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Supercomputer multiscale modeling of composite structures strength

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Abstract. A method for multiscale supercomputer calculations of the composite structures strength has been developed. A feature of the proposed methodology is of division of the solution algorithm into 2 parts: solving problems at the micro level (in turn, these problems can consist of several sub-levels of calculation) and solving the problem at the macro level. Such a division, in which the solution of some problems is the input to problems at a higher level, helps to significantly reduce the consumption of computing resources. When solving problems, curvilinear anisotropy is taken into account at the macro level (structures), as well as at the micro level (composite material). The 3D finite element method was used for the numerical solution. To take into account curvilinear anisotropy, a special assembly algorithm is used, which requires the construction of anisotropy blocks (cells). A method is proposed for taking into account integral boundary conditions when solving problems of the linear theory of elasticity. A finite element modeling of the stress-strain state and damageability of a cylindrical structure with power ring elements has been carried out. As an example, textile composite materials (CM) with carbon and glass fibers are considered. **Key words**: supercomputer, composite structures, finite element.

1 Introduction

At present, there is more interest for multiscale problems, the solution of which requires significant computing power. The hierarchical multilevel structure is clearly seen in modern composite materials. Each previous structural level is included in the next higher level. Such a structure is especially clearly realized in composites based on reinforcing fibers of various weaves: fabric, winding, spatially reinforced, in which the fibers themselves are bundles of a large number of monofilaments [1]. Methods based on approximate analytical approaches [2–6] do not provide acceptable strength characteristics in the transverse directions of the composite and in shear. A detailed calculation of structures, taking into account all the real microstructure of such structures, is currently impossible to carry out in the foreseeable time even on the most powerful modern computing tools, including supercomputer technologies. In this regard, a multilevel model was developed for calculating the effective elastic and

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strength characteristics of composites, within which calculations are carried out only for representative elements of each structural level (periodicity cells), and then for a homogenized structure with effective properties.

2 Simulation of the stress-strain state in composite structures

The proposed calculation method is divided into three stages:

- modeling of effective elastic and strength properties of construction materials on the periodicity cells;
- finite element modeling of macroscopic stress-strain state (SSS) of a composite structure for homogenized material;
- simulation of material damage as part of a structure.

To calculate the effective elastic and strength characteristics, the method of asymptotic averaging (MAA) is used [7-12]. After obtaining the necessary material constant, the macroproblem of the linear theory of elasticity for an anisotropic deformable solid is considered [13,14] in Cartesian basis $\vec{e}_i$ with Cartesian coordinates x_i, which are also called global:

$$\begin{cases} \nabla_j \sigma_{ij} = 0, \\ \sigma_{ij} = C_{ijkl}(z^{(n)})\varepsilon_{kl}, \\ \varepsilon_{ij} = \dfrac{1}{2}(\nabla_j u_i + \nabla_i u_j), \\ \Sigma_\sigma : \sigma_{ij} n_j = S_i, \Sigma_u : u_i = u_{ei}, \\ \Sigma_S : \sigma_{kj} n_j = S_{ek}, u_l = u_{el}, k = 1,...,J, l = 1,...,L, J + L = 3. \end{cases} \tag{1}$$

where u_i – components of the displacement vector (unknown functions of the problem), σ_{ij}, ε_{ij} – components of stress and strain tensors respectively, operators of differentiation with respect to global coordinates: $\nabla_i = \partial / \partial x_i$, $C_{ijkl}(z^{(n)}, x_m)$ – components of the elastic moduli tensor of the composite, which are functions of the damage parameters $z^{(n)}$ and coordinates x_m due to curvilinear anisotropy, n_i – surface normal vector components, S_{ek} – components of the force vector on a part of the boundary Σ_S, u_{ei} – displacement vector components on a part of the boundary Σ_u, u_{el} – displacement vector components on a part of the boundary Σ_S, S_i – components of the force vector on a part of the boundary Σ_σ.

3 Accounting for curvilinear anisotropy in the model for calculating the components of the elastic modulus tensor

The structure has a curvilinear anisotropy, i.e. there are curvilinear coordinates q_i, that are related to global coordinates $q_i(x_m)$. The coordinate line q_1 is chosen orthogonal to the middle surface of the structure at the point of intersection with it. We introduce local Cartesian coordinates ξ_i, which are tangent to the coordinate lines q_i at the point of intersection with the structure. The coordinates ξ_i will form the principal axes of curvilinear anisotropy [15], in which the elastic modulus tensor ${C_{ijkl}}^{(0)}(z^{(n)})$ is orthotropic and is related to the components $C_{ijkl}(z^{(n)}, x_m)$ in global coordinates x_m by the relations:

$$C_{ijkl}(z^{(n)}, x_m) = {C_{i'j'k'l'}}^{(0)} Q_{ii'} Q_{jj'} Q_{kk'} Q_{ll'}, \tag{2}$$

where $Q_{ii'} = \dfrac{\partial x_i}{\partial q_{i'}}$ – Jacobian matrix [15], with the help of which local anisotropy bases are introduced $\vec{r}_j = Q_{ij'} \vec{e}_i$. Let us denote the orthonormal basis as $\hat{\vec{r}}_j$.

