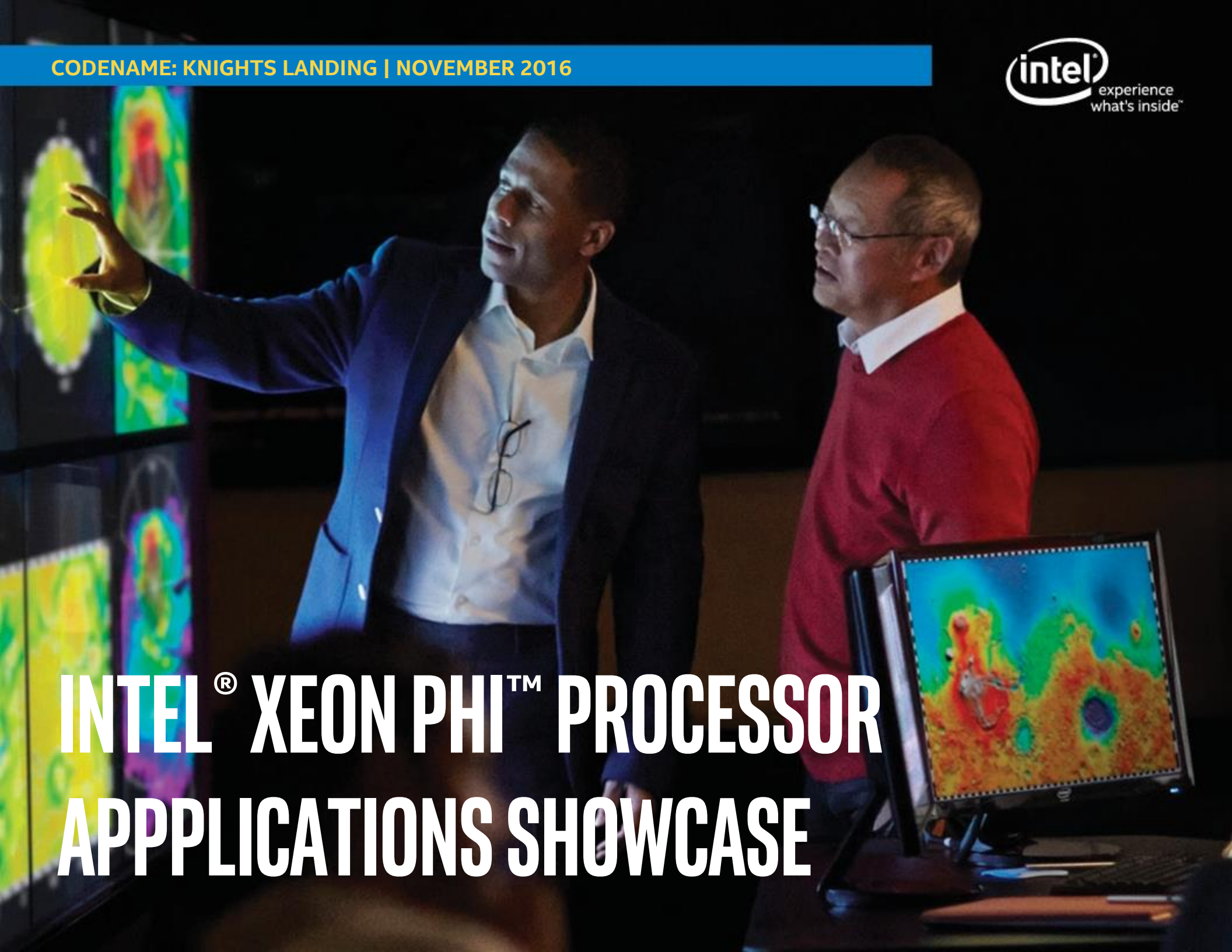


CODENAME: KNIGHTS LANDING | NOVEMBER 2016



INTEL® XEON PHI™ PROCESSOR APPLICATIONS SHOWCASE





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Go to <http://intel.ly/2ejslgj>



HPCG

RESULTS: HIGHER IS BETTER

2.25X higher performance with the Intel® Xeon Phi™ processor 7290 compared to the Intel® Xeon® processor E5-2697 v4.

INTEL TECHNOLOGIES:

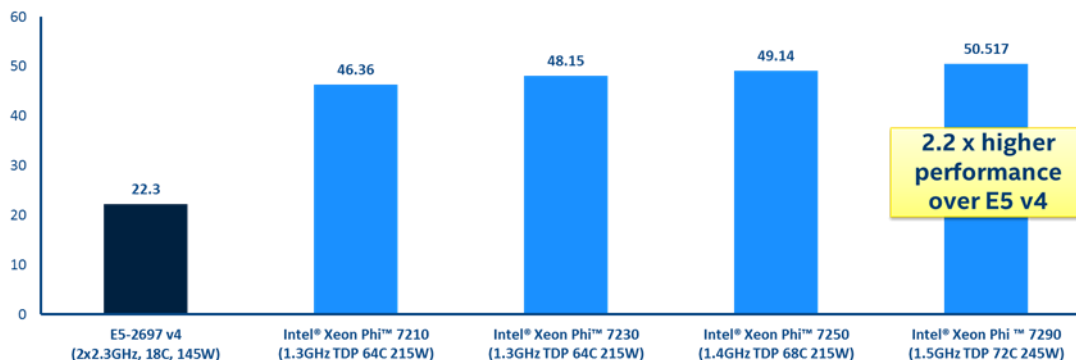
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High Performance Conjugate Gradient (HPCG) (GF/s)



2.2 x higher performance over E5 v4



OPTIMIZED PARALLEL PERFORMANCE



BENCHMARKS



HPL

RESULTS: HIGHER IS BETTER

1.6X faster with the Intel® Xeon Phi™ processor 7290 compared to the Intel® Xeon® processor E5-2697 v4.

INTEL TECHNOLOGIES:

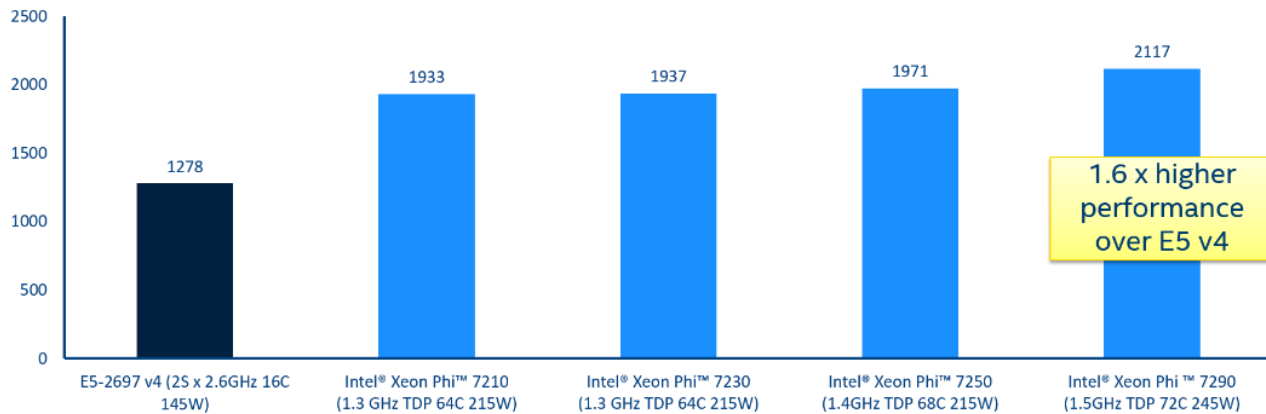
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LINPACK single node (GF/s)



1.6 x higher performance over E5 v4



OPTIMIZED PARALLEL PERFORMANCE



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CORE LIBRARIES

PETSC

PETSc—the Portable, Extensible Toolkit for Scientific Computation—is a suite of data structures and routines for the scalable (parallel) solution of scientific applications modeled by partial differential equations.

RESULTS: LOWER IS BETTER

Up to 1.8X faster with the Intel® Xeon Phi™ processor 7250 compared to the Intel® Xeon® processor E5-2697 v4.

GET THE CODE:

[Code](#)

INTEL TECHNOLOGIES:



INTEL® AVX 512 INSTRUCTIONS



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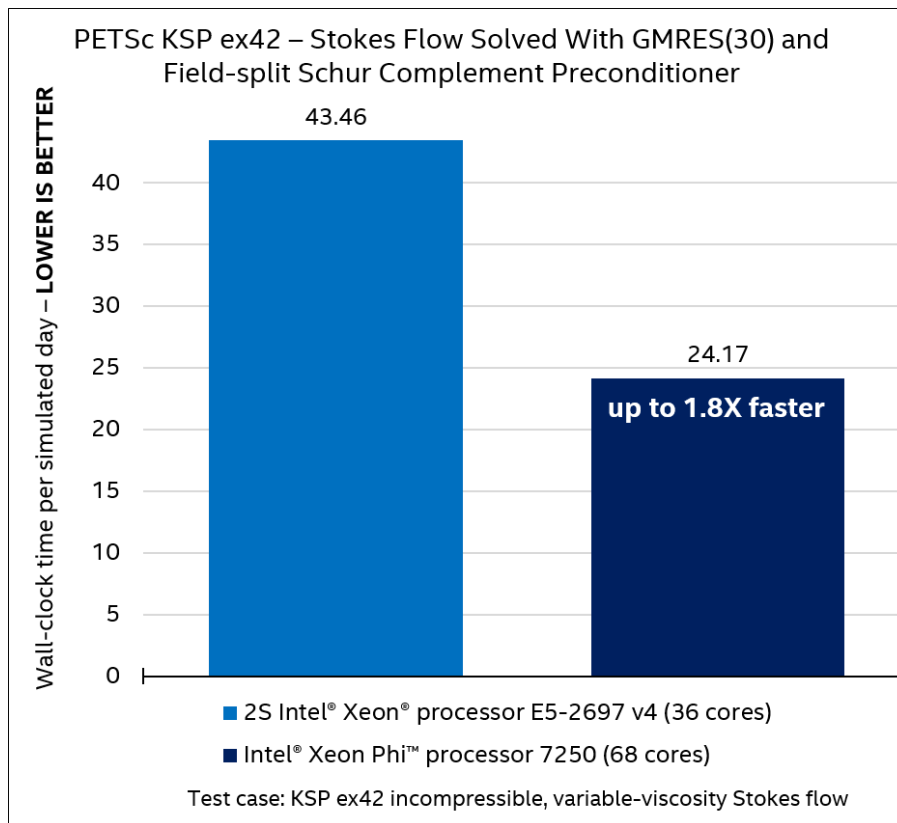
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DMI HIROMB-BOOS-MODEL

The Danish Meteorological Institute (DMI) institute was founded to make observations, communicate them to the general public, and to develop scientific meteorology.

RESULTS: HIGHER IS BETTER

Up to 1.7X performance improvement compared to the Intel® Xeon® processor E5-2697 v4.

