



# INTEL® XEON PHI™ PROCESSOR (CODENAMED KNIGHTS LANDING) SOFTWARE ECOSYSTEM MOMENTUM GUIDE





# INTEL® XEON PHI™ PROCESSOR

## A HIGHLY-PARALLEL CPU THAT TRANSCENDS GPU ACCELERATORS

### No PCIe Dependency

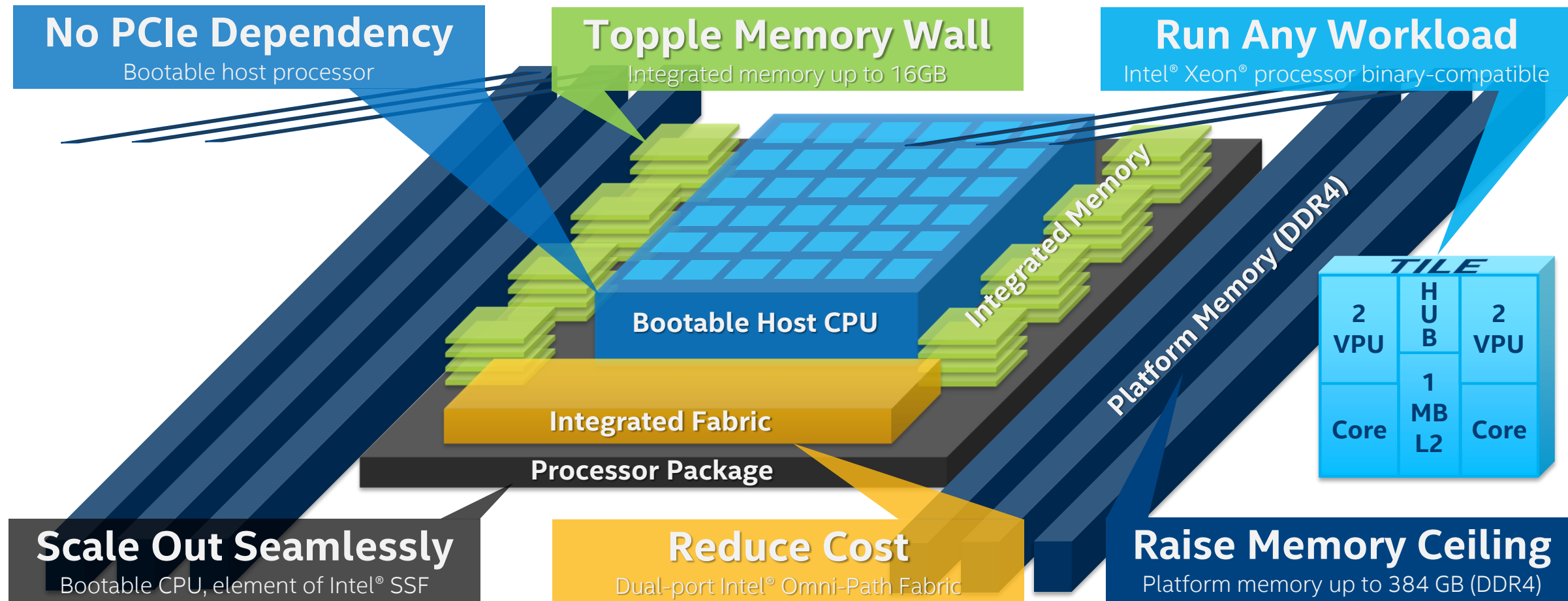
