A Preliminary Report on Application Performance With Intel Woodcrest & QLogic InfiniPath

WHITE PAPER

A Preliminary Report on Application Performance using Intel Woodcrest Processors & QLogic InfiniPath InfiniBand Adapters

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Executive Summary

Intel's new Core 2 micro-architecture provides a substantial performance improvement over previous generations of processors. This whitepaper contains real application benchmarks out to 128 cores for the Intel "Woodcrest" cpu combined with QLogic's InfiniPath InfiniBand interconnect. Comparisons to other processors and interconnects are also included. Wherever possible, published data is used for comparisons.

Finding comparable real application data is always difficult. We would like to work with anyone interested in producing accurate benchmark numbers for modern cpus and interconnect. Please contact us if your organization is interested.

The Woodcrest/InfiniPath numbers in this paper are necessarily preliminary and were run on servers provided by Dalco AG, a leading server supplier in Switzerland. We expect to improve these numbers before the end of this year (2006), and when we do, we will publish a new whitepaper revision with these improved results.

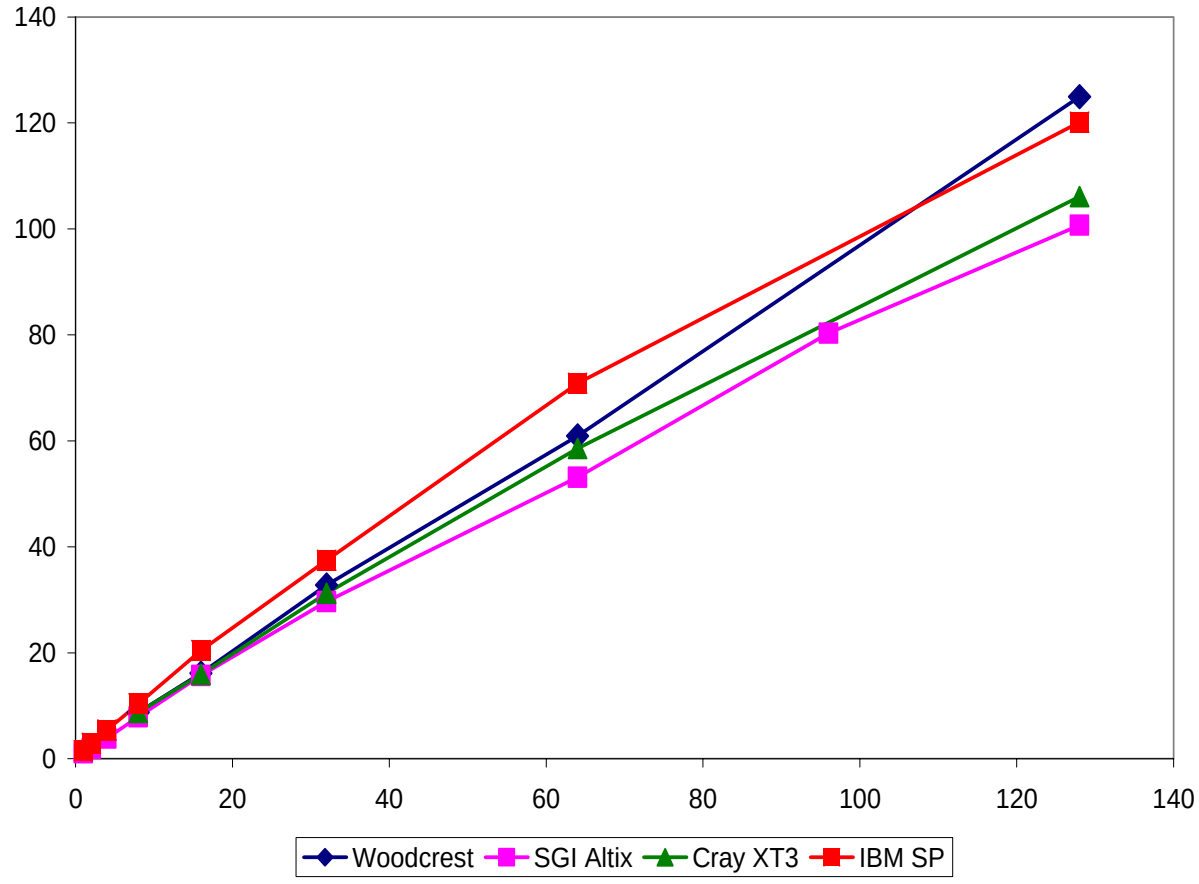
Despite the preliminary nature of these results, the comparisons are quite striking. Clusters using Woodcrest processors and InfiniPath InfiniBand interconnect are faster and scale better than competing solutions such as Opteron with Mellanox InfiniBand, the SGI Altix, and the IBM SP.

