotropy plane Oxy.

$\bar{\lambda}_2$, q_s - hardening coefficients and elastic deformation limits along the isotropy axis Oz.

In the elastic area, the parameters σ_{ij} are determined from Hooke's law. In the area of plastic deformation, the parameters σ_{ij} are determined on the basis of the A. Ilyushin's deformation theory;

λ_i - elastic constants of a transversally-isotropic medium;

(P_{ij}, p_{ij}) - components of the deviator parts of the transversely-isotropic stress and strain tensors in the isotropy plane Oxy;

(Q_{ij}, q_{ij}) - components of the deviator parts of the transversely-isotropic stress and strain tensors along the isotropy axis Oz:

$$P_u = \sqrt{\frac{1}{2} P_{ij} P_{ij}} = \frac{\sqrt{2}}{2} \sqrt{(\sigma_{11} - \sigma_{22})^2 + 4\sigma_{12}^2},$$
$$p_u = \sqrt{\frac{1}{2} p_{ij} p_{ij}} = \frac{\sqrt{2}}{2} \sqrt{(\varepsilon_{11} - \varepsilon_{22})^2 + 4\varepsilon_{12}^2}, \quad (7)$$

$$Q_u = \sqrt{\frac{1}{2} Q_{ij,} Q_{ij}} = \sqrt{\sigma_{13}^2 + \sigma_{23}^2},$$
$$q_u = \sqrt{\frac{1}{2} q_{ij} q_{ij}} = \sqrt{\varepsilon_{13}^2 + \varepsilon_{23}^2}, \tag{8}$$

where

$$p_{ij} = \varepsilon_{ij} + \frac{\tilde{\theta}}{2}\left(\delta_{i3}\delta_{j3} - \delta_{ij}\right) + \varepsilon_{33}\delta_{i3}\delta_{j3} - \left(\varepsilon_{i3}\delta_{j3} + \varepsilon_{3j}\delta_{i3}\right), \tag{9}$$

$$q_{ij} = \varepsilon_{i3}\delta_{j3} + \varepsilon_{3j}\delta_{i3} - 2\varepsilon_{33}\delta_{i3}\delta_{j3}, \tilde{\theta} = \varepsilon_{11} + \varepsilon_{22} \tag{10}$$

$$P_{ij} = \sigma_{ij} + \tilde{\sigma}\left(\delta_{i3}\delta_{j3} - \delta_{ij}\right) + \sigma_{33}\delta_{i3}\delta_{j3} - \left(\sigma_{i3}\delta_{j3} + \sigma_{3j}\delta_{i3}\right), \tag{11}$$

$$\tilde{\sigma} = \left(\sigma_{11} + \sigma_{22}\right)/2, \quad Q_{ij} = \sigma_{i3}\delta_{j3} + \sigma_{3j}\delta_{i3} - 2\sigma_{33}\delta_{i3}\delta_{j3} \tag{12}$$

The mechanical parameters of the transversely isotropic material are related to the modules λ_i by the following relations:

$$\lambda_1 = E'_{ef}\left(1 - \mu_{tf}\right)/l, \quad \lambda_2 = E_{ef}(\mu_{ef} + k\mu_{ef}^{\ 2})/\left[(1 + \mu_{ef})/l\right], \quad \lambda_3 = E_{ef}\mu'_{ef}/l,$$
$$\lambda_4 = G_{ef} = E_{ef}/\left[2(1 + \mu_{ef})\right], \quad \lambda_5 = G'_{ef}, \quad l = 1 - \mu - 2\mu'^2_{ef}k, \quad k = E_{ef}/E'_{ef}.$$

where

μ_{ef} - effective Poisson's ratio and E_{ef} - effective elastic moduli in the isotropy plane of the transversely isotropic material;

μ'_{ef} - effective Poisson ratios and E'_{ef} - effective elastic moduli along the isotropy axis of the transversely isotropic material.

It is assumed that the transversal isotropy plane coincides with the plane Oxy, and the isotropy axis with the axis Oz. The studied medium is homogeneous with effective mechanical parameters both along the isotropy axis and along the isotropy plane. Based on this, the iterative process of the initial stress method is used to solve the elastoplastic problem (Brovko *et al.* 2011).

The effective mechanical parameters of the transversely isotropic material are related to the modules λ_i with the following relations:

$$\lambda_1 = E'_{ef}\left(1 - \mu_{ef}\right)/l; \quad \lambda_2 = E_{ef}(\mu_{ef} + k\mu_{ef}^{\ 2})/\left[(1 + \mu_{ef})/l\right];$$
$$\lambda_3 = E_{ef}\mu'_{ef}/l; \lambda_4 = G_{ef} = E_{ef}/\left[2(1 + \mu_{ef})\right];$$
$$\lambda_5 = G'_{ef}; l = 1 - \mu - 2\mu'^{\,2}_{ef}k; k = E_{ef}/E'_{ef}.$$

Here μ_{ef} and μ'_{ef} – are the effective Poisson coefficients, E_{ef} and E'_{ef} – are the effective Young's modul, G_{ef} and G'_{ef} - are the effective longitudinal shear moduli, respectively, along the transverse isotropy plane and the transverse isotropy axis.