Bootable host processor

### Topple Memory Wall

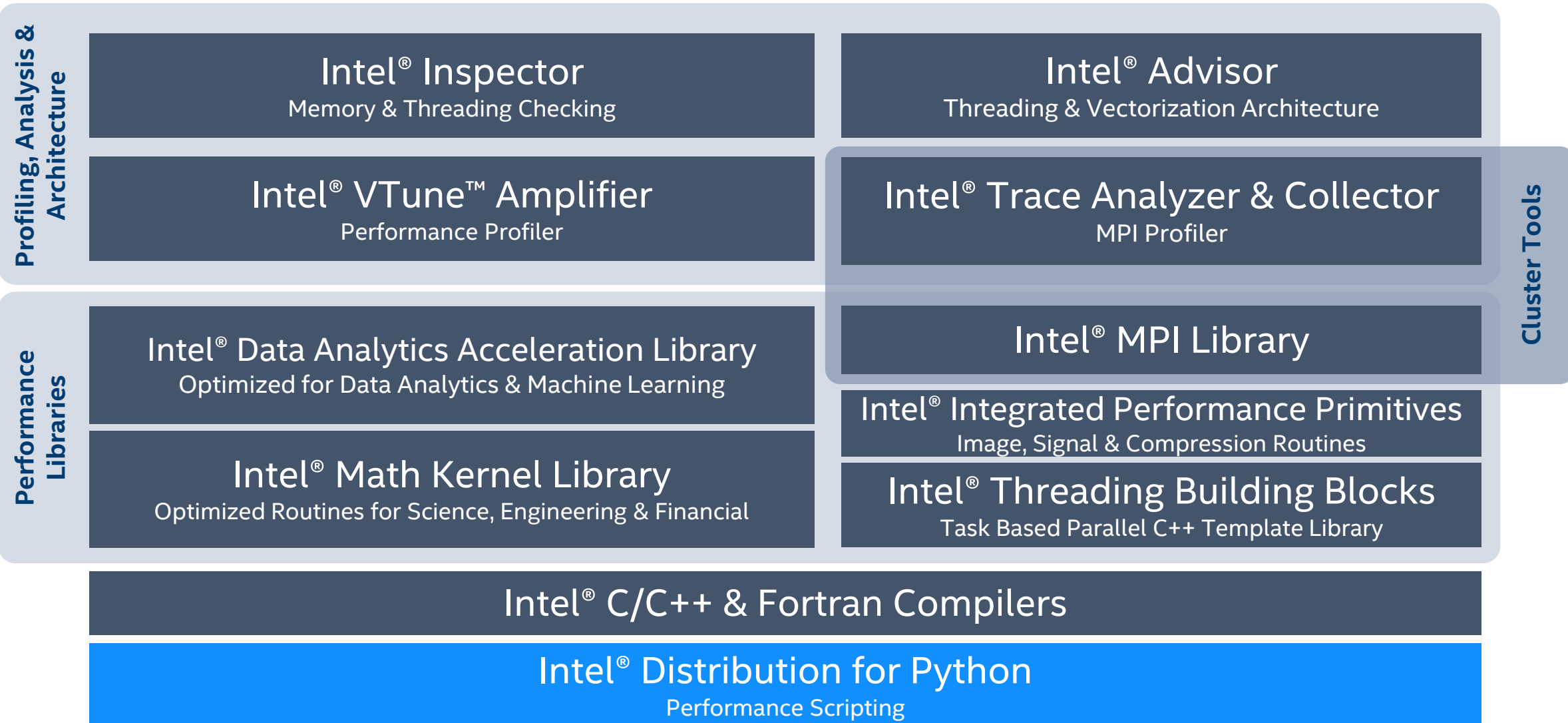
Integrated memory up to 16GB

### Run Any Workload

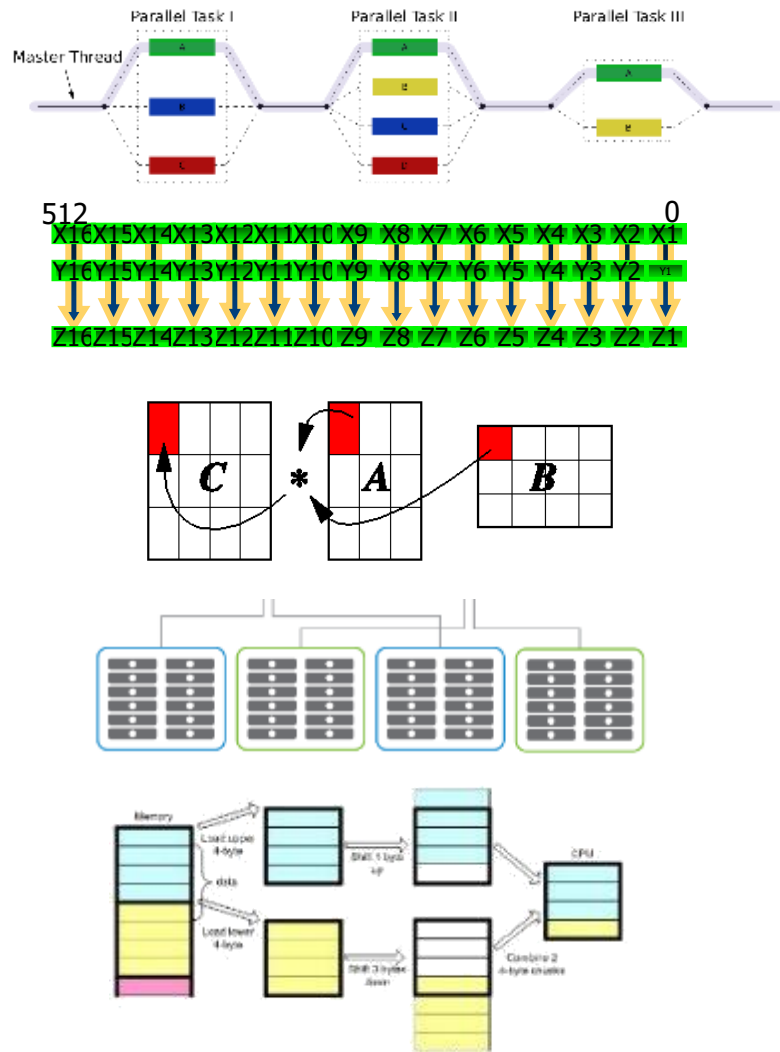
Intel® Xeon® processor binary-compatible



