X-DMS 2015
eXtended Discretization MethodS
September 9-11, 2015, Ferrara, Italy

A Multiscale Model of Synaptic Contacts between Brain Cells

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Key words: multi-scale modeling, finite volumes, molecular dynamics, calcium diffusion, synaptic cleft, cell adhesion, synaptic plasticity

ABSTRACT

Biological processes are typically active on multiple, coupled scales. An example are the chemical contacts between brain cells. We present a multiscale model of chemical synapses, that couples the molecular dynamics of cell-adhesion Cadherin molecules interacting with calcium ions and the continuum scale model representing synaptic function. For this purpose we developed a tetrahedral volume grid representation of a synapse used in a Finite Volume discretization of the synaptic model (described by a system of PDEs [VRR$^+$13]). On the molecular scale we use molecular dynamics (MD) [Gon10], [PBW$^+$05] simulations and couple these to the discrete function space of the PDE-problem, using transfer operators that map between the cartesian space and function space. The three-dimensional non-linear diffusion-reaction system with non-linear interface conditions is solved using parallel multi-grid methods and time-parallel methods. Simulation results demonstrate the described approach applied to the model intercellular coupling between nerve cells and the necessity to employ a multiscale model to unravel interplay of the involved scales.

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