

GROMACS ON 5TH GEN AMD EPYC™ PROCESSORS

MOLECULAR DYNAMICS SIMULATOR

Powered by 5th Gen AMD EPYC™ Processors

October 2024

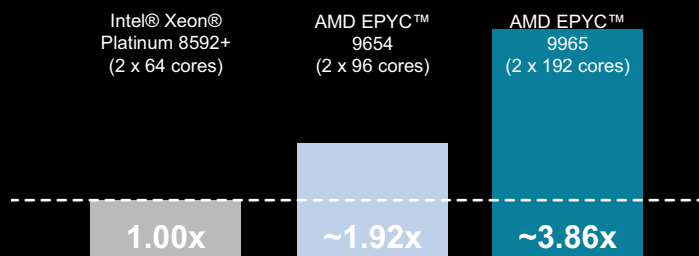
AT A GLANCE

A 2P system powered by 192-core 5th Gen AMD EPYC™ processors demonstrate outstanding performance uplifts versus a 2P system powered by 5th Gen Intel® Xeon® Platinum 8592+ processors running selected GROMACS benchmarks.

PERFORMANCE HIGHLIGHTS

A 2P 192-core 5th Gen AMD EPYC 9965 system (384 total cores) demonstrates a composite average ~3.86x uplift on GROMACS workloads vs. a 2P 64-core Intel® Xeon® Platinum 8592+ system (128 total cores). A 2P 96-core AMD EPYC 9654 system (192 total cores) outperforms the same Intel system by a composite average of ~1.92x. Please see Page 2 for detailed per-benchmark results.

2P 4TH AND 5TH GEN AMD EPYC™ VS.
2P 5TH INTEL XEON PLATINUM 8592+



KEY TAKEAWAYS

A 2P system powered by 192-core 5th Gen AMD EPYC 9965 processors (384 total cores) demonstrates a maximum uplift of ~4.05x versus a 2P system powered by a 64-core 5th Gen Intel Xeon 8592+ processors (128 total cores) running the GROMACS benchPEP workload. A 2P system powered by 96-core 4th Gen AMD EPYC 9654 processors (192 total cores) demonstrates a maximum uplift of ~1.94x running the GROMACS gmx_water1536K_PME workload versus the same Intel system. Detailed per-benchmark results appear on Page 2.

5th Gen AMD EPYC processors are available in 1P and 2P configurations and feature:

- Up to 128 “Zen 5” or 192 “Zen5c” cores.
- Up to 512 MB L3 cache in “Zen 5” AMD EPYC processors.
- Up to 4 links of Gen 3 Infinity Fabric™ at up to 32 Gbps.
- 12 memory channels that support up to 9 TB of DDR5-6000 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.¹

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DETAILED RESULTS

This section presents the detailed per-benchmark results for the systems described in Tables 1 and 2, below. Please see the chart at the top of Page 1 for the composite average performance results for both AMD EPYC processors.

Figure 1: Relative 2P 4th Gen AMD EPYC 9654 per-benchmark GROMACS results vs. 2P 5th Gen Intel Xeon 8592+

