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AN APPROACH FOR THE MICRO-MECHANICAL SIMULATION OF BIOPOLYMER NETWORKS BASED ON GEOMETRICALLY EXACT BEAM ELEMENTS

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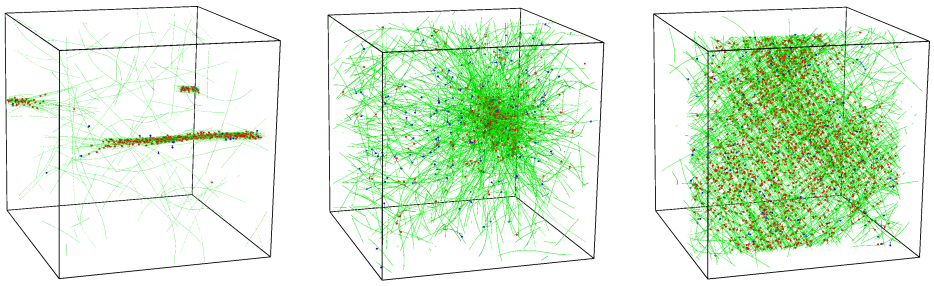
The simulation of biopolymer networks, i.e. polymer filaments and crosslinkers immersed in a viscous fluid, has attracted significant research interest in recent years [1, 3, 4]. A phenomenologically accurate model of biopolymer networks can lead to a deeper understanding of numerous processes in biological systems at different length scales, where experiments and theoretical predictions reach their limitations. At subcellular scale, the dynamic restructuring ability of cytoskeletal networks can be explored. Consecutively, events linked to cytoskeletal kinetics, such as, cell division, cell migration, mechanosensing and mechanotransduction, can be better understood [3].

Since single semi-flexible polymer filaments are extremely slender, they can be modeled as 1D Cosserat continua and be discretised using geometrically exact beam elements. This coarse-grained description yields high computational efficiency and together with other advanced computational techniques as outlined in [1], allows for the study of phenomena occurring on the biologically most relevant time-scale of $10s$ to several $100s$.

Recently, we proposed a micro-mechanical model with minimal assumptions for the simulation of biopolymer networks [1]. This model accounts for three major constituents,

- Semi-flexible filaments, such as F-actin.
- Linker molecules, e.g., filamin, α - actinin.
- Surrounding viscous fluid phase (modeled implicitly).

While, the filaments and the linkers are explicitly modeled using beam elements, their interaction with the surrounding viscous fluid is implicitly captured. This interaction between filaments and linkers with the fluid phase has two components: a deterministic viscous drag component, which, e.g., can be observed when a filament is moved through the fluid, and a stochastic part, which accounts for intermolecular collisions. The viscous effects are captured by an anisotropic friction model. Simultaneously, the stochastic forces are modeled as space-time white noise excitations. It has been observed, that by discretising the filaments and linkers with Reissner beam elements, we can efficiently simulate the polymorphism of semi-flexible biopolymer networks (Fig. 1).



(a) Bundle (b) Cluster (c) Layer

Figure 1: Equilibrium phase models of biopolymer newtworks using Reissner beam elements

At very high slenderness ratios, which is the case for the species of filaments under consideration, shear deformation becomes negligible in many cases. Therefore, modeling semi-flexible filaments with shear free beam elements can further increase computational efficiency. Here, we introduce a novel geometrically exact Kirchhoff beam element [2] to discretise the filaments and linkers. This shear-free element contains less degrees of freedom as compared to a Reissner beam element. Several numerical experiments are conducted to establish the suitability of the Kirchhoff beam element to model the dynamics of semi-flexible filaments.

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