Hewlett Packard Enterprise

Technical brief

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HPE APOLLO 2000 GEN10 PLUS SYSTEM AND GROMACS

Key takeaways

- High-density, flexible infrastructure for high-performance computing (HPC)
- Up to 1.2x (see Figure 1) speed up from one generation of CPUs to the next for GROMACS

HPE Apollo systems with rack-scale efficiency deliver just the right amount of performance and adaptability with flexible systems that are optimized for HPC and AI workloads. The CPU tests for GROMACS were run on an HPE Apollo 2000 Gen10 Plus system.

Configurations

The HPE Apollo 2000 Gen10 Plus system consisted of an HPE ProLiant XL225 node with either AMD EPYC 7002 or 7003 Series processors (two sockets per node). The first configuration below is AMD EPYC 7002 series based while the remainder is AMD EPYC 7003 series based.

- AMD EPYC 7702 CPU (64 cores, 2.0 GHz), with 512 GB of 3200 MT/s memory
- AMD EPYC 7713 CPU (64 cores, 2.0 GHz), with 256 GB of 3200 MT/s memory
- AMD EPYC 7742 CPU (64 cores, 2.5 GHz), with 256 GB of 3200 MT/s memory
- AMD EPYC 7642 CPU (48 cores, 2.3 GHz), with 256 GB of 3200 MT/s memory

All tests used GROMACS 2021.3 with the HECBioSim Benchmark Suite available at hecbiosim.ac.uk/access-hpc/benchmarks.

EXECUTIVE SUMMARY

GROMACS is a molecular dynamics program designed primarily for the modeling and simulation of proteins, lipids, and nucleic acids. It is typically used for biochemistry research and can be used for development of medical drugs and vaccines. The HPE Apollo 2000 Gen10 platform is a high-density, price-performant solution for running HPC workloads such as GROMACS. The HPE Apollo 2000 Gen10 Plus system with AMD EPYC™ 7003 Series CPUs can accelerate GROMACS molecular dynamic simulations by over 1.2x compared to using prior generation CPUs.

CUSTOMER VALUE WITH HPE

HPE Apollo 2000 Gen10 Plus system offers a high-density, shared infrastructure with a flexible scale-out architecture to support a variety of workloads, from remote site systems to large high-performance computing (HPC) clusters and everything in between.

HPE Apollo 2000 Gen10 Plus system supports up to four individually serviceable 1U, half-width servers per 2U chassis for increased density and system uptime. Flexible infrastructure offers multiple storage options, eight memory channels with 3200 MT/s, PCIe Gen4, and support for over 240W processors for enhanced application performance. In addition, there is a choice of three power supply capacities to best match unique data center power strategies.

