Computer Simulations of Membranes and Proteins

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Gruppens kerneforskningsområder

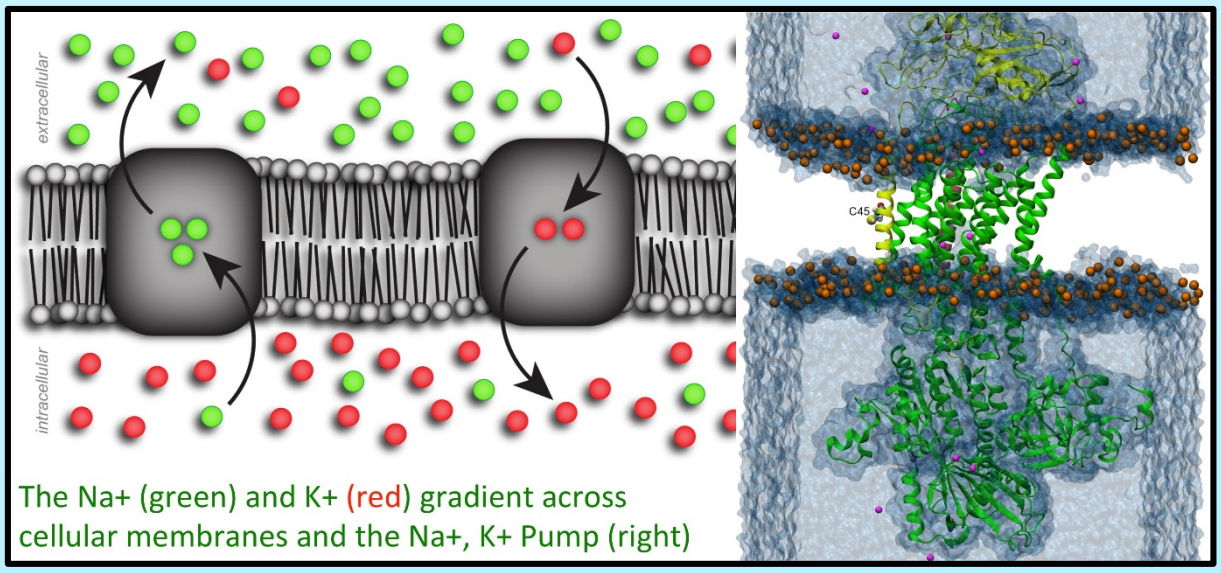
My group uses Molecular Dynamics Simulations and related computational methods to explore a wide range of problem in biological systems, particularly near membranes, and in close collaboration with experiments. Examples of topics:

- The physics of biological membranes: impact of electrical potentials on membrane curvature
- Drug-membrane and drug-protein interactions
- Mechanisms of Ion transport across membranes through Ion Pumps and Channels
- The role of membrane repair in cancer
- The molecular basis of disease (particularly neurological disorders)
- Biogenesis of droplets and nanoparticles
- Techniques to accelerate simulation

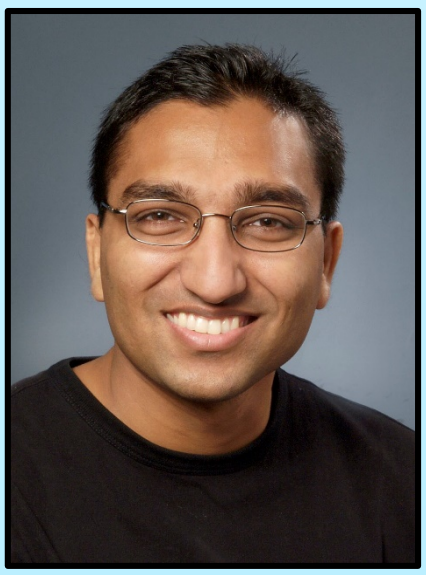
We are housed at FKF and PHYLIFE: Physical Life Sciences, and use ABACUS 2.0: the largest supercomputer in Northern Europe housed at SDU, for our simulations.

YOU WILL LEARN THE FOLLOWING

- about the fundamental physical and chemical forces that drive self-assembly and interactions of biomolecules, i.e. the physicochemical basis of life
- Molecular Dynamics Simulations: To simulate biomolecular interactions and self-assembly
- how to work in a truly interdisciplinary environment with both experimentalists and simulation experts



The Na+ (green) and K+ (red) gradient across cellular membranes and the Na+, K+ Pump (right)



Er du interesseret i at skrive projekt i gruppen, så kontakt:
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Projekter	Beskrivelse
Coupling of Electrical Potential and Curvature in Lipid Membranes	Cellular membrane are highly curved, and the potential across membranes affects key cellular properties. We investigate the relationship between curvature and transmembrane electrical potential in lipid bilayers, and examine if this can have an impact on the gating of voltage-sensitive and tension-sensitive ion channels
Molecular Basis of Neurological Disorders and Ion Selectivity Mechanisms in Ion Pumps	The Na+ K+ pump exchanges 3 Na+ for 2K+ ions to maintain membrane potentials critical for life. We want to know: 1 How is the pump selective to Na+ over K+ on one side, and K+ over Na+ on the other? 2 What is the molecular mechanism of neurological disorders caused by mutations in the pump? We also work on the H+ K+ pump, which transport protons across a million-fold pH gradient
The Transport Mechanism of an Evolutionarily Unique Transport Complex	Some bacteria employ a unique molecular machine (KdpFABC), which integrates functional units of both ion channels (ICs) and ion pumps (IPs) for K+ uptake. KdpFABC is neither an IC, or an IP, and therefore has a unique evolutionarily lineage amongst ion transporting proteins. The goal of this project is to unravel the molecular mechanism by which this unusual protein complex transports K+ across the bacterial membrane using computer simulations. Knowledge of the ion transport mechanism of KdpFABC is key to comprehending how and why proteins transporters evolved into two, rather than three major branches.