A Cellular Automata System with Reconfigurable Hardware: Towards a Whole Cell Simulation

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1 Introduction

Recently, in order to understand the dynamic behavior of living cells, elucidation of gene networks or protein interaction networks becomes one of the hot topics in bioinformatics. Gene products, namely proteins, organize complex interaction networks for both metabolism and gene expression regulation in a living cell. In addition, protein distribution is also complicated because each organelle, such as endoplasmic reticulum, Golgi apparatus, mitochondria, tends to hold proteins specific to its matrix and/or membrane. In this sense, non-uniformity is also a key factor of complex cell behaviors.

This importance of microscopic phenomena in living cells makes it very difficult to describe the total behaviors of proteins in cells using differential equations. Cellular automata are another approach to simulate the total behaviors by dividing the whole area into very small grids and describing only the relationships between the adjacent grids. This approach is very flexible and suitable for simulating very complex systems like cells. However, the amount of computation required to run cellular automata is very large, and it is not realistic to simulate large systems like cells on desktop computers.

The performance and the size of reconfigurable hardwares such as Field Programmable Gate Arrays (FPGAs) have been drastically improved in last several years. With the latest FPGA chips, we can compute more than one hundreds of grids in one clock cycle (less than 50 nano second), and the reconfigurability of FPGAs makes it possible to compute any kind of cellular automata on the same chip. In this paper, we show that an off-the-shelf FPGA board can achieve a speedup of more than one hundred in the context of fluid dynamics simulation.

2 Cellular Automata for Fluid Dynamics

In cellular automata, the target space for the simulation is divided into small grids. The status of grids are updated at the same time using a rule which represents relationships between the grid and its neighborhood. By repeating this procedure, we can simulate many kinds of complex behaviors.

Lattice gas automata are a class of cellular automata designed for simulating fluid dynamics. Many of lattice gas models are based on FHP model [1]. In FHP models, hexagonal grids (Fig. 1) are used. In the figure, bold lines show the borders of each grid, and the dots show particles on the grids. The particles travel over the grids at unit speed. If particles collide at each grid, then they change their

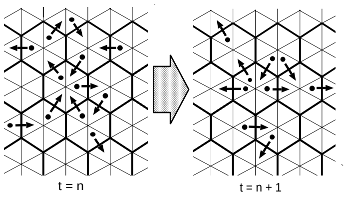

Figure 1: hexagonal grids.

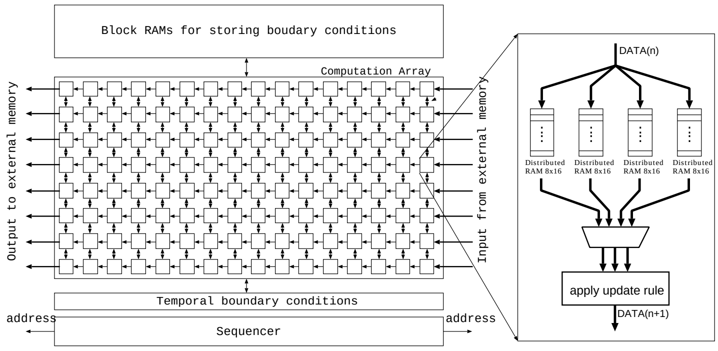

Figure 2: Block Diagram of the Circuit.

directions. In the computation of the lattice gas models, the hexagonal grid is transformed into two dimensional array, and the status of each grid is repeatedly updated based on the status of the grid and its six neighbors. The operations for computing the new status of each grid are very simple, but the need to process many grids many times makes it unrealistic to simulate large grids on desktop computers.

3 A Cellular Automata System with Reconfigurable Gate Array

We have implemented the lattice gas model on an off-the-shelf FPGA board (ADC RC1000) for preliminary experimentation for living cell simulation [2]. Figure 2 shows the block diagram of the circuit. There are 8×16 units in the computation array, and each unit computes next status of each grid. The right part of the Figure 2 shows the structure of the unit. Each unit stores the status of three grids (a cell and its left and right grids), and computes new status of the cell using data of the grids in upper and lower units. The output of each unit is transferred to its left unit. The effective parallelism of this circuit is 112 (with 128 units) because boundary conditions for the lower 16 units are not given correctly owing to the limited I/O bandwidth of the FPGA chip. The speed gain for a lattice gas FHP-III model with 2048×1024 lattice is 143 times faster than with Pentium-III 700MHz.

4 Future Works

We have shown that one off-the-shelf FPGA board can achieve a speedup of more than one hundred compared with a desktop computer in the simulation of fluid dynamics. We are now implementing a cellular automaton model for living cell simulation. The update rule for living cell simulation is more complex than the rule for FHP models. This means that the living cell simulation requires larger size of FPGAs. The size of FPGAs have been steadily improved, and in several years, will become more than 10 times. We believe that this drastic improvement will make it possible to simulate total behaviors of proteins in living cells in reasonable amount of time.

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