4 Setting integral boundary conditions in moments

In engineering practice, it is necessary to model the boundary conditions (BC) in (1) not only in terms of displacement vectors, forces, but also in moments. This boundary condition makes sense only for structures such as cylindrical bodies [], on their flat surfaces Σ. The moment vector is represented in the basis attached to these planes Σ:

$$\vec{M}_e = M_e^i \vec{e}_i^{\,'}. \tag{3}$$

Let $\vec{e}_3^{\,'}$ be orthogonal to plane Σ to which the moment is applied, then M_e^1, M_e^2 are bending moments, and M_e^3 – torque.

The moment is defined as follows [13]:

$$\vec{M} = \int_\Sigma \vec{\bar{x}} \times \vec{t}_n d\Sigma, \tag{4}$$

where $\vec{\bar{x}} = \overrightarrow{O'M}$ the radius vector of point $M \in \Sigma$, $\vec{t}_n$ – the force vector on Σ

$$\vec{t}_n = \sigma_{n1} \overrightarrow{e'_1} + \sigma_{n2} \overrightarrow{e'_2} + \sigma_{nn} \overrightarrow{e'_3}, \tag{5}$$

where σ_{n1} σ_{n2} - shear stresses on Σ, and σ_{nn} – normal stress.

Let us consider possible cases of specifying the moments:

$$M_e^1, M_e^2 \neq 0,\ M_e^3 = 0, \tag{6}$$

then the BSc are given in terms of the stress tensor as follows [13]:

$$\sigma_{nn} = A_0 + A_1 x^1 + A_2 x^2, \sigma_{n1} = \sigma_{n2} = 0, \tag{7}$$

where A_0, A_1, A_2 are calculated by the formulas obtained as a result of solving the problem of bending a cylindrical body by moments [13]:

$$\begin{aligned}
&A_\alpha = a_{\alpha 1} M_e^1 + a_{\alpha 2} M_e^2, \quad \alpha = 0,1,2,\\
&a_{01} = (S_1 I_{12} - S_2 I_{11})\frac{1}{\Delta}, a_{02} = (S_1 I_{22} - S_2 I_{12})\frac{1}{\Delta},\\
&a_{11} = -(S I_{12} - S_1 S_2)\frac{1}{\Delta}, a_{12} = -(S I_{21} - S_2{}^2)\frac{1}{\Delta},\\
&a_{21} = (S I_{12} - S_1{}^2)\frac{1}{\Delta}, a_{22} = (S I_{12} - S_1 S_2)\frac{1}{\Delta},\\
&S = \int_\Sigma d\Sigma, S_1 = \int_\Sigma x^1 d\Sigma, S_2 = \int_\Sigma x^2 d\Sigma,\\
&I_{11} = \int_\Sigma (x^2)^2 d\Sigma, I_{22} = \int_\Sigma (x^1)^2 d\Sigma, I_{12} = \int_\Sigma x^1 x^2 d\Sigma,\\
&\Delta = \det\begin{pmatrix} S & S_1 & S_2 \\ S_1 & I_{11} & I_{12} \\ S_2 & I_{12} & I_{22} \end{pmatrix}.
\end{aligned}$$

$$M_e^3 \neq 0, \qquad M_e^1 = 0, M_e^2 = 0, \tag{8}$$

then the BCs are given in terms of the displacement vector as follows, obtained when solving the problem of beam torsion:

$$\begin{aligned}
&u_1 = -\vartheta x_2 x_3, u_2 = \vartheta x_1 x_3, \sigma_{33} = 0,\\
&\vartheta = \frac{M_e^3}{I_{22} G_{23} + I_{11} G_{13}}.
\end{aligned} \tag{6}$$

where G_{23}, G_{13} - shear moduli.

It should be noted that in the case of bending moments, the final result will be independent of the choice of $O' \in \Sigma$, in the case of torsion, such a statement will be incorrect.

