io-port 06047860

Katsimitsoulia, Zoe; Taylor, William R.

Coarse-grained simulation of myosin-V movement.

Comput. Math. Methods Med. 2012, Article ID 781456, 15 p. (2012).

Summary: We describe the development of a hierarchic modelling method applied to simulating the processive movement of the myosin-V molecular motor protein along an actin filament track. In the hierarchic model, three different levels of protein structure resolution are represented: secondary structure, domain, and protein, with the level of detail changing according to the degree of interaction among the molecules. The integrity of the system is maintained using a tree of spatially organised bounding volumes and distance constraints. Although applied to an actin-myosin system, the hierarchic framework is general enough so that it may easily be adapted to a number of other large biomolecular systems containing in the order of 100 proteins. We compared the simulation results with biophysical data, and despite the lack of atomic detail in our model, we find good agreement and can even suggest some refinements to the current model of myosin-V motion.

doi:10.1155/2012/781456