GET THE CODE:

[Code](#)

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INTEL TECHNOLOGIES:



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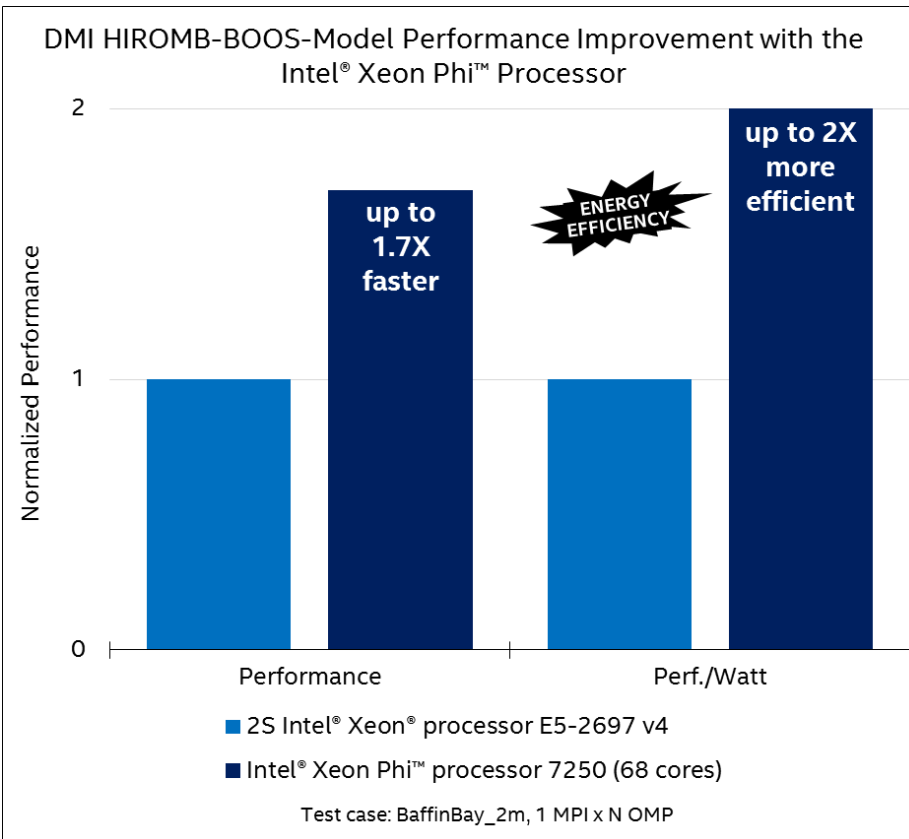
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MPAS OCEAN 4.0*

MPAS (Model for Prediction Across Scales) is a suite of programs for atmosphere, ocean, and other earth-system simulation. LANL is primarily responsible for the MPAS Ocean (MPAS-O) model. MPAS-O has demonstrated the ability to accurately reproduce mesoscale activity. (Workload contact: Doug Jacobson, LANL, jacobson.douglas@gmail.com).

RESULTS: HIGHER IS BETTER

Up to 1.96X performance/power compared to the Intel® Xeon® processor E5-2697 v4 for EC_60to30_forward workload.

GET THE CODE:

[Code](#)

[Recipe](#)

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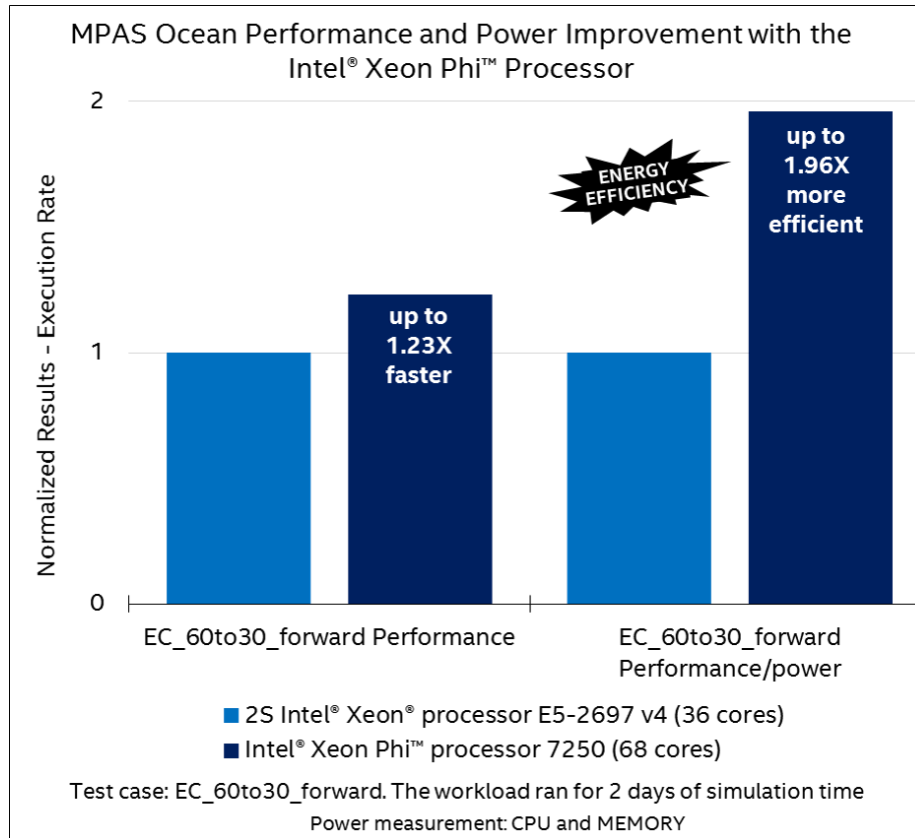
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NUCLEUS FOR EUROPEAN MODELLING OF THE OCEAN*

Nucleus for European Modelling of the Ocean (NEMO) is an ocean modelling framework composed of "engines" in an "environment." The "engines" provide numerical solutions of ocean, sea-ice, tracers, and biochemistry equations and their related physics.



RESULTS: LOWER IS BETTER

Up to 2.1X improved performance compared to the Intel® Xeon® processor E5-2697 v4.

GET THE CODE:

[Code](#)

[Recipe](#)

INTEL TECHNOLOGIES:



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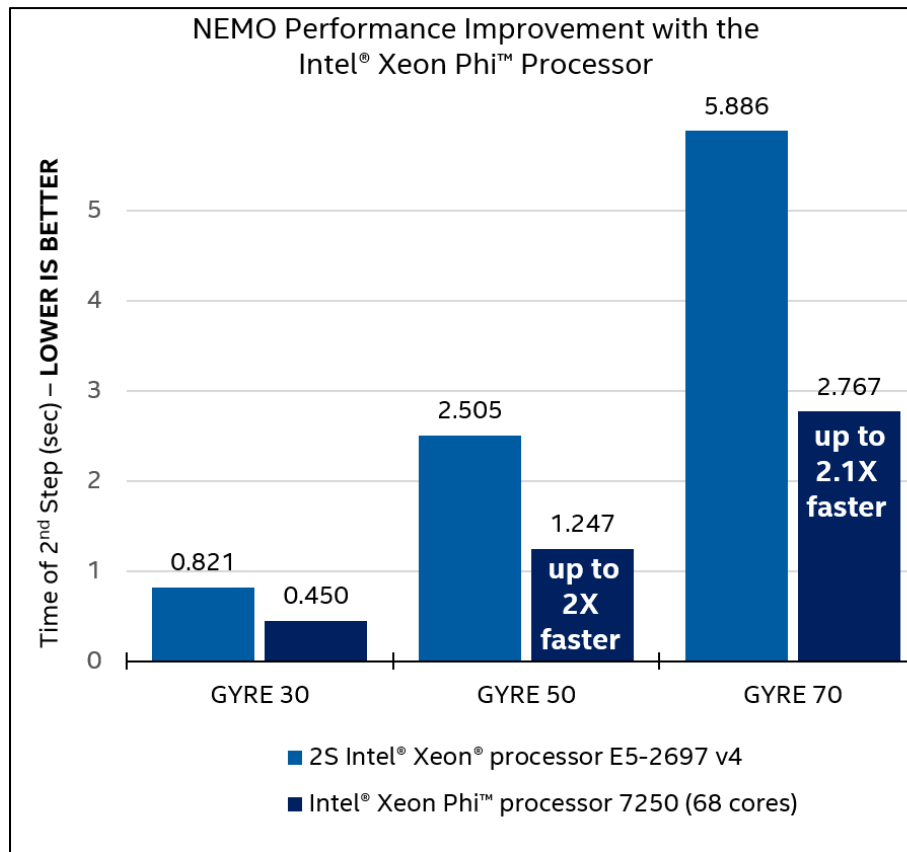
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WEATHER & RESEARCH FORECAST MODEL*

The WRF Model is a numerical weather prediction system designed to serve atmospheric research and operational forecasting needs. Currently in operational use at NCEP, AFWA, NASA, NOAA, etc.

RESULTS: LOWER IS BETTER

Up to 1.7X faster compared to the Intel® Xeon® processor E5-2697 v4.

GET THE CODE:

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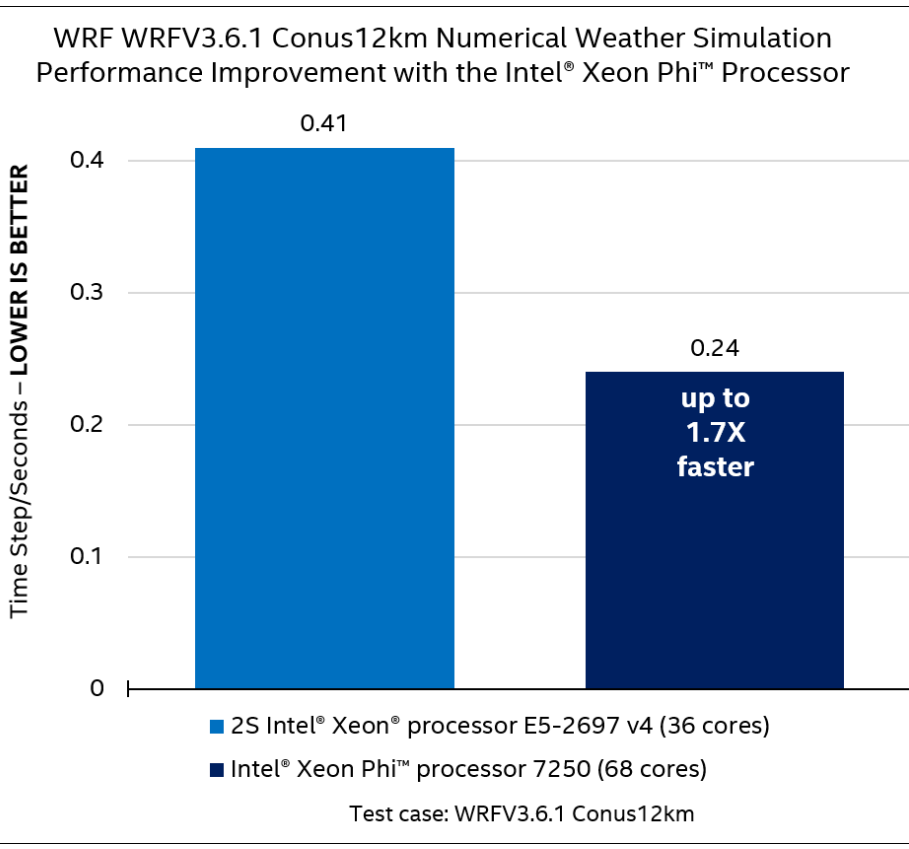
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ISO3DFD (3D ACOUSTIC ISOTROPIC FINITE DIFFERENCE)*

Iso3DFD—The Iso-3D 16th order Isotropic kernel is at the heart of RTM algorithm. It plays a major role on accurate imaging of complex subsurfaces. This kernel computes the wave propagation used in seismic imaging. The code is in-house code.

RESULTS: HIGHER IS BETTER

Up to 1.71X faster with the Intel® Xeon Phi™ processor 7250 compared to the Intel® Xeon® processor E5-2697 v4.

