UNIVERSITY of HOUSTON | ENGINEERING

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Multi-scale computational models of spatial and dynamic properties of biological systems: protein functions, protein-protein interactions, stochastic networks, chromosome folding, and wound healing

Understanding the working machineries of cells and tissues requires a multi-scale approach that examines details of individual gene/protein, interactions of multiple proteins, and genetic circuit networks to elucidate complex behavior of cellular and tissue states and their spatio-temporal pattern formation. At the molecular level, we discuss how new insight can be gained by computation of protein geometric structures, including predicting protein functions from structures at large scale through reconstruction of the evolutionary history of binding surfaces using a Bayesian Monte Carlo method. We also describe a new method for predicting 3D structure and assembly of beta barrel membrane proteins, as well as general strategies for engineering bionanopores. At the network level, we describe how to account for the full stochasticity of rare and small copy number events important for cell fate by characterizing the full state space and by solving the chemical master equation accurately without Gillespie simulation or Fokker-Planck/Langevin approximation. We show how to relate the computed landscape probability to phenomenological characterization of networks such as bi-stability, epigenetic states, and the robustness of wild type versus mutant lambda phages. At the chromosome and epigenetic level, we discuss the important roles of spatial confinement in shaping the scaling and folding landscape of chromosome folding. At the cellular level, we describe a geometric model and an algorithm for simulating dynamic spatio-temporal pattern formation of cell populations and how the process of wound healing can be studied through simulation. It is our belief that this multi-scale approach will be useful for future engineering of biological systems.
(Please visit http://www.uic.edu/~jliang for further information).