COMP3750 Project work in computer systems
Semester 2 2008

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

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Task Description

- Things to implement
  - Extend an existing system that has implemented a simple particle simulation on the Cell Broadband Engine to include some more complex particle interactions, such as charge effects and chemical bonds, which will enable us to provide a basic molecular dynamics simulation of water

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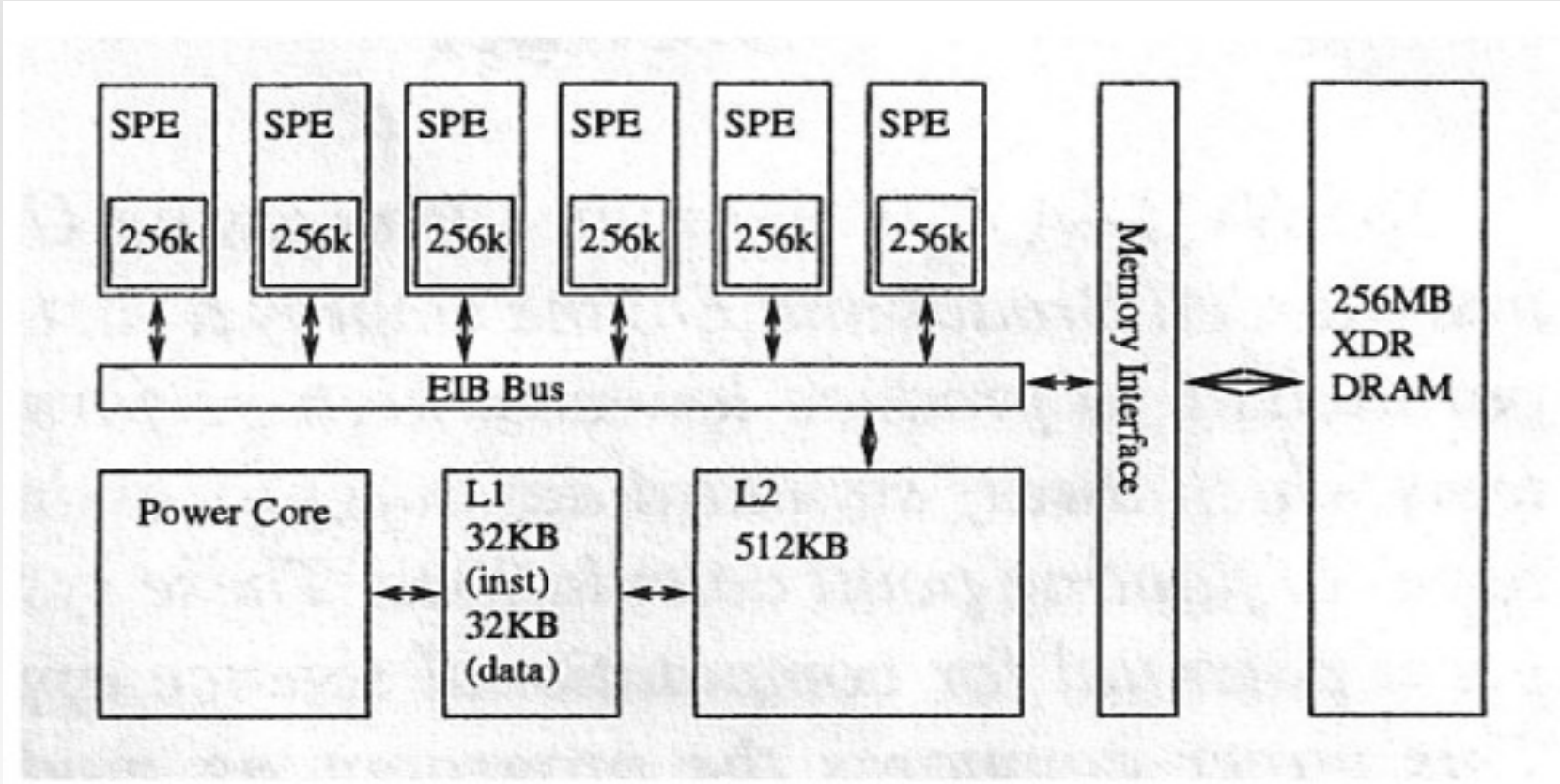
Cell on the PlayStation 3



What is the Cell?

