Mechanical numerical model of deoxyribonucleic acid

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Molecules of deoxyribonucleic acid can be used as components of advanced electronic devices [1]. Electronic nanobiochips have a number of advantages over modern silicon chips. They are miniature, fast and accurate. It is also possible to use deoxyribonucleic acid (DNA) molecules in memory and logic devices [1, 2]. The success of the use of DNA in electronics depends on the ability to provide its electric conductivity, largely determined by the properties of open states. The formation of open states (bubbles of denaturation) and their propagation can be numerically simulated on the basis of mechanical models of the Peyrard–Bishop–Dauxois type [3]. In this work, a numerical realization of such a model is proposed, based on an implicit integration scheme. The system of finite-difference equations obtained as a result of approximation of the model relations is solved by the tridiagonal matrix algorithm at each time step. The results of calculations of mechanical disturbances of various types propagating along a non-uniform DNA molecule are presented.

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