6th European Conference on Computational Mechanics (ECCM 6)
7th European Conference on Computational Fluid Dynamics (ECFD 7)
11 – 15 June 2018, Glasgow, UK

FINITE ELEMENT FORMULATIONS FOR MOLECULAR INTERACTIONS OF FLEXIBLE FIBERS

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Key words: *geometrically exact beam theory, beam finite elements, (biopolymer) fibers, molecular interactions, van der Waals interaction, Lennard-Jones potential, electrostatic interaction*

(Bio)polymer fibers (e. g. collagen, DNA), carbon fibers/nanotubes or glass fibers are examples for slender flexible structures to be found on the scale of nano to micrometers that recently gained massive attention across various research communities. On these length scales, molecular interactions such as electrostatic or van der Waals forces are of utmost importance for the overall system behavior. This is in strong contrast to the macroscale where relevant interactions between bodies are mostly limited to contact. Accordingly, existing numerical methods for beam-to-beam interactions focus on contact described either point-pair-wise or along a line interval [1].

Motivated by the importance and inspired by the manifoldness of molecular interactions, we propose several new numerical methods to accurately and efficiently model the interactions between 3D slender elastic bodies described by the geometrically exact beam theory. All our methods are based on first principles of pair-wise atom or unit charge interactions that suggest well-known potential laws for the point-pair interaction energy. Considering two 3D bodies, this leads to a six-dimensional integral over both volumes to arrive at the two-body interaction potential. This strategy has been applied by Argento et al. [2] and Sauer et al. [3] for solids and is the key concept of one of our methods using full numerical integration over the two beams' deformed geometries. Unfortunately, the computational cost of such high-dimensional numerical integration is tremendous. Adhering to the underlying idea of beam models, namely reduced dimensionality, we therefore propose more efficient formulations using semi-analytical expressions and reduce the need for numerical integration to two or even one dimension(s). Moreover, we propose a new categorization for beam-to-beam interactions suggesting that the novel methods may be regarded as an extension of existing approaches for beam-to-beam contact. A study of the mechanics of collagen fibers will serve as an exemplary application of the methods to real-world biomechanical systems.

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