Comparison of Molecular Dynamics Simulation Speed Using a Sony Playstation 3

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Abstract

Molecular dynamics is a powerful tool to study biological and biochemical systems at a microscopic level. Performing simulations using molecular dynamics is computer-intensive and typically requires tens to thousands of processors several days to generate data for analysis. Recent advances in gaming hardware, e.g. PS3, have the potential to reduce the cost of performing these simulations. A PS3 was chosen to perform simulations of an ice/water/bilayer system. These simulations would be compared to home computing, another possible solution.

Introduction

Physical experiments can be expensive. Because of this cost, companies are looking to perform simulations that yield similar results without major expenses. This need led to molecular dynamics (MD). MD is a way to perform simulations of experiments without actually conducting them, eliminating materials fees and the need for lab time. MD makes use of computers, but that limits the speed and efficiency of the “experiment” to that of the computer(s). As various industries (gaming, in particular) create a demand for more powerful hardware, a strong and cost-effective candidate has appeared in Sony’s Playstation 3 (PS3).

The goal of this research was to determine if a PS3 is faster compared to other computers for MD simulations. If it is, how much faster is it and whether or not the costs are justified.

Method

For the timings, the same simulation was conducted on both platforms. This involved water surrounding a segment of ice in contact with a standard section of a lipid bilayer. The simulation resulted in a melting of the ice block. Later, the simulation will be modified to progress without melting the ice so that interaction can better be observed.

Results

As of this poster production, only results for the PC have been obtained. Timings for the aforementioned simulations are:

- 2.7347 seconds per step and 31.6516 days per nanosecond

Results with the PS3 will be several times faster than the PC.

All future work will be directed towards work with the PS3. Results are expected within the coming weeks.

Conclusion

Results from the dual-core computer were expected. It is estimated that the PS3 will be several times faster especially as the software is optimized for its Cell Broadband Engine (CBE) processor.

Further research will be conducted with the end goal being further study into ice-membrane interactions.

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References