# Intel® Parallel Studio XE



# What is “Modernized” Code?



	What	Defined	Tools of the trade
1	Thread Scaling	Increase concurrent thread use across coherent shared memory	OpenMP, TBB, Cilk Plus
2	Vector Scaling	Use many wide-vector (512-bit) instructions	Vector loops, vector functions, array notations
3	Cache Blocking	Use algorithms to reduce memory bandwidth pressure and improve cache hit rate	Blocking algorithms
4	Fabric Scaling	Tune workload to increased node count	MPI
5	Data Layout	Optimize data layout for unconstrained performance	AoS→SoA, directives for alignment

# Next Steps for Knights Landing Enablement

Your Code



**Modernize Code** using Intel® Xeon Phi™ coprocessor (threading, vectorization, cache-blocking, fabric scaling, data layout)



## Evaluate Code Modernization

- Plot OpenMP thread scaling (concurrency)
- Plot performance vs. SIMD vector length (profitability)
- Plot performance vs # ranks/node (scalability)
- Use [Intel® Parallel Studio XE 2017 tools](#) to further profile and optimize your code

## Code Modernization Enablement Program

**SPECIAL OFFER**



**ACME**  
MICRO SYSTEMS

advanced clustering  
technologies, inc.

**COLFAX**  
Customized Solutions

DACHAN  
CONSULTING GROUP