GET THE CODE:

[Code](#)

Recipe: -O3 -xMIC-AVX512
-fp-model fast -fma -
qopenmp -lmemkind

INTEL TECHNOLOGIES:



INTEL® AVX 512
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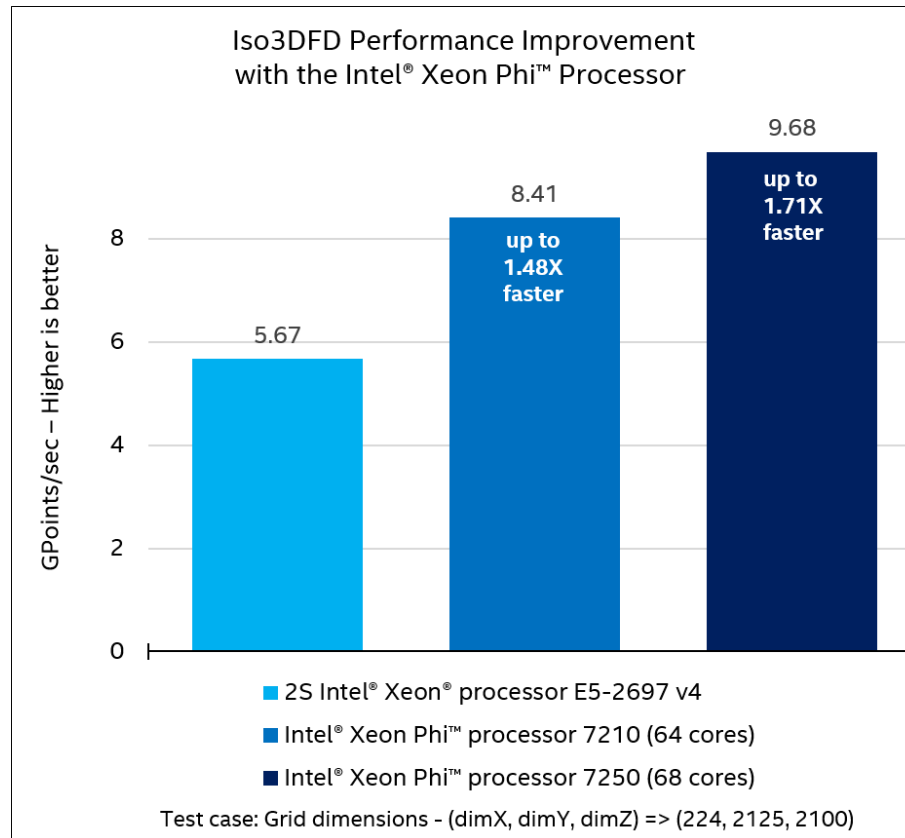
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STAC-A2* BENCHMARK

The STAC-A2 Benchmark suite is the industry standard created by the financial community to test technology stacks used for compute-intensive analytic workloads involved in pricing and risk management.



RESULTS: LOWER IS BETTER

The Intel® Xeon Phi™ 7250 processor system is up to 2X more power efficient (not in chart) compared to the IBM Power8* system.

GET THE CODE:

[Code](#)

[Recipe](#)

INTEL TECHNOLOGIES:



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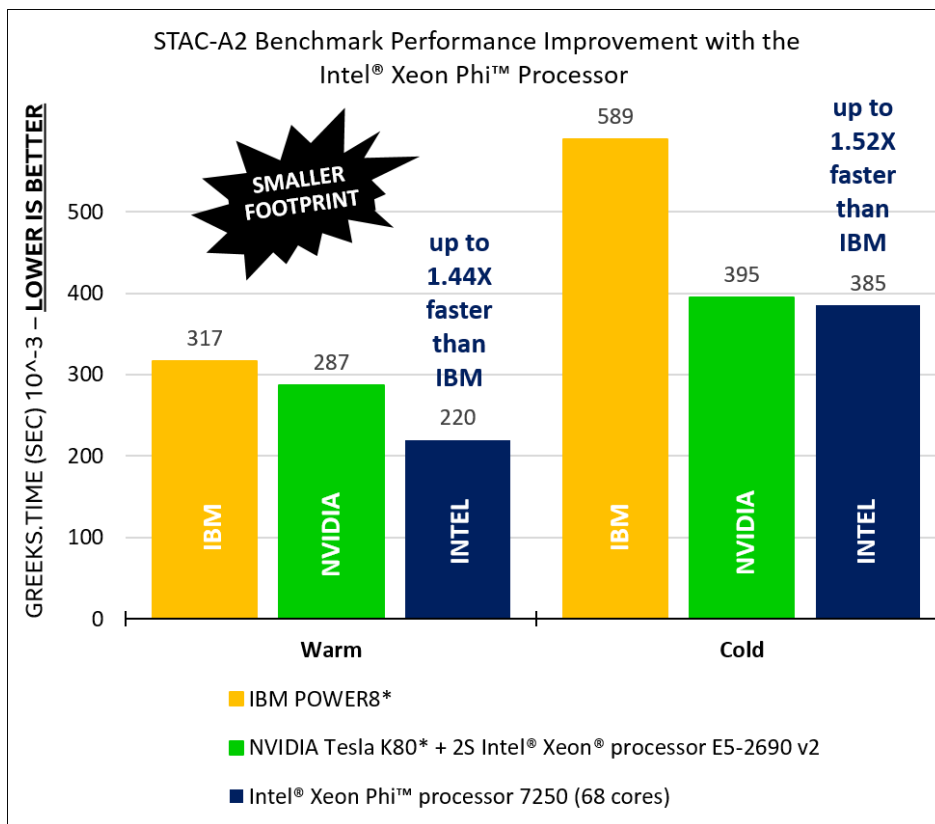
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GROMACS*

GROMACS (GROningen MACHine for Chemical Simulations) is a versatile package to perform classical molecular dynamics simulations. Heavily optimized for most modern platforms and provides extremely high performance compared to all other MD codes.

RESULTS: HIGHER IS BETTER

Up to 1.45X better energy efficiency compared to the 2S Intel® Xeon® processor E5-2697 v4.

GET THE CODE:

[Code](#)

Recipe: All optimizations merged in GROMACS 2016 branch, MKL FFT

INTEL TECHNOLOGIES:



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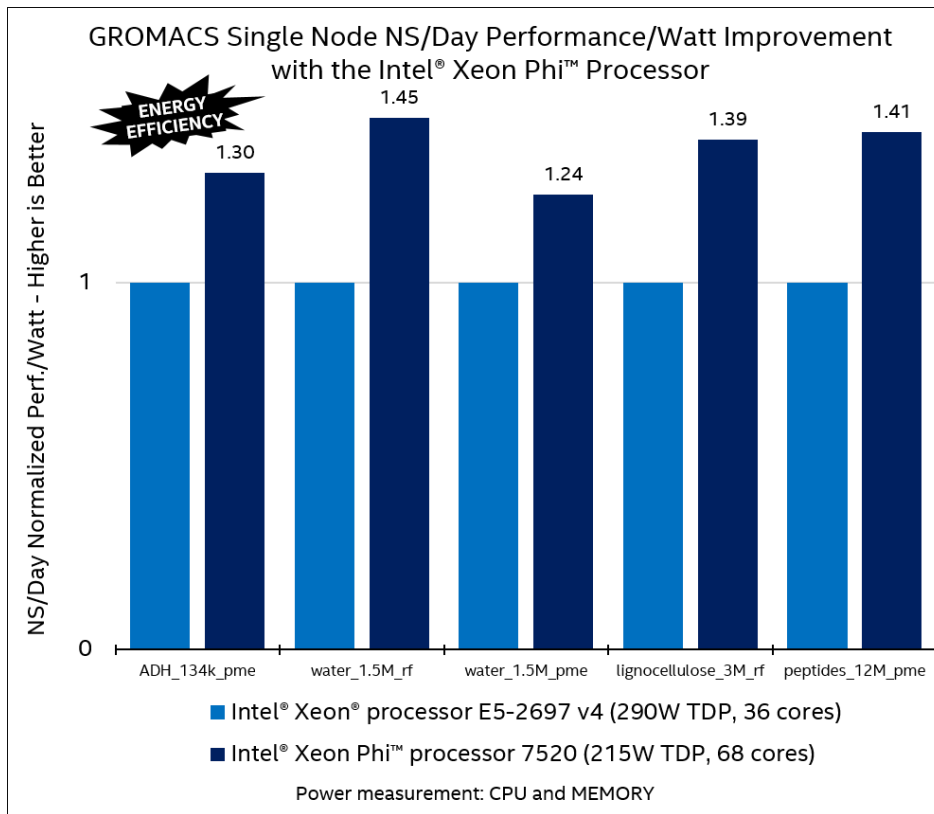
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LAMMPS COARSE-GRAIN WATER SIMULATION

LAMMPS is a classical molecular dynamics code, and an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator. It is used to simulate the movement of atoms to develop better therapeutics, improve alternative energy devices, develop new materials, and more.

RESULTS: HIGHER IS BETTER

Up to 1.67X performance per watt compared to the Intel® Xeon® processor E5-2697 v4.

GET THE CODE:

[Code](#)

[Recipe](#)

INTEL TECHNOLOGIES:



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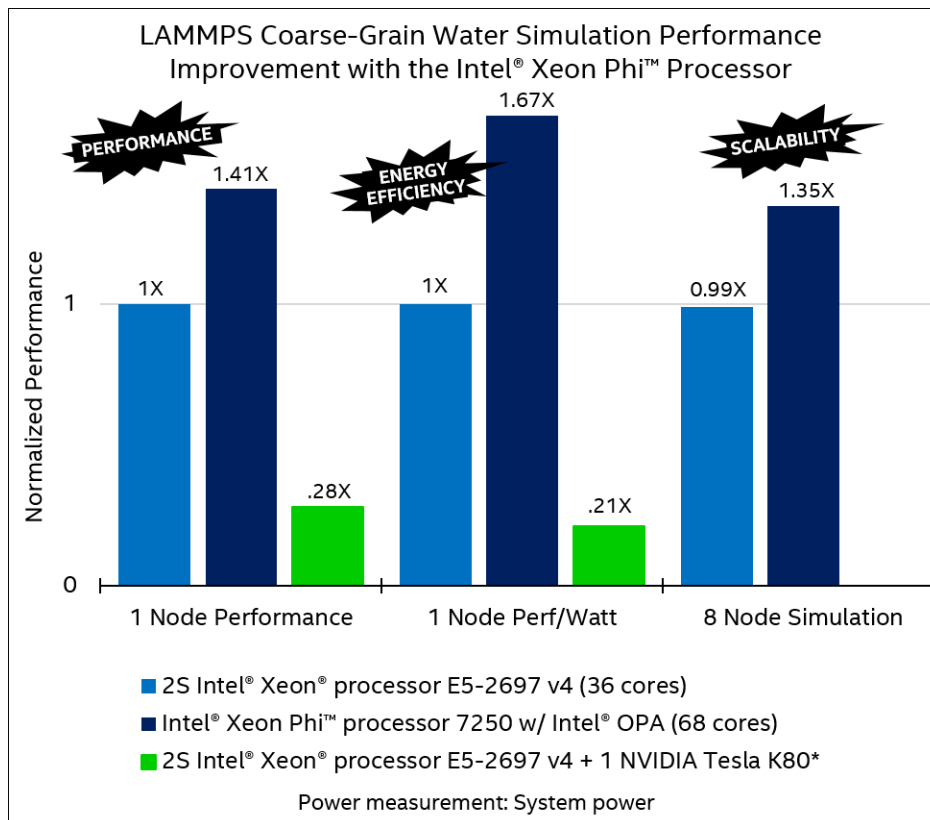
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NANOSCALE MOLECULAR DYNAMICS PROGRAM*

Nanoscale Molecular Dynamics program (NAMD) is a parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems. Based on Charm++ parallel objects, NAMD scales to hundreds of cores for typical simulations and beyond 200,000 cores for the largest simulations.

