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