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Molecular Dynamics Modeling and Analysis of Actin Network Formation RONALD PANDOLFI, UC Merced — Actin filaments are ubiquitous and critical in cellular functions. The polymeric protein F-actin is a semi-flexible filament that forms networks in the presence of binding proteins (i.e. α -actinin, Filamin, Fascin). Molecular dynamics modeling and simulation of the formation of these networks informs the dependence of network structure on the length and flexibility of these filaments. In comparative experimental work, filament length is controlled by the addition of Gelsolin. The calculation of radial pair distribution functions of simulated actin systems allows quantitative characterization of the network structure by bundling and mesh size.

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