**EXXACT**

**FUJITSU**

**hp**

**inspur**

**KSC**  
KING STAR COMPUTER  
Rackmount Server Specialist

**Lenovo**

NAVIGARE  
誠海通波

**NorTech**  
www.nor-tech.com

**PowerLeader**  
宝德

**Puget**  
systems

**THINKMATE**  
HIGH PERFORMANCE SOLUTION

No

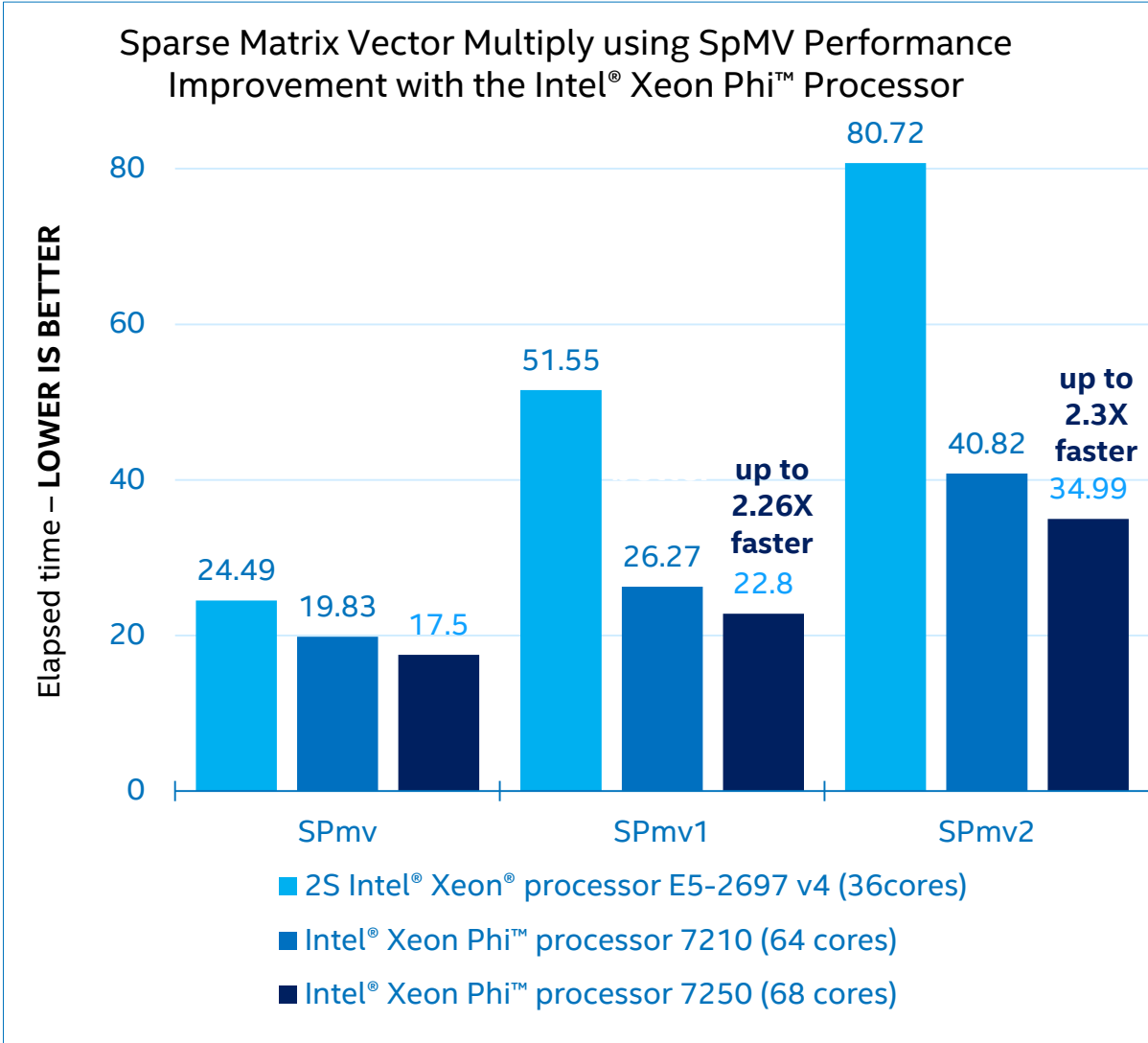
**Performs well?**

Yes

## Prepare for KNL

1. Recompile for KNL (ICC with -MIC-AVX512)
2. Run on [Intel® Software Development Emulator \(SDE\)](#) with Intel® AVX-512 enabled to identify opportunities
3. Experiment with [High Bandwidth \(HBW\) malloc API](#)

# SPARSE MATRIX VECTOR MULTIPLY\*



See next slide for configuration details. SOURCE: INTEL MEASURED RESULTS AS OF APRIL, 2016

*Sparse matrix-vector multiplication (SpMV) is an important kernel for a diverse set of applications in which systems with sparse pattern are used, such as scientific computing, engineering, economic modeling, information retrieval, oil & gas, weather consulting, animation, aero-spacing, recommender systems in machine learning, and earthquake prediction.*

**Application:** Sparse Matrix Vector Multiply

**Code:** [Available here.](#) **Recipe:** In development

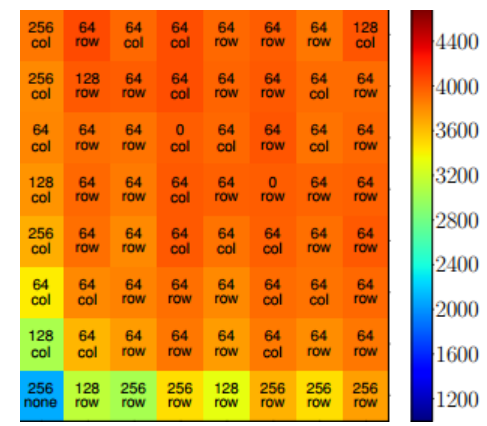


Image Source: US gov.