To calculate the effective mechanical parameters of fibrous materials, we use relations that allow to take into account the internal structure of the material for the calculation of periodically inhomogeneous materials based on the asymptotic averaging method and are suitable for any values of properties and volume fractions of components (Bolshakov *et al*. 2008):

$$E_{ef} = EE'/(\upsilon_2 E + (1-\upsilon_2)E'),$$
$$E'_{ef} = \upsilon_2 E' + (1-\upsilon_2)E + 4\upsilon_2(1-\upsilon_2)(\mu'-\mu)^2/r,$$

where

υ_2, υ_1 - is the Poisson's ratio of the fiber and matrix (υ_1= 1-υ_2),

$$r = (1-\upsilon_2)/K_2 + \upsilon_2/K_1 + 2(1+\mu)/E,$$
$$K_1 = \frac{E}{2(1+\mu)(1-2\mu)}, \quad K_2 = \frac{E'}{2(1+\mu')(1-2\mu')}$$

- effective longitudinal Young modulus of the matrix and fiber:

$$G_{ef} = -(c_2 + \sqrt{c_2^2 - c_1 c_3})G/c_1,$$
$$G'_{ef} = GG'/((1-\upsilon_2)G' + \upsilon_2 G)),$$

where

$$c_1 = 3\upsilon_2(1-\upsilon_2)^2(l-1)(l+d_2) + (ld_1 + d_1 d_2 - (ld_1 - d_2)\upsilon_2^3)(d_1(l-1)\upsilon_2 - (ld_1+1)),$$
$$c_2 = -3\upsilon_2(1-\upsilon_2)^2(l-1)(l+d_2) + (ld_1 + (l-1)\upsilon_2 + 1)((d_1-1)(l+d_2)/2 -$$
$$-2(ld_1 - d_2)\upsilon_2^3) + (d_1+1)(l-1)(l+d_2 + (ld_1-d_2)\upsilon_2^3)\upsilon_2/2,$$
$$c_3 = 3\upsilon_2(1-\upsilon_2)^2(l-1)(l+d_2) + (ld_1 + (l-1)\upsilon_2 + 1`)(l+d_2 + (ld_1-d_2)\upsilon_2^3,$$
$$l = G_2/G_1, \quad d_1 = 3-4\mu, \quad d_2 = 3-4\mu';$$

- effective longitudinal Poisson's ratio of matrix and fiber:

$$\mu_{ef} = E_{ef}/(2G_{ef}) - 1,$$
$$\mu'_{ef} = (1-\upsilon_2)\mu_1 + \upsilon_2\mu' + \upsilon_2(1-\upsilon_2)(1/K_1 - 1/K_2)(\mu'-\mu)/r.$$

In the general case, by representing the relationship between the stress tensor σ_{ij} and the strain tensor ε_{kl} as a function $\sigma_{ij} = F(\varepsilon_{kl})$, the Cauchy relation and displacement vector of each particle in the coordinate system $Ox_1x_2x_3$ as $\vec{u}(u_1, u_2, u_3)$, one can imagine a nonlinear relationship between the stress tensor and displacement vector u_i (Pobedrya 1994):

$$\sigma_{ij} = F\{\varepsilon_{ij}(\vec{u})\} = \sigma_{ij}(\vec{u}).$$

In this case, the equilibrium equation (1) defines a system of three partial differential equations for the three components of the displacement vector. For this system of equations, one can put three types of boundary conditions: in displacements (3), stresses (4) or a mixed type. Thus, the process of deformation of a solid body in equilibrium under the action of external forces can be reduced to the determination of the displacement vector $\vec{u}$. Based on the solution of boundary value problems, it is possible to determine the components of the displacement vector. From the known values of the components of the displacement vector, one can determine the components of the strain tensor and the stress tensor.

3. A finite element model of a multiply - connected area

The finite element mesh of a multiply connected area is formed by “stitching” (merging) the canonical subdomains. By canonical is meant the area for which there is an algorithm for constructing a finite element mesh. A quadrilateral (in the case of a two-dimensional body) and a quadrilateral prism (for a three-dimensional body) are chosen as the final elements, since filling the real area with these elements is very effective.

