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Extended discretization and smooth subdivision of hybrid tetra-/octahedral grids with application in neuroscientific numerical simulations

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ABSTRACT

An important goal in neuroscience is understanding how networks of neurons are processing information. Chemical synapses define interfaces where signals are exchanged between neurons and other (neural) cells and thus play an essential role in this context. To pursue this goal we are developing detailed mathematical models of time- and space-dependent synaptic processes. Amongst others the models comprise the description of three-dimensional reaction-diffusion dynamics with non-linear (inner) boundary conditions. This leads to systems of coupled partial differential equations, which have to be discretized in time and space. Multigrid methods are a highly efficient way of finally solving the resulting and in practice vast systems of linear equations.

However, realistic neurobiological applications of numerical simulation occur on arbitrarily complex domains including neuron networks, single neurons, cell structures like axons, dendrites, dendritic spines or cell organelles facing the challenge of unstructured computational grids with severe anisotropies, invaginations, nestings and branches. To meet this challenge a combination of both accurate and robust discretization and refinement techniques is essential.

Motivated by the use of novel refinement strategies to enhance the element qualities of computational grids, which approximate complex neurobiological domains, we present an extended discretization approach of hybrid tetra-/octahedral grids. Based on the splitting of an octahedral element into four tetrahedrons we first provide piecewise multi-linear polynomial shape functions p_i, $i = 0, ..., 5$, which fulfill the conditions $p_i(a_j) = \delta_{ij}$ in the element corners a_i, $i = 0, ..., 5$ and are linear restricted to the triangular faces. This is inspired by an analogue approach for pyramids by Wieners in [1]. Corresponding to the tetrahedral splitting, we then create a vertex-centered finite volume geometry inside the octahedron using the barycenter method [2]. This enables a conforming combination with standard Lagrange $\mathbb{P}1$ tetrahedral elements [3] either using the finite element or finite volume method of first order.

The hybrid tetra-/octahedral grid discretization at hand we are able to introduce a modified multigrid method with a new refinement strategy based on grid hierarchies which are generated by using Loop's smooth subdivision surface refinement [4] of the boundary combined with

Schaefer's smooth subdivision volumes refinement [5] of the inner grid. These Subdivision schemes are based on the B-spline theory and define smooth subdivision surfaces or volumes resp. as unique limits of successive grid refinements and vertex repositionings by distinct position masks.

Starting with a triangulated surface geometry, which approximates the boundary of the corresponding neurobiological domain, the vertices are first projected onto their final position on the subdivision surface and then a constrained Delaunay tetrahedrization [6] is generated as coarse grid. The multigrid hierarchy is now created by successive linear refinement operations. Tetrahedrons are split into four outer tetrahedrons and one inner octahedron. Octahedrons are split into six outer octahedrons and the remaining cavities are filled with eight tetrahedrons. Subsequent to that, the boundary vertices of each refinement level are projected onto their final position on the subdivision surface and the inner vertices onto their final position on the subdivision volume. This procedure results in a particularly smooth approximation of the computational domain and prevents degenerate volume elements to emerge especially in the vincinity of the boundary at the same time.

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