Diffusion in inhomogeneous systems: Avoiding pitfalls when using Lattice Monte Carlo (LMC) simulations

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Lattice Monte Carlo (LMC) methods are frequently used to model diffusion controlled drug delivery systems. In a typical case, the drug, initially encapsulated in a porous material (e.g., a hydrogel), is released via diffusive escape. One way to control this process is to design layered materials with regions that have different porosities or properties. However, modelling inhomogeneous systems where both the porosity and the diffusivity are space-dependent is ambiguous in LMC simulations. In this talk, I examine five fundamental issues: 1) How to build reliable LMC algorithm for simple problems; 2) How to replace connected regions with different porosities by free-solution regions of different effective viscosities; 3) How to treat the LMC jumps between regions with different effective viscosities; 4) The relative roles of obstructed volume and tortuosity in diffusion problems; 5) How to fit drug release data and predict the Weibull (or stretched exponential) exponent from first principles.