The computational algorithm for constructing a finite element mesh of a multiply connected region consists of a sequence of the following steps:

1) the formation of a finite element mesh of canonical subareas;
2) “stitching” (merging) subdomains;
3) determine the initial front;
4) ordering node numbers based on the frontal method;
5) minimization of the tape width of the system of equations.

Finite element representation of the area is described by the set

$$\Omega = \{N, M, MK, MN\},$$

where

N - number of nodes;
M - quantity of finite elements;
MK –coordinate nodes array;
MN - array of node numbers of finite elements.

The definition is given, according to which the area is called "canonical" if there is an algorithm for constructing its finite element mesh. Further a ratio which by combining ("stitching") of elementary sub-areas forms a finite element representation of the configuration area complex is given:

$$\Omega = \sum_{i=1}^{k} \Omega_i ,$$

where Ω_i - finite element representation of the *i*-th elementary subarea, k - number of sub-areas which to be combined.

At the initial stage of solving the problem, a library of finite element meshes of canonical areas is formed. The merging of areas is based on the criterion of coincidence of boundary nodes by establishing a simple hierarchy of volumes, surfaces, lines and points. The formation of elements of the set of initial fronts is carried out by determining the numbers of vertices and boundary nodes of the finite element representation of a multiply connected area. Renumbering nodes and finite elements is carried out on the basis of the frontal method (Kamel and Eisenstein 1974), taking into account the fact that vertices and faces of the structure are used as the initial front. It is known that the tape width of nonzero coefficients of the system of resolving equations of the FEM depends on the ordering of the nodes and finite elements of the finite element mesh. Identifying the numbering at which the width of the tape has the smallest value is determined by conducting a computational experiment. As the variation parameter, elements of the set of initial fronts are used. The developed algorithm for constructing a finite element mesh allows, by ordering the node numbering, determining such a sequence in which the width of the tape of nonzero coefficients of the resolving system of equations of the FEM is locally minimal (Polatov 2013).

4. Construction of the resolving system of symmetric-tape equations

The most significant and largely determining the quality of the FEM calculation scheme is the construction of the stiffness matrix coefficients and the formation of a system of resolving equations.

Each hexagon element from the family of finite elements into which the body is divided can be mapped into a three-dimensional element of regular shape, for example, into a cube. For a linear finite element with 8 nodes, the functions of the form N_i in the local coordinate system ξ, η, ζ can be represented as given expressions that satisfy all necessary criteria (Zienkiewicz and Taylor 2005):

$$N_i = \frac{1}{8}(1+\xi_0)(1+\eta_0)(1+\zeta_0),$$

where

$$\xi_0 = \xi * \xi_i, \quad \eta_0 = \eta * \eta_i, \quad \zeta_0 = \zeta * \zeta_i,$$

ξ_i, η_i, ζ_i - coordinates of the $i-$ node, $i = \overline{1,n}$.

To this end, global coordinates, in this case Cartesian, are associated with local coordinates by the relation:

$$\begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = f \begin{Bmatrix} \xi \\ \eta \\ \zeta \end{Bmatrix}.$$

$$\begin{Bmatrix} \frac{\partial N_i}{\partial \xi} \\ \frac{\partial N_i}{\partial \eta} \\ \frac{\partial N_i}{\partial \zeta} \end{Bmatrix} = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & \frac{\partial z}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & \frac{\partial z}{\partial \eta} \\ \frac{\partial x}{\partial \zeta} & \frac{\partial y}{\partial \zeta} & \frac{\partial z}{\partial \zeta} \end{bmatrix} * \begin{Bmatrix} \frac{\partial N_i}{\partial x} \\ \frac{\partial N_i}{\partial y} \\ \frac{\partial N_i}{\partial z} \end{Bmatrix} = [J] * \begin{Bmatrix} \frac{\partial N_i}{\partial x} \\ \frac{\partial N_i}{\partial y} \\ \frac{\partial N_i}{\partial z} \end{Bmatrix},$$

where $|J|$ – is the Jacobi matrix.

Here

$$x = N_1 x_1 + N_2 x_2 + \cdots + N_n x_n = [N]\{x_1, x_2, \ldots, x_n\}',$$
$$y = N_1 y_1 + N_2 y_2 + \cdots + N_n y_n = [N]\{y_1, y_2, \ldots, y_n\}',$$
$$z = N_1 z_1 + N_2 z_2 + \cdots + N_n z_n = [N]\{z_1, z_2, \ldots, z_n\}',$$

where the points with coordinates x_i, y_i, z_i by definition of the properties of the form function coincide with the corresponding points of the border of the element (i=1,2,…,n; n - is the number of nodes in the element).

