HIGH PERFORMANCE COMPUTING

AMD EPYC™ 7002 SERIES PROCESSORS AND NAMD MOLECULAR DYNAMICS SIMULATION

AMD EPYC

AUGUST 2019

AMD EPYC for HPC

Utilizing the x86-architecture, and built on 7nm technology, the AMD EPYC™ 7002 Series processors bring together high core counts, large memory capacity, extreme memory bandwidth and massive I/O with the right ratios to enable exceptional HPC workload performance.

Standards Based Architecture

Continuing the AMD commitment to industry standards, AMD EPYC™ 7002 generation processors offer you a choice in x86 architecture. x86 compatibility means you can run your x86 based applications on AMD EPYC processors.

Exceptional Scalability

Scaling is critical to HPC applications. AMD EPYC 7002 Series processors provide high bandwidth between nodes with support for PCIe Gen 4 enabled network devices. Within node, take advantage of up to 64 cores per socket, including 8 memory channels utilizing speeds up to DDR4-3200[2]. Add incredible floating point and integer compute within each core and the AMD EPYC 7002 generation delivers exceptional performance and scalability for HPC.

Fully Tested and Validated

AMD's broad partner ecosystem and collaborative engineering provide tested and validated solutions that help lower your risk and total cost of ownership.

NAMD

NAMD, recipient of a 2002 Gordon Bell Award and a 2012 Sidney Fernbach Award, is a parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems.

AMD EPYC™ 7002 Processors: Architectural Innovations Deliver Exceptional Performance and Scalability

The high-performance computing (HPC) market has grown to a point where it is a critical component of new technology advancements in academia and a wide array of industries in both the public and private sectors. Scientific research, public health, climate modeling, as well as oil and gas exploration are just a few examples where HPC is the driving force behind new innovations and knowledge discovery.

7 nm	PCIe® Gen 4	DDR4 3200
64 Cores per socket	**128** PCIe® Gen 4 lanes per socket	**8** Memory channels per socket
World's first 7 nm x86 server CPU Highest available core count[1] to maximize parallelism	World's first PCIe® Gen 4 ready x86 server CPU[2] Doubles the bandwidth of the previous generation	World's first x86 architecture with DRR4 3200[2] Up to 4 TB of memory capacity per socket

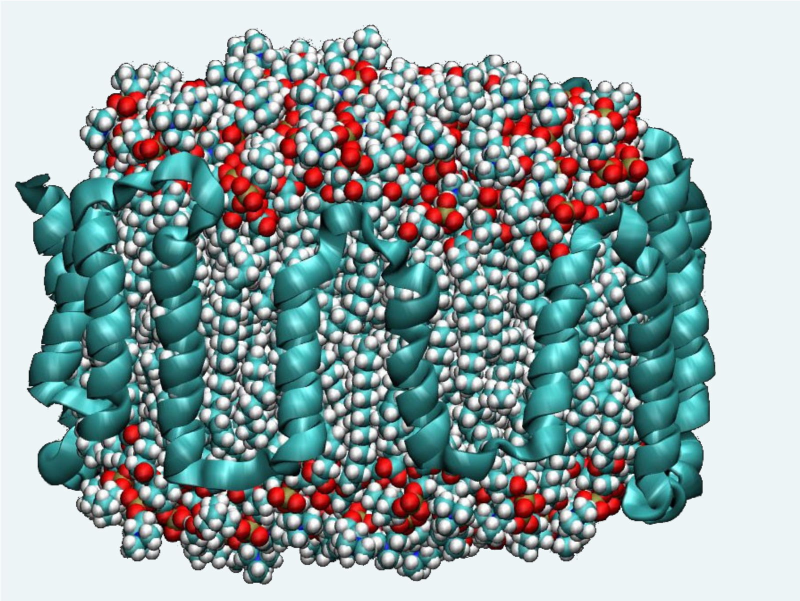
The second generation of the AMD EPYC™ processor extends AMD innovation leadership for HPC. Built with leading-edge 7nm technology, the AMD EPYC™ SoC offers a consistent set of features across a range of choices from 8 to 64 cores, including 128 lanes of PCIe® Gen 4[2] and 8 memory channels with access to up to 4 TB of high-speed memory.

The AMD EPYC™ 7002 Series processor's innovative architecture translates to tremendous performance and scalability for HPC applications, offering you a choice in x86 architecture while optimizing total cost of ownership.