RESULTS: HIGHER IS BETTER

Up to 1.91X improved energy efficiency compared to the Intel® Xeon® processor E5-2697 v4.

GET THE CODE:

[Code](#)

INTEL TECHNOLOGIES:



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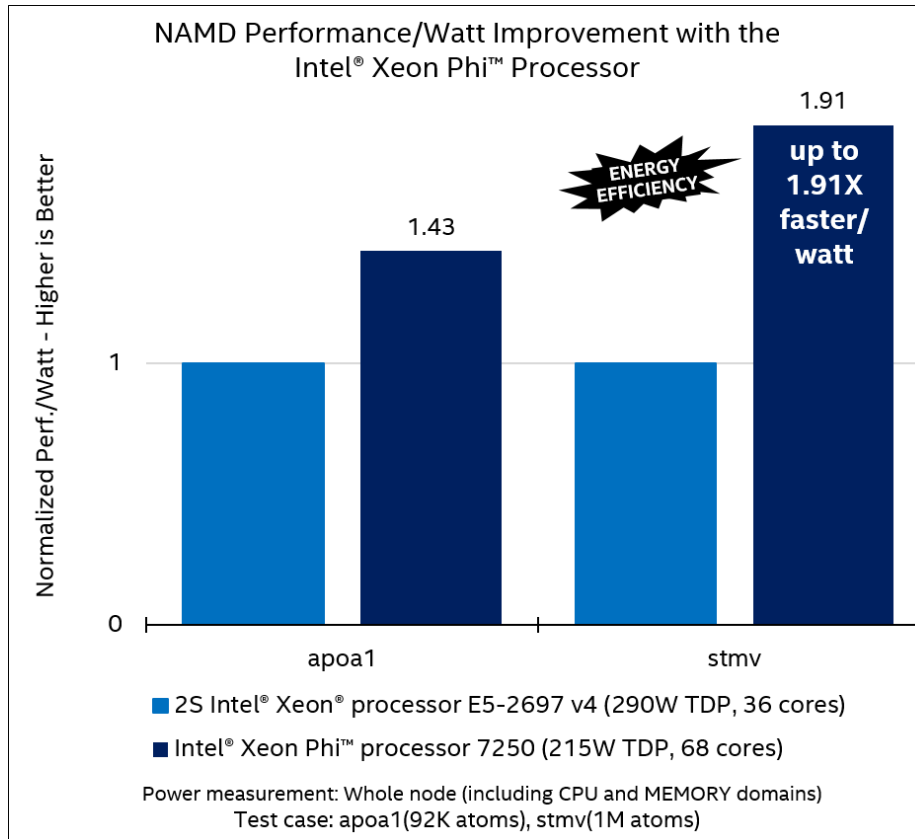
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ROME/SML

ROME (Refinement and Optimization via Machine Learning for cryo-EM) is one of the major research software packages from Dana-Farber Cancer Institute. ROME is a parallel computing software system dedicated to high-resolution cryo-EM structure determination and data analysis, implementing advanced machine learning approaches optimized for HPC clusters.

RESULTS: LOWER IS BETTER

Up to 2.36X improved performance compared to the Intel® Xeon® processor E5-2697 v4.

GET THE CODE:

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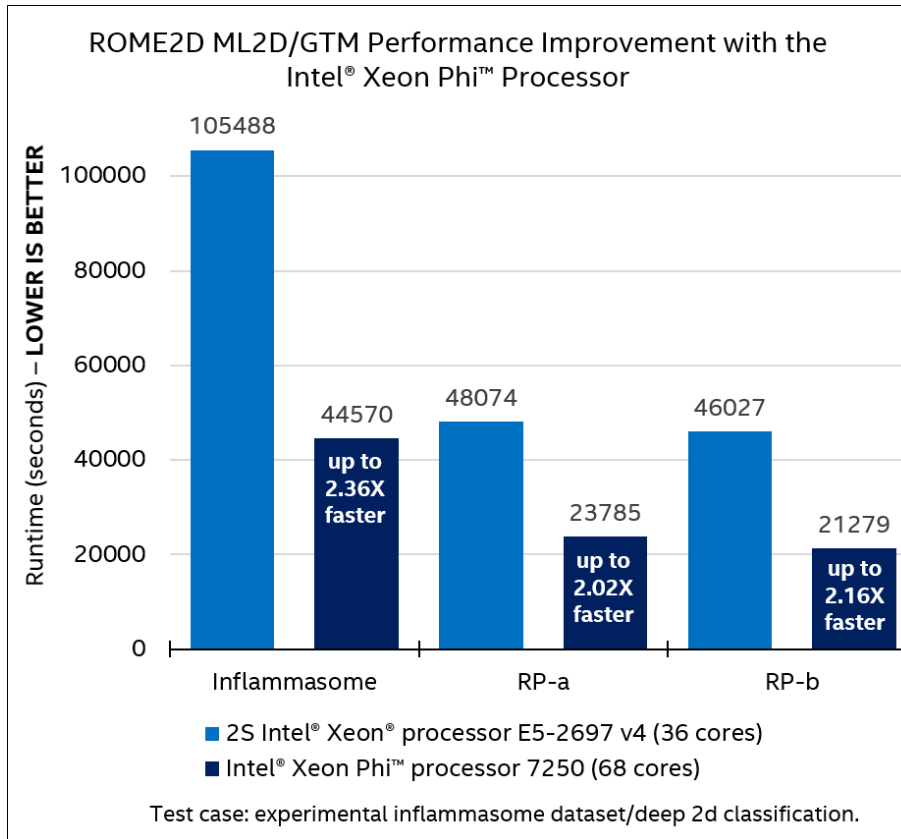
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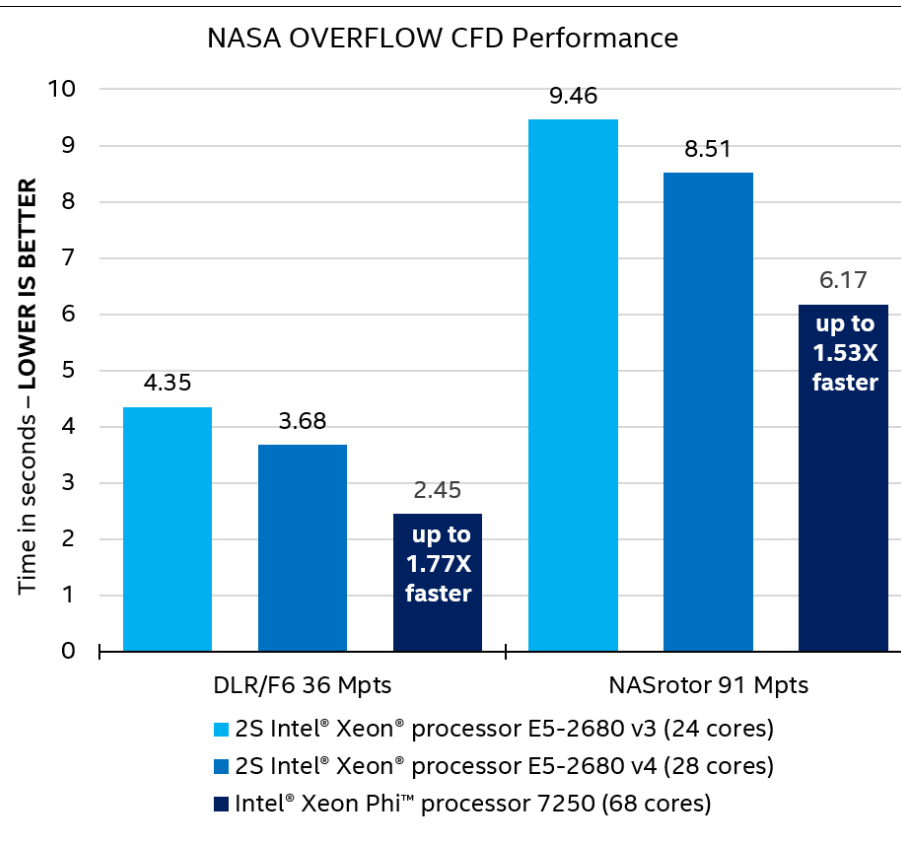


NASA OVERFLOW*

OVERFLOW is a 3D time marching implicit Navier-Stokes computational fluid dynamics simulator developed by NASA and used across aerospace and other industries.

RESULTS: LOWER IS BETTER

Up to 1.77X performance improvement compared to the Intel® Xeon® processor E5-2680v3.



GET THE CODE:

[Code](#)

Recipe: No code changes were required. Recompile with Intel® AVX-512.

INTEL TECHNOLOGIES:



INTEL® AVX 512 INSTRUCTIONS



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OPENFOAM*

OpenFOAM (for "Open source Field Operation And Manipulation") is a C++ toolbox for the development of customized numerical solvers, and pre-/post-processing utilities for the solution of continuum mechanics problems, including computational fluid dynamics (CFD).

RESULTS: LOWER IS BETTER

Up to 1.71X faster compared to the 2S Intel® Xeon® processor E5-2697 v4.

GET THE CODE:

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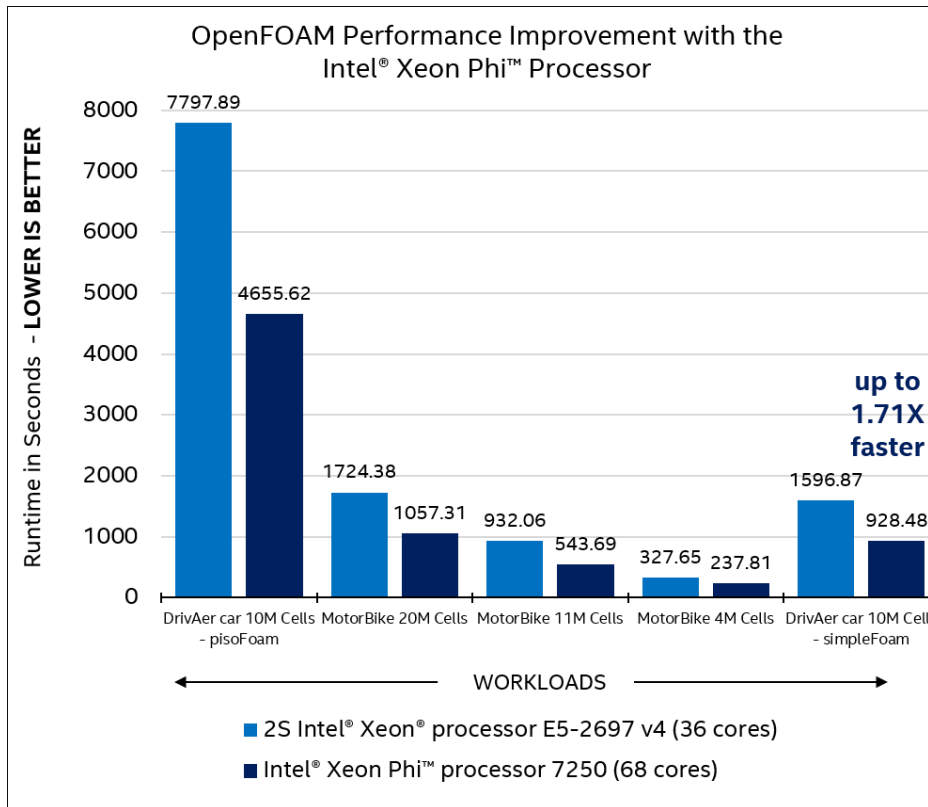
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BERKELEYGW*

BerkeleyGW Package is a set of computer codes that calculates the quasiparticle properties and the optical responses of a large variety of materials from bulk periodic crystals to nanostructures such as slabs, wires, and molecules. It is a massively parallel computational package for electron excited state properties.