Where can we write:

$$\begin{Bmatrix} \frac{\partial N_i}{\partial x} \\ \frac{\partial N_i}{\partial y} \\ \frac{\partial N_i}{\partial z} \end{Bmatrix} = [J]^{-1} \begin{Bmatrix} \frac{\partial N_i}{\partial \xi} \\ \frac{\partial N_i}{\partial \eta} \\ \frac{\partial N_i}{\partial \zeta} \end{Bmatrix} \tag{13}$$

Further, taking into account the one-to-one correspondence between the local and global coordinate systems, we can write the components of the Jacobi matrix in the following form:

$$[J] = \begin{bmatrix} \sum_{i=1}^{n} \frac{\partial N_i}{\partial \xi} x_i & \sum_{i=1}^{n} \frac{\partial N_i}{\partial \xi} y_i & \sum_{i=1}^{n} \frac{\partial N_i}{\partial \xi} z_i \\ \sum_{i=1}^{n} \frac{\partial N_i}{\partial \eta} x_i & \sum_{i=1}^{n} \frac{\partial N_i}{\partial \eta} y_i & \sum_{i=1}^{n} \frac{\partial N_i}{\partial \eta} z_i \\ \sum_{i=1}^{n} \frac{\partial N_i}{\partial \zeta} x_i & \sum_{i=1}^{n} \frac{\partial N_i}{\partial \zeta} y_i & \sum_{i=1}^{n} \frac{\partial N_i}{\partial \zeta} z_i \end{bmatrix} = \begin{bmatrix} \frac{\partial N_1}{\partial \xi} & \frac{\partial N_2}{\partial \xi} & \cdots & \frac{\partial N_n}{\partial \xi} \\ \frac{\partial N_1}{\partial \eta} & \frac{\partial N_2}{\partial \eta} & \cdots & \frac{\partial N_n}{\partial \eta} \\ \frac{\partial N_1}{\partial \zeta} & \frac{\partial N_2}{\partial \zeta} & \cdots & \frac{\partial N_n}{\partial \zeta} \end{bmatrix} * \begin{bmatrix} x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \\ \vdots & \vdots & \vdots \\ x_n & y_n & z_n \end{bmatrix} \tag{14}$$

We denote the components of the inverse matrix $[J]^{-1}$ as follows:

$$[J]^{-1} = \begin{bmatrix} c_{11} & c_{12} & c_{13} \\ c_{21} & c_{22} & c_{23} \\ c_{31} & c_{32} & c_{33} \end{bmatrix} \tag{15}$$

Using the obtained relations (13-15), the deformation vector of the finite element ***e*** can be written in the local coordinate system:

$$\{\varepsilon\}^e = \begin{bmatrix} c_1 & 0 & 0 \\ 0 & c_2 & 0 \\ 0 & 0 & c_3 \\ c_2 & c_1 & 0 \\ 0 & c_3 & c_2 \\ c_2 & 0 & c_1 \end{bmatrix} * \begin{bmatrix} \Phi & \emptyset & \emptyset \\ \emptyset & \Phi & \emptyset \\ \emptyset & \emptyset & \Phi \end{bmatrix} \{g\}^e$$

where $c_i=\{c_{i1}, c_{i2}, c_{i3}\}$, i=(1,2,3)– the components of the inverse matrix $[J]^{-1}$,

$\{g\}^e$ - is the displacement vector of e-th finite element;

$$\Phi = \begin{bmatrix} \frac{\partial N_1}{\partial \xi} & \frac{\partial N_2}{\partial \xi} & \cdots & \frac{\partial N_n}{\partial \xi} \\ \frac{\partial N_1}{\partial \eta} & \frac{\partial N_2}{\partial \eta} & \cdots & \frac{\partial N_n}{\partial \eta} \\ \frac{\partial N_1}{\partial \zeta} & \frac{\partial N_2}{\partial \zeta} & \cdots & \frac{\partial N_n}{\partial \zeta} \end{bmatrix};$$

0 - zero vector, dimension 3;

$\emptyset$ - zero matrix, of dimension 3×8.

Using the obtained relations (13-15), the deformation vector of the finite element e can be written in the local coordinate system:

The stress vector associated with the deformation vector by the Hooke law can also be represented:

$$\{\sigma\}^e = [D] \begin{bmatrix} c_1 & 0 & 0 \\ 0 & c_2 & 0 \\ 0 & 0 & c_3 \\ c_2 & c_1 & 0 \\ 0 & c_3 & c_2 \\ c_2 & 0 & c_1 \end{bmatrix} * \begin{bmatrix} \Phi & \emptyset & \emptyset \\ \emptyset & \Phi & \emptyset \\ \emptyset & \emptyset & \Phi \end{bmatrix} \{g\}^e ,$$

where $[D]$ - elastic matrix of transversely isotropic material with effective mechanical parameters.

