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Atoms-to-beam homogenization, applied to DNA

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Abstract:

Mechanical properties of DNA are of great biological interest, as duplication and expression are, as a rule, processes involving force-driven deformations. Traditionally, DNA sequences are considered as cylindrical straight isotropic beams[1], but this lead to unrealistic ratios between torsional and bending stiffnesses[2].

The deformation characteristics of long biological macromolecules, such as DNA or collagen, can be lucidly described by the terms "bending", "stretching", "torsion" and "shearing". These terms appear in a subset of continuum mechanics, called beam theory, while the standard numerical modelling procedure for macromolecules, which is molecular dynamics, does not allow for a direct introduction of these deformation characteristics.[3].

This deficit has motivated the theoretical development of a transition or upscaling procedure from molecular dynamics to beam theory[4]. It consists of two steps: (i) translation of potential energies into systems of equilibrated forces and moments; (ii) upscaling, through the principle of virtual power, the forces and moments arising from (i), to the scale where the macromolecule itself is considered as a beam structure.

As a first application, the above-described novel strategy is realised for a sequence of DNA base pairs, elucidating the source of the somehow paradox stretching-torsion coupling these molecules are known for.

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[3]Li, Ch. and Chou, T.-W. (May 2003). *A structural mechanics approach for the analysis of carbon nanotubes.* International Journal of Solids and Structures, 40(10):2487–2499.
[4]Kalliauer, J.; Kahl, G.; Scheiner, St.; and Hellmich, Ch. (October 2020). *A new approach to the mechanics of DNA: Atoms-to-beam homogenization.* Journal of the Mechanics and Physics of Solids, 143:104040.