NAMD Molecular Dynamics Simulation on 3rd Generation Intel® Xeon® Scalable Processors

up to **1.27x**

faster with fewer cores[1]

Intel® Xeon® Platinum 8380 processor versus AMD EPYC 7763 processor

up to **2.43x**

speedup with optimizations[2]

3rd Generation Intel® Xeon® Scalable processors versus prior generation

NAMD on Intel

Nanoscale Molecular Dynamics (NAMD) is one of the most widely used applications in high-performance computing (HPC). University of Illinois at Urbana-Champaign engineers collaborated with Intel to optimize NAMDs on Intel® Xeon® Scalable processors to provide significant improvements that can help save millions of node hours of time for researchers.[3] These optimizations accelerate workload processing by using a "tile" algorithm that increases the computational efficiency of each node. As a result, researchers can achieve longer timescales in simulating molecules that are relevant in COVID-19 research, increasing understanding at the atomic level.

Intel® Xeon® Scalable processors boost the performance of compute-bound applications like NAMD, increasing the computational efficiency of each node by using Intel® Advanced Vector Extensions 512 (Intel® AVX-512) vector units and a large cache. NAMD also benefits from the increased instructions per clock (IPC) and increased core counts of 3rd Generation Intel® Xeon® Scalable processors.

Key Intel® Xeon® Scalable Processor Features

- 20% higher instructions per clock[6]
- Built-in AI inference and training acceleration with DL Boost
- Built-in HPC acceleration with Intel® AVX-512

Intel for Health and Life Sciences

Intel's unmatched portfolio and broad ecosystem help life sciences researchers:

- Handle complex, diverse workloads and massive, sensitive datasets
- Achieve greater throughput with increased system utilization and availability
- Drive insight and discovery via accelerated computing

Outstanding Performance

3rd Generation Intel® Xeon® Scalable processors deliver a **60%** geomean improvement across top life and material sciences applications, compared to previous generations.[7] In addition, 3rd Generation Intel® Xeon® Scalable processors deliver **27%** better NAMD performance at fewer cores than AMD EPYC Milan processors.[1] Built-in Intel® Speed Select Technology supports three configurations in one CPU for granular control over performance.

Built-in Acceleration

Only Intel® Xeon® processors support Intel® AVX-512 instructions to handle the most demanding computational tasks. NAMD on 3rd Generations Intel® Xeon® Scalable processors optimized for Intel® AVX-512 runs **2.43x faster** than the non-optimized versions on the previous-generation processors.[2]

Unmatched Ecosystem

Intel has engaged for decades with software developers who contribute to open-source scientific applications like NAMD in order to optimize these applications for Intel® architecture. As a result, users can innovate faster on high-performing and scalable Intel® architecture.

Optimizing NAMD Performance with Intel

NAMD optimizations on Intel® Xeon® Scalable processors provide significant improvements that can help save millions of node hours for researchers.[3] These optimizations accelerate workload processing by using a "tile" algorithm that increases the computational efficiency of each node through Intel® AVX-512. These improvements are due to increased vector widths, improved masking support for complex nested loops, instructions that expand the functionality for vector computation, and an increase in vector registers.

NAMD software was optimized using Intel® software tools targeted explicitly for providing outstanding performance on Intel® architecture.

Intel® Math Kernel Library (Intel® MKL) simplifies development with highly optimized, extensively threaded routines.

Intel® MPI Library and high-performance fabrics also help improve scalability.

Intel® C++ Compiler targets CPUs and accelerators, and it aids with efficient tuning code for performance.

The University of Illinois at Urbana-Champaign and Intel developers are collaborating to support oneAPI in future NAMD releases. oneAPI support will allow heterogeneous development on a variety of platforms using accelerators in addition to CPUs. NAMD also benefits from the increased instructions per clock (IPC) and increased core counts of 3rd Generation Intel® Xeon® Scalable processors.

Figure 1. Generational Performance Gains[2]

Single-socket performance per core (STMV and Apoa1 geomean)

