

MOLECULAR DYNAMICS ON AMD EPYC™ 9754 PROCESSORS

MOLECULAR DYNAMICS

Powered by 4th Gen AMD EPYC™ 9754 Processors

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AT A GLANCE

A 2P system powered by 128-core 4th Gen AMD EPYC™ 9754 CPUs show strong high core count competitive performance uplifts on several molecular dynamics workloads vs. a 2P system powered by comparable² Intel® Xeon® Platinum 8480+ CPUs.

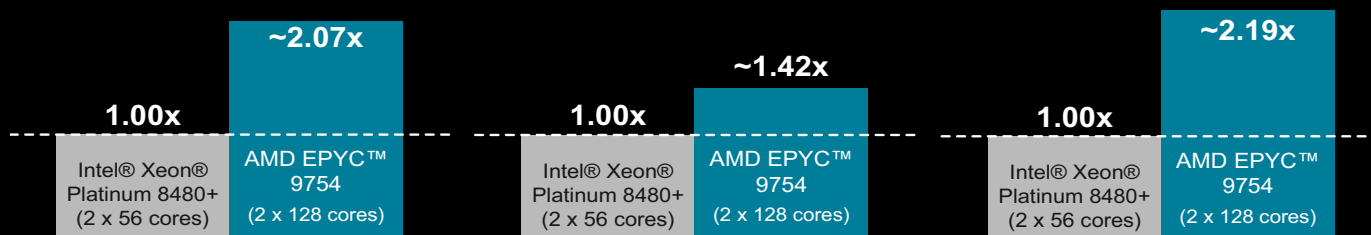
PERFORMANCE HIGHLIGHTS

A single 2P 128-core 4th Gen AMD EPYC 9754 system demonstrates the following uplifts vs. a comparable² single 2P Intel® Xeon® 8480+ system on the following molecular dynamics workloads: ~2.07x (NAMD), ~1.42x (Quantum ESPRESSO), and ~2.19x (GROMACS).

AMD EPYC™ 9754 VS. INTEL XEON PLATINUM 8480+ (NAMD)

AMD EPYC™ 9754 VS. INTEL XEON PLATINUM 8480+ (QUANTUM ESPRESSO)

AMD EPYC™ 9754 VS. INTEL XEON PLATINUM 8480+ (GROMACS)



KEY TAKEAWAYS

A 2P server powered by 4th Gen AMD EPYC 9754 (128-core) processors delivered competitive molecular dynamics performance uplifts compared to a 2P server powered by a Intel Xeon Platinum 8480+ (56-core) processors of ~2.07x on NAMD, ~1.42x on Quantum ESPRESSO, and ~2.19x on GROMACS.

4th Gen AMD EPYC 97x4 processors are available in 1P and 2P configurations and feature:

- Up to 128 cores (256 threads) per processor.
- Up to 256MB L3 cache.
- Up to 4 links of Gen 3 Infinity Fabric™ at up to 32 Gbps.
- 12 memory channels that support up to 6TB of DDR5-4800 memory.
- Support for PCIe® Gen 5 at up to 32 Gbps.
- AVX-512 instruction support for enhanced HPC and ML performance.
- AMD Infinity Guard technology to defend your data.³

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SYSTEM CONFIGURATION

AMD SYSTEM CONFIGURATION	
CPUs	2 x AMD EPYC 9754
Frequency: Base Boost ⁴	2.25 GHz 3.10 GHz (up to)
Cores	128 cores/socket (256 threads)
L3 Cache	256 MB per CPU
Memory	1.5 TB (24x) Dual-Rank DDR5 4800 64 GB DIMMs 1 DPC
NIC	25 Gb Ethernet CCX512-A ConnectX-5 (fw 16.35.2000)
InfiniBand	200 Gb HDR ConnectX-6 VPI (fw 20.35.2000)
Storage: OS Data	Samsung MZQL21T9HCJR-00A07 1.92 TB
BIOS Version	1007D
BIOS Settings	SMT=OFF; NPS=4; Determinism=Power
OS	RHEL 8.7 (kernel 4.18.0-425.3.1.el8.x86_64)
OS Settings	amd_iommu=ON; iommu=pt; mitigations=off; clear caches; NUMA balancing=0; THP=on; CPU governor=Performance; C2 states=disabled

