IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project title: *Biomembrane hydrodynamics*

Project number: IMURA0089

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Research Academy theme: ***Biotechnology & Stem-cell Research; Advanced computational engineering, simulation and manufacture***

The research problem

Membranes are ubiquitous in living cells. For a long time, it was thought that cellular membranes played a largely structural role in biological processes. However, in the last decade or so, it has become increasingly apparent that lipid bilayer membranes are not just passive compartment walls, but in fact take an active part in the entire gamut of cellular processes, ranging from cell signalling, intracellular transport, and enzymatic regulation, to cell division, and cell death.

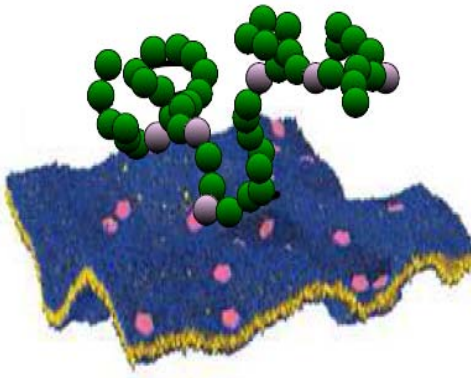

Fig.: Polymer adsorption on membrane: the polymer has a few sites (lighter spheres) that are attracted to sites on the membrane surface (lighter patches on membrane surface). Only a section of the membrane is shown. Both membrane and polymer are subject to thermal fluctuations, and disturb the ambient fluid as they move. Does the coupling of their motions due to the fluid flow hasten the process of adsorption in any way?

A common theme in several of these diverse activities that biomembranes engage in involves the adsorption of small and large molecules to multiple target sites (typically membrane proteins or sugar residues) on the membrane surface. Flows driven by the fluctuating surface may modify the motion of particles at a distance so as to increase its chances of locating specific heterogeneities on the membrane surface. The simulations proposed in this Project will examine this possibility in detail, and will lead to a deeper understanding of the dynamics of adsorption on to fluctuating membrane surfaces.

Project aims

The primary objective of this Project is to use computer simulations to study the dynamic processes leading to the adsorption of a single polymer molecule on the surface of a semi-flexible biomembrane. The simulations in this study will involve the following typical scenario (see figure). The polymer molecule of interest is a flexible chain of segments, a few of which

possess an electrostatic charge. The membrane is an infinite nearly elastic, nearly two-dimensional, fluid of a much higher viscosity than the ambient fluid. Scattered in the membrane are target sites with a charge opposite to the charged segments in the polymer. The attraction between the polymer segments and the target sites is however strongly screened because of the presence of ions in the fluid. The target sites may be fixed, or alternatively, may be free to diffuse within the membrane. Thermal fluctuations in the ambient fluid give rise to randomly fluctuating forces on the polymer, membrane and the diffusing target sites. The motions of the polymer and membrane in turn drive flows through the ambient fluid, which strongly affect, and couple, their dynamics.

Freely diffusing polymer molecules in solution can be thought of as long, flexible, stringy objects that are in constant random motion because of the continuous thermal buffeting they receive from the surrounding solvent molecules. Further, as any segment of the polymer molecule moves in response to the noisy Brownian forces exerted by the solvent, it experiences frictional resistance from the fluid that is proportional to its velocity relative to that of fluid in its vicinity. But the motion of the segment also perturbs the fluid. This perturbation decays slowly with distance, and thus modifies the motion of all the other polymer segments in the fluid. In recent years, computer simulations have clearly established the importance of such “hydrodynamic interactions” (HI) in determining the dynamical properties of polymer solutions.

Simulations of polymer molecules near rigid walls have only recently demonstrated that the presence of boundaries affect how polymers move near interfaces. The dynamics of polymers near deformable surfaces that are also subject to thermal fluctuations–the central theme of the current proposal–remains to be explored.

Expected outcomes

The immediate impact of the proposed research will be a deeper understanding of the process of adsorption of polymers on membranes. More generally, this study will be a valuable contribution towards a growing body of work on the dynamics of membranes, and their role in biological processes. A knowledge of the hydrodynamics of membranes would also be particularly useful in the design of advanced microfluidic devices and reactors. Currently, microfluidic applications are still grounded in the macroscopic paradigm that reactors and piping must be rigid, whereas solid bounding walls and sharp corners are conspicuously absent in the biological cell, the very apotheosis of a complex microfluidic device.

This Project is an ideal stepping-stone for a rewarding academic or industrial career in bioengineering and advanced computer simulations, and will provide in-depth training in biophysics, numerical methods, modern simulation techniques, fluid mechanics, and statistical mechanics.