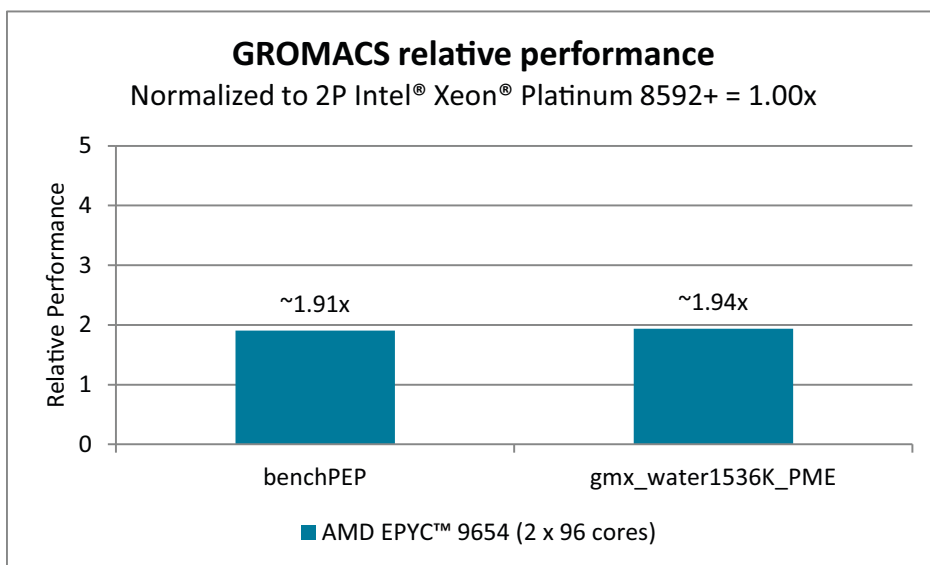
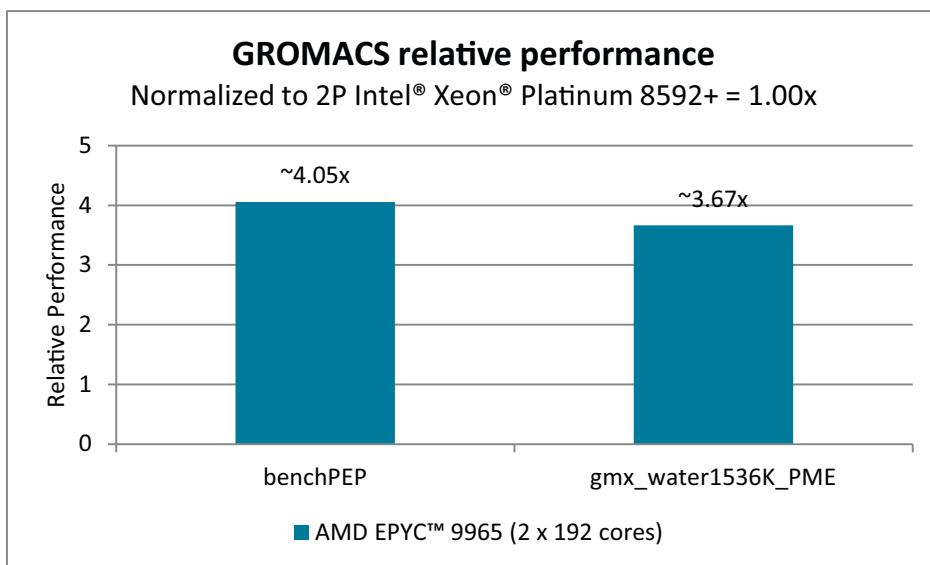


Figure 2: Relative 2P 5th Gen AMD EPYC 9965 per-benchmark GROMACS results vs. 2P 5th Gen Intel Xeon 8592+



AMD EPYC 9005 PROCESSORS

5th Gen AMD EPYC processors are the newest generation of the powerful and efficient AMD EPYC processor family for servers that have set hundreds of [world records](#) for performance and efficiency. The AMD EPYC 9005 processor family is built on the breakthrough high performance, highly efficient “Zen 5” processor core architecture and advanced microprocessor process technologies to better meet the needs of the modern AI-enabled data center. The complete line of 5th Gen AMD EPYC processor offerings include a wide range of core counts (up to 192 cores and 384 threads per processor), max boost frequencies up to 5 GHz², generous L3 cache capacities, high energy efficiency, and competitive cost points. These cutting-edge technologies and features are all backed by the familiar x86 software compatibility that allows servers powered by AMD EPYC 9005 processors to readily support almost any business need.

