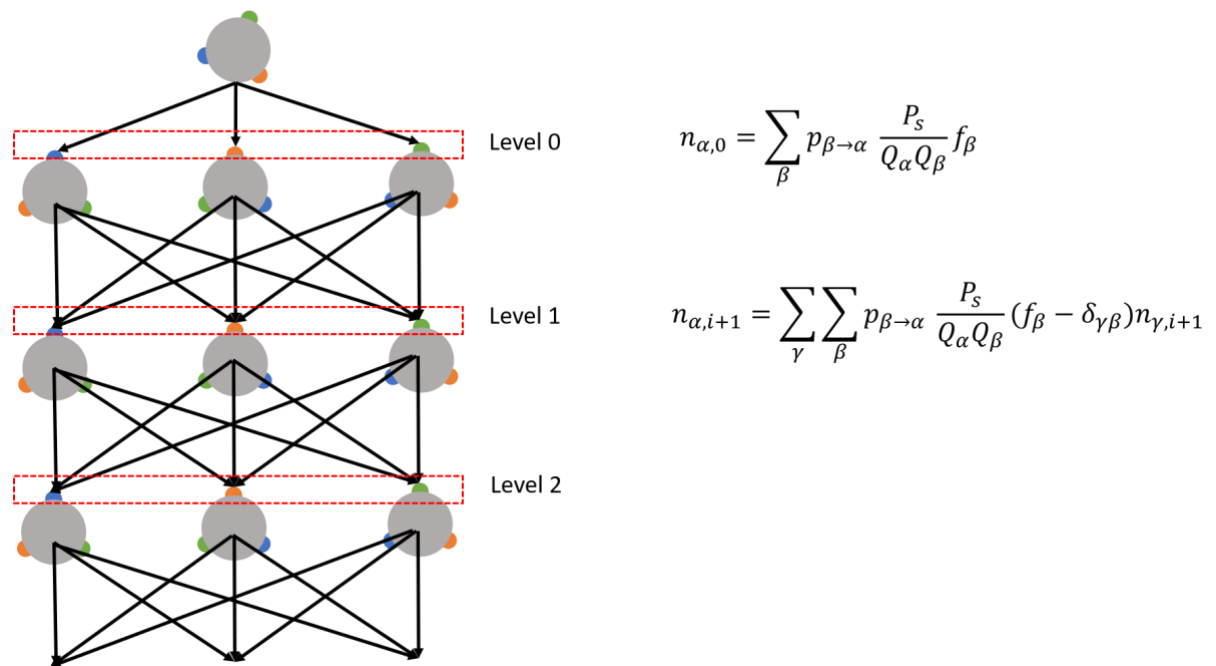


Title: Distinct connectivity states in actomyosin networks described using the Flory-Stockmayer theory

Presenting Author: Carlos Bueno

In this work we model the actomyosin networks using a mean field model based on the Flory-Stockmayer theory and compare it to a mechanochemical coarse-grained model. We find that Arp2/3 modulates the connectivity of the networks in a non-monotonic way. We also describe rigidity percolation in actomyosin networks and propose different connectivity states that give rise to distinct dynamical behaviors.

Figure:



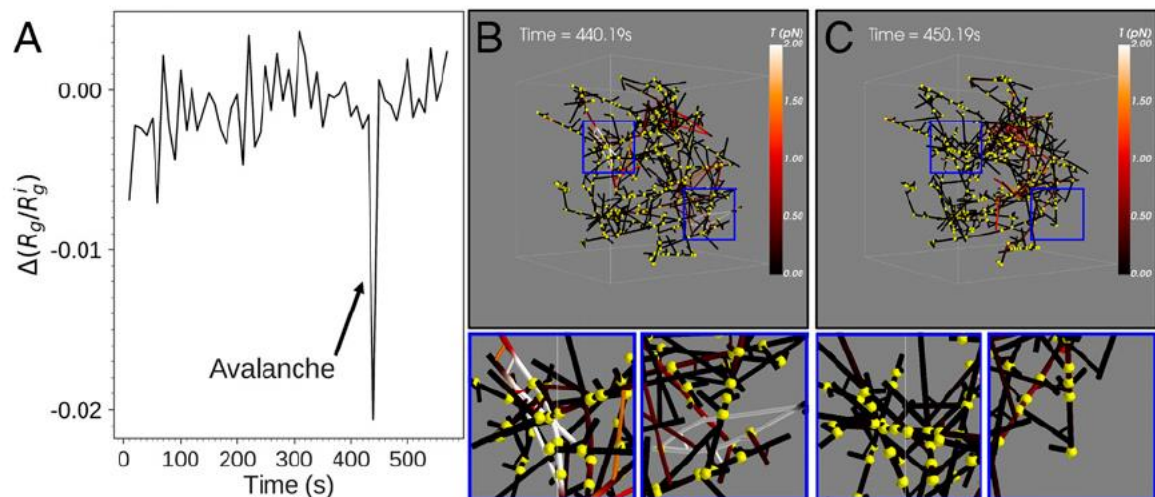
Connectivity of an actomyosin cluster in a Bethe lattice. Each actin monomer is represented by a gray circle and the connections are represented by black arrows. The equations on the right describe the average number of connections on each layer as a function of the probability of forming a connection between two monomers and the probability that the connections percolate the actin network. [Link to the abstract.](#)

Title: Rare convulsive movements observed in simulations of motorized actin networks with the Arp2/3 complex

Presenting Author: James Liman

We model the structural rearrangements of motorized actin network, both in the presence of and in the absence of actin-related protein 2/3 (Arp2/3) complex. In this model, we incorporate motor proteins (non-muscle myosin IIA heavy chain (NMIIA)) and cross-linking proteins (α -actinin) in the two actin systems. We observe that the relaxation times of the branched actomyosin networks are significantly longer than those of their unbranched counterparts, by as much as a factor of 4. We also observe that the branched networks exhibit rare convulsive movements, which we call avalanches. These avalanches release tension in the network. Recent experimental evidence of “cytoquakes” are consistent with the results of our simulations. [Link to the abstract.](#)

Figure:



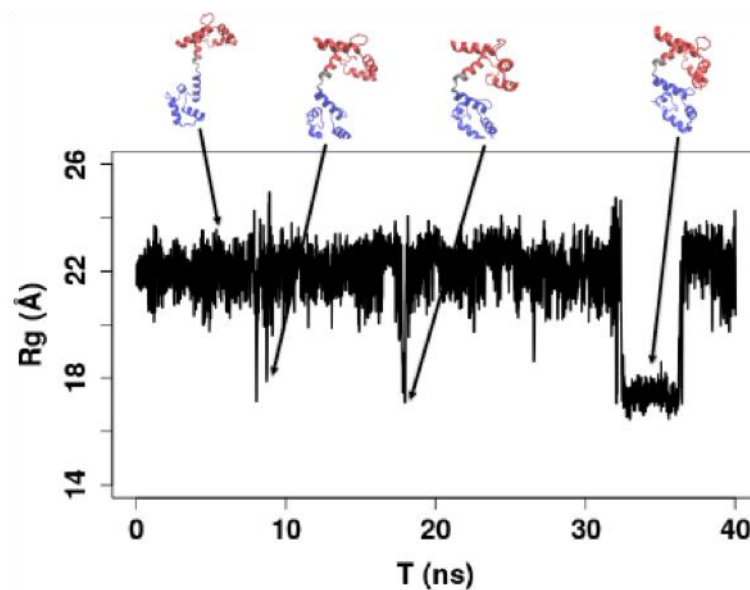
An example of a branched network simulation trajectory consisting of 33 motors and 1500 linkers with an avalanche. (A) The time series of changes over a 10-s time interval in the ratio of the radius of gyration normalized by the Rg value at 10 s. (B) and (C) Two snapshots of actin filaments, motors, and linkers where the tension is indicated by color; these show the morphology of the network before (B) and after (C) the abrupt drop of $\Delta(R_g/R_g^i)$ when an avalanche occurs. The dimensions of the cubic simulation box are $1 \mu\text{m} \times 1 \mu\text{m} \times 1 \mu\text{m}$. A blue square highlights a concentrated high-tension region that can be seen prior to the $\Delta(R_g/R_g^i)$ drop which then becomes a dispersed low-tension area after the $\Delta(R_g/R_g^i)$ drop.

