Fast but not Furious

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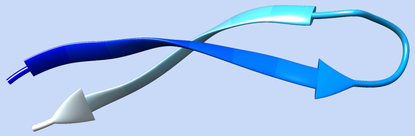
Aims

- To test a variety of workstation computer parts with Gromacs, a molecular dynamics simulation program
- To propose the most cost effective workstation computer for use with Gromacs from the parts and configurations tested

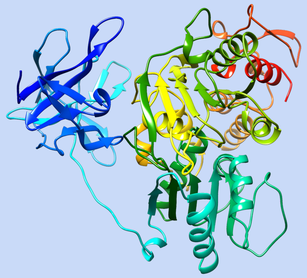
Introduction

The use of computers in chemistry has progressed through the years, coming closer and closer to being a substitute for lab experimentation. Saving both time and money on expensive reagents and laborious procedures.

This allows chemists to test the basic viability of a new drug designed to bind to a particular enzyme via docking software such as DOCK6 or to examine the configuration a molecule will adopt when in a particular solvent via Gromacs.



Alpha-synuclein, 4BXL1

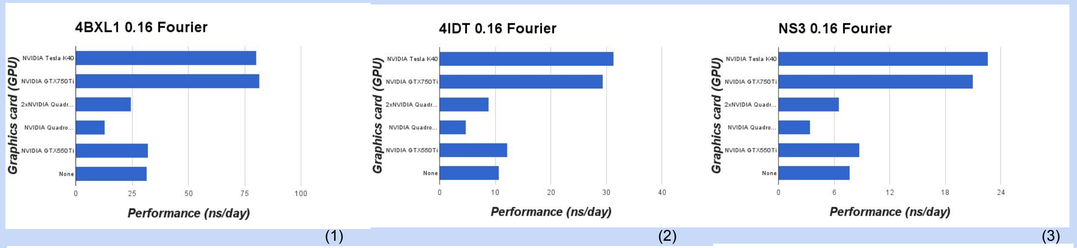


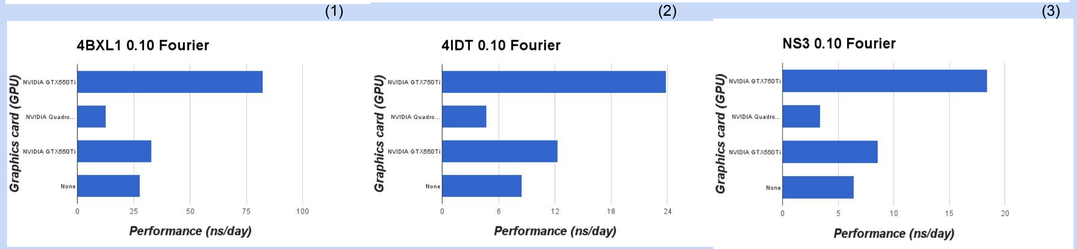
Nonstructural protein 3, NS3

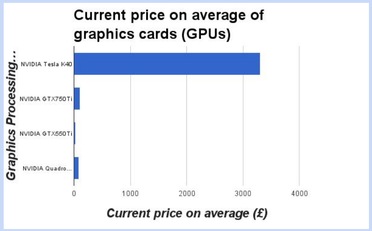
Method

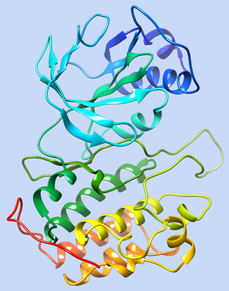
Three proteins were selected because of their varying size. They were then simulated using gromacs under the parameters of a nm^3 box of water at an energy minimum and when completely ionically neutral This was performed on various workstations and with various graphics cards (GPUs) in the workstations, from the lower end gtx 210 and Quardo 600 to the high end Tesla k40. In each case the relative speed of each simulation was noted in the form of nanoseconds per day (ns/day). This represents the amount of time over which the system's movements could be simulated per day of running the simulation. After/this, attempts were made to refine the process via adjusting the parameters of the simulation. The Fourier distance was altered from the default of 0.16 to 0.10. A variety of cards were then tested with this new parameter.

Results









NF-kappa-B-inducing kinase (NIK), 4IDT

Analysis

The results, shown left, give the performance of a variety of GPUs for the three systems. Graphs 1-3 show use of Fourier spacing of 0.16, 4-6 show 0.10.

The amount of time simulated for any of the three systems is either near identical for the very expensive Tesla K40 and the years old mid range GTX750Ti card, or in some cases even slightly superior. This seems to indicate that gromacs does not benefit substantially from research grade GPUs as there is a clear case of diminishing returns for further monetary investment. There also appears to be certain scenarios with particularly old or low end GPUs, for example the Quadro 600, where the GPU can hold back simulation times. In these cases it is best to command that gromacs uses solely the CPU. Attempts to refine the process by changing fourier spacing failed to net any gains in performance.

Conclusion

The most efficient computer at present would be one that includes a top of the line consumer grade CPU and GPU. This is cheaper by an order of magnitude than a research grade workstation and would currently achieve similar results.The altering of parameters such as fourier spacing to boost performance warrants further study to find refinements that result in performance gains without greatly sacrificing quality of results.

Further reading

G. H. Grant, W. G. Richards, Computational Chemistry, Oxford University Press, Great Clarendon Street Oxford OX2 6DP, 1999

P. Biggs, Computers in Chemistry, Oxford University Press, Great Clarendon Street Oxford OX2 6DP, 1995

Acknowledgments

Dr Mark Garner. Computing officer at the school of chemistry.