5 Composite structure damage calculation

For isotropic materials, the Mises criterion is most often used to calculate strength and damage [13]. For orthotropic composites, this criterion is not applicable; instead, the Tsai-Wu and Tsai-Hill strength criteria are most often used [3,5,13]. These criteria are mainly used for fabric and layered composites. In the principal axes of anisotropy, the criterion of the Tsai-Hill type, written with the help of sign-constant stress tensor invariants [4], has the form:

$$z^{(1)} = \sum_{\alpha=1}^{2}\left(\left(\frac{\sigma_{\alpha\alpha}^{+}}{\sigma_{T\alpha}}\right)^2 + \left(\frac{\sigma_{\alpha\alpha}^{-}}{\sigma_{C\alpha}}\right)^2\right) - \left(\frac{\sigma_{11}^{+}}{\sigma_{T1}} - \frac{\sigma_{11}^{-}}{\sigma_{C1}}\right)\left(\frac{\sigma_{22}^{+}}{\sigma_{T2}} - \frac{\sigma_{22}^{-}}{\sigma_{C2}}\right) + \left(\frac{\sigma_{12}}{\sigma_{S12}}\right)^2,$$
$$z^{(2)} = \left(\frac{\sigma_{33}^{+}}{\sigma_{T3}}\right)^2 + \left(\frac{\sigma_{33}^{-}}{\sigma_{C3}}\right)^2 + \left(\frac{\sigma_{13}}{\sigma_{S13}}\right)^2 + \left(\frac{\sigma_{23}}{\sigma_{S23}}\right)^2, \quad (7)$$

where $z^{(1)}$ – the damage parameter responsible for the rupture or crushing of the fibers in the plane Oe_1e_2,

$z^{(2)}$ – damage parameter responsible for delamination during interaxial shear, or transverse separation or collapse.

$$\sigma_{\alpha\alpha}^{\pm} = \frac{1}{2}\left(\sigma_{\alpha\alpha} \pm \left|\sigma_{\alpha\alpha}\right|\right) \ \ \alpha = 1,2,3$$

sign-constant invariants of the stress tensor, and $\sigma_{T\alpha}, \sigma_{C\alpha}$ - limits of tensile strength, compression in various directions, $\sigma_{S12}, \sigma_{S13}, \sigma_{S23}$ - shear strength limits in various planes.

The algorithm for calculating the damage of an orthotropic composite with a layered structure is implemented as follows:

1) The SSS of the structure is calculated without taking into account damage, which corresponds to the solution of the of the linear theory of elasticity problem (1);

2) The strength criterion is selected depending on the type of material and the field of parameters $z^{(i)}$ is calculated;

3) The safety factor is calculated:

$$\eta = 1/\max_{\vec{x}\in\Omega}\{z^{(i)}(\vec{x})\}, \quad (9)$$

where Ω – construction area together with boundary surfaces

4) after condition $z^{(2)} = 1$ is reached in any finite element (or node), a partial change in the elastic modulus of the composite occurs in the plane of laying the composite layers;

5) after reaching condition $z^{(1)} = 1$ in the FE (or node), all components of the elastic modulus tensor turn to zero in this FE.

6 Results of numerical simulation of the strength of a cylindrical composite structure

For the finite element solution of problem (1) using the proposed algorithm, the SMCM software package developed at the Scientific and Educational Center "Supercomputer Engineering Modeling and Development of Software Complexes" of Bauman Moscow State Technical University [16,17] (SIMPLEX) was used. The software package allows modeling on supercomputer technology:

- using distributed nodes with CPU and using MPI,
- using GPU;
- using hybrid computing tools based on GPU+CPU.

Calculations were carried out on the SIMPLEX supercomputer complex.

The input data for modeling the properties of fabric composites in microlevel problems are the effective elastic and strength characteristics of matrices and monofilaments located in the matrix (a bundle of monofilaments is impregnated with a polymer binder). Table 1 shows the values of the matrix and monofilament constants used in the calculations. in turn, to obtain the second one, it is required to make a calculation at a lower level, for which it is necessary to know the characteristics of only monofilaments and matrices shown in Table 1.

Table 1. Elastic and strength properties of materials [4] used in calculations.

