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Simulating Biological Cells[1]

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Cells interact with their environment via a cascade of biochemical reactions that invoke a signaling, metabolic, or regulatory response. The properties of these reaction networks can be modeled at various levels of detail from continuum to stochastic, and steady-state to kinetic. Our group (and others) have been developing tools that attempt to simulate these networks in cellular geometries with spatio-temporal detail. In our model a single particle represents a protein, complex, or other biomolecule. Membranes and cellular compartments are represented as idealized or triangulated surfaces. Particles diffuse via 3d Brownian motion within the cytoplasm, or in 2d on membrane surfaces. When particles are near each other, they interact in accord with Monte Carlo rules to perform biochemical reactions which represent complex formation, dissociation events, ligand binding, etc. In this talk, I'll describe the reaction algorithms we use and the underlying physics they attempt to capture. I'll illustrate the effects stochasticity and spatial organization have on biochemical networks at the cellular scale and show some simple examples of how such models can address biological questions. This is an emerging field of simulation, so there are many issues still to be addressed, but the eventual goal is to enable whole-cell models of protein networks with realistic numbers of biomolecules.

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