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”Computers? They are useless.” On the importance of a computational simulation

Computational simulation is an integral part of any research on life science. It gives a powerful tool to build a realistic model, investigate it in detail and analyze experimental observations, and therefore, is widely used in systems biology and life sciences.

As a part of my Bachelor studies in Applied mathematics, I faced the several interdisciplinary problems. In the present work, I want to focus on my final project on the Numerical Analysis of the Model of Thin Shell. Initially, the problem in biology was considered as a typical problem of structural mechanics. The mechanical properties of tissues, living cells, and cellular components play an important role in determining the overall functioning of a plant. Hence, it is crucial to consider firstly structural model of cell walls which can be described in terms of the Kirchhoff-Love shell theory.

Following traditional assumptions, the shell is described in terms of its middle surface (thickness is constant under the deformation, normal stress in the thickness direction is negligible). Moreover, for the thin shell, the following relation holds

max(h$\overline{R)\ \frac{1}{20}}$

Hence we can reduce the problem to a 1-dimensional case. Following the classical theory of shells in terms of forces, displacements, stresses, and strains by Timoshenko we obtain the following nonlinear problem on the domain Ω=[a,b].

$$\frac{1}{A_1}\frac{dT_{11}}{d\xi_1} - k_1T_{13} = p_1; \quad -\frac{1}{A_1}\frac{dT_{13}}{d\xi_1} + k_1T_{11} = p_3; \quad -\frac{1}{A_1}\frac{dM_{11}}{d\xi_1} + T_{13} = m_1;$$

M$_{11}$ $=$ $\frac{E_2h^3}{12(1-\nu_2^2)}\chi_{11}$;T$_{11}, T_{13}$ are expressed in terms of the following variables similarly to M_{11} $\varepsilon_{11} = \frac{1}{A_1}\frac{dv_1}{d\xi_1} + k_1w + \frac{1}{2}w_{13}^2$;$\varepsilon_{13} = \frac{1}{A_1}\frac{dw}{d\xi_1} + \gamma_1 - k_1v_1$;$\chi_{11} = \frac{1}{A_1}\frac{d\gamma_1}{d\xi_1} + w_{13}\tau_{13} - \frac{1}{2}k_1w_{13}^2$;$w_{13} = \frac{1}{2}(-\frac{1}{A_1}\frac{dw}{d\xi_1} + k_1v_1 + \gamma_1)$;$\tau_{13} = k_1\gamma_1$;

where v_1, w - tangential and normal displacements; γ_1- the angle of rotation; T_{11}, T_{13}, M_{11} – stresses and the bending moment in the shell; A_1,k_1– Lamé and curvature parameters, respectively; $_2$ – Young's modulus, ν_2–Poisson's ratio; p_1, p_3, m_1 are expressed in terms of components of Cauchy tensor.

The problem was completed with boundary conditions and linearized by the Newton-Kantorovich method. An iterative process was obtained at each step of which the linear system of equation is to be solved. The Finite Element Method was applied. Following the standard procedure, the variational formulation of the problem was presented. The set of shape functions was chosen as an approximation of the discretized solution. It was shown that in case of piecewise linear shape functions the locking effect occurs. Hence to avoid this, on each element a continuum approximation using the integrated Legendre polynomials was introduced.

To sum up, a typical biological model was solved from the point of view of structural mechanics with FEM. The convergence and stability analysis was performed.

At this point, I can fully agree with Pablo Picasso, who said

> Computers are useless. They can only give you answers.

because it is a mathematician, who is always behind the model and who analyses the results. However, mathematical modelling, numerical analysis and computer simulation are integral parts of any scientific research and this is what I am willing to dedicate my life to.

Summary

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