Table 1: AMD system configurations

INTEL SYSTEM CONFIGURATION	
CPUs	2x Intel Xeon Platinum 8480+
Frequency: Base Boost	2.00 GHz 3.80 GHz (up to)
Cores	56 cores per socket (112 threads)
L3 Cache	105 MB per CPU
Memory	1.0 TB (16x) Dual-Rank DDR5 4800 64 GB DIMMs 2 DPC
NIC	25 Gb Ethernet CCX512-A ConnectX-5 (fw 16.35.2000)
InfiniBand	200 Gb HDR ConnectX-6 VPI (fw 20.35.2000)
Storage: OS Data	Samsung MZQL21T9HCJR-00A07 1.92 TB
BIOS Version	ESE110Q-1.10
BIOS Settings	Hyperthreading=Off, Profile = Maximum Performance
OS	RHEL 8.7 (kernel 4.18.0-425.3.1.el8.x86_64)
OS Settings	processor.max_cstate=1; intel_idle.max_cstate=0; iommu=pt mitigations=off; clear caches; NUMA Balancing=0; randomize_va_space 0; THP=ON; CPU Governor=Performance

Table 2: Intel system configurations

TEST METHODOLOGY

All three molecular dynamics codes tested in this paper provided their own standard sets of benchmarks to evaluate performance on different platforms. These benchmark cases represent typical usage and cover a range of sizes. The uplift is calculated as the ratio of the systems under test (*sut*) to the reference systems (*ref*). In this Performance Brief, the Intel Xeon Platinum 8480+ is the *ref* system, and the 4th Gen AMD EPYC 9754 is the *sut*. With an industry-leading 128 cores per x86 socket, this processor is able to exhibit compelling performance uplifts across all these different molecular dynamics applications. The total amount of variability between individual runs was <1%.

The results presented in this Performance Brief are:

- **NAMD:** apoa1, flotpase, stmv, stmv20m
- **Quantum ESPRESSO:** ausurf, ta205
- **GROMACS:** benchpep, water1536k_pme

The systems tested were configured as shown in Tables 1 and 2, above.

FOR ADDITIONAL INFORMATION

Please see the following additional resources for more information about 4th Gen AMD EPYC features, architecture, and available models:

- [AMD EPYC™ 9004 Series Processors](#)
- [AMD EPYC™ Products](#)
- [AMD EPYC™ Tuning Guides](#)

REFERENCES

1. "Technical Computing" or "Technical Computing Workloads" as defined by AMD can include: electronic design automation, computational fluid dynamics, finite element analysis, seismic tomography, weather forecasting, quantum mechanics, climate research, molecular modeling, or similar workloads. GD-204
2. The Intel Xeon Platinum 8480+ is the highest-performing processor listed in the Performance General-Purpose category for 4th Gen Intel Xeon CPU models at https://download.intel.com/newsroom/2023/data-center-hpc/Intel-4th-Gen-Xeon_product_SKUs.jpg.
3. AMD Infinity Guard features vary by EPYC™ Processor generations. Infinity Guard security features must be enabled by server OEMs and/or Cloud Service Providers to operate. Check with your OEM or provider to confirm support of these features. Learn more about Infinity Guard at <https://www.amd.com/en/technologies/infinity-guard>. GD-183
4. Maximum boost for AMD EPYC processors is the maximum frequency achievable by any single core on the processor under normal operating conditions for server systems. EPYC-18

AUTHORS

Alvaro Fernandez and Ashok Manikonda contributed to this Performance Brief.

RELATED LINKS

- [NAMD*](#)
- [Quantum ESPRESSO*](#)
- [GROMACS*](#)
- [AMD EPYC Processors](#)
- [AMD EPYC Technical Briefs](#)

**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.*

AMD EPYC 9004 FOR CFD

4th Gen AMD EPYC CPUs deliver excellent per-core performance by taking advantage of fast CPU frequencies, low latency memory, and a unified cache structure. Design engineers can use AMD EPYC processors to perform complex finite element analysis tasks with ground-breaking high-performance computing and robust security features to deliver excellent results.

“ZEN 4” CORE & SECURITY FEATURES

Support for up to:

- 128 physical cores, 256 threads
- 256 MB of L3 cache per CPU
- 96 MB of L3 cache per CCD
- 6 TB of DDR5-4800 memory
- Up to 128 1P, up to 160 2P PCIe® Gen 5 lanes

Infinity Guard security features³

- Secure Boot
- Encrypted memory with SME

MOLECULAR DYNAMICS

NAMD is a free parallel molecular dynamics application for large biomolecular systems. Quantum ESPRESSO is an integrated open-source suite calculating electronic structures and nanoscale materials modeling. GROMACS is a free, open-source software suite for high-performance molecular dynamics and output analysis.

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