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Biofisica Computazionale
Simulating transport phenomena at the molecular scale

The modern simulation techniques combined with the potent hardware available allow the investigation of transport phenomena at the molecular scale. Two different algorithms available for performing virtual electrophysiology with ion channels and pores will be presented and compared. Virtual electrophysiology is useful on one side to gain detailed information on permeation of ions, on the other as a very sensitive technique for transport of small molecules. Taking as a model a bacterial porin, we developed the landscape theory of transport applying multiscale simulations: permeability coefficients, thermodynamics and kinetic parameters can be obtained through the application of the diffusion equation.