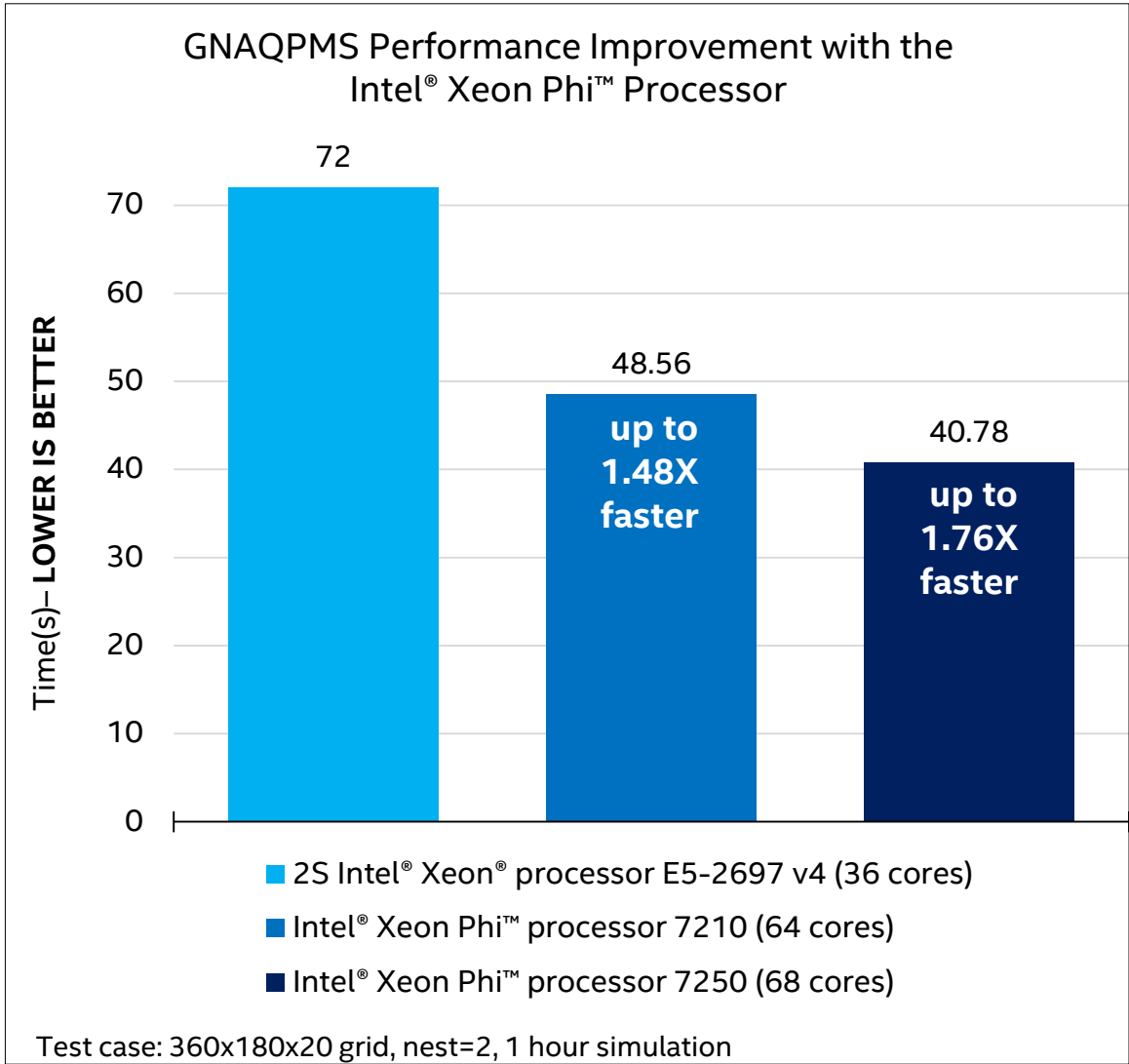
**Value Proposition:** The SpMV benchmark validates the Intel Xeon Phi Processor's generational performance improvement. SpMV is a high-bandwidth LINPACK-like workload for Sparse Matrix Multiplication seen in many codes.

**Results:** Up to 2.3X faster compared to the Intel® Xeon® processor E5-2697 v4.

Software and workloads used in performance tests may have been optimized for performance only on Intel microprocessors. Performance tests, such as SYSmark and MobileMark, are measured using specific computer systems, components, software, operations and functions. Any change to any of those factors may cause the results to vary. You should conduct your own evaluation and performance tests to assist you in fully evaluating your contemplated purchases, including the performance of that product when combined with other products. For more information go to <http://www.intel.com/performance> \*Other names and brands may be claimed as the property of others



