Biophysical Journal (1993) **64:** p. A22
in Issue 2 Part 2, February, Abstracts of Annual Meeting of (American) Biophysical Society

Workshop 5
FROM STRUCTURE TO PERMEATION IN OPEN IONIC CHANNELS

M-PM-WS4-1
FROM STRUCTURE TO PERMEATION IN OPEN IONIC CHANNELS
Organizer: Robert S. Eisenberg

The anatomy of channel proteins is becoming better known as the techniques of molecular biology yield structural results. The functions of channels are quite well known from measurements in the Hodgkin-Huxley and Neher-Sakmann traditions. A hierarchy of theories should be needed to link atomic structure of channels to their macroscopic function, starting with simulations of molecular dynamics of channel proteins and their contents, proceeding through stochastic analysis of ions in the channel's pore, ending with a macroscopic description of single channel currents as actually measured. Bob Eisenberg will present a Poisson-Nernst-Planck theory in which the electric field within the pore is calculated from channel structure, instead of being assumed a priori. This PNP theory predicts many characteristics of biological channels, although it describes a channel of just one conformation in which ionic points flow through each other. Duanpin Chen will show that the electric field—the barriers and wells of potential-in such a theory varies substantially with experimental conditions, producing many coupling phenomena and some gating phenomena observed in real channels and transporters. Olaf Andersen will describe the currents and fluxes in a gramicidin channel that a useful theory must predict.