Mathematical Biology Seminar

Monday, November 15, 2021
3 pm – 457 CAB (in person)
To join via Zoom Meeting -
https://ualberta-ca.zoom.us/j/92284917292?pwd=UnZrSTZrRE5LQ250Tk5hekVrUG9adz09

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The stochastic Weighted Ensemble method to understand T Cell Receptor activation

The activation of T cells, key players of the immune system, involves local evacuation of molecules (phosphatases) from the nearby region of the cell surface, segregating them from the T cell receptor. What drives this evacuation? This phenomenon involves the Brownian motion of particles with stochastic rare events, the fluid dynamics of the thin layer of extracellular environment, and the polymer properties of the receptors. We use a computational rare event method called Weighted Ensemble and spatial stochastic particle-based simulation to study the surface motion of phosphatases. The method provides the ability to simulate a full range of rare events from (unphysiological) 300-year timescales down to 1-second timescales. Among other results, we find that oligomerization (attachment of multiple molecules together) leads to order-of-magnitude acceleration of evacuation. This provides a biological example in which an increase in stochastic correlations (with little change in stochastic amplitude) provides a functional benefit to the cell.