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## **(G\*) Stochastic Simulations of Protein Clustering on Tubular Networks**

*Tuesday 7 June 2022 09:30 (15 minutes)*

Protein clustering occurs in living cells, often involving phase transitions, and can be an essential step in signal transduction in cells. Protein-protein interaction strength and diffusion times dictate when and how clusters occur, and with diffusion times dependent on geometric properties of cell compartments. The evolution of protein cluster sizes, and any signals sent by the clusters, can be controlled by coarsening dynamics.

We investigate the effects of geometry on controlling phase behaviour of proteins on the endoplasmic reticulum (ER), a tubular network that spans much of the cell. The protein IRE1 $\alpha$  resides on the surface of the ER and performs essential signaling as part of the Unfolded Protein Response, which is critical for the healthy function of the cell.

Using stochastic simulations, we explore how the geometry of the tubular surface of the ER, and the network that they form, affects the diffusion and the clustering of the IRE1 $\alpha$  proteins on the ER's tubular surface. The simulation applies a kinetic Monte Carlo algorithm to represent the IRE1 $\alpha$  proteins as a lattice gas on a single tube. We find that clustering substantially increases on tubes that are narrower than the typical ER tube diameter of 100nm. Furthermore, the simulations yield IRE1 $\alpha$  protein clustering at physiological IRE1 $\alpha$  protein concentrations, estimated to be only 1 ~ 10 proteins per micrometre of tube length. We also explore the role of tube geometry in determining the typical cluster formation times.

IRE1 $\alpha$  signaling is integral to cell health and function, and its malfunction is tied to the development of neurodegenerative diseases and cancer. We aim to further our understanding of protein clustering on the ER to provide insight into geometric regulation of phase behaviour and cellular signaling.

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