

Abstract View

MCELL3: A NEXT-GENERATION SIMULATOR OF CELLULAR MICROPHYSIOLOGY

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MCell3 is a new version of MCell, a program for spatially realistic Monte Carlo simulation of molecular diffusion and chemical signaling. MCell3 expands on previous versions in three important ways. First, it allows simulation of bimolecular reactions between diffusing molecules, in addition to reactions between diffusing and immobile molecules. Second, the Model Description Language used to define simulations has been enhanced accordingly, and now allows input of chemical reactions in familiar "A+B->C+D [rate]" format. Third, the new computational core uses an event queue to schedule unimolecular state transitions and also includes an adaptive spatial partitioning scheme, improving speed and accuracy, and reducing memory usage. Two examples that highlight these changes will be shown. The first is an analysis of the spatial extent, time-course, and variability of calcium microdomains near a channel, incorporating static and mobile calcium buffering proteins as well as small molecule calcium buffers. The second is a simulation of a reaction-diffusion model of oscillations of the MinD and MinE cell division proteins in *E. coli*.

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