Application of Partial Differential Equations in Modelling of Motion of Molecular Motors

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In biological systems, molecular motors are motor proteins that consume chemical energy and move along polymer filaments of the cytoskeleton, which act as macromolecular tracks. Their collective dynamics plays a major role in various intracellular processes/functions such as cellular trafficking, protein synthesis, cell division etc. In order to analyze the collective properties of interacting molecular motors and other driven stochastic transport problems, totally asymmetrically simple exclusion process (TASEP) model is found to be a paradigmatic model to study such problems in the last decade. TASEP model comprises of single species of particles performing biased hopping with uniform rate in a preferred direction along a 1D lattice. The particles obey certain preassigned rules under hard-core exclusion principle, due to which a lattice site cannot have more than one particle.

In this presentation, I will be talking about usage of computational partial differential equations in modeling the motion of motor proteins. To mimic this phenomena more realistically, we propose a three-channel system instead of a single channel system with a non-conserving dynamics namely Langmuir-Kinetics. After modeling this biological problem into mathematical form, we get system of non-linear coupled partial differential equations which we solve numerically. Using this numerical solution, we calculate various important characterizes, including phase diagrams and density profiles to understand the system dynamics deeply.