# SUMMARY OF Ph.D. DISSERTATION

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Title

An FPGA-Based Acceleration Method for Biochemical Simulations


Abstract

Biochemical simulators are now essential for understanding of cellular systems. Cellular systems are modeled as a network of substances and reactions, and the models are refined in repetition of experiments and simulations.

Reaction pathways are expressed as set of ordinal differential equations (ODEs), which have concentrations of molecular species as their variables and kinetic parameters as their coefficients. Since it's not possible to know the complete pathway, concentration and kinetic parameters from experiments, simulations have to be run again and again to find an ideal parameter set to present reasonable behavior.

Parameter optimization process is a time consuming task, and usually takes over 1 week. Current solutions for parameter optimization are parallel systems, such as PC/WS clusters or SMP systems. However, computers are still bottleneck for biologists, because expensive parallel systems can't be the "personal" computing environment for them. To relax this bottleneck, a cheaper and smaller solution for biocomputing is required.

This research introduces an efficient solution for acceleration of biochemical simulations, by using an FPGA as the simulation engine. FPGA can provide optimized hardware and performance, but it's usually difficult to use. Mostly common problems with FPGA-based biochemical simulations are: 1) limited bandwidth of PCI bus between the FPGA and host processor, 2) existence of various rate-law functions, and 3) users without any knowledge in hardware design. The method developed here provides solutions to these problems by modules by 1) describing reaction pathway by pointers among memory blocks on FPGA, 2) modular design of various rate-law functions, and 3) software-friendly design of hardware modules.

This thesis describes the background of this work, basic structure of the FPGA-based biochemical simulator ReCSiP, and the result of its basic performance evaluation. Result of the evaluation showed that ReCSiP is suitable for parameter optimization, by exploiting the potential of its deep-pipelined structure. The peak performance gain reached to 80-fold speedup, and its effective throughput was 10 to 50-fold speedup compared to Intel's Pentium4 processor at 3.2GHz. This result shows that FPGA is now hopeful candidate as the engine for future biocomputing.