# GNAQPMS\*



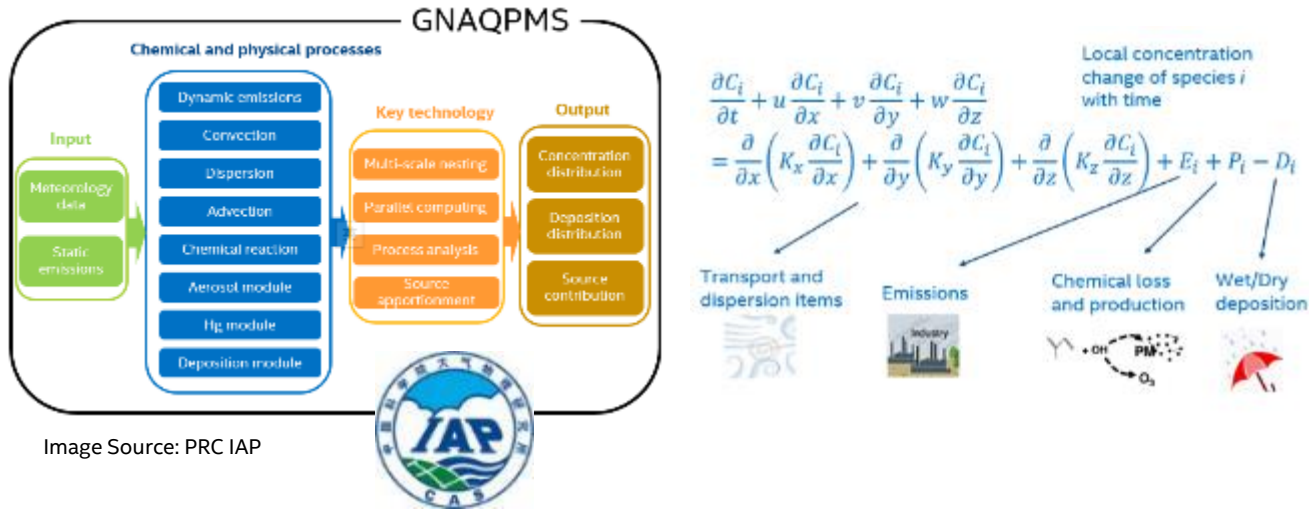
See next slide for configuration details. SOURCE: INTEL MEASURED RESULTS AS OF April,2016

*GNAQPMS is an in-house code from the Institute of Atmospheric Physics (IAP), China Academy of Sciences (CAS), parallelized with hybrid MPI+OpenMP and written in Fortran. The application is the global multi-scale chemistry transport model which can simulate the trace gases including ozone, NO<sub>x</sub>, CO and main aerosols including dusts, sea salts, BC, OC, sulfate and nitrate in multi-special resolutions.*

**Application:** GNAQPMS.

**Code:** In-house code. To access, please contact [tangxiao@mail.iap.ac.cn](mailto:tangxiao@mail.iap.ac.cn)

**Recipe:** Please contact [tangxiao@mail.iap.ac.cn](mailto:tangxiao@mail.iap.ac.cn)



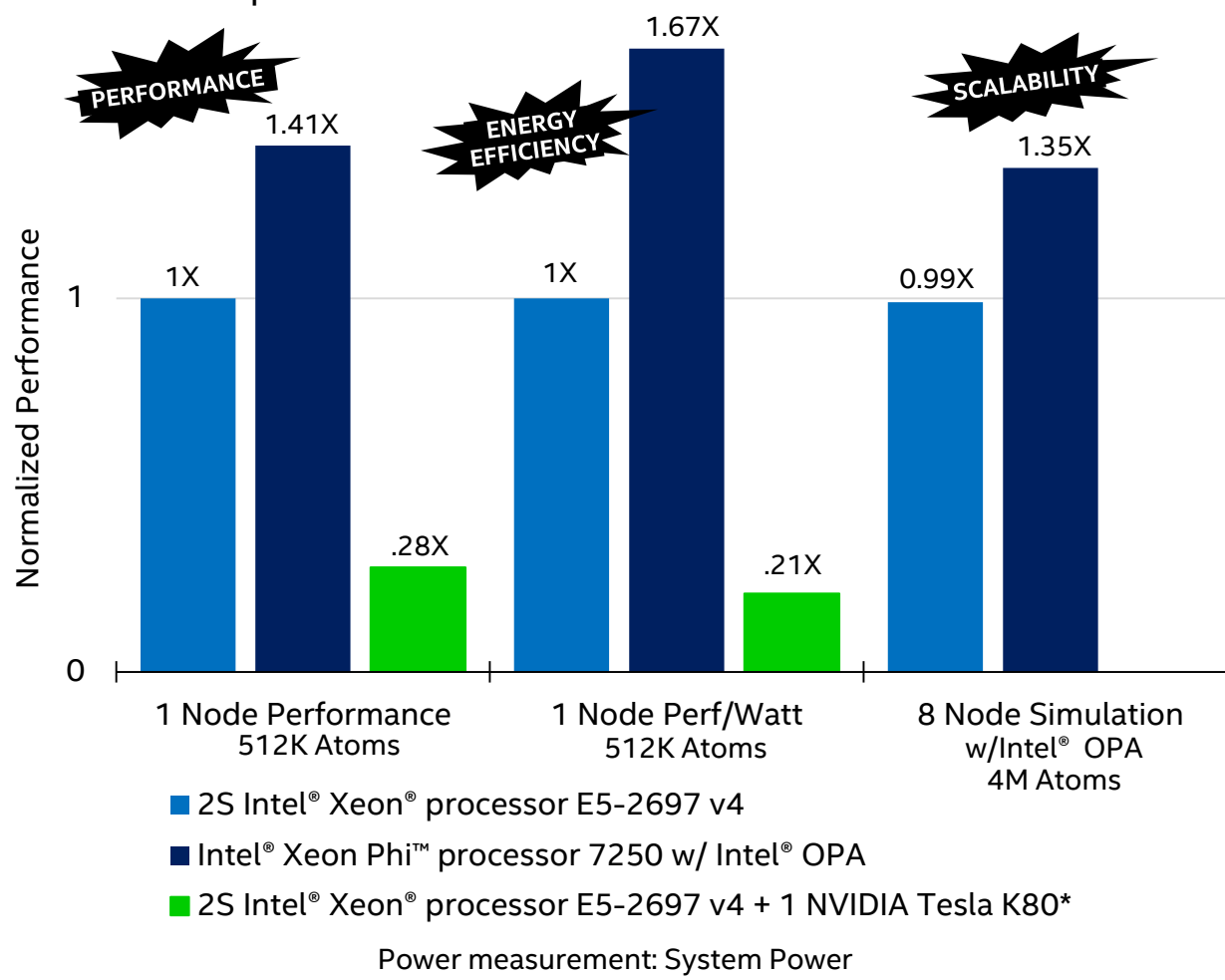
**Value Proposition:** Performance is enhanced by Intel® AVX512.