Now, making the appropriate substitution, we can write an expression to calculate the stiffness matrix

$$[K]^e = \int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1} \left\{ \begin{bmatrix} c_1 & 0 & 0 \\ 0 & c_2 & 0 \\ 0 & 0 & c_3 \\ c_2 & c_1 & 0 \\ 0 & c_3 & c_2 \\ c_2 & 0 & c_1 \end{bmatrix} * \begin{bmatrix} \Phi & \emptyset & \emptyset \\ \emptyset & \Phi & \emptyset \\ \emptyset & \emptyset & \Phi \end{bmatrix} \right\}^T [D] \begin{bmatrix} c_1 & 0 & 0 \\ 0 & c_2 & 0 \\ 0 & 0 & c_3 \\ c_2 & c_1 & 0 \\ 0 & c_3 & c_2 \\ c_2 & 0 & c_1 \end{bmatrix} * \begin{bmatrix} \Phi & \emptyset & \emptyset \\ \emptyset & \Phi & \emptyset \\ \emptyset & \emptyset & \Phi \end{bmatrix} * \left|\det[J]\right| d\xi\, d\eta\, d\zeta ,$$

given that

$$dV = \left|\det[J]\right| d\xi d\eta\, d\zeta \cdot$$

To calculate the integral of surface loads, it is necessary to consider each surface of the final element separately. Depending on which surface the load is given, six different values of this integral can be written. Suppose that a uniformly distributed load $\xi=1$ is applied on the surface $F=\{F_x,F_y,F_z\}$ and the four first nodes of the finite element are located on it. Then the vector of nodal forces can be represented in the form:

$$\{F\}^e = -\int_{-1}^{1}\int_{-1}^{1} [N^p]^T \{F\} \left|\det\left[J^p\right]\right| \partial\xi \partial\eta ,$$

where

$$[N^p]^T = \begin{bmatrix} N_1 & 0 & 0 & N_2 & 0 & 0 & N_3 & 0 & 0 & N_4 & 0 & 0 \\ 0 & N_1 & 0 & 0 & N_2 & 0 & 0 & N_3 & 0 & 0 & N_4 & 0 \\ 0 & 0 & N_1 & 0 & 0 & N_2 & 0 & 0 & N_3 & 0 & 0 & N_4 \end{bmatrix} ,$$

$$\left[J^{p}\right]=\begin{bmatrix}\frac{\partial N_1}{\partial \xi} & \frac{\partial N_2}{\partial \xi} & \frac{\partial N_3}{\partial \xi} & \frac{\partial N_4}{\partial \xi}\\ \frac{\partial N_1}{\partial \eta} & \frac{\partial N_3}{\partial \eta} & \frac{\partial N_3}{\partial \eta} & \frac{\partial N_4}{\partial \eta}\end{bmatrix}\bullet\begin{bmatrix}x_1 & y_1\\ x_2 & y_2\\ x_3 & y_3\\ x_4 & y_4\end{bmatrix}.$$

The coefficients of the stiffness matrix of isoparametric finite elements and components of the vector of nodal loads are calculated by means of Gaussian quadratures, since it ensures the greatest accuracy for a given number of integration points. Using the Gauss formula three times to integrate the function of one variable, you can write:

$$\int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1} f(\xi,\eta,\zeta)\, d\xi d\eta\, d\zeta=\sum_{i=1}^{t}\sum_{j=1}^{t}\sum_{k=1}^{t} H_i H_j H_k f(\xi_i,\eta_j,\zeta_k)$$

where

t - is the number of integration points; H_i,H_j,H_k – weights.

Such an approach is especially effective in the three-dimensional case, since it allows to approximately halving the number of integration points as compared to the standard $t{\times}t{\times}t$– point formula.

For the integration of expressions $[B]^T[D][B]$ and $[N^p]^T\{F\}$ sufficient quadrature second order. The coordinates of the nodes and the weighting factors for the Gauss quadrature are given in paper (Laurie 2007).

The constructed stiffness coefficients for all finite elements are used in the formation of the resolving system of equations. Usually several elements converge in one node. The essence of the assembly is to sum up the corresponding coefficients of the stiffness matrices of adjacent elements for each node in each direction and place this sum in the right place of the global stiffness matrix.

Quantifying the stress-strain state of spatial bodies requires a breakdown of the area occupied by the body into a large number of finite elements. This leads to the construction of a system of high-order algebraic equations and is fraught with certain difficulties when implemented on computer systems. For this purpose, we used the method of line-by-line data preparation for each node separately, which ensures the construction of a tape system of high order algebraic equations taking into account the symmetry of its coefficients.

