Informal Seminar on Mathematics and Biochemistry-Biophysics

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Insight into Molecular through Subcellular Calcium Signaling via Multi-Scale Simulation

Abstract:
Calcium is critical to a wide range of physiological processes, including neurological function, immune responses, and muscle contraction. Calcium-dependent signaling pathways enlist a variety of proteins and channels that must rapidly and selectively bind calcium against thousand-fold higher cationic concentrations. Frequently these pathways further require the co-localization of these proteins within specialized subcellular structures to function properly. Our lab has developed multi-scale simulation tools to elucidate how protein structure and co-localization facilitate intracellular calcium signaling. Developments include combining molecular simulations with a statistical mechanical model of ion binding, a homogenization theory to upscale molecular interactions into micron-scale diffusion models, and reaction-diffusion simulations that leverage sub-micron microscopy data. In this seminar, I will describe these tools and their applications toward molecular mechanisms of calcium-selective recognition and cross-talk between co-localized calcium binding proteins inside the cell.

Hosts: Li-Tien Cheng and Bo Li

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