NAMD and AMD EPYC: Power Without Compromise

Core IPC is a critical factor in optimizing performance of NAMD. AMD EPYC server processors employing the "Zen2" microarchitecture help ensure that you get the most out of your system, optimizing execution time and overall utilization of your deployment.

Based on Charm++ parallel objects, NAMD scales to hundreds of cores for typical simulations and beyond 500,000 cores for the largest simulations. NAMD uses the popular molecular graphics program VMD for simulation setup and trajectory analysis, but is also file-compatible with AMBER, CHARMM, and X-PLOR. NAMD is distributed free of charge with source code. You can build NAMD yourself or download binaries for a wide variety of platforms.



Many High-Performance Compute (HPC) workloads require you to balance performance vs per-core license costs to manage your overall cost. AMD EPYC processors offer a consistent set of features across the product line, allowing users to optimize the number of cores required for their workloads without sacrificing features, memory channels, memory capacity, or I/O lanes. Whether you need 8 or 64 physical cores per socket, you will have access to 8 channels of memory per processor across all EPYC server processors

As workloads demand more processor cores, the communications between processor cores becomes critical to efficiently solving the complex problems faced by customers. As cluster sizes increase, the communication requirements between nodes rises quickly and can limit scaling at large node counts.
AMD addresses this scaling limitation by partnering with leading network providers, such as Mellanox®, to offer high performance solutions based on PCIe Gen 4. PCIe Gen 4 allows incredible performance on Infiniband HDR 200Gb/s fabric when run on 2nd Generation EPYC processor-based clusters.

Performance Testing

This document focuses on performance and scaling of the EPYC 7002 Series Processors. Testing was performed on a cluster of dual-socket EPYC 7742-based systems and dual-socket EPYC 7542-based systems.

Each EPYC™ 7742 processor has 64 cores with a base frequency of 2.25 GHz and a boost frequency of 3.4 GHz. Each EPYC™ 7542 processor has 32 cores with a base frequency of 2.9 GHz and boost of 3.4 GHz.

The compute nodes in the cluster are each populated with 1 DIMM per channel of 64-GB, dual-rank, DDR4-3200 DIMMs from Micron®, for a total of 1TB of memory per node.

A Mellanox® ConnectX-6 200 Gb/s HDR InfiniBand adapter, utilizing EPYC processors' support for PCIe Gen 4, is also populated on each EPYC processor-based system.

Single-node testing was performed across all platform configurations and multi-node scaling was tested on the EPYC 7742 processor.

Single-node testing was also performed on 2-socket platform using 1st Gen EPYC 7601 processors to show generational comparisons.

Results from each run were calculated using a script from the benchmarking page of the NAMD website, located here:

https://www.ks.uiuc.edu/Research/namd/2.13/benchmarks/ns_per_day.py

This script finds the nanoseconds per day simulation rate from the log file by averaging time per step using "TIMING:" lines.

The EPYC Advantage: AMD EPYC server processors offer 8 memory channels of DDR4-3200[2] and support for up to 4 TB of memory per processor, yielding exceptional memory bandwidth and capacity.

Tested Hardware and Software Configuration

AMD 2nd Generation EPYC Compute Nodes		
CPUs	2 x EPYC 7742	2 x EPYC 7542
Cores	64 cores per socket (128 per node)	32 cores per socket (64 per node)
Memory	1TB (16x) Dual-Rank DDR4-3200, 1DPC	
Network Adapter	Mellanox® ConnectX-6 HDR 200Gb HDR InfiniBand x16 PCIe® Gen 4	
Storage: OS | Data	1 x Micron 1100 256 GB SATA | 1 x 1 TB NVMe	
Software		
OS	RHEL 7.6 (3.10.0-862.el7.x86_64)	
Mellanox OFED Driver	MLNX_OFED_LINUX-4.5-1.0.1.0 (OFED-4.5-1.0.1)	
Network		
Switch	Mellanox 200Gb/s HDR InfiniBand Switch (MQM8790)	
Configuration Options		
BIOS Setting	NPS = NPS4, SMT = Off, Boost = On, X2APIC = On, Determinism Slider = Performance, Preferred IO=Enabled	
OS Settings	Governor=Performance, CC6 = Disabled	

