Coarse-grained simulation of actin self-assembling.

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We have developed a grand canonical 2D Montecarlo coarse-grained simulation that mimics the self assembling of the actin to study the effect of the actin bundling cross-linkers. This simulation reproduces the bundling process only considering energy stability obtained by the formation and destruction of contact bonds between the proteins, we do not consider remote interactions (forces).

Our new approach is to consider the direct formation of the bundles without a previous phase of actin single chains. In this simulation, we only have considered three proteins: the actins the cross-linkers and the nucleators (called caps during this work). The actins bond one to each other in the direction of growing to form a filament, the cross-linkers bond two actin chains and the caps bond with the weak end of the actin chains to increase their stability.

The results of several simulations show that the bundle formation is strongly related to the cross-linker concentration, as you can see in the two adjunted snapshots of the system with two diferent ratios of Actin/Cross-Linkers (Figures 1 and 2).

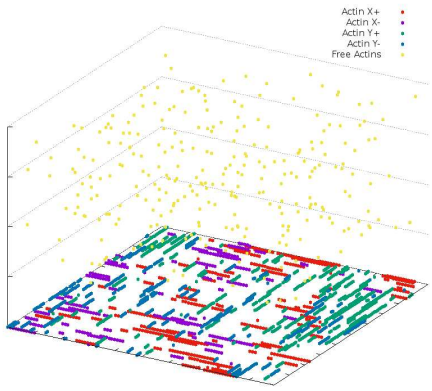

Figure 1: State of the system for a ratio actin/cross-linker of 1000.

One can observe that in the system with the 1/1000 (Figure 1) despite having aproximatelly the same fraction of linked actins ($\simeq 0.8$) the actin filaments are dispersed in the system while in the snapshot with a larger Cross-Linker/Actin ratio (Figure 2) the filaments form large bundles.

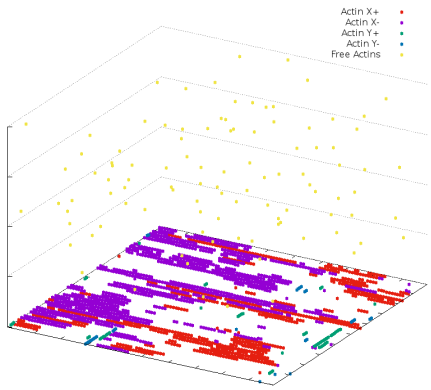

Figure 2: State of the system for a ratio actin/cross-linker of 2.

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