RESULTS: HIGHER IS BETTER

Up to 38% speedup compared to the Intel® Xeon® processor.

GET THE CODE:

[Code](#)

INTEL TECHNOLOGIES:



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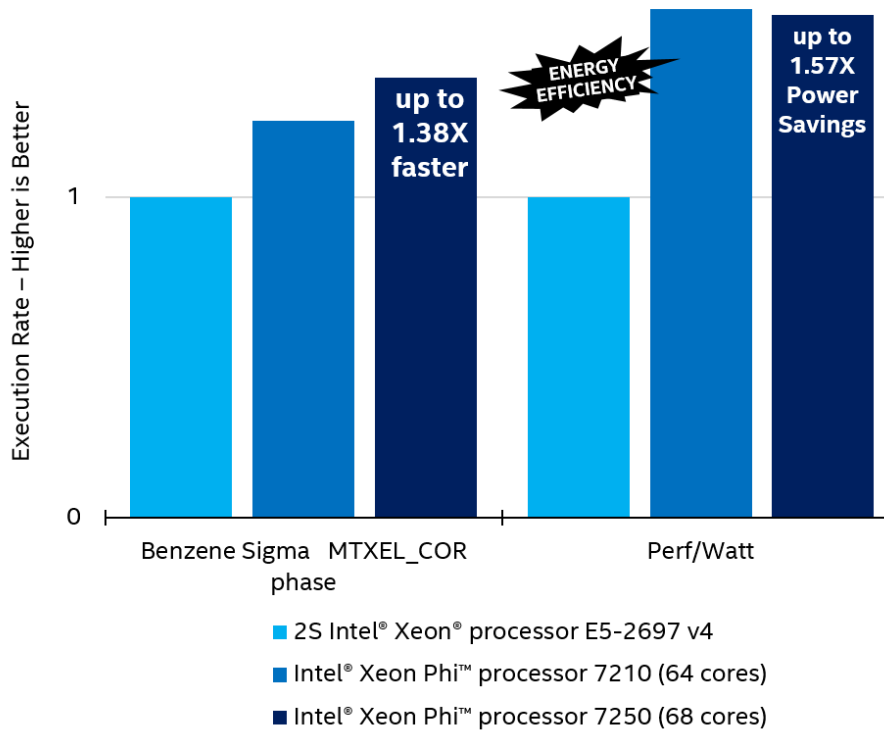
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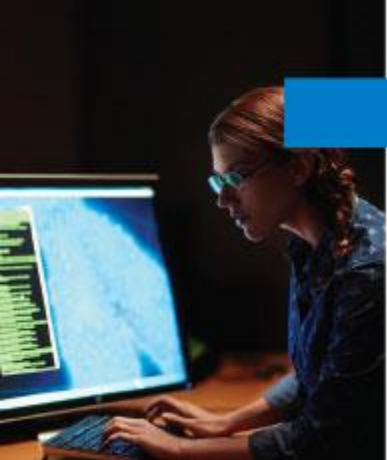
BerkeleyGW Performance Improvement with the Intel® Xeon Phi™ Processor





QUANTUM ESPRESSO* AUSURF112

Quantum ESPRESSO is an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials.



RESULTS: LOWER IS BETTER

Up to 1.17X improved energy efficiency compared to the Intel® Xeon® processor E5-2697 v4.

GET THE CODE:

[Code](#)

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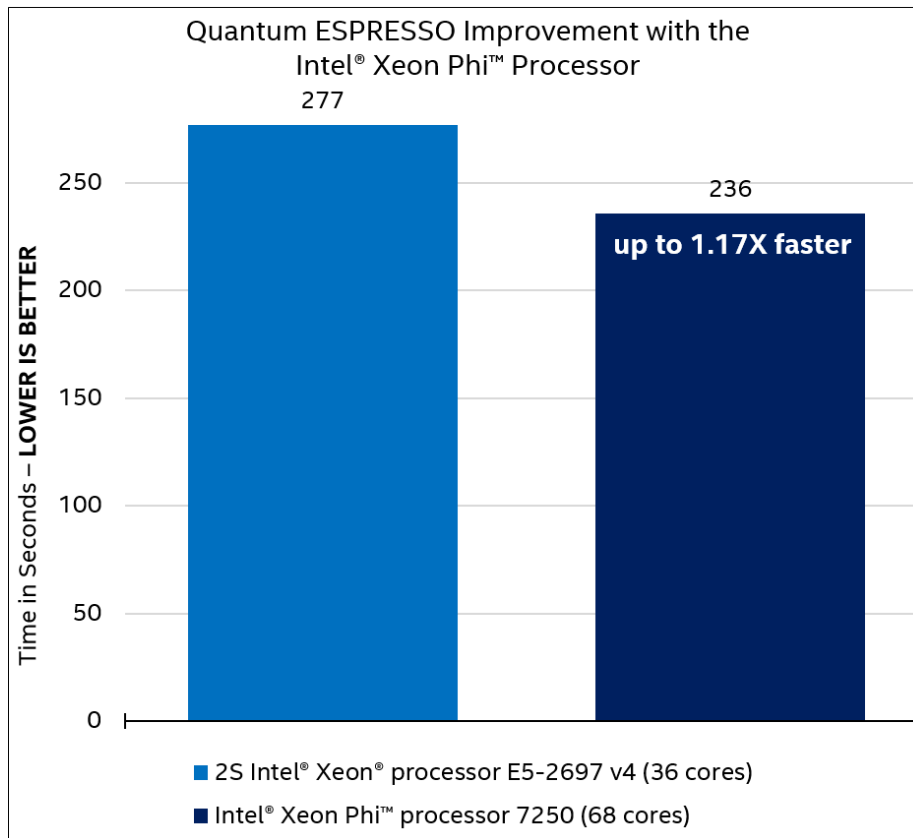
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CLOVERLEAF*

The CloverLeaf* code investigates the behavior of fluids under high temperatures and pressures, which potentially cause shock fronts to form. It is common for hydrocodes to be constructed using one of two formulations—Lagrangian, in which a mesh is constructed and evolved through time, or Eulerian, where material flow is calculated relative to a fixed spatial grid.

RESULTS: LOWER IS BETTER

Up to 2.3X improved performance compared to the Intel® Xeon® processor E5-2697 v4.

GET THE CODE:

[Code](#)

INTEL TECHNOLOGIES:



INTEL® AVX 512 INSTRUCTIONS



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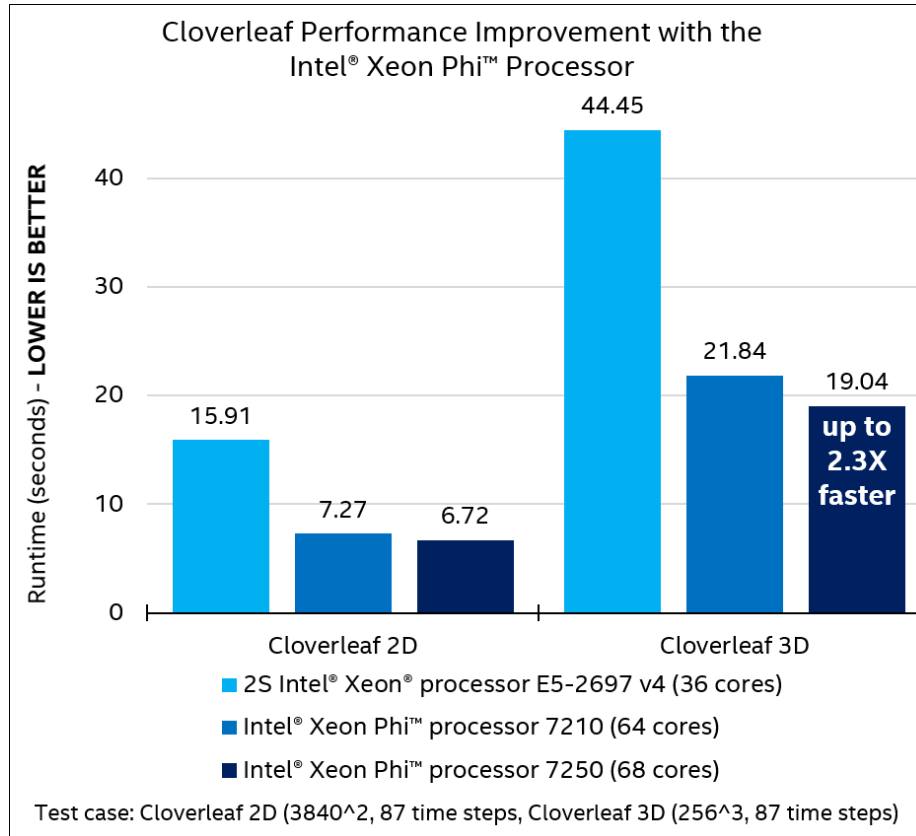
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MILC*

The MILC Code is used to study quantum chromodynamics (QCD), the theory of the strong interactions of subatomic physics and is written by the MIMD Lattice Computation (MILC) collaboration.

RESULTS: LOWER IS BETTER

The Intel® Xeon Phi™ processor 7250 improved performance by up to 1.58X compared to the NVIDIA Titan X*.

GET THE CODE:

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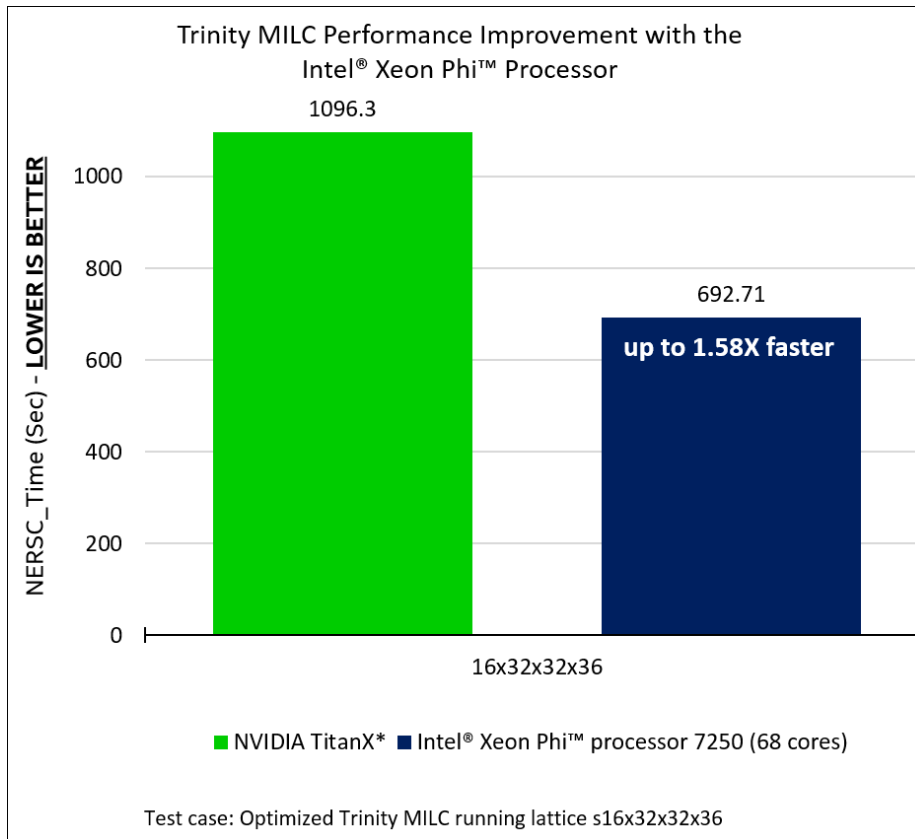
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INTEL EMBREE V2.9.0

Embree is a collection of high-performance ray tracing kernels, developed at Intel. The target user of Embree are graphics application engineers that want to improve the performance of their application by leveraging the optimized ray tracing kernels of Embree. Embree supports runtime code selection to choose the traversal and build algorithms that best matches the instruction set of the CPU.