5. Solutions of a symmetric-tape system of equations of high order

The use of FEM leads to a resolving system of linear algebraic equations of high order. To solve the system of equations, the square root method is used, modified for the symmetric - tape structure of the coefficient matrix (Polatov 2019). Since each finite element is associated with a limited number of other finite elements, the matrix of the system of equations always turns out to be rarely filled. The arrangement of the coefficients in the matrix is closely related to the order of the numbering of the nodes in the body. In the case of random numbering, nonzero components are also distributed randomly in the matrix, which leads to an increase in the calculation time of the problem. Therefore, it is necessary to choose an order of numbering in which non-zero elements would be grouped around the main diagonal of the matrix, that is, would form a strip (ribbon). The procedure of ordering the node numbers in the finite element model allows minimizing the width of the tape of nonzero coefficients of the resolving system of equations. Since the coefficients of

$$T^{'} = \begin{bmatrix} t_{11} & & & & & & & & \\ t_{21} & t_{22} & & & & & & & \\ t_{31} & t_{32} & t_{33} & & & & & & \\ t_{41} & t_{42} & t_{43} & t_{44} & & & & & \\ 0 & t_{52} & t_{53} & t_{54} & t_{55} & & & & \\ 0 & 0 & t_{63} & t_{64} & t_{65} & t_{66} & & & \\ 0 & 0 & 0 & t_{74} & t_{75} & t_{76} & t_{77} & & \\ 0 & 0 & 0 & 0 & t_{85} & t_{86} & t_{87} & t_{88} & \\ 0 & 0 & 0 & 0 & 0 & t_{96} & t_{97} & t_{98} & t_{99} \end{bmatrix} \quad S = \begin{bmatrix} 0 & 0 & 0 & s_{14} \\ 0 & 0 & s_{23} & s_{24} \\ 0 & s_{32} & s_{33} & s_{34} \\ s_{41} & s_{42} & s_{43} & s_{44} \\ s_{51} & s_{52} & s_{53} & s_{54} \\ s_{61} & s_{62} & s_{63} & s_{64} \\ s_{71} & s_{72} & s_{73} & s_{74} \\ s_{81} & s_{82} & s_{83} & s_{84} \\ s_{91} & s_{92} & s_{93} & s_{94} \end{bmatrix}$$

Fig. 1 The location of the coefficients of the system of equations

the matrix of such a system of equations and the coefficients of the stiffness matrix of finite elements are symmetric, then at the stage of solving the system of equations it is advisable to use only the diagonal elements and the elements located below it, that is, the lower triangular matrix. In this case, the coefficients of the last matrix also have a tape structure.

In the square root method transformations, the operation of matrix-vector multiplication is mainly used. In this regard, an algorithm for multiplying the matrix by the vector has been developed for the case when only the coefficients of the lower band of the triangular matrix are given. If we arrange these coefficients line by line, a rectangular matrix S_{ij} is formed with dimensions $n\times l$, where n - is the order of the system of equations, l is the half width of the tape of nonzero coefficients, including diagonal elements. Moreover, the diagonal elements of the original matrix are located on the last l - th column of the matrix S_{ij}.

To illustrate the transformations, assume that $n = 9$, $l = 4$. In this case, the lower triangular and rectangular S_{ij} matrices have the following representations (Fig. 1).

For the formation of the process of multiplying the matrix S_{ij} by the vector x_j in the case when the transformed coefficients of the matrix, located diagonally and below, are taken as a basis, the following relation is developed and used:

$$y_i = \sum_{j=1}^{p} s_{i,q} x_r + \sum_{j=i}^{m} s_{j,i+l-j} x_j \ ,$$

where

$$p = \begin{Bmatrix} i-1, if\ 1 \le i \le l \\ l-1, else \end{Bmatrix} \qquad q = \begin{Bmatrix} l+j-i, if\ 1 \le i \le l \\ j, else \end{Bmatrix}$$

$$r = \begin{Bmatrix} j, if\ 1 \le i \le l \\ i-l+j, else \end{Bmatrix} \qquad m = \begin{Bmatrix} i+l-1, if\ 1 \le i \le n-l+1 \\ n, else \end{Bmatrix}$$

The relation given makes it possible in the algorithm of the square root method, by using the coefficients of the lower triangular matrix, to dispense with the zero coefficients of the nonzero elements located outside the ribbon and the coefficients of the upper triangular matrix. On the basis of the obtained solutions of the system of resolving equations, which correspond to the nodal displacements, the parameters of the stress state are calculated using the relation (5, 6).

6. Visualization of calculation results

To visualize the resulting parameters the algorithms that allow display a picture of object's deformation-stress state are developed. Since the values of the displacement is smaller compared with the dimensions of construction the values multiplied by the correction coefficient *k*: $(u', v', w')=k\cdot(u, v, w)$ is used in the algorithm.