Title: Coarse-grained molecular dynamics simulations of Ca²⁺-Calmodulin

Presenting Author: Jules Nde

Calmodulin is the primary calcium binding protein that regulates the activities of over 300 binding partners in the calcium dependent manner. Those binding partners may either increase or decrease the calcium's affinity to calmodulin. The main question we want to answer in this work is how such a small protein like calmodulin binds, activates, or regulates the activities of so many diverse targets. We try to answer this question using the computational approach based on the coarse-grained simulations with the associative memory, water mediated, structure and energy model (AWSEM), a transferable protein force field. We were able to show that calmodulin exists in multiple conformations in solution and each conformation maybe specific to a target protein.

Figure:



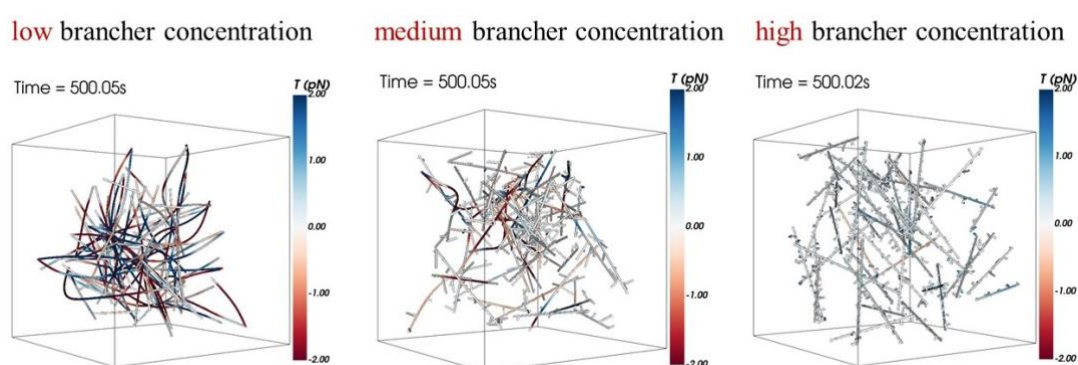
Different conformations of calmodulin in solution. Coarse-grained molecular dynamics simulation shows that calmodulin exists in the extended, intermediate, and collapsed conformations. Each conformation may be proper to a specific target protein. [Link to the abstract.](#)

Title: Exploring the impact of Arp2/3 concentration on actomyosin dynamics

Presenting Author: Chengxuan Li

Using a coarse-grained active network model MEDYAN, we simulate the branched actomyosin networks in the size of dendritic spine and explore the impact of the concentration of Arp2/3 complex on the network structure and dynamics. Our results show that high concentration of Arp2/3 complex inhibits the network contraction by saturating the binding sites on actin filaments, and an emergent phenomenon 'avalanche' tend to happen in branched networks with medium Arp2/3 concentrations. We utilized graph theory parameters to describe hierarchical properties of the actomyosin network, in which the assortativity proves to be able to capture the morphology change during the network evolution.

Figure:



Tension snapshots at 500 seconds for simulations with same high motor and linker concentrations but various brancher concentrations. The contraction of actomyosin networks with high brancher concentration is inhibited because of the saturation of binding sites on actin filaments by Arp2/3 complexes, and the morphology of the network is changed from 'centered' structure when brancher concentration is low to multiple 'stared' structure, which is revealed by the graph theory parameter assortativity. [Link to the abstract.](#)