

Project Plan for COMP3750
Project Work in Computer System

Particle Simulation
on the Cell Broadband Engine
- Extending types of interactions

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1 Background

The Cell Broadband Engine is a novel microprocessor architecture jointly developed by Sony Computer Entertainment, Toshiba and IBM. The Cell architecture is widely regarded as a challenge for software development due to its design focus on prioritise bandwidth over latency and favours peak computational throughput over simplicity of code. This unique design of the Cell increases the difficulty for programming. However, it also gives high computational potential. This project aims to evaluate the performance and limitation of using the Cell on the PlayStation for high performance computing. This is done by implementing a particle simulation program on the PlayStation 3.

A simple particle simulation program that implements a Lennard-jones potential has been developed by a previous student. The task of this project is to extend this program to include more types of particle interactions and therefore be able to provide a basic simulation of water.

2 Task Description

2.1 Implementation Task

This project will extend an existing system that has implemented a simple particle simulation on the Cell Broadband Engine to include some more complex particle interactions. The first one is the electrostatic interaction. This will be based on the Coulomb's Law, which energy of a particle can be written in the following form:

$$E_{elect} = C \frac{q_1 q_2}{r_{12}}$$

Electrostatic interaction plus the Lennard-jones potential will enable us to build the TIP3P model of water, which energy of the whole system can be written in the following form:

$$E_{ab} = \sum_i^{ona} \sum_j^{onb} K_c \frac{q_1 q_2}{r_{ij}} + \frac{12}{r_{OO}^{12}} - \frac{6}{r_{OO}^6}$$

2.2 Research Task

The research aim is to evaluate the performance of the above implementation on the Cell on the PlayStation 3 and find out the potential limitations of it.

A final report and a final presentation regarding the implementation and research result will be produced as per course requirements.

3 Schedule

- Electrostatic interaction finished by 10am Thursday 21 August (week 5).
- TIP3P water model finished by 10am Thursday 11 September (week 8).
- Performance evaluation by 10am 25 September (week 10)
- Draft final report by 10am 16 October Thursday (week 11)
- Final report by 10am 30 October Thursday (week 12)

4 Reference

- A. Leach. Molecular modelling: principles and applications.
- E.C.McCreath, A.E.Zein, J.Imholz, A.P. Rendell, E. Wong. Using the Cell Broadband Engine and NVIDIA8800 GPU for Computational Science Applications: A Particle Dynamics Comparison.
- [http://en.wikipedia.org/wiki/Cell_\(microprocessor\)](http://en.wikipedia.org/wiki/Cell_(microprocessor))
- http://en.wikipedia.org/wiki/water_model