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2022-07-15-0850

KVM testing on AlmaLinux 8.6 via the Phoronix Test Suite.

Test Systems:

16 x AMD EPYC

Processor: 16 x AMD EPYC (with IBPB) (16 Cores), Motherboard: RDO OpenStack Compute (1.11.0-2.el7 BIOS), Chipset: Intel 440FX 82441FX PMC, Memory: 2 x 16 GB RAM, Disk: 100GB, Graphics: Cirrus Logic GD 5446, Network: Red Hat Virtio device

OS: AlmaLinux 8.6, Kernel: 4.18.0-305.3.1.el8_4.x86_64 (x86_64), Compiler: GCC 8.5.0 20210514, File-System: xfs, Screen Resolution: 1024x768, System Layer: KVM

Kernel Notes: Transparent Huge Pages: always
Compiler Notes: --build=x86_64-redhat-linux --disable-libmpx --disable-libunwind-exceptions --enable-__cxa_atexit --enable-bootstrap --enable-cet --enable-checking=release --enable-gnu-indirect-function --enable-gnu-unique-object --enable-initfini-array --enable-languages=c,c++,fortran,lto --enable-multilib --enable-offload-targets=nvptx-none --enable-plugin --enable-shared --enable-threads=posix --mandir=/usr/share/man --with-arch_32=x86-64 --with-gcc-major-version-only --with-isl --with-linker-hash-style=gnu --with-tune=generic --without-cuda-driver
Processor Notes: CPU Microcode: 0x1000065
Security Notes: SELinux + itlb_multihit: Not affected + l1tf: Not affected + mds: Not affected + meltdown: Not affected + spec_store_bypass: Mitigation of SSB disabled via

prctl and seccomp + spectre_v1: Mitigation of usercopy/swapgs barriers and __user pointer sanitization + spectre_v2: Mitigation of Full AMD retpoline IBPB: conditional STIBP: disabled RSB filling + srbds: Not affected + tsx_async_abort: Not affected

	16 x AMD EPYC
miniFE - Small (CG Mflops)	9282
Standard Deviation	0.8%
GROMACS - MPI CPU - water_GMX50_bare (Ns/Day)	1.029
Standard Deviation	0.8%
LAMMPS Molecular Dynamics Simulator - 20k Atoms (ns/day)	8.071
Standard Deviation	0.9%
LAMMPS Molecular Dynamics Simulator - Rhodopsin Protein	8.040
Standard Deviation	0.7%
LULESH (z/s)	6158
Standard Deviation	0.6%
NAMD - ATPase Simulation - 327,506 Atoms (days/ns)	2.14576
Standard Deviation	0.1%
Pennant - sedovbig (Hydro Cycle Time - sec)	49.00870
Standard Deviation	0.3%
Pennant - leblancbig (Hydro Cycle Time - sec)	36.44773
Standard Deviation	1.8%
CloverLeaf - L.E.H (sec)	62.73
Standard Deviation	1.8%
CP2K Molecular Dynamics - Fayalite-FIST (sec)	1101
Dolfyn - C.F.D (sec)	30.064
Standard Deviation	0.6%
NWChem - C240 Buckyball (sec)	8328
Xcompact3d Incompact3d - i.i.1.C.P.D (sec)	19.4648781
Standard Deviation	0.4%
Xcompact3d Incompact3d - i.i.1.C.P.D (sec)	77.0652186
Standard Deviation	1.2%
OpenFOAM - motorBike - Mesh Time (sec)	72.26
OpenFOAM - motorBike - Execution Time (sec)	153.24

