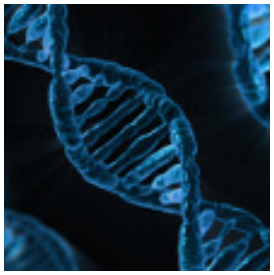

Contribution ID: **61** Type: **Oral presentation**

KEYNOTE 8 - Interplay of gating and hydrodynamic interactions in crowded protein solutions

Tuesday 5 June 2018 14:00 (40 minutes)

An outstanding challenge in computational biophysics is the simulation of a living cell at molecular detail. Over the past several years, using Stokesian Dynamics, progress has been made in simulating coarse grained molecular models of the cytoplasm. Since macromolecules comprise 20-40% of the volume of a cell, one would expect that steric interactions dominate macromolecular diffusion. However, the reduction in cellular diffusion rates relative to infinite dilution is due, roughly equally, to steric and hydrodynamic interactions, HI, with nonspecific attractive interactions likely playing rather a minor role. HI not only serve to slow down long time diffusion rates but also cause a considerable reduction in the magnitude of the short time diffusion coefficient relative to that at infinite dilution. More importantly, the long range contribution of the Rotne-Prager-Yamakawa, RPY, diffusion tensor results in temporal and spatial correlations that persist up to microseconds and for intermolecular distances on the order of protein radii. While HI slows down the bimolecular association rate in the early stages of lipid bilayer formation, they accelerate the rate of large scale assembly of lipid aggregates. This is suggestive of an important role for HI in the self-assembly kinetics of large macromolecular complexes such as tubulin. Since HI are important, questions as to whether continuum models of HI are adequate. Nevertheless, the stage is set for the molecular simulations of ever more complex subcellular processes and we discuss one such case, the diffusion of lac repressor in a packed cellular nucleoid.

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Session Classification: Dynamics of Proteins in Crowded and Confined Geometry

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