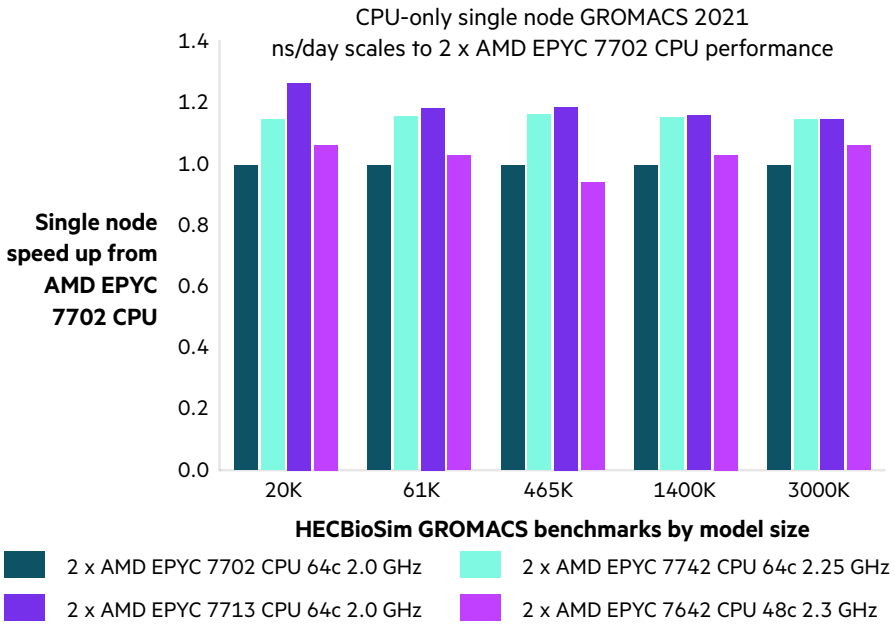

FIGURE 1. Absolute performance of single node GROMACS 2021.3 scaled to 2 x AMD EPYC 7702 CPU performance using HECBioSim data sets

From this data, we can see that in all five cases, GROMACS performance increases from one generation of the processor to the next and benefits from more cores and higher frequency depending on the systems.

GROMACS SOFTWARE

GROMACS is a molecular dynamics program designed primarily for the modeling and simulation of proteins, lipids, and nucleic acids. Originally developed at the University of Groningen in the Netherlands, GROMACS is a free, open-source solution and is available at gitlab.com/gromacs/gromacs.

THE HECBIOSIM DATA SET

HECBioSim Benchmark Suite available at hecbiosim.ac.uk/access-hpc/benchmarks has been set up for a number of different molecular dynamics packages, which represent examples of the types and sizes of simulations that scientists would typically run in production. It includes a 20K atom system, a 61K atom system, a 465K atom system, a 1.4M atom system, and a 3M atom system. These packages can be run on several molecular dynamic codes including GROMACS. The details for the various models are in Figure 2.

MODEL DETAILS

20K atom system—3NIR Crambin
Total number of atoms = 19,605
Protein atoms = 642
Water atoms = 18,963
rcsb.org/structure/3NIR

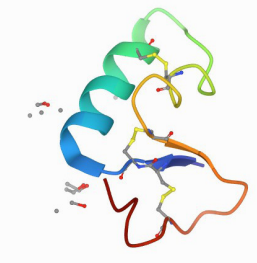

FIGURE 2. 3NIR Crambin

1.4M atom system—A pair of hEGFR Dimers of 1IVO and 1NQL
Total number of atoms = 1,403,182
Protein atoms = 43,498
Lipid atoms = 235,304
Water atoms = 1,123,392
Ions = 986
rcsb.org/structure/1IVO
rcsb.org/structure/1NQL

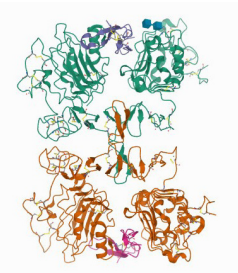

FIGURE 4. 1IVO

61K atom system—1WDN Glutamine-Binding Protein
Total number of atoms = 61,153
Protein atoms = 21,749
Lipid atoms = 134,268
Water atoms = 309,087
Ions = 295
rcsb.org/structure/1WDN

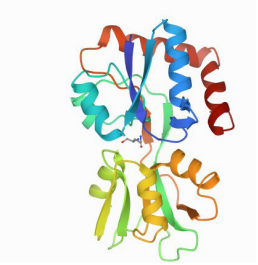

FIGURE 3. 1WDN Glutamine-Binding Protein

3M atom system—A pair of hEGFR tetramers of 1IVO and 1NQL
Total number of atoms = 2,997,924
Protein atoms = 86,996
Lipid atoms = 867,784
Water atoms = 2,041,230
Ions = 1,914
rcsb.org/structure/1IVO
rcsb.org/structure/1NQL

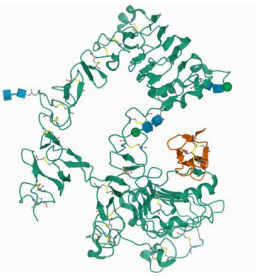

FIGURE 5. 1NQL

SUMMARY

Performance benchmarks such as these highlighted in this brief show the power of HPE servers and provide insight into how to configure HPE Apollo 2000 Gen10 Plus platforms that include GROMACS molecular dynamic simulations as part of their workloads.

LEARN MORE AT

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