Nomination	Elastic constants	Values
Carbon fiber	E . GPa	260
	ν	0.2
	$\bar{\sigma}$	2.2
	H_0	3
	s	0.07
	ω	0.33
	r	0.25
Fiberglass	E . GPa	60
	ν	0.25
	$\bar{\sigma}$	2
	H_0	2.2
	s	0.13
	ω	0.38
	r	0.35
Epoxyphenol matrix	E . GPa	3
	ν	0.35
	σ_C	0.07
	σ_S	0.042
	σ_T	0.062

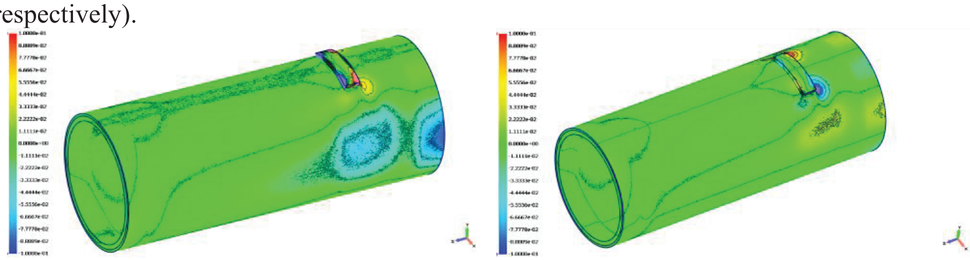
where E – Young's modulus, ν – Poisson's ratio, $\bar{\sigma}$ – average tensile strength of fibers, H_0, s, ω, r - temperature-independent constants that characterize the statistical spread in the strength of monofilaments in a fiber [4], σ_C – ultimate compressive strength, σ_S – ultimate shear strength, σ_T – ultimate tensile strength. The constants H_0 s ω r are used in the model for calculating the strength of threads of 1D composites consisting of monofilaments [4].

To calculate the properties of tissue CM, the method of asymptotic averaging was used, the description of which is given in [10-12], as well as the software [16,17], which is an integral part of the SMCM complex.

After solving the microlevel problems, we obtain data on materials that are necessary for calculating the stress-strain state of a structure made of composite materials.

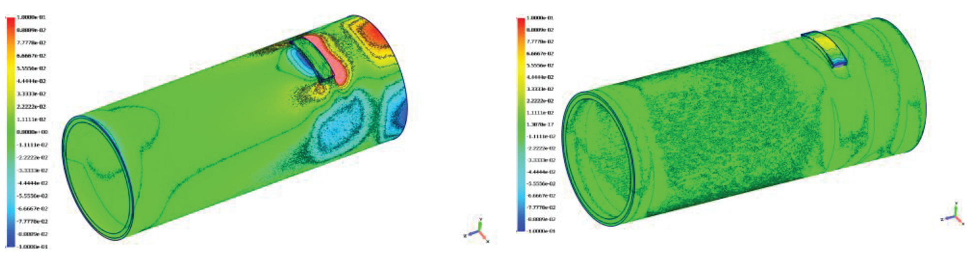
A cylindrical structure with reinforcing ring elements and a local fastening zone was considered. The following boundary conditions were considered: forces are applied tangentially along the end surfaces of the front and rear power elements, respectively, moments are also set on these surfaces.

Figures 1-3 show some calculation results: Figure 1 shows the fields of dimensionless stress values σ_{yy} and σ_{xy} in the global coordinate system, and Figure 2 shows the stress fields σ_{xx}^{loc} and σ_{yz}^{loc} in their own coordinate system. Figure 3 shows the maximum fields of the damage parameters z_1 and z_2 and the type of destruction (partial or complete, respectively).



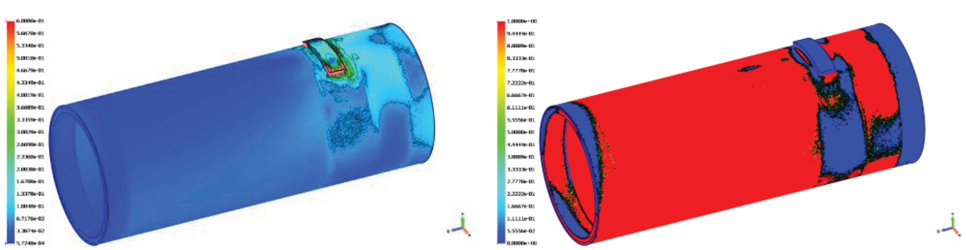
a) b)

Fig. 1. Stress fields σ_{yy} (a) and σ_{xy} (b).



a) b)

Fig. 2. Stress fields σ_{xx}^{loc} and σ_{yz}^{loc} .



a) b)

Fig. 3. The maximum of the damage parameters z_1 and z_2 (a) and the type of destruction (b).

7 Conclusions

A technique for solving multiscale strength problems for composite materials structures has been developed. A method of taking into account integral boundary conditions for problems of elasticity theory is considered. An example of the application of the developed technique for modeling stress fields in a cylindrical composite structure is given. It is shown that the developed technique makes it possible to successfully calculate stress fields both in the global coordinate system and in the local system associated with the local basis of anisotropy. The technique allows us to calculate the fields of damage parameters that determine various types of structural failure made of layered composite materials.

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