**Results:** up to 1.76X improved performance by up to 1.76X compared to the Intel® Xeon® processor E5-2697 v4.



# LAMMPS COARSE-GRAIN WATER SIMULATION

LAMMPS Coarse-Grain Water Simulation Performance Improvement with the Intel® Xeon Phi™ Processor

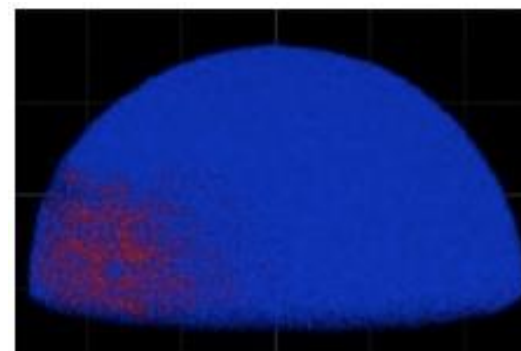


SOURCE: INTEL MEASURED RESULTS AS OF JUNE, 2016

*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.*

**Application:** Coarse-grain water simulation with LAMMPS using Stillinger-Weber potential. More at <http://lammps.sandia.gov/>

**Code:** In main [LAMMPS repository](#). **Recipe:** In development



Ice formation in water droplet wetting a flat surface with coarse-grain model in LAMMPS