QLOGIC

WRF 2.1.1

WRF (pronounced like “wharf”) is a next-generation weather code used for both mesoscale and continental US weather prediction. It is a joint project between weather forecasting and research organizations including NCAR, NCEP, FSL, AFWA, NRL, Oklahoma University, and the FAA. WRF is currently used for operational weather forecasts at the US National Weather Service.

The results shown below are for the 12km CONUS test-case, which can be downloaded from http://www.mmm.ucar.edu/wrf/WG2/bench/. Comparative numbers were provided by John Michalakes from his presentation to the GARPA conference, June 1-2, 2006. As you can see, the Intel Woodcrest cluster is best-in-class at 128 cores. A price/performance comparison would show a huge advantage to the Intel Woodcrest cluster.



Intel Woodcrest, 3.0 Ghz, InfiniPath PCI Express HCAs, PathScale compiler.

Cray XT3, Opteron 2.6 Ghz, SeaStar interconnect, PGI compiler

SGI Altix, Itanium2 1.6 Ghz 9 meg L2, Intel Fortran compiler

IBM SP Power5, 1.9 Ghz, Federation Switch, XLF compiler.

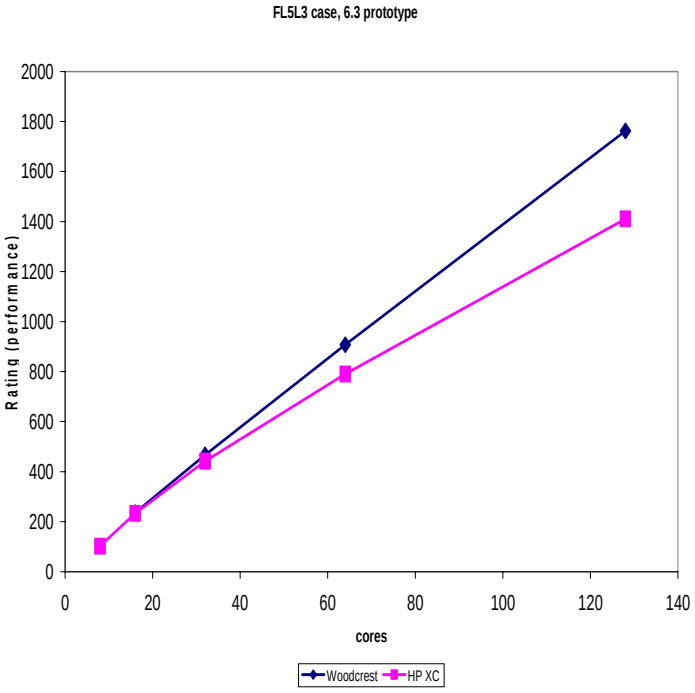
Fluent

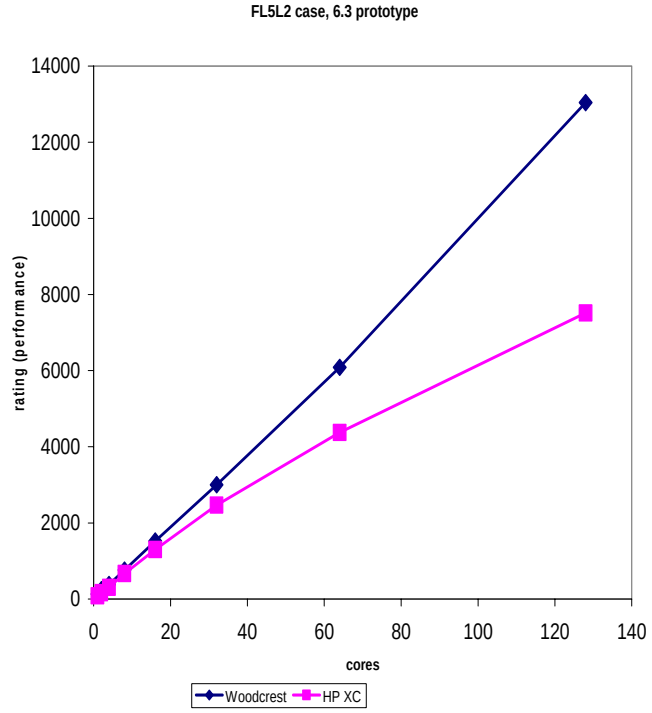
Fluent is a commercial code used for CFD (computational fluid dynamics) applications. Fluent's website contains 9 benchmarks with data of small, medium, and large sizes, which represent the types of computations done by Fluent's users. We ran 2 of the "large" test cases, FL5L2 and FL5L3. Comparison data is taken from Fluent's website, for the "version 6.3 prototype", http://fluent.org/software/fluent/fl5bench.