This coefficient is selected by the user depending on the problem. To improve the visualization, the coordinate values of nodes are also multiplied by the correction factor. The correspondence between the parameter and the fill color is determined from the following relationship:

$$c = C\left(\begin{cases} \dfrac{p}{p_{max}}, & if\ p \geq 0 \\ \dfrac{p}{p_{min}}, & if\ p < 0 \end{cases}\right), \tag{20}$$

$$c = \begin{cases} c_1, & if\ p < \iota_1 \\ c_2, & if\ p < \iota_2 \\ \dots \\ c_n, & if\ p < \iota_n \\ c^*, & if\ p \geq \iota_n \end{cases}, \tag{21}$$

where

p_{min}, p_{max} - respectively, the minimum and maximum values of parameter;

C - machine-dependent function that linearly maps the numerical interval [-1; 1] in the space of colors from dark blue to dark red.

Then the process of gradient fill is beginning. In this case the dependence between the values of parameter and color is given by relationship (21), where n - number of isolines, $c_1, \dots, c_n$ - the color values by which will be used while painting cross section areas. The remaining area will be colored in the color c*. For user convenience, the color is specified as a numbers from -100 to +100.

7. Software package

For performing computational experiments, the ARPEK - special software package is developed. Software has a modular structure; data exchange between modules is executed through configuration files and data files. Further, scheme of functioning calculation modules of ARPEK

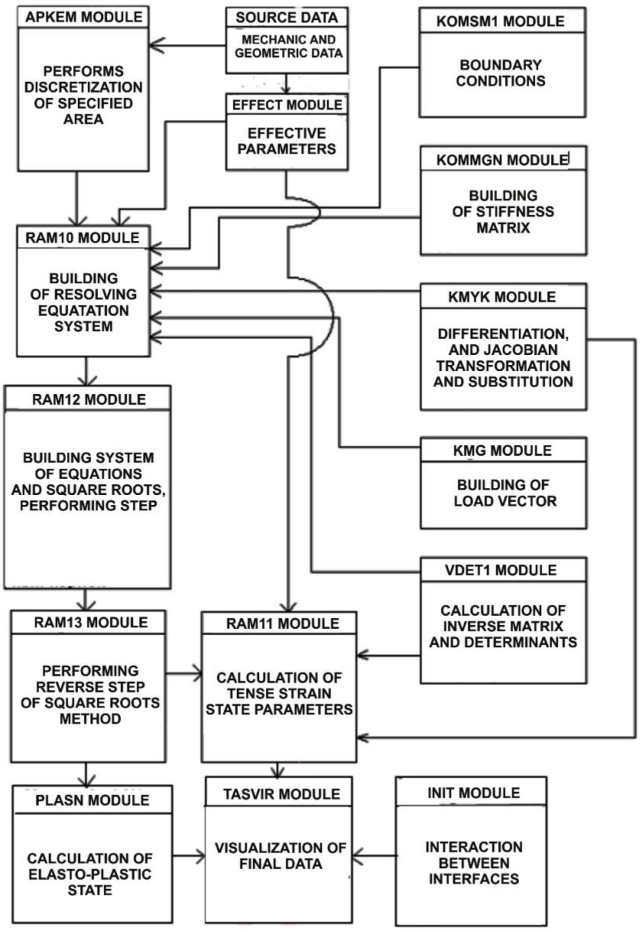


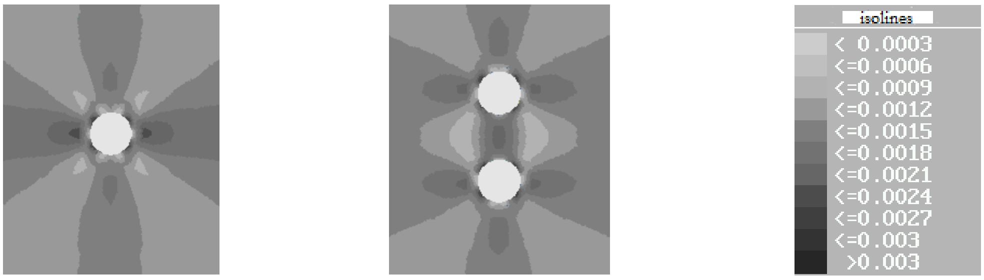
Fig. 2 Architecture of ARPEK - software package

software (Fig. 2) is described. Construction of finite element mesh is carried out in APKEM - software module.