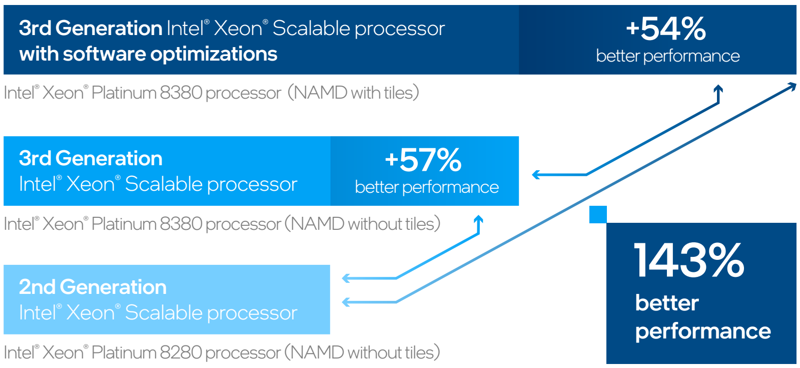
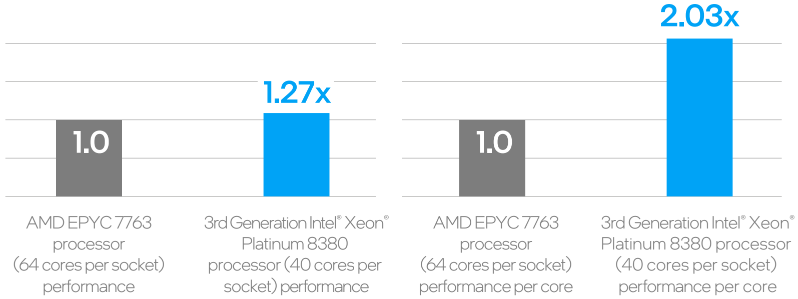


Figure 2. Competitive Performance Advantage[1]

Single-socket performance and performance per core (STMV and Apoa1 geomean)



Conclusion

Only Intel combines a comprehensive hardware and software portfolio with a mature global ecosystem to help the scientific community solve complex problems. The increased core counts and IPC of 3rd Generation Intel® Xeon® Scalable processors provide the performance needed for HPC applications like NAMD. In addition, collaborations between Intel and the University of Illinois at Urbana-Champaign have produced Intel® AVX-512 optimizations for NAMD that save data centers millions of CPU node hours.[3]

Learn more

For more information about 3rd Generation Intel® Xeon® Scalable processors for HPC, visit intel.com/hpc.

For details on Intel® Software tools and libraries, visit intel.com/content/www/us/en/software/software-overview.html.

For more information about NAMD, visit www.ks.uiuc.edu/research/namd.

Figure 1. NAMD normalized performance with and without tiles optimization, running benchmark tests on systems powered by Intel® Xeon® Scalable processors; perforance increases significantly with each successive generation[3]

Figure 2. NAMD performance on systems powered by AMD EPYC 7763 processors compared to systems powered by 3rd Generation Intel® Xeon® Scalable processors[2]

1 See [36] at intel.com/3gen-xeon-config. Results may vary.

2 See [107] at intel.com/3gen-xeon-config. Results may vary.

3 HPCwire. "Intel Speeds NAMD by 1.8x: Saves Xeon Processor Users Millions of Compute Hours." August 2020. hpcwire.com/2020/08/12/intel-speeds-namd-by-1-8x-saves-xeon-processor-users-millions-of-compute-hours/.

4 Intel® Advanced Vector Extensions 512 (Intel® AVX-512) has double the width of data registers, double the number of registers, and double the width of FMA units, compared to Intel® Advanced Vector Extensions 2 (Intel® AVX2). Source: Intel. "Accelerate Your Compute-Intensive Workloads." intel.com/content/www/us/en/architecture-and-technology/avx-512-overview.html.

5 This image was made with VMD and is owned by the Theoretical and Computational Biophysics Group, NIH Center for Macromolecular Modeling and Bioinformatics, at the Beckman Institute, University of Illinois at Urbana-Champaign. Source: John Stone. "VMD: Preparation and Analysis of Molecular and Cellular Simulations." NIH Center for Macromolecular Modeling and Bioinformatics, University of Illinois at Urbana-Champaign. 2017. www.ks.uiuc.edu/Research/vmd/publications/VMD-PRACE2017.pdf

6 20% IPC improvement: 3rd Gen Intel® Xeon® Scalable processor: 1-node, 2x 28-core 3rd Gen Intel® Xeon® Scalable processor, Wilson City platform, 512GB (16 slots / 32GB / 3200) total DDR4 memory, HT on, ucode=x270, RHEL 8.0, Kernel Version4.18.0-80.el8.x86_64, test by Intel on 3/30/2021. 2nd Gen Intel® Xeon® Scalable processor: 1-node, 2x 28-core 2nd Gen Intel® Xeon® Scalable processor, Neon City platform, 384GB (12 slots / 32GB / 2933) total DDR4 memory, HT on, ucode=x2f00, RHEL 8.0, Kernel Version4.18.0-80.el8.x86_64, test by Intel on 3/30/2021. SPECrate2017_int_base (est). Tests at equal frequency, equal uncore frequency, equal compiler.

7 See [108] at intel.com/3gen-xeon-config. Results may vary.