INTERNATIONAL SOLVAY INSTITUTES BRUSSELS

2016 International Solvay Chair in Chemistry

Professor Raymond Kapral
(University of Toronto, Canada)

Programme

Lecture 1: Monday 11 April (4 - 6 P.M., Solvay Room)

Quantum Dynamics in Complex Systems

Quantum processes, such as electron, proton and coherent energy transfer, often take place in large complex many-body environments. While the dynamics of a subsystem of the entire system is often of primary interest, its interaction with the remainder of the system is responsible for decoherence and other environmental effects. Coupling between the subsystem and environment can lead to the breakdown of the Born-Oppenheimer approximation. The resulting nonadiabatic dynamics plays an important role in many physical phenomena, such as population relaxation following initial preparation of the system in an excited electronic state. The talk will focus on a mixed quantum-classical description of nonadiabatic dynamics and discuss how coherence and decoherence are accounted for in this framework, and how it can be used to simulate the quantum dynamics of chemical rate processes.

Inaugural Lecture: Tuesday 19 April (4 - 5 P.M., Solvay Room)

Molecular Machines and Synthetic Motors: Active Motion on the Nanoscale

Molecular machines operate far from equilibrium and are subject to strong thermal fluctuations. They use chemical energy to perform a variety of tasks, acting as motors, enzymes or pumps, and in doing so play important roles in the operation of the cell. Synthetic chemically-powered nanomotors, with and without moving parts, operate under similar conditions and are being studied because of their potential applications involving active transport on small scales and the challenges they pose for theory and simulation. Two examples will be used to illustrate the phenomena that such systems display: synthetic chemically-powered nanomotors and hydrodynamic collective effects arising from active protein machines. The kinds of synthetic nanomotors that have been constructed and their potential applications will be described, and the mechanisms they use for propulsion and how their dynamics may be simulated will be discussed. Experimental observations have shown that transport in the cell is influenced by protein activity. It will be shown that one mechanism that may contribute to the enhanced transport of passive particles and other enzymes in the cell and in solution is due to the hydrodynamic flows that are generated by the nonequilibrium conformational changes of active enzymes.

FOR THE INAUGURAL LECTURE, COFFEE AND TEA WILL BE SERVED AT 3.45 P.M.
AND DRINKS AT 5.00 P.M. IN FRONT OF THE SOLVAY ROOM

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Lecture 2: Monday 25 April (4 - 6 P.M., Solvay Room)

Chemically-Powered Nanomotors

Synthetic chemically-powered motors that do not make use of conformational changes for their propulsion will be described. They operate under far-from-equilibrium conditions and are subject to strong fluctuations from the environment in which they move. In particular, motors that operate by diffusiophoresis, where a self-induced chemical gradient is responsible for motion, will form the focus of the discussion. The propulsion mechanism based on the continuum reaction-diffusion and hydrodynamic equations will be given, as well as a mesoscopic model for motor motion. The properties of these motors will be described. The manner in which different chemical reactions on the catalytic sites of the motor and in its environment influence motor propulsion properties will be considered. In collections of such motors, the individual motors interact through forces that arise from concentration gradients,hydrodynamic coupling and direct intermolecular forces. Motors self-assemble into transient aggregates with distinctive structural correlations and exhibit swarming where the aggregates propagate through the system. These phenomena will be illustrated by simulations of the dynamics of many-motor systems.

Lecture 3: Wednesday 27 April (4 - 6 P.M., Solvay Room)

Protein Dynamics and Hydrodynamics

The dynamics of proteins in solution and in crowded molecular environments, which mimic some features of the interior of a biochemical cell, will be discussed. The translational and internal dynamics and catalytic activity of enzymes that utilize chemical energy to effect cyclic conformational changes to carry out their catalytic functions will be described. Proteins often function when bound to lipid membranes and the nature of the mutual interactions between the lipid membrane and active protein will be discussed. The emphasis in these studies is on the role that hydrodynamics plays in determining the protein dynamics. The investigation of the dynamics of such complex systems requires knowledge of the time evolution on physically relevant long distance and time scales, necessitating a coarse grained or mesoscopic treatment of the dynamics.

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