Abstract

Complex biochemical systems such as gene regulation networks are often represented as delay differential equations (DDEs). However, unlike ordinary differential equations (ODEs), there are few large-scale systems available for simulating DDEs, and fewer still for high-performance simulations. To meet the growing need for simulating tissue-level systems of intercellular signaling gene regulation networks, I present a high-performance DDE simulation framework. By using compile-time specialization and optimization, my framework creates highly compact and efficient data structures with a small amount of configuration for the model being simulated. It also supports GPU acceleration of highly parallel models, which can be used to increase the simulation speed of large tissues, or increase the search speed among independent simulations in a reaction parameter search. I demonstrate congruence of my simulation results with prior special-purpose simulations, and the superior CPU and GPU performance of my framework over those same frameworks, while also supporting greater flexibility and configurability of the systems being modeled.