miniFE 2.2

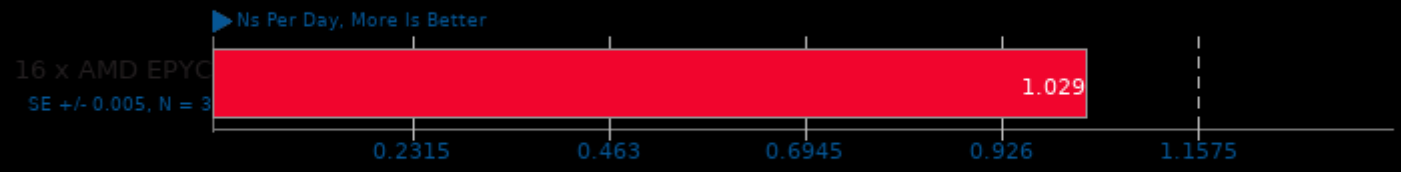
Problem Size: Small



1. (CXX) g++ options: -O3 -fopenmp -pthread -lmpi_cxx -lmpi

GROMACS 2022.1

Implementation: MPI CPU - Input: water_GMX50_bare



1. (CXX) g++ options: -O3 -pthread

LAMMPS Molecular Dynamics Simulator 29Oct2020

Model: 20k Atoms



1. (CXX) g++ options: -O3 -pthread -lm

LAMMPS Molecular Dynamics Simulator 29Oct2020

Model: Rhodopsin Protein

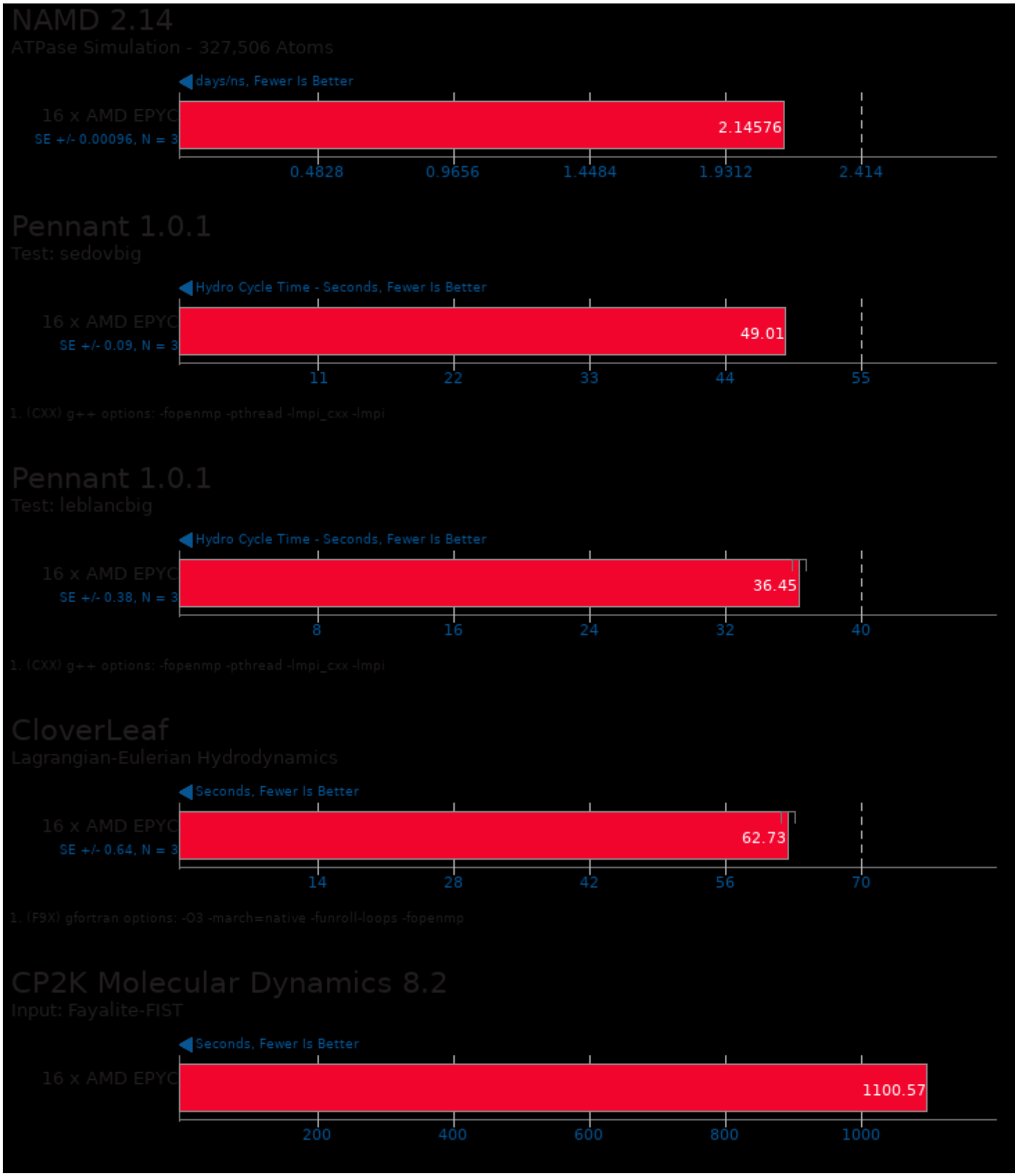


1. (CXX) g++ options: -O3 -pthread -lm

LULESH 2.0.3



1. (CXX) g++ options: -O3 -fopenmp -lm -pthread -lmpi_cxx -lmpi


NAMD 2.14
ATPase Simulation - 327,506 Atoms
days/ns, Fewer Is Better
16 x AMD EPYC
SE +/- 0.00096, N = 3
2.14576
0.4828
0.9656
1.4484
1.9312
2.414
Pennant 1.0.1
Test: sedovbig
Hydro Cycle Time - Seconds, Fewer Is Better
16 x AMD EPYC
SE +/- 0.09, N = 3
49.01
11
22
33
44
55
1. (CXX) g++ options: -fopenmp -pthread -lmpi_cxx -lmpi
Pennant 1.0.1
Test: leblancbig
Hydro Cycle Time - Seconds, Fewer Is Better
16 x AMD EPYC
SE +/- 0.38, N = 3
36.45
8
16
24
32
40
1. (CXX) g++ options: -fopenmp -pthread -lmpi_cxx -lmpi
CloverLeaf
Lagrangian-Eulerian Hydrodynamics
Seconds, Fewer Is Better
16 x AMD EPYC
SE +/- 0.64, N = 3
62.73
14
28
42
56
70
1. (F9X) gfortran options: -O3 -march=native -funroll-loops -fopenmp
CP2K Molecular Dynamics 8.2
Input: Fayalite-FIST
Seconds, Fewer Is Better
16 x AMD EPYC
1100.57
200
400
600
800
1000