SYSTEM CONFIGURATION

AMD SYSTEM CONFIGURATION		
CPUs	2 x AMD EPYC™ 9654	2 x AMD EPYC™ 9965
Frequency: Base Boost ²	2.4 GHz 3.7 GHz	2.25 GHz 3.7 GHz
Cores	96 cores/socket (192 threads)	192 cores/socket (256 threads)
L3 Cache	256 MB per CPU	384 MB per CPU
Memory	1.5 TB (24 x 64 GB DDR5-4800)	1.5 TB (24 x 64 GB DDR5-6000)
Storage	SAMSUNG MZQL21T9HCJR-00A07	SAMSUNG MZWLO3T8HCLS-00A07
BIOS Version	RTI1009C	RVOT1000C
BIOS Settings	SMT=Off, NPS=4, Determinism=Power	
OS	RHEL 9.4 (kernel 5.14.0- 427.16.1.el9_4.x86_64)	
OS Settings	amd_iommu=on, iommu=pt, mitigations=off	

Table 1: AMD system configurations

INTEL SYSTEM CONFIGURATION	
CPUs	2 x Intel® Xeon® PLATINUM 8592+
Frequency: Base Boost	1.9 GHz 3.9 GHz
Cores	64 cores/socket (128 threads)
L3 Cache	320 MB per CPU
Memory	1.0 TB (16 x 64 GB DDR5-5600)
Storage	KIOXIA KCMYXRUG3T84
BIOS Version	ESE122V-3.10
BIOS Settings	Hyperthreading=Off, High Performance Mode
OS	RHEL 9.4 (kernel 5.14.0-427.16.1.el9_4.x86_64)
OS Settings	processor.max_cstate=1, intel_idle.max_cstate=0, iommu=pt, mitigations=off

Table 2: Intel system configurations

TEST METHODOLOGY

GROMACS provides a standard set of benchmarks that evaluate the performance of different platforms running GROMACS applications. 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*) based on an average of three test runs per benchmark. In this Performance Brief, the Intel Xeon Platinum 8592+ processor is the *ref* system, and 4th and 5th Gen AMD EPYC processors are the *sut*. The total amount of variability between individual runs was <1%. The results presented in this Performance Brief are the GROMACS benchmarks shown in Figures 1 and 2, above. 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 5th Gen AMD EPYC features, architecture, and available models:

- [AMD EPYC™ Processors](#)
- [AMD Documentation Hub](#)

REFERENCES

1. AMD Infinity Guard features vary by EPYC™ Processor generations and/or series. 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 <http://www.amd.com/en/products/processors/server/epyc/infinity-guard.html>. GD-183A
2. 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

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RELATED LINKS

- [GROMACS*](#)
- [AMD EPYC™ Processors](#)
- [AMD Documentation Hub](#)

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AMD EPYC 9005 FOR MOLECULAR DYNAMICS

5th Gen AMD EPYC CPUs deliver excellent performance by taking advantage of fast CPU frequencies, low latency memory, and a unified cache structure. Biologists and geneticists can use AMD EPYC processors to perform complex DNA sequencing and other molecular dynamics simulations with ground-breaking high-performance computing and robust security features to deliver excellent results.

“ZEN 5” CORE & SECURITY FEATURES

AMD EPYC 9005 Series Processors support up to:

- 192 physical cores, 384 threads
- Up to 512 MB of L3 cache per CPU
- 32 MB of L3 cache per CCD
- 9 TB of DDR5-6000 memory
- Up to 128 (1P) or 160 (2P) PCIe® Gen 5 lanes

Infinity Guard security features¹

- Secure Boot
- Encrypted memory with SME

GROMACS

GROMACS simulates the Newtonian equations of motion for systems with hundreds to millions of particles. It is primarily designed for biochemical molecules like proteins, lipids and nucleic acids that have a lot of complicated bonded interactions. GROMACS is also fast at calculating the nonbonded interactions (that usually dominate simulations), and many groups are thus using it for research on non-biological systems, e.g. polymers and fluid dynamics.

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