E-Cell 3D: 3-Dimensional Visualization of Dynamic Cell Simulation

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The E-Cell Project is an international research project aiming to model and reconstruct biological phenomena *in silico*, and to develop necessary theoretical supports, technologies, and software platforms to allow precise whole cell simulation. Cell simulation realizes theoretical experiments *in silico*, in order to enhance our understandings of dynamic cellular activities through systems biology approaches. E-Cell Simulation Environment version 3 (E-Cell SE 3) is a potential platform for this purpose, which allows multi-algorithm and multi-timescale simulation that is scriptable with Python programming language.

E-Cell 3D is a novel 3D visualization interface for the simulation results of E-Cell SE3. Given a model, this system automatically lays out all molecular entities (corresponding to "species" in SBML) and displays all connections between them (corresponding to "reactions" in SBML) in 3-D space. Then the time-course changes in concentration and reaction rates are animated according to the simulation results, where molecular concentrations are represented by the size and brightness (changing from blue to yellow) of the nodes, and the flux is represented by the speed of particles traveling along the edges that connect the molecular entities. Since every component of a model is present in this visualization, system biologists can capture the dynamic workings of the entire system at a glance. Moreover, when there is large amount of flux in or out of a node, the coordinates of the node are altered, allowing rapid identification of controlling factors within the cellular network. In highly dynamical models such as the circadian clock, we can clearly observe the synchronization of oscillations within the network, and identify the controlling molecules of feedback oscillators. Although still experimental, this type of visualization approach may complement the use of graphs for the interpretation of modeling and simulation. E-Cell 3D is developed using Quartz Composer (graphical programming environment for 3D animations available on MacOS X) and OpenGL API.

Software and source code: http://ecell3d.iab.keio.ac.jp