DIFFUSION OF SMALL LIGANDS IN COMPLEX CONFINING AND REACTIVE LANDSCAPES: THE GEOMETRY OF CHEMORECEPTION

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The rate constant that describes the diffusive encounter/reaction between a particle and a large sphere can be computed easily by solving the stationary diffusion (i.e. Laplace) equation for the particle density with appropriate boundary conditions imposed on the surface of the sphere. In one classic, textbook example, this calculation is used to estimate the binding rate constant of a ligand to a receptor-covered cell.

But what happens if the particles are diffusing in the presence of many reactive boundaries of different strength (intrinsic reaction rate), which compete for the same ligands and amidst a landscape of inert obstacles? In spite of the apparent overwhelming complexity, the same mathematical framework as the two-body problem can be used to solve the N-body problem exactly, by resorting to addition theorems for the appropriate fundamental solutions of the Laplace equation.

This powerful mathematical framework allows one to investigate fundamental issues that are central in cell biology and modern nano- sciences, such as how the specific geometric configurations of many reactive boundaries shape the overall reaction rate constant. We will illustrate several examples, including applications to the study of small ligand binding to arrays of receptors on the surface of a cell and the action of many nano-catalysts embedded within a core-shell nano-reactor.

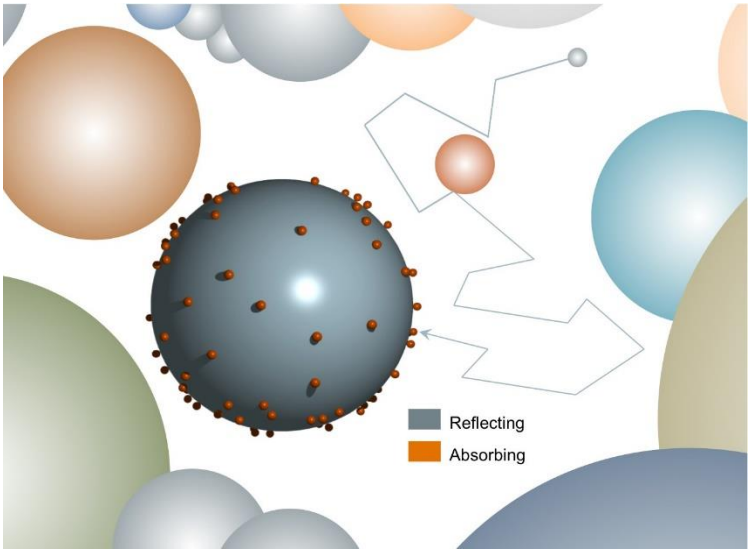

Figure 1 – Diffusion of a small ligand to a receptor-covered cell in a crowded and confining environment. The rate to capture can be computed exactly as a function of the geometrical and chemical parameters