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DNA Nanostructure Modelling and Simulation

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Extended Abstract

Recently, various DNA nanostructures have been designed and synthesized mostly relying on their self-assembly feature. Once a unit tile structure is précised designed, numerous copies are produced and self-assembled into 2D or 3D nanostructures. However, lack of information about its dynamic characteristics sometimes fails to reach the anticipated DNA nanostructure. For example, planar unit cross-tiles do not form a 2D lattice nanostructure but a 3D nanotube [1]. Modal analysis of DNA nanostructures successfully explained this self-assembly mechanism in terms of mechanical vibration [2]. In this talk, I will briefly introduce a theoretical framework how to model and simulate DNA nanostructure in order to understand its dynamic characteristics which play an important role in DNA nanostructure design and synthesis. First, a DNA nanostructure, either a unit tile or an assembly, is represented by a coarse-grained mass-spring network which contains DNA's structural information including mass and chemical interaction [3]. Then, a mechanical vibration theory, called normal mode analysis, is applied to the given DNA coarse-grained model to simulate its intrinsic vibrational characteristics. In addition, it will be discussed how to relate intrinsic vibration modes with self-assembly process successfully for various exampled DNA nanostructures including 2D lattice, 2D ring, and 3D bulky ball. Consequently, the proposed theoretical approach enables us to design DNA nanostructures much more precisely and systematically, compared to the conventional trial and error method.

References

[1] H. Yan, S. H. Park, G. Finkelstein, J. H. Reif, and T. H. LaBean, "DNA-templated self-assembly of protein arrays and highly conductive nanowires," *Science*, vol. 301, no. 4, pp. 1882-1884, 2003.
[2] P. Qian, S. Seo, J. Kim, S. Kim, B. S. Lim, W. K. Liu, B. J. Kim, T. H. LaBean, S. H. Park, and M. K. Kim, "DNA nanotube formation based on normal mode analysis," *Nanotechnology*, vol. 23, no. 105704, 2012.
[3] M. K. Kim, G. S. Chirikjian, and R. L. Jernigan, "Elastic models of conformational transitions in macromolecules," *J. Mol. Graph.*, vol. 21, pp. 151-160, 2002.