The following charts compare Intel Woodcrest 3.0 Ghz, dual-socket dual-core servers with InfiniPath InfiniBand HCAs to HP XC Opteron 2.2 Ghz, dual-socket dual-core servers with Mellanox IB HCAs

In both cases the Intel Woodcrest cluster has the best absolute performance, and also scales better than the competing Opteron with Mellanox-based HCAs.

In the FL5L3 case, the Woodcrest/InfiniPath has super-linear scaling from 64 to 128 cores, primarily caused by the problem fitting into Woodcrest's large 4 megabyte L2 cache.





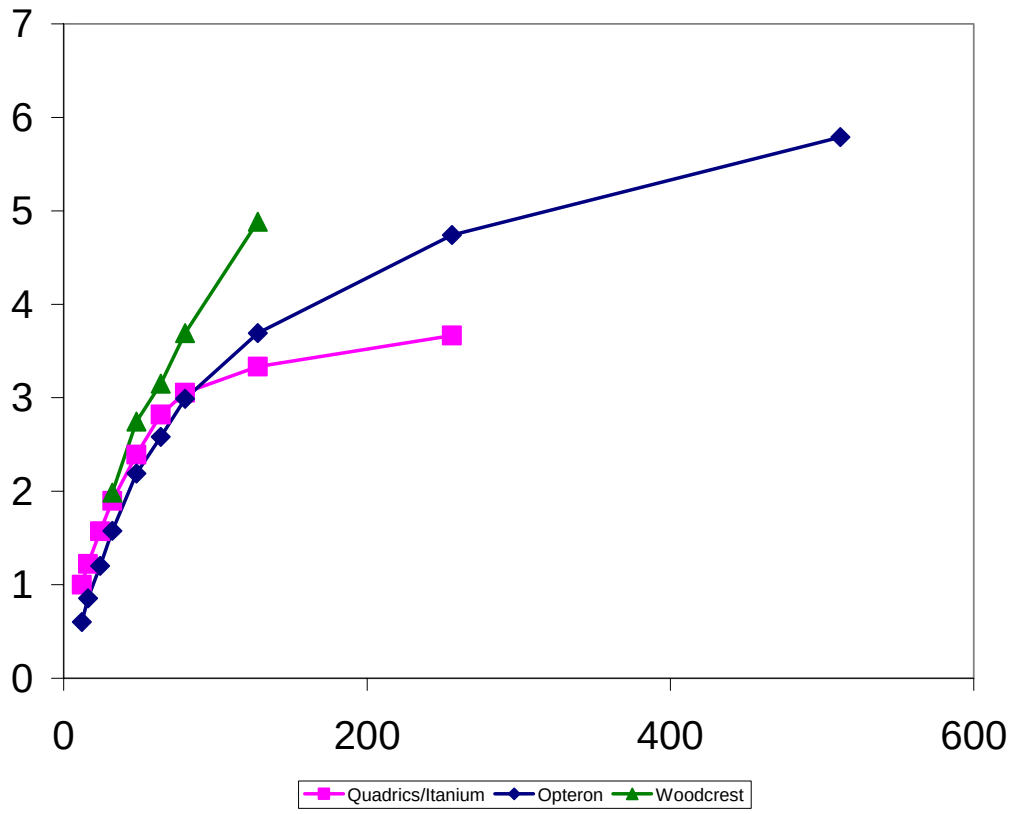
Note: At the time of this publication, Fluent has not completed certification on InfiniPath.

NWChem

NWChem is a computational chemistry code developed at the Molecular Sciences Software group of the Environmental Molecular Sciences Laboratory at the Pacific Northwest National Laboratory. NWChem is built on top of a one-sided messaging library named ARMCI, and many interconnects such as Quadrics have specially-written ARMCI drivers.

We modified ARMCI to implement one-sided operations using two-sided MPI messages. While this isn't the most efficient implementation, it was good enough to allow an InfiniPath-equipped cluster to out-scale PNNL's Itanium2 1.5 Ghz + Quadrics cluster. PNL's data is in pink, the Intel Woodcrest 3.0 Ghz InfiniPath cluster is green, and Opteron 2.4 Ghz InfiniPath data is dark blue.