RESULTS: HIGHER IS BETTER

Up to 5.17X improved compared to the NVIDIA Titan X*.

GET THE CODE:

[Code](#)

[Recipe](#)

INTEL TECHNOLOGIES:



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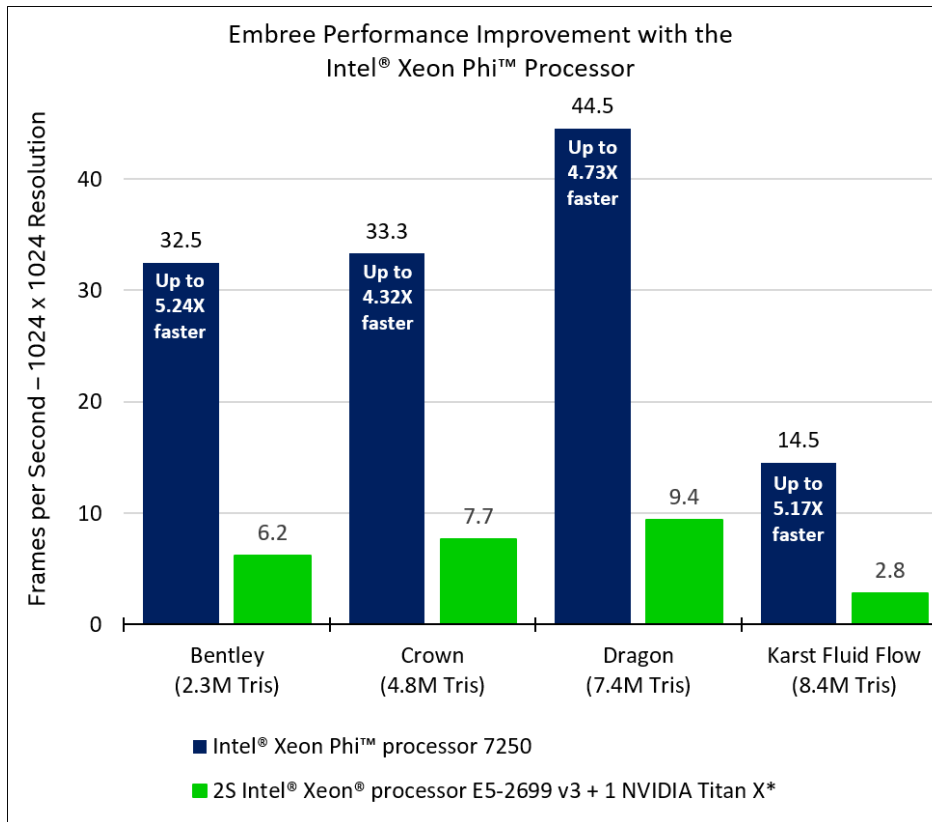
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Benchmarks

HPCG

Processor	Intel® Xeon® Processor E5-2697 v4 (45M Cache, 2.30 GHz)	Intel® Xeon Phi™ Processor 7210 (16GB, 1.30 GHz, 64 core)	Intel® Xeon Phi™ Processor 7230 (16GB, 1.30 GHz, 64 core)	Intel® Xeon Phi™ Processor 7250 (16GB, 1.40 GHz, 68 core)
Vendor	Intel	Intel	Intel	Intel
Nodes	1	1	1	1
Sockets	2	1	1	1
Cores	18	64	64	68
Logical Processors	36			
Platform	Grantley-EP (Wellsburg)	Groveport (Knights Landing)	Groveport (Knights Landing)	Groveport (Knights Landing)
Slots	8	6	6	6
Total Memory	128 GB	192 GB	192 GB	192 GB
Memory Configuration	8 slots / 16 GB / 2400 MT/s / DDR4 RDIMM	6 slots / 32 GB / 2400 MT/s / DDR4 RDIMM	6 slots / 32 GB / 2400 MT/s / DDR4 RDIMM	6 slots / 32 GB / 2400 MT/s / DDR4 RDIMM
Memory Comments		running @ 2133 MHz		
OS	Red Hat Enterprise Linux* 7.2-kernel 3.10.0-327	SUSE Linux Enterprise Server* 12	SUSE Linux Enterprise Server* 12	SUSE Linux Enterprise Server* 12
OS/Kernel Comments		SP2 Beta1	SP2 Beta1	SP2 Beta1
Storage Number	400 GB, Intel S3710 SSD	400 GB, Intel S3710 SSD	400 GB, Intel S3710 SSD	400 GB, Intel S3710 SSD
Other Configurations		GVPRCRB1.86B.0009.R02.1604071 525, Quad/Flat	GVPRCRB1.86B.0009.R02.1604071 525, Quad/Flat	GVPRCRB1.86B.0010.R00.160325173 2, Quad/Flat
HT	No	Yes	Yes	Yes
Turbo	Yes	Yes	Yes	Yes
Computer Type	server	server	server	server
Benchmark	High Performance Conjugate Gradient (HPCG) - GF/s	High Performance Conjugate Gradient (HPCG) - GF/s	High Performance Conjugate Gradient (HPCG) - GF/s	High Performance Conjugate Gradient (HPCG) - GF/s
Data Source	Request Number: 2362	Request Number: 2362	Request Number: 2362	Request Number: 2362
Configuration Summary	1-Node, 2 x Intel® Xeon® Processor E5-2697 v4 on Grantley-EP (Wellsburg) with 128 GB Total Memory on Red Hat Enterprise Linux* 7.2-kernel 3.10.0-327 using (No Software). Data Source: Request Number: 2362, Benchmark: High Performance Conjugate Gradient (HPCG), Score: 22.25 Higher is better	1-Node, 1 x Intel® Xeon Phi™ Processor 7210 (16GB, 1.30 GHz, 64 core) on Groveport (Knights Landing) with 192 GB Total Memory on SUSE Linux Enterprise Server* 12 using (No Software). Data Source: Request Number: 2362, Benchmark: High Performance Conjugate Gradient (HPCG), Score: 46.36 Higher is better	1-Node, 1 x Intel® Xeon Phi™ Processor 7230 (16GB, 1.30 GHz, 64 core) on Groveport (Knights Landing) with 192 GB Total Memory on SUSE Linux Enterprise Server* 12 using (No Software). Data Source: Request Number: 2362, Benchmark: High Performance Conjugate Gradient (HPCG), Score: 48.15 Higher is better	1-Node, 1 x Intel® Xeon Phi™ Processor 7250 (16GB, 1.40 GHz, 68 core) on Groveport (Knights Landing) with 192 GB Total Memory on SUSE Linux Enterprise Server* 12 using (No Software). Data Source: Request Number: 2362, Benchmark: High Performance Conjugate Gradient (HPCG), Score: 49.14 Higher is better

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Benchmarks, continued

HPL

Processor	Intel® Xeon® Processor E5-2697 v4 (45M Cache, 2.30 GHz)	Intel® Xeon Phi™ Processor 7210 (16GB, 1.30 GHz, 64 core)	Intel® Xeon Phi™ Processor 7230 (16GB, 1.30 GHz, 64 core)	Intel® Xeon Phi™ Processor 7250 (16GB, 1.40 GHz, 68 core)
Vendor	Intel	Intel	Intel	Intel
Nodes	1	1	1	1
Sockets	2	1	1	1
Cores	18	64	64	68
Logical Processors	36			
Platform	Grantley-EP (Wellsburg)	Groveport (Knights Landing)	Groveport (Knights Landing)	Groveport (Knights Landing)
Slots	8	6	6	6
Total Memory	128 GB	192 GB	192 GB	192 GB
Memory Configuration	8 slots / 16 GB / 2400 MT/s / DDR4 RDIMM	6 slots / 32 GB / 2400 MT/s / DDR4 RDIMM	6 slots / 32 GB / 2400 MT/s / DDR4 RDIMM	6 slots / 32 GB / 2400 MT/s / DDR4 RDIMM
Memory Comments		running @ 2133 MHz		
OS	Red Hat Enterprise Linux* 7.2-kernel 3.10.0-327	SUSE Linux Enterprise Server* 12	SUSE Linux Enterprise Server* 12	SUSE Linux Enterprise Server* 12
OS/Kernel Comments		SP2 Beta1	SP2 Beta1	SP2 Beta1
Storage Number	400 GB, Intel S3710 SSD	400 GB, Intel S3710 SSD	400 GB, Intel S3710 SSD	400 GB, Intel S3710 SSD
Other Configurations		GVPRCRB1.86B.0009.R02.160407 1525, Quad/Flat	GVPRCRB1.86B.0009.R02.16040715 25, Quad/Flat	GVPRCRB1.86B.0010.R00.160325173 2, Quad/Flat
HT	No	Yes	Yes	Yes
Turbo	Yes	Yes	Yes	Yes
Computer Type	server	server	server	server
Benchmark	DGEMM - GF/s	DGEMM - GF/s	DGEMM - GF/s	DGEMM - GF/s
Data Source	Request Number: 2356	Request Number: 2356	Request Number: 2356	Request Number: 2356
Configuration Summary	1-Node, 2 x Intel® Xeon® Processor E5-2697 v4 on Grantley-EP (Wellsburg) with 128 GB Total Memory on Red Hat Enterprise Linux* 7.2-kernel 3.10.0-327 using (No Software). Data Source: Request Number: 2356, Benchmark: DGEMM, Score: 1279.25 Higher is better	1-Node, 1 x Intel® Xeon Phi™ Processor 7210 (16GB, 1.30 GHz, 64 core) on Groveport (Knights Landing) with 192 GB Total Memory on SUSE Linux Enterprise Server* 12 using (No Software). Data Source: Request Number: 2356, Benchmark: DGEMM, Score: 1976.64 Higher is better	1-Node, 1 x Intel® Xeon Phi™ Processor 7230 (16GB, 1.30 GHz, 64 core) on Groveport (Knights Landing) with 192 GB Total Memory on SUSE Linux Enterprise Server* 12 using (No Software). Data Source: Request Number: 2356, Benchmark: DGEMM, Score: 1999.07 Higher is better	1-Node, 1 x Intel® Xeon Phi™ Processor 7250 (16GB, 1.40 GHz, 68 core) on Groveport (Knights Landing) with 192 GB Total Memory on SUSE Linux Enterprise Server* 12 using (No Software). Data Source: Request Number: 2356, Benchmark: DGEMM, Score: 2057.83 Higher is better

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Core Libraries

PETSc

Intel® Xeon® processor E5-2697 v4: Dual Socket Intel® Xeon® processor E5-2697 v4 2.3 GHz (Turbo OFF), 18 Cores/Socket, 36 Cores, 72 Threads (HT on), DDR4 128GB, 2400 MHz, Red Hat 6.5.

