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An Efficient Single-Molecule Resolution Method for Simulating Spatio-Temporal Dynamics of Protein Interaction Networks that Involve the Cell Membranes[1] OSMAN N. YOGURTCU, MARGARET E. JOHNSON, Johns Hopkins University — A significant number of the cellular protein interaction networks, such as the receptor mediated signaling and vesicle trafficking pathways, includes membranes as a molecular assembly platform. Computer simulations can provide insight into the dynamics of complex formation and help identify the principles that govern recruitment and assembly on the membranes. Here, we introduce the Free-Propagator Re-weighting (FPR) algorithm, a recently developed method that efficiently simulates the spatio-temporal dynamics of multiprotein complex formation both in the solution and on the membranes. In the FPR, the position of each protein is propagated using the Brownian motion and the reactions between pairs of proteins can occur upon collisions. Depending on the dimensionality of the interaction, the association probabilities are determined by solving the Smoluchowski diffusion equations in 2D or 3D and trajectory reweighting allows us to obtain the exact association rates for all the reactive pairs. Using the FPR, in this presentation, we investigate the interaction dynamics of the receptor mediated endocytic network as a case study and discuss the possible effects of membrane binding and molecular crowding on the formation of complexes.

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