Dolfyn 0.527

Computational Fluid Dynamics



NWChem 7.0.2

Input: C240 Buckyball



1. (F9X) gfortran options: -lnwctask -lccsd -lmcscf -lselci -lmp2 -lmoints -lstepper -ldriver -loptim -lnwdft -lgradients -lcphf -lesp -lddscf -ldangchang -lgue

Xcompact3d Incompact3d 2021-03-11

Input: input.i3d 129 Cells Per Direction



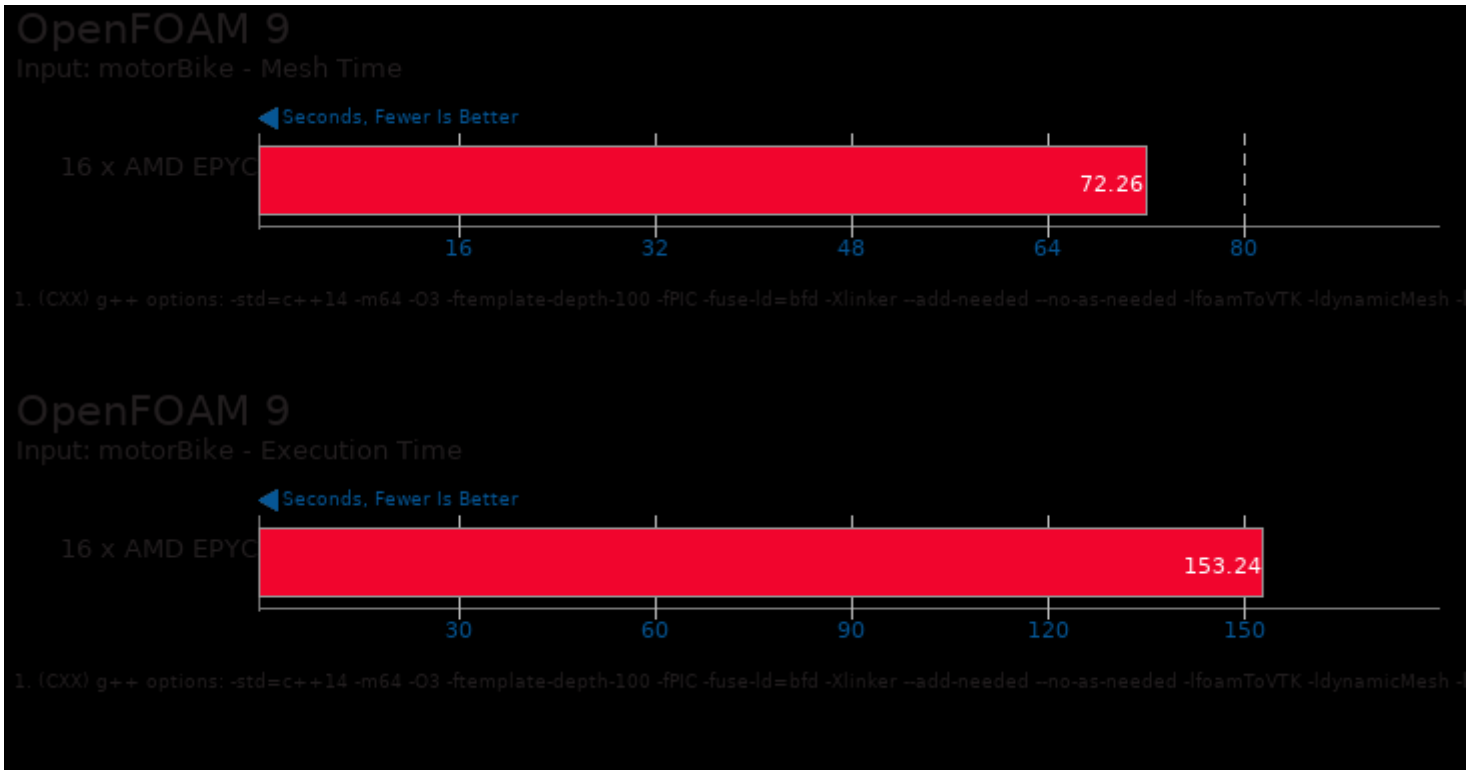
1. (F9X) gfortran options: -cpp -O2 -funroll-loops -floop-optimize -fcray-pointer -fbacktrace -pthread -lmpi_usempif08 -lmpi_mpifh -lmpi

Xcompact3d Incompact3d 2021-03-11

Input: input.i3d 193 Cells Per Direction



1. (F9X) gfortran options: -cpp -O2 -funroll-loops -floop-optimize -fcray-pointer -fbacktrace -pthread -lmpi_usempif08 -lmpi_mpifh -lmpi



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