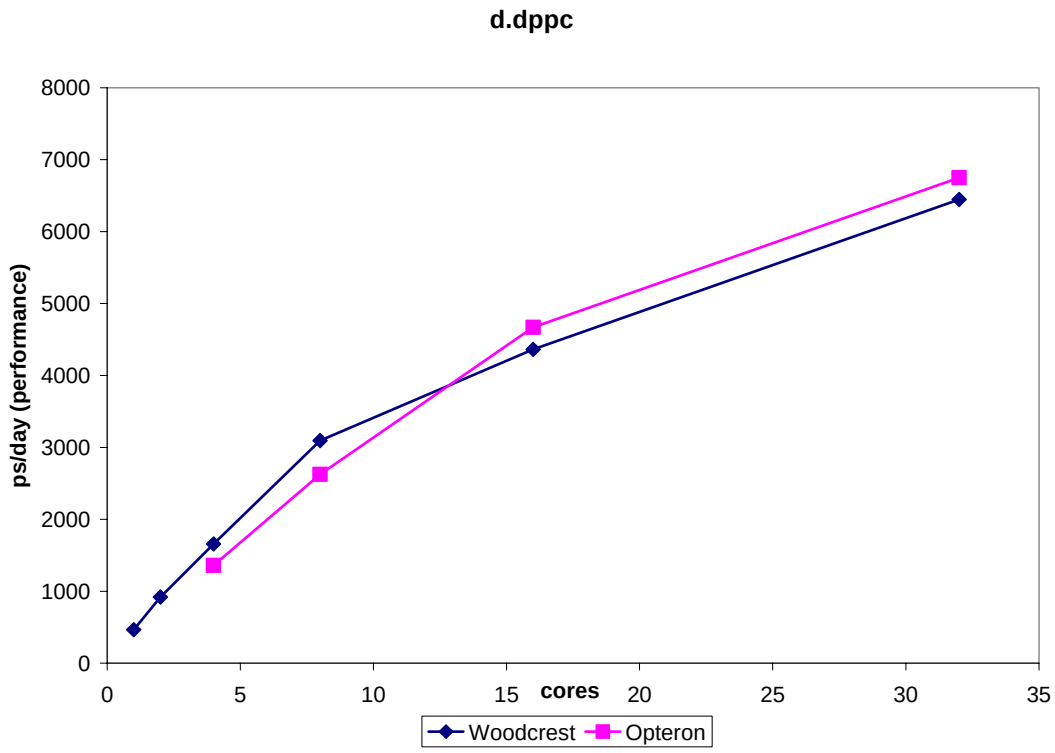
This test case is Siosi6. Comparable results may be found at:
http://www.emsl.pnl.gov/docs/nwchem/benchmarks/

