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Spatial stochastic modeling of intracellular Ca<sup>2+</sup> dynamics using two-regime methods<sup>1</sup> ULRICH DOBRAMYSL, MARTIN ROBINSON, RADEK ERBAN, University of Oxford — The signaling pathways in many cell types depend on the controlled release of calcium ions from the endoplasmatic reticulum (ER) into the cytoplasm, via clusters of inisitol triphosphate  $(IP_3)$  receptor channels. At low concentrations,  $Ca^{2+}$  ions facilitate channel activation, while acting as inhibitory agents at high concentrations. An activation event causes the opening of other channels in a cluster, resulting in a calcium puff. We simulate calcium ion dynamics using a recently-developed hybrid two-regime technique, wherein the positions of calcium ions in the vicinity of a channel cluster are tracked by employing an offlattice Brownian dynamics algorithm. An efficient compartment-based algorithm is used in the remainder of the computational domain to correctly capture the diffusive spread of ions. We characterize calcium puffs via the distributions of inter-puff times and amplitudes and investigate the influence of diffusive noise on the puff characteristics by comparing our results with data obtained from an effective nonspatial model.

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