Next the EFFECT module performs calculations the effective mechanical properties of the material. Formation of equations' system resolving is performed in FEM RAM10 module. To solve equations' system method of square roots, modified for equations' system with symmetric-band structure, is used. The solution process consists of two stages: first stage - RAM12 module, performs calculations in accordance with direct path algorithm, second stage - RAM13 module – reverse path of solution method. As result - vector of nodal displacements is formed. In operation stage, RAM11 module counts values of the stress-strain state component, which are recorded in the output module - PARAMS. While physically nonlinear problems solving, for clarification of elastoplastic solution based on iterative process based on Initial stress method - PLASN module is used. The output values of elastoplastic stress-strain state are recorded in PARAMS file. Visualization of calculation results is performed in TASVIR software module.

Table 1 Comparison of calculation results

Model	u	σ_{xx} [MPa]	p_u	P_u [MPa]
Transversely-isotropic	-10.20*10^{-2}	-0.997*10^{4}	0.1494	0.705*10^{4}
(Khaldjigitov 2003)	-09.57*10^{-2}	-1.003*10^{4}	0.1500	0.707*10^{4}



(a) (b) (c)

Fig. 3 Distribution of deformation intensity p_u (fragments)

8. The computational experiment

The results of numerical simulation of solving the three-dimensional problem of elastoplastic deformation of structural elements made of fibrous materials are given.

Validation of the newly created program is performed by comparing the numerical results with some of the results available in the literature. In the paper (Polatov 2019), the accuracy of the numerical results of the calculation is confirmed by graphically comparing the solution of the elastic problem of stretching a fiber composite plate with a hole in the center (Karpov 2002).

To test the software, the results of the calculation of the problem of two-sided compression of a transversely isotropic elastoplastic single cube from a magmatic with uniformly distributed loads $P_{xx} = \pm 10^4$ MPa along the axis OX are considered. Construction material has a linear hardening. The main axis of transversal isotropy is directed along the OZ axis. For a given load, a uniaxial stress state is observed throughout the cube. The material is completely in plastic state. In the first line of Table 1 presents the results of solving the above elastoplastic problem. To substantiate the reliability of the obtained results of the calculation, the second line contains the solutions of a similar problem based on the variation-difference method (Khaldjigitov 2003). Comparison of results confirms the correctness of the results obtained and it should be noted that with uniaxial stress, there is a steady convergence of the iterative process.

Being considered the process of reducing stress by changing the shape of the construction contour with the minimum distortion of stress state is considered. The geometrical dimensions of structures and stress concentrators are dimensionless relative to the side of a square plate.

The deformed condition of infinite lengthy strip of fibrous material with the system of uniaxial holes is considered. The fibers are arranged in the direction of the OZ-axis. Volume content of boron fibers is taken as 35%., mechanical parameters have:

$E = 0.9964 * 10^5$ MPa, $E' = 1.8532 * 10^5$ MPa, $G = 0.4311 * 10^5$ MPa, $G' = 0.3802 * 10^5$ MPa,
$\mu = 0.1558$, $\mu' = 0.2762$, the limit of elastic deformation of duralumin is $p_s = 0.003$.

Strip is stretched in the direction of the fibers (P_{zz} = 950 MPa). The centers of the holes of radius R = 0.05 placed along the OX-axis (hereinafter all linear dimensions are given relative to the unit size plate). The distance between the centers of holes is *h* = 0.2, width of the strip – 1,0 , thickness – 0.1 . Analysis of the deformation intensity indicates to the presence of mutual influence of horizontally located holes (fig.3.a). The vicinities of holes are unloaded and no plastic zone is presented. The increasing values of deformation are observed along the axis of holes' system.

Stretching of endless strip with a system of vertically arranged pair holes is investigated as well. The distance between of holes along the vertical $h = 0.2$, along horizontal - $l = 0.5$. Unloading of strip's deformed state is the result of mutual influence of holes both, along vertical, as well as horizontal (fig. 3.b). The values of deformation intensity of the strip in this case are bit lower than in the case of uniaxial holes' system.

Thus, analysis of the results of computational experiments allow to design a rational structure of fiber composites, to determine placement of the structural holes and to reduce the concentration of stress in constructions.

9. Conclusion

In the course of the research produced the following results:

- on the basis of finite element method and the theory of small elastic-plastic deformations for a transversely isotropic environment the numerical model, computational algorithms and software for solve three-dimensional problems of physically nonlinear deformation of structural materials are developed.
- analysis of the results of computational experiments allows designing a rational structure of fiber composites, to determine placement of constructional holes and to reduce the concentration of stress in constructions.
- method has been created, computational algorithms and software for formation grid of finite element representation of three-dimensional constructions is developed that enables automation of 3D representation on user computer monitor.
- on the basis of numerical modeling and computational experiments three-dimensional elastoplastic problems connected with the study of the presence of stress concentrators on the deformation structures of fiber composite materials are solved.

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