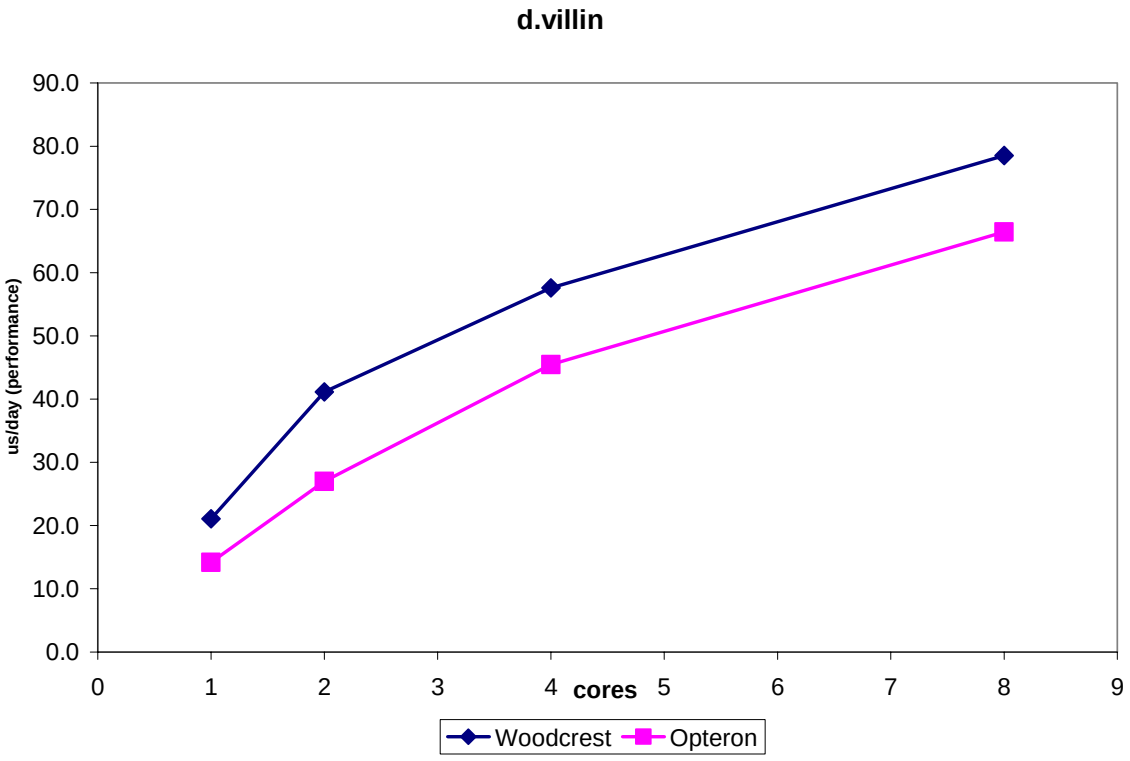


These results are quite interesting, as the Woodcrest+InfiniPath cluster is able to beat the Itanium2+Quadrics cluster at all sizes. The Opteron+InfiniPath cluster is slower than the Itanium2 cluster at small sizes (64 cores and below.)

Gromacs

Gromacs is a commonly-used molecular dynamics code. The two test cases below are both difficult to scale. In “d.dppc”, the Intel Woodcrest cluster (3.0 Ghz) begins with a big scalar advantage (Woodcrest is 50% faster at one core), but is eventually outscaled by the Opteron cluster (2.6 Ghz single-core). This is an illustration of an area where InfiniPath with Intel Woodcrest scales similar to InfiniPath with Opteron. In the other test case, “d.villin,” both clusters stop scaling above 8 cores due to a limitation in the algorithm, and the Intel Woodcrest scalar performance advantage translates into a large win. See http://biowulf.nih.gov/apps/gromacs/bench.html for comparison data. Gromacs performance is measured in “us/day” or “ps/day”, pico- or micro-seconds of simulation time per day of compute time.




d.villin
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0.0
us/day (performance)
0
1
2
3
4
cores
5
6
7
8
9
Woodcrest
Opteron

NWChem Citation

NWChem's license requires the following citation in any paper giving NWChem results:

Aprà, E.; Windus, T.L.; Straatsma, T.P.; Bylaska, E.J.; de Jong, W.; Hirata, S.; Valiev, M.; Hackler, M.; Pollack, L.; Kowalski, K.; Harrison, R.; Dupuis, M.; Smith, D.M.A; Nieplocha, J.; Tipparaju V.; Krishnan, M.; Auer, A.A.; Brown, E.; Cisneros, G.; Fann, G.; Fruchtl, H.; Garza, J.; Hirao, K.; Kendall, R.; Nichols, J.; Tsemekhman, K.; Wolinski, K.; Anchell, J.; Bernholdt, D.; Borowski, P.; Clark, T.; Clerc, D.; Dachsel, H.; Deegan, M.; Dyall, K.; Elwood, D.; Glendening, E.; Gutowski, M.; Hess, A.; Jaffe, J.; Johnson, B.; Ju, J.; Kobayashi, R.; Kutteh, R.; Lin, Z.; Littlefield, R.; Long, X.; Meng, B.; Nakajima, T.; Niu, S.; Rosing, M.; Sandrone, G.; Stave, M.; Taylor, H.; Thomas, G.; van Lenthe, J.; Wong, A.; Zhang, Z.; "NWChem, A Computational Chemistry Package for Parallel Computers, Version 4.7" (2005), Pacific Northwest National Laboratory, Richland, Washington 99352-0999, USA. A modified version.

"High Performance Computational Chemistry: an Overview of NWChem a Distributed Parallel Application", Kendall, R.A.; Aprà, E.; Bernholdt, D.E.; Bylaska, E.J.; Dupuis, M.; Fann, G.I.; Harrison, R.J.; Ju, J.; Nichols, J.A.; Nieplocha, J.; Straatsma, T.P.; Windus, T.L.; Wong, A.T. Computer Phys. Comm., 2000, 128, 260-283

A special thanks to Dalco AG of Switzerland for providing the Intel Woodcrest-based servers. Info on Dalco servers can be found at www.dalco.ch.

For More Information

Additional information on QLogic InfiniPath InfiniBand products can be obtained by visiting http://www.qlogic.com/pathscale on the World Wide Web, or by contacting:

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