

Abstract View

COMPUTER SIMULATION OF SYNAPTIC ULTRASTRUCTURE AND MICROPHYSIOLOGY IN THE CHICK CILIARY GANGLION

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Using MCell, a general Monte Carlo simulator of subcellular signaling (<http://mcell.cnl.salk.edu>), it is now possible to simulate the process of synaptic transmission on actual 3D microanatomy derived from serial electron microscopic tomography. Here we present the methods used to construct a realistic MCell model of a chick ciliary ganglion (CG) synapse. A $96 \mu\text{m}^3$ region of synaptic ultrastructure was obtained by segmentation of active zone locations, and pre- and postsynaptic membranes within a tomographic volume with better than 10 nm resolution. Published and estimated values for the numbers and distributions of nicotinic acetylcholine (ACh) receptors and ACh-esterase enzymes, together with reaction mechanisms and rate constants, were mapped onto membranes. Via the MCell Model Description Language, these data were combined with the 3D structure and estimates of the number of ACh molecules in a quantum. The resulting MCell model can be used to run a simulation of miniature postsynaptic current generation at the CG in about 90 seconds on a 1 GHz Pentium III workstation. The model allows parameter sweep studies evaluating the behavior of this in-silico CG system and thereby estimate difficult to determine parameters such as the rate constant for agonist binding and the number of competent receptors accessible. This permits results from laboratory and computational experiments to be compared quantitatively.

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