Intel® Xeon Phi™ processor 7250: Intel® Xeon Phi™ processor 7250 68 core, 272 threads, 1400 MHz core freq. Turbo mode ON, 1700 MHz uncore freq., MCDRAM 16 GB 7.2 GT/s, BIOS 10R00, DDR4 96GB 2400 MHz, Red Hat 7.2, quad cluster mode, MCDRAM flat memory mode. Adams Pass Platform BMC version 12.9511 FRU/SDR Package 1.10. 1 1-TB SATA disk installed.

Earth Science and Weather

Danish Meteorological Institute HIROMB-BOOS-Model

Intel® Xeon® processor E5-2697 v4: Dual Socket Intel® Xeon® processor E5-2697 v4 2.3 GHz (Turbo ON), 18 Cores/Socket, 36 Cores, 72 Threads (HT on), DDR4 128GB, 2400 MHz, Red Hat 6.7.

Intel® Xeon Phi™ processor 7250: Intel® Xeon Phi™ processor 7250 68 core, 272 threads, 1400 MHz core freq. (Turbo OFF), 1700 MHz uncore freq., MCDRAM 16 GB 7.2 GT/s, BIOS 09D10, DDR4 96GB 2400 MHz, Red Hat 6.7 (Santiago), quad cluster mode, MCDRAM flat memory mode.

MPAS Ocean 4.0*

Intel® Xeon® processor E5-2697 v4: Dual Socket Intel® Xeon® processor E5-2697 v4 2.3 GHz, Turbo mode ON, 18 Cores/Socket, 72 Threads (HT on), DDR4 128GB, 2400 MHz, Red Hat 7.2. BIOS 86B0271.R00. Wildcat Pass Platform BMC version 1.33.9832 FRU/SDR Package 1.09. 1 1-TB SATA disk (Western Digital WD1003FZEX-00MK2A0) installed.

Intel® Xeon Phi™ processor 7250: Intel® Xeon Phi™ processor 7250 68 core, 272 threads, 1400 MHz core freq. Turbo mode ON, 1700 MHz uncore freq., MCDRAM 16 GB 7.2 GT/s, BIOS 10R00, DDR4 96GB 2400 MHz, Red Hat 7.2, quad cluster mode, MCDRAM Cache memory mode. Adams Pass Platform BMC version 12.9511 FRU/SDR Package 1.10. 1 1-TB SATA disk (Western Digital WD1003FZEX-00MK2A0) installed.

Recipe for The Intel® Xeon Phi™ processor:

1. Building all the 3rd party libraries (NetCDF, ParallelNetCDF, PIO) are same as Intel Xeon.
2. Compilation of MPAS: In the Makefile, for ifort target, -xMIC-AVX512 is used as additional flag.

```
"FFLAGS_OPT = -O3 -xCORE-AVX2 -convert big_endian -FR"
```

```
"CFLAGS_OPT = -O3 -xCORE-AVX2 "
```

```
"CXXFLAGS_OPT = -O3 -xCORE-AVX2 "
```

Command: make ifort CORE=ocean MODE=forward

3. Running instructions:

Intel® Xeon Phi™ processor memory mode: cache, cluster mode: quadrant.

Following environment variables should be set:

```
export I_MPI_PIN_DOMAIN=core
```

```
export I_MPI_FABRICS=shm
```

```
ulimit -s unlimited
```

1 MPI rank/core is used for 68 core Intel® Xeon Phi™ processor 7250. "mpirun" command is same as the Intel Xeon processor.

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Earth Science and Weather, continued

NEMO

Intel® Xeon® processor E5-2697 v4: Dual Socket Intel® Xeon® processor E5-2697 v4 2.3 GHz, Turbo OFF, 18 Cores/Socket, 36 Cores, 36 Threads (HT off), DDR4 128GB, 2400 MHz, Red Hat 7.2.

Intel® Xeon Phi™ processor 7250: Intel® Xeon Phi™ processor 7250 68 core, 272 threads, 1400 MHz core freq., Turbo OFF, 1700 MHz uncore freq., MCDRAM 16 GB 7.2 GT/s, BIOS 10R00, DDR4 96GB 2400 MHz, quad cluster mode, MCDRAM cache memory mode, Memory mode = quadrant, Red Hat 7.2.

Weather & Research Forecast Model*

Intel® Xeon® processor E5-2697 v4: Dual Socket Intel® Xeon® processor E5-2697 v4 2.3 GHz, 18 Cores/Socket, 36 Cores, 72 Threads (HT and turbo on), DDR4 128GB, 2400 MHz, Red Hat 6.7.

Intel® Xeon Phi™ processor 7250: Intel® Xeon Phi™ processor 7250 68 core, 272 threads, 1400 MHz core freq. (turbo on), 1700 MHz uncore freq., MCDRAM 16 GB 7.2 GT/s, BIOS 09D10, DDR4 96GB 2400 MHz, Red Hat 6.7 (Santiago), quad cluster mode, MCDRAM flat memory mode.

Energy

ISO3D

Intel® Xeon® processor E5-2697 v4: Dual Socket Intel® Xeon® processor E5-2697 v4 2.3 GHz, 18 Cores/Socket, 36 Cores, 72 Threads (HT ON, Turbo OFF), DDR4 128GB, 2400 MHz, Oracle Linux Server release 6.7.

Intel® Xeon Phi™ processor 7210: Intel® Xeon Phi™ processor 7210 64 core, 256 threads, 1300 MHz core freq. (HT and Turbo ON), 1600 MHz uncore freq., MCDRAM 16 GB 6.4 GT/s, BIOS 10D28, DDR4 96GB 2133 MHz, CentOS 7.2, quad cluster mode, MCDRAM flat memory mode, MPSP 1.3.1.

Intel® Xeon Phi™ processor 7250: Intel® Xeon Phi™ processor 7250 68 core, 272 threads, 1400 MHz core freq. (HT and Turbo ON), 1700 MHz uncore freq., MCDRAM 16 GB 7.2 GT/s, BIOS 10D28, DDR4 96GB 2400 MHz, CentOS 7.2, quad cluster mode, MCDRAM flat memory mode, MPSP 1.3.1.

Financial Services

STACA2

STAC SUT ID INTC160428 - Intel® Xeon Phi™ processor 7250: Intel® Xeon Phi™ processor 7250 68 core, 272 threads, 1400 MHz core freq. (Turbo ON), MCDRAM 16 GB 7.2 GT/s, DDR4 96GB 2400 MHz, CentOS 7.2, quadrant cluster mode, flat memory mode. See www.STACresearch.com/INTC160428.

STAC SUT ID INTC160314 - Intel® Xeon® processor E5-2699 v4: Supermicro* Superserver SYS-1028GR-TR, Dual Socket Intel® Xeon® processor E5-2699 v4 2.2 GHz (Turbo ON), 22 (HT on) Cores/Socket, 44 Cores, 88 Threads, DDR4 256GB, 2133 MHz, Red Hat 7.2. See www.STACresearch.com/INTC160314.

STAC SUT ID IBM150305 - IBM POWER8™: IBM Power System* sever, 2x 12-core POWER8* @ 3.52 GHz, 24 cores / 192 Threads (only 96 used), 1 TB DDR3, RH 7.0, IBM XL C/C++ for Linux v13.1. See www.STACresearch.com/IBM150305.

STAC SUT ID NVDA141116 - NVidia® Tesla® K80: Supermicro* SYS-2027GR-TRHF, Intel Xeon E5-2690 v2, 3.00GHz, 128GB DDR3, 2XGK210B PCI Express* GEN3 Dual GPU 2496 Processor cores Base Clock 560MHz Boost Range 562-875MHz 12GB GDDR5 Memory Clock 2.5GHz. NVIDIA CUDA* 6.5 (Driver 340.58), CentOS 6.6 + Intel® Xeon® processor E5-2690 v2: 10 Cores/Socket, 20 Cores (HT off), DDR3 128GB. See www.STACresearch.com/NVDA141116.

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Life Sciences

GROMACS

Intel® Xeon® processor E5-2697 v4: Dual Socket Intel® Xeon® processor E5-2697 v4 2.3 GHz (Turbo ON), 18 Cores/Socket, 36 Cores, 72 Threads (HT on), Wildcat Pass, DDR4 128GB, 2400 MHz, BMC ver. 1.33.9832, Red Hat 7.2, BIOS 86B0271.R00, FRU/SDR Package 1.09, kernel 3.10.0-327.el7.x86_64, 1 1.0 TB SATA drive WD1003FZEX-00MK2A0, Idle Power measurement 89W.

Intel® Xeon Phi™ processor 7250: Intel® Xeon Phi™ processor 7250 68 core, 272 threads, 1400 MHz core freq. 6 x 16 GB 2400 MHz DDR4, BMC ver. 12.951, Red Hat 7.2, BIOS 10R00, FRU/SDR Package 1.1, kernel 3.10.0-327.el7.x86_64, 1 1.0 TB SATA drive WD1003FZEX-00MK2A0, Idle Power measurement 125W.

LAMMPS Coarse-Grain Water Simulation*

Intel® Xeon® processor E5-2697 v4: Dual Socket Intel® Xeon® processor E5-2697 v4 2.3 GHz, 18 Cores/Socket, 36 Cores, 72 Threads (HT and turbo on), DDR4 128GB, 2400 MHz, Red Hat 6.7, Wildcat Pass Motherboard, BMC 1.33.9832, FRU/SDR Package 1.09, 1.0 TB SATA Western Digital* 1003FZEX-00MK2A0 System Disk, 448W mean power consumption for LAMMPS water simulation, Scalability tests performed on nodes with Intel® Omni-Path Host Fabric Interface Adapter 100 Series 1 Port PCIe x16.

Intel® Xeon Phi™ processor 7250: Intel® Xeon Phi™ processor 7250, 68 core, 272 threads, 1400 MHz core freq. (turbo on), 1700 MHz uncore freq., MCDRAM 16 GB 7.2 GT/s, BIOS 09D10, DDR4 96GB 2400 MHz, Red Hat 6.7 (Santiago), quad cluster mode, MCDRAM flat memory mode, Adams Pass Motherboard, BMC 12.951, FRU/SDR Package 1.1, 1.0 TB SATA drive Western Digital* 1003FZEX-00MK2A0 System Disk, 378W mean power consumption for LAMMPS water simulation, Scalability tests performed on nodes with Intel® Omni-Path Host Fabric Interface Adapter 100 Series 1 Port PCIe x16.

NVIDIA Tesla K80*: Dual Socket Intel® Xeon® processor E5-2697 v4 2.3 GHz, 18 Cores/Socket, 36 Cores, 72 Threads (HT and turbo on), DDR4 128GB, 2400 MHz, Red Hat 7.2, Super Micro* SuperServer 1028GR-TR, Bios Version 2.0a, Super Micro* X10DRG-H Motherboard, CSE-118GHTS-R1K66BP FRU, 500GB SATA Seagate* ST9500423AS System Disk, NVIDIA Tesla* K80 GPU, NVIDIA CUDA* 7.5.17 (Driver: 352.39), ECC enabled, persistence mode enabled. Number of MPI tasks on host varied to give best performance. CUDA MPS* used where possible. 608W mean power consumption for LAMMPS water simulation.

