NAMD Performance Analysis on Skylake Architecture

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The purpose of this blog is to provide a comparative performance analysis of the Intel® Xeon® Gold 6150 processor and the previous generation Xeon® E5-2697 v4 processors using the NAMD benchmark. The Xeon® Gold 6150 CPU features 18 physical cores or 36 logical cores when utilizing hyper threading. This processor is based on Intel's new micro-architecture codenamed "Skylake". Intel significantly increased the L2 cache per core from 256 KB on Broadwell to 1 MB on Skylake. The 6150 also touts 24.75 MB of L3 cache and a six channel DDR4 memory interface.

Nanoscale Molecular Dynamics (NAMD) is an application developed using the Charm++ parallel programming model for molecular dynamics simulation. It is popular due to its parallel efficiency, scalability, and the ability to simulate millions of atoms.

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Test Cluster Configurations:

	Dell EMC PowerEdge C6420		**Dell EMC PowerEdge C6320**
CPU	*2x Xeon® Gold 6150 18c 2.7 GHz (Skylake)*		*2x Xeon® E5-2697 v4 16c 2.3 GHz (Broadwell)*
RAM	*12x 16GB @2666 MHz*		*8x 16GB @2400 MHz*
HDD	*1TB SATA*		*1 TB SATA*
OS	*RHEL 7.3*		*RHEL 7.3*
InfiniBand	*EDR ConnectX-4*		*EDR ConnectX-4*
CHARM++	*6.7.1*		
NAMD	*2.12_Source*		

BIOS Options	**Settings**
System Profile	*Performance Optimized*
Logical Processor	*Disabled*
Virtualization Technology	*Disabled*

The benchmark dataset selected for this series of tests was the Satellite Tobacco Mosaic Virus, or STMV. STMV contains 1,066,628 atoms, which makes it ideal for demonstrating scaling to large clustered environments. The performance is measured in nanoseconds per day (ns/day), which is the number of days required to simulate 1 nanosecond of real-time. A larger value indicates faster performance.

The first series of benchmark tests conducted were to measure the CPU performance. The test environment consisted of a single node, two nodes, four nodes, and eight nodes with the NAMD STMV dataset run three times for each configuration. The network interconnect between the nodes used was EDR InfiniBand as noted in the table above. Average results from a single node showed 0.70 ns/day. While for a two-node run performance increased by 80% to 1.25 ns/days. The trend of an average of 80% increase in performance for each doubling of node count remained relatively consistent as the environment was scaled to eight nodes, as seen in Figure 1.

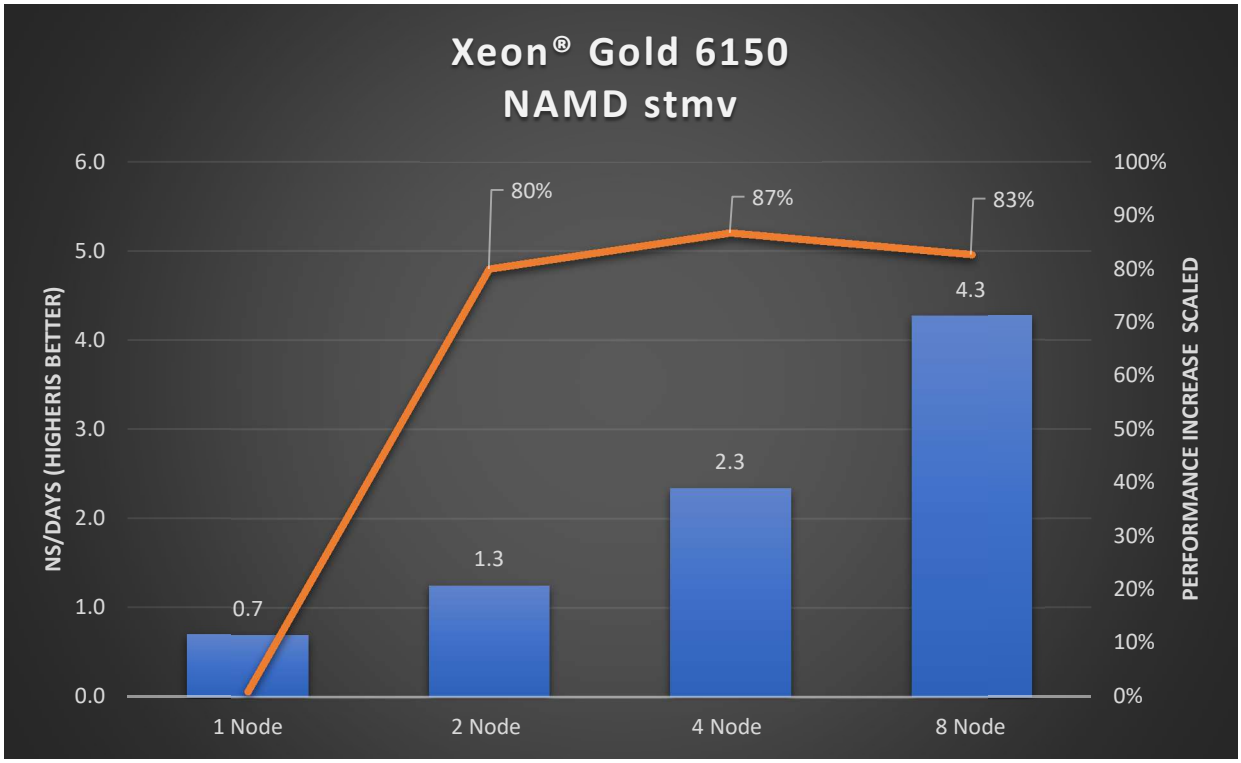

Figure 1.