AMD 1st Generation EPYC Compute Nodes	
CPUs	2 x EPYC 7601
Cores	32 cores per socket (64 per node)
Memory	256GB (16x 16GB Dual-Rank) DDR4-2666
NIC	Mellanox ConnectX-5 EDR 100Gb InfiniBand x16 PCIe
Storage: OS | Data	1 x 256 GB NVMe | 1 x 1 TB NVMe
Software	
OS	RHEL 7.6 (3.10.0-862.el7.x86_64)
Mellanox OFED Driver	MLNX_OFED_LINUX-4.5-1.0.1.0 (OFED-4.5-1.0.1)
Network	
Switch	Mellanox HDR 200Gb/s Unmanaged Switch (MQM8790)
Configuration Options	
BIOS Setting	SMT = Off, Boost = On, Determinism Slider = Performance, Global C-State Control = Enabled
OS Settings	Governor=Performance, CC6 = Disabled

NAMD Compilation

NAMD version 2.12 was compiled from source on RHEL 7.6 using the AOCC 2.0 compiler and OpenMPI 4.0.0. The default optimization flags were used. No further compile time optimizations were done. The FFTW and TCL libraries used are the precompiled versions from the NAMD website. The same binary was used for all benchmarks across all configurations.

NAMD Benchmarks

NAMD benchmarks provide a basis for evaluating hardware performance. The industry standard benchmarks for NAMD include STMV, ApoA1, and f1atpase. These benchmarks are well established NAMD workloads that allow users to compare performance of different hardware solutions to determine which solutions are best for their needs.

A larger public model was used from PRACE to show scalability, since the standard benchmarks are relatively small. The STMV.28M model from PRACE can be found here:

https://repository.prace-ri.eu/git/UEABS/ueabs/#namd

NAMD: Single-node Performance

Single node performance was compared between the 1st Generation EPYC 7601 processor (32 cores) and the 2nd Generation EPYC 7542 (32 cores) and EPYC 7742 (64 cores) processors.

Figure 1 details the performance of all 4 benchmarks on single-node, two-socket systems across each of the AMD EPYC processors. The 1st Gen EPYC 7601 and the 2nd Gen EPYC 7542 both have 32 cores per socket for a total of 64 cores per node. The 2nd Gen EPYC 7742 has 64 cores per socket for a total of 128 cores per node.

The performance shows a strong generational average improvement of ~29% between the EPYC 7601 and the EPYC 7542. However, you can see that NAMD can take advantage of the higher core count of the 2nd Gen EPYC 7742, with an impressive ~99% average performance boost over the 1st generation EPYC 7601.

Multi-threading was disabled in the cluster during these tests. Planned follow-up testing will include Simultaneous Multi-Threading (SMT) enabled, via BIOS.