LAMMPS CONFIGURATION: 22 Mar 2016 (Git Hash: 154eb1f886fde), Intel® Compiler 16.0.2, Intel® MPI 5.1.2.150, Optimization Flags: "-O2 -fp-model fast=2 -no-prec-div -qoverride-limits"

Nanoscale Molecular Dynamics program* (perf./watt)

Intel® Xeon® processor E5-2697 v4: Dual Socket Intel® Xeon® processor E5-2697 v4 2.3 GHz (Turbo OFF), 18 Cores/Socket, 36 Cores, 72 Threads (HT on), DDR4 8x16GB 2400 MHz, BIOS 86B0271.R00, Motherboard Wildcat Pass, BMC 1.33.9832, FRU/SDR package 1.09, Red Hat 7.2 kernel 3.10.0-327.el7.x86_64, System Disk 1 1.0 TB SATA drive WD1003FZEX-00MK2A0, coprocessor N/A, Idle Power measurement 129W, energy usage to complete benchmark calculation in Joules: APOA1 – 4,565; STMV – 61,138.

Intel® Xeon Phi™ processor 7250: Intel® Xeon Phi™ processor 7250 68 core, 272 threads, 1400 MHz core freq. (Turbo ON), 1700 MHz uncore freq., DDR4 6x16GB 2400 MHz quadrant cluster mode, MCDRAM 16 GB 6.4 GT/s flat memory mode, BIOS 10R00, Motherboard Adams Pass, Sleds per Chassis 1, BMC 12.951, FRU/SDR package 1.1, Red Hat 7.2 kernel 3.10.0-327.el7.x86_64, System Disk 1 1.0 TB SATA drive WD1003FZEX-00MK2A0, coprocessor N/A, Idle Power measurement 89W, energy usage to complete benchmark calculation in Joules: APOA1 – 3,899; STMV – 43,218.

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Life Sciences, continued

ROME*/SML

Intel® Xeon® processor E5-2697 v4: Dual socket Intel® Xeon® processor E5-2697 v4, @2.3GHz 145W, 18 cores/socket HT enabled, 128GB RAM, Red Hat® Enterprise Linux® Server release 6.7 (Santiago).

Intel® Xeon Phi™ processor 7250: Intel® Xeon Phi™ processor 7250 68 core, 272 threads, 1400 MHz core freq. MCDRAM 16 GB 7.2 GT/s, DDR4 96GB 2400 MHz, Red Hat Enterprise Linux Server release 6.7 (Santiago), quad cluster mode, MCDRAM cache mode.

Workload: provided by Intel® PCCSB, Contact Youdong Mao youdong_mao@dfci.harvard.edu. (Performance data is based on 30 iterations). Workload Descriptions: Inflammasome data: 16306 images of NLRC4/NAIP2 inflammasome with a size of 2502 pixels.

RP-a: 57001 images of proteasome regulatory particles (RP) with a size of 1602 pixels.

RP-b: 35407 images of proteasome regulatory particles (RP) with a size of 1602 pixels.

Manufacturing

NASA OVERFLOW

Intel® Xeon® processor E5-2680 v3: Dual Socket Intel® Xeon® processor E5-2680 v3 2.5 GHz (Turbo ON), 12 Cores/Socket, 24 Cores, 48 Threads (HT on), DDR4 128GB, 2133 MHz, SUSE Linux*.

Intel® Xeon® processor E5-2680 v4: Dual Socket Intel® Xeon® processor E5-2680 v4 2.4 GHz (Turbo ON), 14 Cores/Socket, 28 Cores, 56 Threads (HT on), DDR4 128GB, 2400 MHz, SUSE Linux.

Intel® Xeon Phi™ processor 7250: Intel® Xeon Phi™ processor 7250 68 core, 272 threads, 1400 MHz core freq. (Turbo On), 1700 MHz uncore freq., MCDRAM 16 GB 7.2 GT/s, BIOS 10.R00, DDR4 16GB 2400 MHz, SLES 12 SP1, Quadrant cluster mode, MCDRAM cache mode.

Additional details for OVERFLOW configuration: 34x2 (DLR/F6) and 8x8 (NASrotor) MPIxOMP decomposition on Intel Xeon Phi Processor based system. 24x1 and 28x1 MPIxOMP for Intel Xeon processor based platforms.

OpenFOAM

Intel® Xeon® processor E5-2697 v4: Dual Socket Intel® Xeon® processor E5-2697 v4 2.3 GHz (Turbo ON), 18 Cores/Socket, 36 Cores, 72 Threads (HT on), DDR4 128GB, 2400 MHz, Red Hat 6.5.

Intel® Xeon Phi™ processor 7250: Intel® Xeon Phi™ processor 7250 68 core, 272 threads, 1400 MHz core freq. (Turbo ON), 1700 MHz uncore freq., MCDRAM 16 GB 7.2 GT/s, BIOS 09D10, DDR4 96GB 2400 MHz, Red Hat 6.7 (Santiago), quad cluster mode, MCDRAM flat memory mode; MCDRAM cache memory mode used for the 20M Cell Motorbike benchmark.

OpenFOAM software: Development version from GitHub (<https://github.com/OpenFOAM/OpenFOAM-dev>, version-3.0.0-480-gf8f835c*), Intel® MPI Library Version 5.1.3 Build 20160120, Intel® Compiler Version 16.0.1 Build 20151021.

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Material Sciences

BerkeleyGW (Sigma Phase) Benzene

Intel® Xeon® processor E5-2697 v4: Dual Socket Intel® Xeon® processor E5-2697 v4 2.3 GHz (Turbo ON), 18 Cores/Socket, 36 Cores, 72 Threads (HT on), Wildcat Pass, DDR4 128GB, 2400 MHz, BMC ver. 1.33.9832, Red Hat 7.2, BIOS 86B0271.R00, FRU/SDR Package 1.09, kernel 3.10.0-327.el7.x86_64, 1 1.0 TB SATA drive WD1003FZEX-00MK2A0, Idle Power measurement 89W.

Intel® Xeon Phi™ processor 7210: Intel® Xeon Phi™ processor 7250 64 core, 256 threads, 1300 MHz core freq. 6 x 16 GB 2400 MHz DDR4, Memory mode = cache, Cluster mode=quadrant, BMC ver. 12.951, Red Hat 7.2, BIOS 10R00, FRU/SDR Package 1.1, kernel 3.10.0-327.el7.x86_64, 1 1.0 TB SATA drive WD1003FZEX-00MK2A0, Idle Power measurement 122W.

Intel® Xeon Phi™ processor 7250: Intel® Xeon Phi™ processor 7250 68 core, 272 threads, 1400 MHz core freq. 6 x 16 GB 2400 MHz DDR4, Memory mode = cache, Cluster mode=quadrant, BMC ver. 12.951, Red Hat 7.2, BIOS 10R00, FRU/SDR Package 1.1, kernel 3.10.0-327.el7.x86_64, 1 1.0 TB SATA drive WD1003FZEX-00MK2A0, Idle Power measurement 125W.

Quantum ESPRESSO*

Intel® Xeon® processor E5-2697 v4: Dual Socket Intel® Xeon® processor E5-2697 v4 2.3 GHz, 18 cores/socket, 36 cores, 72 threads (HT and Turbo ON), DDR4 64 GB, 2400 MHz, RHEL 6.7.

Intel® Xeon Phi™ processor 7250: Intel® Xeon Phi™ processor 7260, 68 core (272 threads), 1.4 GHz base core freq. (Turbo ON), 1.7 GHz uncore freq., MCDRAM 16 GB 7.2 GT/s, BIOS GVPRCB1.86B.0010.R00, DDR4 96 GB 2400 MHz, quadrant cluster mode, MCDRAM cache memory mode, RHEL 6.7, MPSP 1.3.0, Intel Compiler 2017.

Building Quantum ESPRESSO:

Configure for Intel Compiler and MKL according to http://www.quantum-espresso.org/wp-content/uploads/Doc/user_guide/node14.html#SECTION00037670000000000000

Modify defines in make.sys to

```
-D__INTEL -D__OPENMP -D__DFTI -D__MPI -D__PARA -D__ELPA -D__SCALAPACK
```

Add -xMIC-AVX512 to CFLAGS and FFLAGS

Running Quantum ESPRESSO:

Intel® Xeon Phi™ processor 7250

```
mpirun -n 68 <PATH_TO_BINARY>/pw.x -nk 2 -nt 34 -nd 25 -i ausurf.in
```

Intel® Xeon® processor E5-2697 v4:

```
mpirun -n 36 <PATH_TO_BINARY>/pw.x -nk 1 -nt 36 -nd 36 -i ausurf.in
```

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Physics

Cloverleaf*

Intel® Xeon® processor E5-2697 v4: Dual Socket Intel® Xeon® processor E5-2697 v4 2.3 GHz (Turbo ON), 18 Cores/Socket, 36 Cores, 72 Threads (HT on), DDR4 128GB, 2400 MHz, Red Hat 6.5.

Intel® Xeon Phi™ processor 7210: Intel® Xeon Phi™ processor 7210 64 core, 256 threads, 1300 MHz core freq. (Turbo OFF), 1600 MHz uncore freq., MCDRAM 16 GB 6.4 GT/s, BIOS 09D10, DDR4 96GB 2133 MHz, Red Hat 6.7 (Santiago), quad cluster mode, MCDRAM flat memory mode.

Intel® Xeon Phi™ processor 7250: Intel® Xeon Phi™ processor 7250 68 core, 272 threads, 1400 MHz core freq. (Turbo OFF), 1700 MHz uncore freq., MCDRAM 16 GB 7.2 GT/s, BIOS 09D10, DDR4 96GB 2400 MHz, Red Hat 6.7 (Santiago), quad cluster mode, MCDRAM flat memory mode.

Trinity MILC*

Intel® Xeon® processor E5-2697 v4: Dual Socket Intel® Xeon® processor E5-2697 v4 2.3 GHz (Turbo ON), 18 Cores/Socket, 36 Cores, 72 Threads (HT on), DDR4 128GB, 2400 MHz, Red Hat 6.5.

Intel® Xeon Phi™ processor 7250: Intel® Xeon Phi™ processor 7250 68 core, 272 threads, 1400 MHz core freq. (Turbo OFF), 1700 MHz uncore freq., MCDRAM 16 GB 7.2 GT/s, BIOS 09D10, DDR4 96GB 2400 MHz, Red Hat 6.7 (Santiago), quad cluster mode, MCDRAM flat memory mode.

Visualization

Embree*

Intel® Xeon Phi™ processor 7250: Intel® Xeon Phi™ processor 7250, MCDRAM 16 GB RAM 96 GB 6*16GB 2400MHz, Reg ECC DDR4 BIOS Configuration: L2 HWP patches (same as targeted for production) Software Details: Intel Compiler Version 16.0.1, ISPC Compiler Version 1.9, Embree Version 2.9.0, OS / Kernel CentOS 7.1.

NVIDIA* GPU: NVIDIA Optix* System: Xeon DP Intel® Xeon® processor E5-2699 v3 LGA2011 2.3GHz 45MB 145W Dual socket 18 core RAM 128 GB total 8*16GB 2133MHz Reg ECC DDR4 BIOS SE5C610.86B.01.01.0005.101720141054 Intel SSDSA2M160G2GC, 1x160 GB SATA SSD, NVIDIA* GeForce* GTX* Titan X 3072 CUDA Cores 12GB memory Software Details: CUDA Version 7.5. OptiX Version 3.9.0 NVIDIA Driver Version 346.46 OS / Kernel CentOS release 6.6 / 2.6.32-504.23.4.el6.x86_64.

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