The second series of benchmarks were run to compare the Xeon® Gold 6150 against the previous generation Xeon® E5-2697v4. The same dataset, STMV was used for both benchmark environments. As you can see below in Figure 2, the Xeon® Gold CPU results surpass the Xeon E5 V4 by 111% on a single node, and the relative performance advantage decreases to 63% at eight nodes.

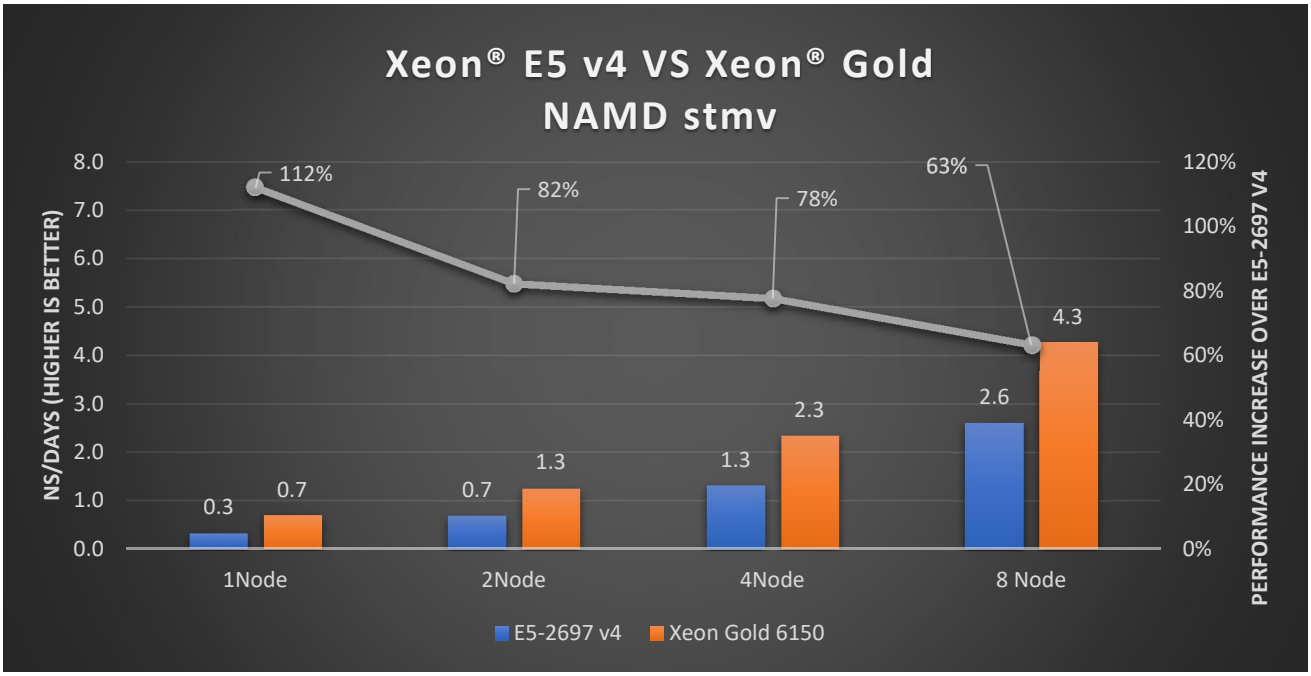

Figure 2.

Summary

In this blog, we analyzed and presented the performance of a Dell EMC PowerEdge C6420 cluster scaling from a single node to eight nodes running NAMD with the STMV dataset. Results show that performance of NAMD scales linearly with the increased number of nodes.
At the time of publishing this blog, there is an issue with the Intel Parallel Studio v, 2017.x and NAMD compilation. Intel recommends using Parallel Studio 2016.4 or 2018 (which is still in beta) with -xCORE-AVX512 under the FLOATOPS variable for best performance.
A comparative analysis was also conducted with the previous generation Dell EMC PowerEdge C6320 server and Xeon® E5 v4 (Broadwell) processor. The Xeon® Gold outperformed the E5 V4 by 111% and maintained a linear performance increase as the cluster was scaled and the number of nodes multiplied.

Resources

- Intel NAMD Recipe: https://software.intel.com/en-us/articles/building-namd-on-intel-xeon-and-intel-xeon-phi-processor
- Intel Fabric Tuning & Application Performance: https://www.intel.com/content/www/us/en/high-performance-computing-fabrics/omni-path-architecture-application-performance-mpi.html