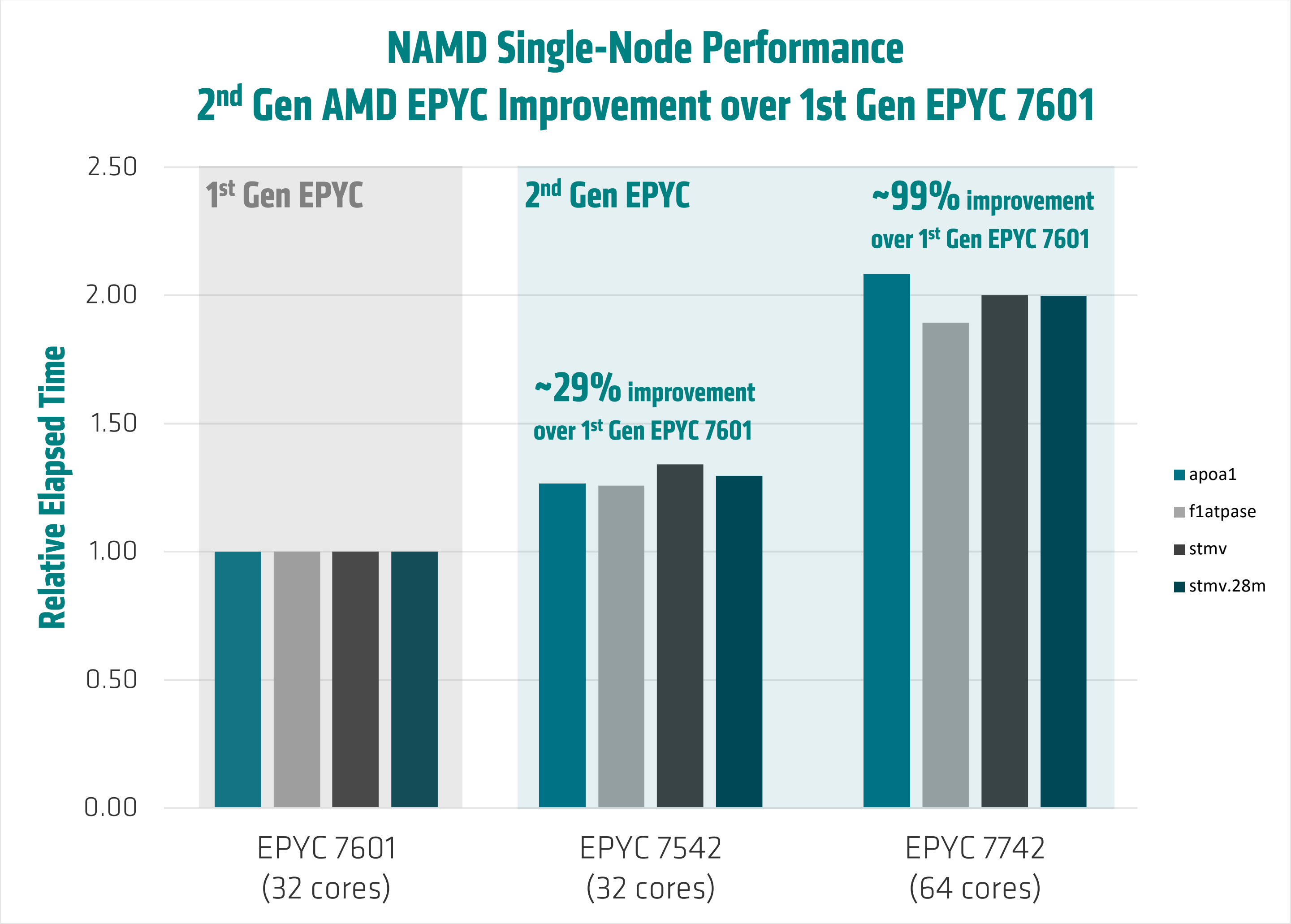


Figure 1

NAMD: Multi-node Scaling

The STMV.28M NAMD model from PRACE is a large model and was used to show how NAMD scales on the 64-core EPYC 7742. Figure 2 shows very clean scaling through 16 nodes (2048 cores).

These results demonstrate the benefits of the balanced architecture of 2nd Generation EPYC processors. Fitting 128 cores into a single node without losing scalability is accomplished by having very high memory bandwidth, bringing PCIe Gen 4 capabilities to the x86 market, and partnering with leading networking partners, such as Mellanox, to utilize the higher speed of PCIe Gen 4 with their InfiniBand HDR 200Gb/s fabric.

The density offered by having the incredible single-node performance of 128 cores per node, combined with the scalability shown in Figure 2, and low power/performance enabled by 7nm technology, makes it easy to see why 2nd Generation EPYC processors are a great solution.

