論文 / 著書情報
Article / Book Information

題目(和文)	GPUを用いた多様な計算プラットフォーム上で動作する実時間制御3次元可視化分子運動シミュレーションに関する研究
Title(English)	A Study of a GPU Based Real-time 3D Live Controlled Molecular Kinetics Simulation on Multiple Computing Platforms
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Category(English)	Doctoral Thesis
種別(和文)	論文要旨
Type(English)	Summary

（博士課程）
Doctoral Program

論 文 要 旨

THESIS SUMMARY

専攻： Department of	Computational Intelligence and Systems Science 専攻	申請学位（専攻分野）： Academic Degree Requested	博士 Doctor of (Engineering)
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要旨（和文 2000 字程度）
Thesis Summary (approx.2000 Japanese Characters 800 English Words)

The purpose of my research is to develop a flexible real-time 3D live controlled molecular kinetics simulation with the aim to assist in the development of molecular robotics. This thesis is composed of six chapters: chapter 1 an introduction to the topic, chapter 2 an overview of our molecular model, chapters 3-5 various GPGPU performance solutions for various systems, and chapter 6 the conclusion.

Chapter 1 Introduction

This chapter begins with an introduction to the research issue faced, gaining more understanding of microtubules and motor protein dynamics for creating molecular actuators to be used in molecular robotics. As well as bringing up our methodology for gaining knowledge, the use of computer simulations utilizing GPGPU processing. This is followed by some background on microtubule gliding assays and GPU units. Then the following research issues and challenges are outlined and explained: creating a new bottom-up large scale model, defining a new type of molecular simulation, finding a solution to the vast amounts of data produced, designing an intuitive simulation for efficiently gaining understanding, and enabling high-performance across many computing platforms.

Chapter 2 Microtubule Gliding Assay Model

This chapter starts by addressing a few related works, and their limitations with regards to our goal are addressed. Then our particle based chain model is explained, followed by an overview of the microtubule snuggling and overriding interactions reproduced by our model with the Lennard-Jones Potential. Next, we take a look at the results of incorporating a past work's algorithms into our model which is able to create original swarm results, but explain why it is not sufficient for our goals. Lastly, we introduce a new explicit model which is able to produce microtubule swarms and present preliminary images.

Chapter 3 Single GPU Performance

This chapter begins by explaining the major challenges with creating a real-time 3D live controlled simulation. For example, rendering performance, computational performance, and linear scalability. Then it discusses the methods being used to achieve linear performance such as a grid sort with a nearest neighbor search, along with memory optimizations being

used to reach a higher degree of performance. Then concludes with a performance evaluation for this sections topics.

Chapter 4 Multi-GPU Performance

This chapter begins by describing the challenges of managing the two different workloads rendering and computation. Then goes into the methods developed to efficiently manage both asynchronously on independent hardware, followed by a performance analysis and a comparison to a related work. Next, this chapter compares a typical distributed computing approach and our master and assist GPGPU computing approach. Our master and assist algorithm was developed as a solution for fully utilizing a system with four GPU, by organizing workloads to specific GPU and using a memory buffer system. Then the chapter concludes with a performance evaluation for this sections topics.

Chapter 5 Distributed Real-time Simulation

This chapter begins by explaining some of the challenges with a distributed real-time simulation, the greatest being memory movement between hardware and systems. The next section goes into detail about our method developed for networking a client/host system together, as well as a solution to the networking limitations. Then the chapter moves on to explain the management tasks performed by the CPU to distribute the computational work to multiple GPU and gather the results. This is followed by a section explaining the work done on the GPU and the GPU-to-GPU data updates. Next, the rendering performance is looked at as well as current limitations. Then the chapter concludes with a performance comparison to a GPGPU fluid simulation which utilizes similar spatial optimizations.

Chapter 6 Conclusion

In the conclusion, the major results of this thesis' research are outlined, as well as the current limitations.