A Multiscale Model of Synaptic Contacts between Brain Cells

Stephan Grein\(^1\), Gillian Queisser\(^2\)

\(^1\) Goethe University, Goethe Center for Scientific Computing, Kettenhofweg 139, 60325 Frankfurt am Main, stephan.grein@gcsc.uni-frankfurt.de

\(^2\) Goethe University, Goethe Center for Scientific Computing, Kettenhofweg 139, 60325 Frankfurt am Main, gillian.queisser@gcsc.uni-frankfurt.de

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**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.

**REFERENCES**