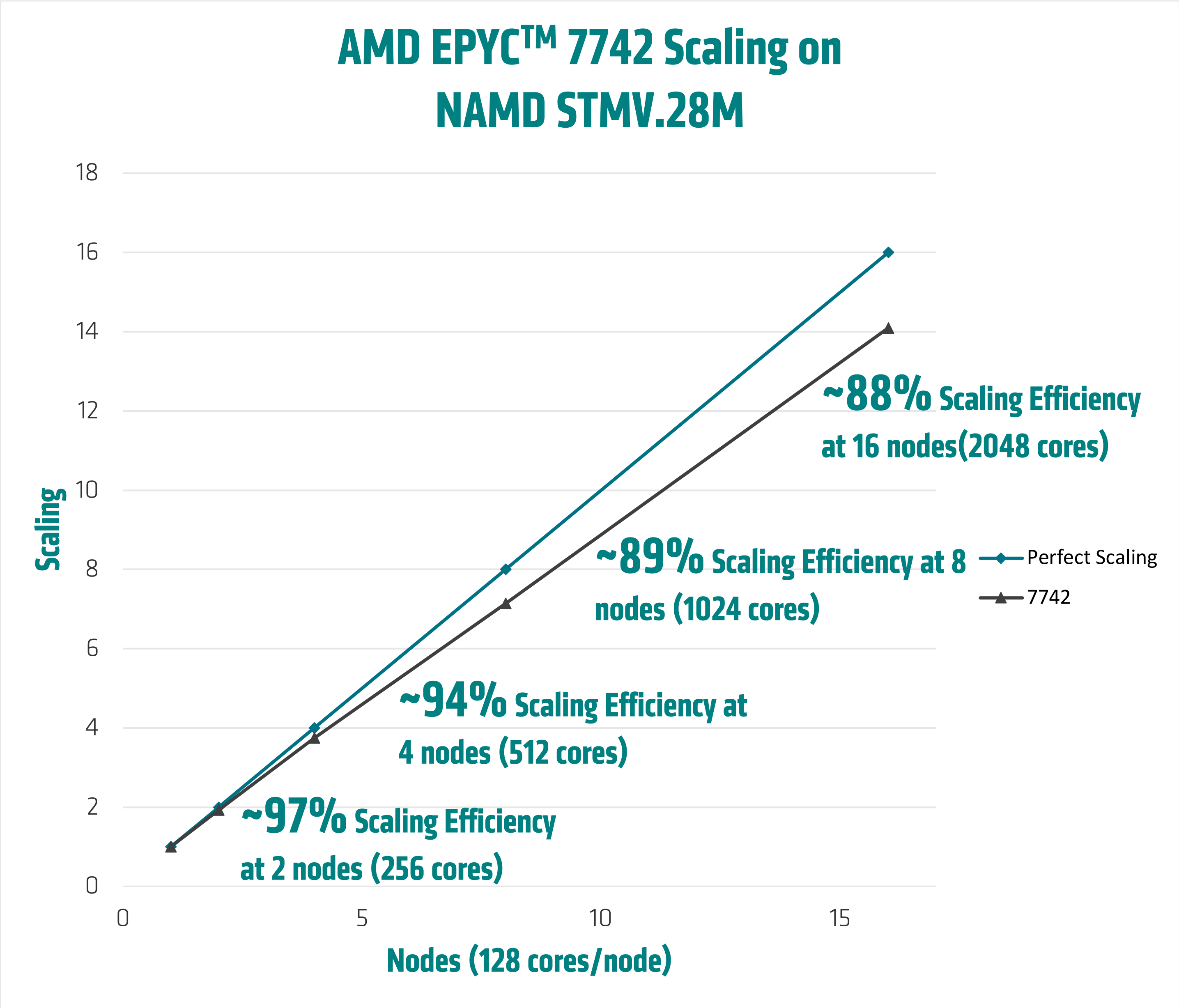


Figure 2

Summary

AMD engineers performed NAMD benchmark testing on single nodes of two-socket systems, running 32-core and 64-core AMD 2nd Gen EPYC processors and showed incredible generational performance gains over the AMD 1st Gen EPYC 7601. Specifically, the 64-core EPYC 7742 showed a ~99% average performance increase over the prior generation.

Scaling tests were then run on the STMV.28M model from PRACE to show scaling of a much larger model running on NAMD. Results demonstrated exceptional scaling of ~88% efficiency through 16 nodes (2048 cores).

Conclusion

Scale-out testing on the EPYC cluster shows impressive results on these benchmarks. Pure performance was highest with the 64-core EPYC 7742. Per-core performance was highest with the 32-core EPYC 7542. Whether you need the dominating system level performance and density of the EPYC 7742 or the equally dominating per-core performance of the EPYC 7542, all products offer exceptional core IPC, and provide your organization a significant advantage. Customers can pick the optimal part based on their unique requirements.

AMD empowers the development of fast, accurate molecular dynamics simulations running on cost-effective clustered systems.

For more information about AMD's EPYC line of processors visit: http://www.amd.com/epyc

For more information about NAMD visit: http://www.ks.uiuc.edu/Research/namd/

FOOTNOTES

1. Best-in-class based on industry-standard pin-based (LGA) X86 processors. NAP-166.
2. Some supported features and functionality of second-generation AMD EPYC™ processors (codenamed "Rome") require a BIOS update from your server manufacturer when used with a motherboard designed for the first-generation AMD EPYC 7000 series processor. A motherboard designed for "Rome" processors is required to enable all available functionality. ROM-06.

NOTE: Links to third party sites are provided for convenience and unless explicitly stated, AMD is not responsible for the contents of such linked sites and no endorsement is implied. GD-5