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Cellular Dynamic Simulator: an event driven molecular simulation environment

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Introduction

In this paper, we present the Cellular Dynamic Simulator (CDS) for simulating crowded molecular environments. CDS is based on an event driven algorithm [1] that allows precise calculation of the timing of collisions, reactions and other events for each individual molecule in the simulated environment. Generic mesh based compartments allow the creation/importation of very simple or detailed intracellular structures that exist in a spatial 3D environment. Multiple levels of convoluted compartments and static obstacles can be used to create a dense environment to mimic the intracellular space. Diffusing molecules move in a Brownian fashion by randomly generating a new velocity vector at specified time intervals. This novel algorithm can address how volume exclusion and molecular crowding impact signaling cascades in small subcellular compartment such as dendritic spines. With the CDS, we can simulate simple enzyme reactions; aggregation, channel transport, as well as highly complicated chemical reaction network of both freely diffusing and membrane bound multi-protein complexes. Components of the CDS are generally defined such that the simulator can be applied to a wide range of environments in terms of scale and level of detail. Through an initialization GUI, a simple simulation environment can be created and populated within minutes yet is powerful enough to design elaborate spaces. The initializer allows visual confirmation of the environment construction prior to execution by the simulator. Design implementation and features of the CDS are detailed in this paper and its utility is highlighted by the specific case of calcium signaling in a dendritic spine.

References

1. Sigurgeirsson H, Stuart A, Wan W-L: **Algorithms for particle-field simulations with collisions.** *Journal of Computational Physics* 2001, **172:**766-807.