Mechanics of active biological materials undergoing growth and remodeling

November 17, 2014

Recent experimental findings report the ability of biological tissues to undergo softening, stiffening and fluidisation. It is becoming increasingly clear that the processes at sub-cellular scale must be taken into consideration to explain these behaviours. At sub-cellular level, the cytoskeletal network is a dynamic mechanical structure which plays a major role in regulating important phenomena including contractility, motility, cell division and mechanotransduction. Therefore, modelling cytoskeletal kinetics at an appropriate length scale encompassing (de-)polymerization, crosslinker dynamics, active force generation is of the utmost importance.

Recently, a computationally efficient micro-mechanical finite element model has been developed [1] which can simulate phenomena well over 1000 s. This state-of-the-art model encompasses stochastic thermal undulations of cytoplasm and dynamic cross-linking. The smallest length scale in this model is a semi-flexible polymer similar to filamentous actin (F-actin). Since the slender-ness ratio of F-actin is very high (10 – 1000), these filaments can be discretised using geometrically exact beam elements. Previous works were developed by discretising the filaments using geometrically exact Reissner type of beam elements.

Current developments of the model are focused on implementing a novel geometrically exact



(a) Change in orientation correlation function (ϑ) along (b) Bundle network architecture formation in a repnormalised length (ξ/L) of a filament resentative volume element

Figure 1: Results of bio-polymer network simulation

Kirchhoff beam element [2] to discretise the filaments. This Kirchhoff beam element yields lower discritisation error compared to Reissner beam element and alleviates ill-conditioning by eliminating shear-stiffness terms. Preliminary simulations using Kirchhoff beam elements show promising results at single filament scale and at network level. At single filament scale, the numerical results are in very good agreement with theoretical predictions of orientation correlation function along the length of a filament (Figure 1a). At network scale, we are able to observe the formation of a bundle network architecture (Figure 1b) in a representative volume element as reported in experimental findings [3]. Future development of this model is directed towards reproduction of phenomena observed in cytoskeletal networks. The interaction of networks with cellular membranes is of particular interest.

References

- [1] C. J. Cyron, K. W. Müller, A. R. Bausch, W. A. Wall. Micromechanical simulations of biopolymer networks with finite elements. J. Comput. Phys., Vol. 244, 236 - 251, 2013.
- [2] C. Meier, A. Popp, W. A. Wall. An Objective 3D Large Deformation Finite Element Formulation for Geometrically Exact Curved Kirchhoff Rods. *Comput. Meth. Appl. Mech. Eng.* Vol. 278, 445 478, 2014.
- [3] O. Lieleg, M. M. A. E. Claessens, C. Heussinger, E. Frey and A. R. Bausch. Mechanics of Bundled Semiflexible Polymer Networks. *Phys. Rev. Lett.*, Vol. 99, 088102–, 2007.