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Multiscale approach to ions in solution, proteins and channels: from brownian dynamics to continuum equations

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The diffusive motion of ions in solution, near proteins and through protein channels of biological membranes involves many length and time scales. In this talk we'll describe a multiscale averaging procedure, that starting from a Brownian dynamics description for the ionic motion of particles, yields a hierarchy of continuum equations for the averaged concentration profiles in the system. This set of equations is a generalization of the well known BBGKY equations of equilibrium statistical mechanics to non-equilibrium. Therefore, as in the equilibrium theory, closure relations are needed to compute explicit solutions. In the context of ionic permeation through protein channels, we show how an analysis of these continuum equations together with simple closures provides a theoretical explanation for experimentally measured phenomena.

[1]Joint work with R.S. Eisenberg and U. Hollerbach (Rush University, Chicago, IL) and Z. Schuss and A. Singer (Tel-Aviv University, Israel)