

# A Multiscale Model of Synaptic Contacts between Brain Cells

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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). On the molecular scale we use molecular dynamics (MD) 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 methods applied to the model of intercellular coupling between nerve cells and the necessity to employ a multiscale model solved with multi-level solvers.