Intelligent Computational Simulation Methods for Biomedical Applications

Shafagh Jafer, Masters Degree Student
Systems & Computer Engineering Department
Carleton University, Ottawa, ON, K1S 5B6

Simulation is becoming increasingly important in the analysis of biological processes. The complexity of these systems makes computer simulation an adequate tool to study them under particular experimental conditions. Our long term goal is to provide realistic simulations of different biological processes when specific internal or external parameters are applied. We want to provide environments that the researchers in biology and medicine could use to understand and control the dynamics of these biological processes through computer simulation in a whole organelle scale. Our approach is based on the use of the DEVS formalism. DEVS provides a framework for the construction of hierarchical models in a modular fashion, which makes DEVS ideal for describing naturally hierarchical systems. DEVS discrete-event nature improves the execution performance of the models, due to the asynchronous nature of the events occurring in the cell. DEVS also uses explicit timing information; hence, we can adequately represent timing of the reactions occurring in the organism.

CD++ is a modeling tool that was defined using the DEVS and Cell-DEVS specifications. The toolkit includes facilities to build DEVS and Cell-DEVS models. DEVS Atomic models can be programmed and incorporated onto a class hierarchy programmed in C++. Coupled models can be defined using a built-in specification language. Cell-DEVS models are built following the formal specifications for DEVS models (informally presented in the previous section), and a built-in language is provided to describe them. CD++ makes use of the independence between modeling and simulation provided by DEVS, and different simulation engines have been defined for the platform.

Our research is based on the DEVS (Discrete Events systems Specification) and Cell-DEVS methodologies, using parallel/distributed computer systems. Our current interest is focused on the definition and analysis of synapsin and actin concentration modeling at the presynaptic nerve terminal. The aim of this model is to predict the number of synaptic vesicles released from the reserve pool as a function of time under the influence of action potentials at differing frequencies. A biochemical model is created, incorporating five key components, namely vesicles, synapsin, protein kinase, protein phosphatase, and actin, and including the effect of exocytosis and endocytosis. The model is used to analyze several phenomena observed in physiological measurements, which will allow us to better understand the synapsis behavior in neurons. The results of the simulation were optimized using a parallel Cell-DEVS simulator based on the Time Warp simulation kernel. The Parallel Cell-DEVS simulator will allow the simulation time to be significantly reduced from hours to minutes providing an “on-line” aspect to the tool in time critical decision-making processes.