A self-contact preventing energy for nonlinear elastic filaments

Lonati Chiara*[1]

[1]Catholic University of Sacred Heart – Italy

Abstract

Nonlinear elastic filaments with small non-vanishing thickness can represent various physical phenomena, such as DNA folding and protein modeling, or, more generally, charged flexible structures. A fundamental notion to obtain physical descriptions is the constraint of non-interpenetration of matter and preservation of the isotopy class of the midline, i.e. its knot type.
Several expressions for local and global injectivity of the configuration map of an inextensible and unshearable closed rod were stated in the last decades (Ciarlet-Nečas, Gonzalez, Schuricht). We prove equivalences between them and a natural constraint on virtual displacements and we stress the similarity between notions of self-intersection and self-distance of knots and the corresponding treatment for thick filaments.
We then present a new repulsive energy functional defined on the surface of tubular neighbourhoods of inextensible curves: it is a generalization to thick filaments of the electrostatic inspired Mobius energy for knots by O'Hara. The functional preserves isotopy classes and degenerates to infinity if and only if self-contact or interpenetration occurs, so it acts as a natural constraint that guarantees physically acceptable configurations, without the necessity of reducing the space of admissible rods with complicated conditions. The main properties that we prove for this energy, supported by numerical simulations, are analogous to the ones proved for knots by O'Hara.

*Speaker