- Microprocessor architecture jointly developed by Sony Computer Entertainment, Toshiba and IBM.
- Combines a general-purpose Power Core with Synergistic Processing Elements (SPE)
- Provides huge computational potential
  - Used in the IBM Roadrunner (rank no.1 Top500, June 2008)
  - Theoretical 25.6 GFLOPS per SPE(single precision)

What is the Challenge?

- Unique system and memory architecture
  - Design focus
    - Bandwidth > Latency
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- Unique system and memory architecture
  - Design focus
    - Bandwidth > Latency
    - Peak computational throughput > Simplicity of code
  - Organise code structure and memory transfer to maximise performance
  - Balance computing load over each SPE

Particle Simulation

- What has been done
  - Lennard-Jones potential

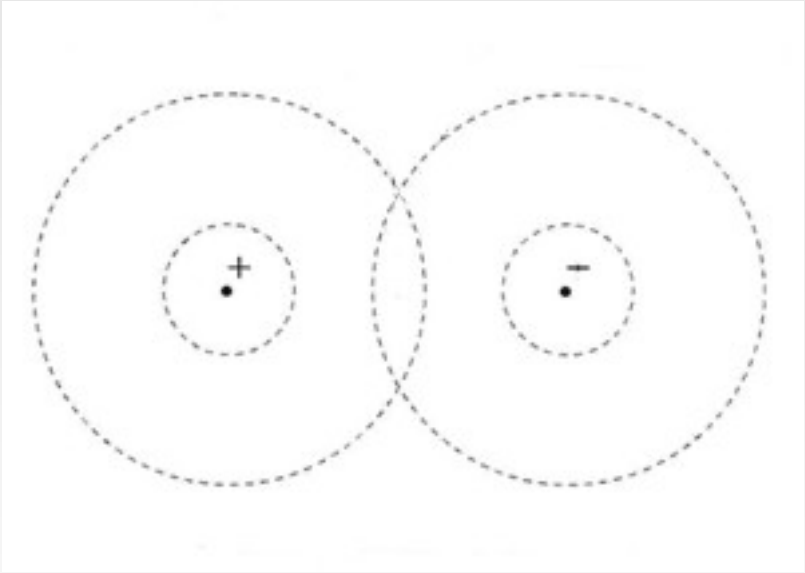
$$E_{elect} = \frac{12}{r_{12}^{12}} - \frac{6}{r_{12}^{6}}$$

Particle Simulation

- What we want to add
  - Electrostatic interactions
    - Coulomb's Law

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

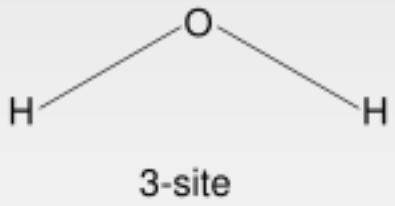
$$F_x^{elect} = C\frac{q_1 q_2}{r_{12}^2}(x_1 - x_2)$$



Particle Simulation

- What we want to add
  - Electrostatic interactions
  - TIP3P water model

$$E_{ab} = \sum_{i}^{on\,a} \sum_{j}^{on\,b} K_c \frac{q_i q_j}{r_{ij}} + \frac{12}{r_{OO}^{12}} - \frac{6}{r_{OO}^{6}}$$



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Evaluation

- Evaluate the performance achieved on the Cell on the PlayStation 3.
- Limitations of such implementation on the Cell?
- Possible improvements?

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/Water_model