

Biochemical simulations connecting the tissue from the cell

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Key Words: RICS, cells, simulation, biochemical reactions, diffusions, advections

The cells have various cell shapes depending on various cell functions. Many intra-cellular proteins are localized in a sub-cellular compartment such as cytosol, nucleus, and mitochondria, so that almost biochemical reactions also are localized and regulated in a cell. We have developed a cells-simulator called RICS. The RICS simulates diffusions and biochemical reactions in a three dimensional space. RICS required the V-Sphere software^[1] in V-CAD system^[2]. V-Sphere is an unsteady physical simulation framework centering on thermal fluids applicable for VCAD, designed for handling multiple solvers integratedly, and supports parallelization for high performance computers.

It is an important for our body homeostasis that the blood flow carries nutrients, waste products, and hormonal signals. In this study, we have applied the advection for RICS system and tried to speed up calculations of reactions.

We implemented advection solvers, which are a second-order finite difference method and a fifth-order WENO^[3] method. An old version RICS had used only the E-Cell biochemical reaction system^[4]. However, many biological scientists have used the SBML system^[5] recently, because SBML is simple. We tried to adapt SBML for RICS and measure calculation accuracy and elapsed time.

The second-order finite difference method accumulated errors on real-time simulation, because diffusion speeds of biomaterials in the blood are significantly slower than blood flow speeds. We suggest that the fifth-order WENO method is a good solver for our body simulation. We implemented SBML solver in RICS. This solver could speed up a reaction part.

It is thought that it becomes a useful tool to understand the disease and the clinical condition, such as on hepatic rubble or brain vessel.

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