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V. L. Leontiev (Saint-Petersburg, SPbPU). **Orthogonal splines in models and methods of nanomechanics.**

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Резюме: The paper considers models and methods of nanomechanics related to the use of localization and orthogonality of splines. The application of the potential of interatomic interaction forces, integral transformations, and mixed numerical methods based on the properties of orthogonal splines increases the efficiency of modeling and spectral analysis of nanosystems, as well as the quality and accuracy of the analysis of the stress-strain state of nanosystems.

Ключевые слова: Nanomechanics, models, orthogonal splines, spectral analysis, stress-strain state, mixed variational-grid method.

This paper considers models and methods of nanomechanics related to orthogonal splines. These models of nanomechanics use the localization and orthogonality of the splines. Such properties allowed creation a new potential for interatomic interaction forces [1], the use of which in molecular dynamics programs significantly reduces the time for computer analysis of nanosystem dynamics. On the basis of orthogonal splines, integral transformations [2] were created, which are an effective tool for spectral analysis of electromagnetic impacts that cause movement of nanosystem, as well as a tool for spectral analysis of radiation generated by nanosystem. The peculiarity of these integral transformations is that they, like integral wavelet transformations, do not lose short-time signal components. At the same time, the quality of the results of spectral analysis with help of these transformations is not inferior to wavelet transformations, and the analysis time on the computer is significantly reduced. When nanosystems consist of a significant number of atoms, models of continuum mechanics are often used. In this case, orthogonal splines can increase the accuracy and smoothness of approximate solutions obtained when analyzing the stress-strain state of nanosystems. For this purpose, mixed variational-grid methods based on the Reissner variational principle and on use of orthogonal splines for simultaneous and independent approximation of kinematic and force factors are used. This approach allows us to obtain approximate solutions for displacements, stresses and deformations that are characterized by the same smoothness and accuracy of the same order. At the same time, the computational cost of these solutions is approximately the same as in the variational-grid method associated with the Lagrange variational principle. This is explained by the fact that the orthogonality of splines makes it possible to exclude nodal values of stresses before solving a system of grid equations. Thus, on the same grid, the variational-grid method based on the Lagrange variational principle and the mixed variational-grid method based on the Reissner variational principle give grid systems of algebraic equations with the same number of unknowns. At the same time, in the variational-grid method based on the Reissner variational principle, there is no numerical differentiation of approximate solutions obtained for displacements at the first stage, and it generates advantages of such

method. Theoretical studies and numerical calculations [3] have confirmed the high accuracy and same smoothness of all approximate solutions obtained with help of such mixed variational-grid method for displacements and for stresses.

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