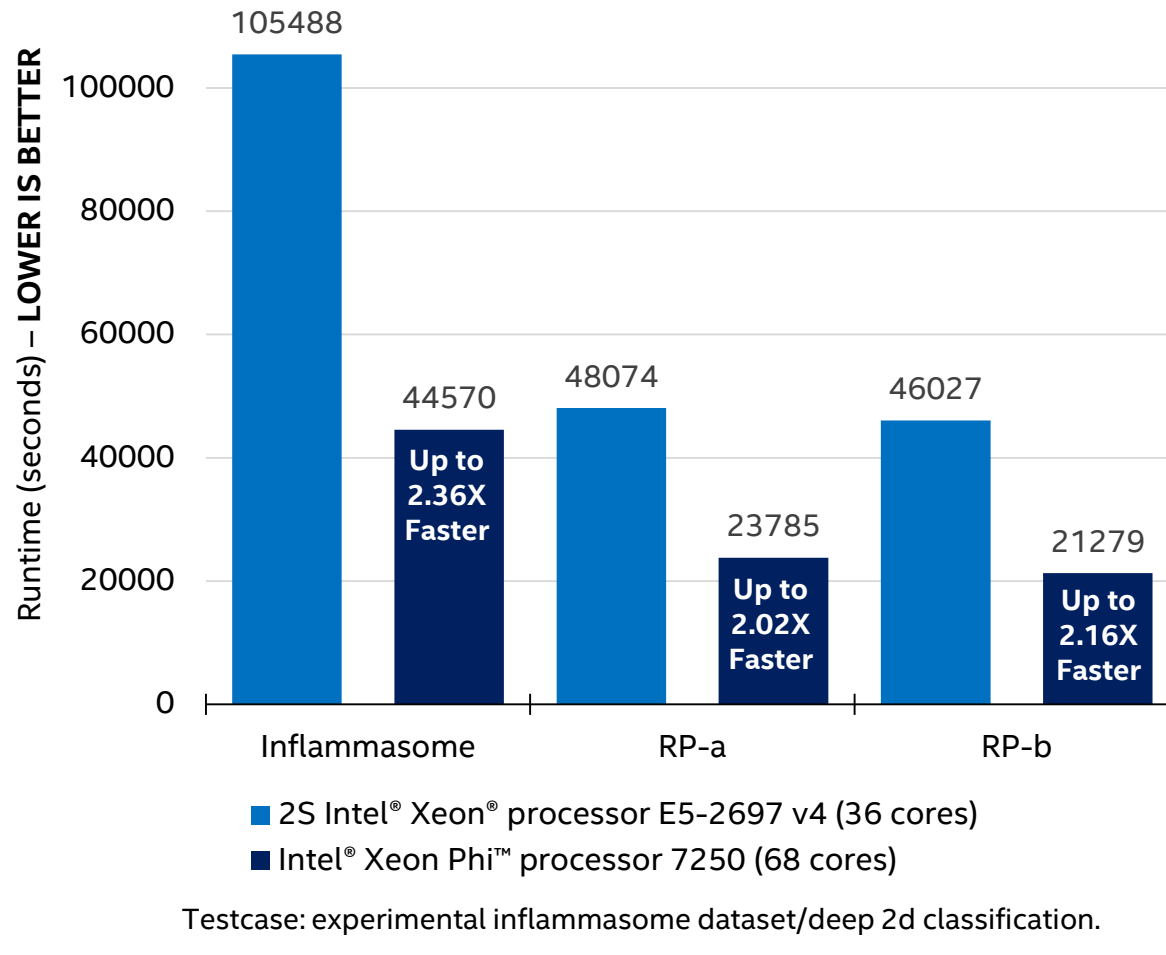
Image Source: Comput. Phys. Commun., 2013, 184, 2785-2793

**Value Proposition:** Intel continues to advance the capabilities of HW and SW necessary for scientists to solve new and more complex problems that could not previously be achieved. The Intel® Xeon Phi™ processor improves power-efficient performance for scalable workloads.

**Results:** Up to 1.41X improved coarse-grain water simulation rate (Performance result) with up to 1.67X performance per watt compared to the Intel® Xeon® processor E5-2697 v4. 96% parallel efficiency with Intel® Omni-Path Architecture (8 Node chart result).



ROME2D ML2D/GTM Performance Improvement with the Intel® Xeon Phi™ Processor



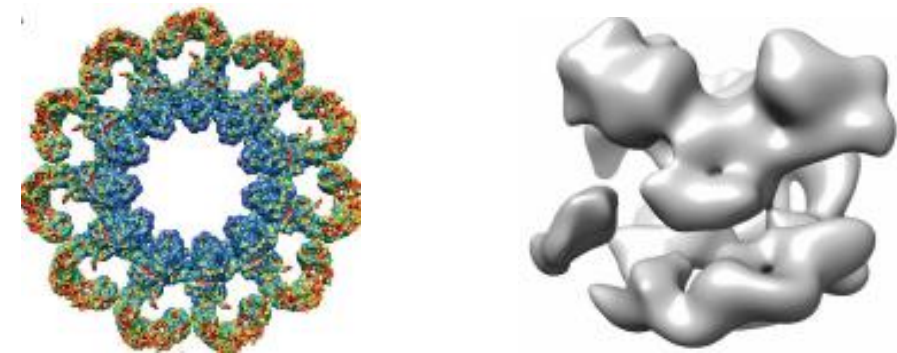
See next slide for configuration details.

SOURCE: INTEL MEASURED RESULTS AS OF JUNE 2016

**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. ROME 1.0 introduces SML (statistical manifold learning)-based deep classification, following MAP-based (maximum a posteriori) image alignment.

**Application:** ROME/SML

**Code:** [Available here](#) **Recipe:** [Available here](#)



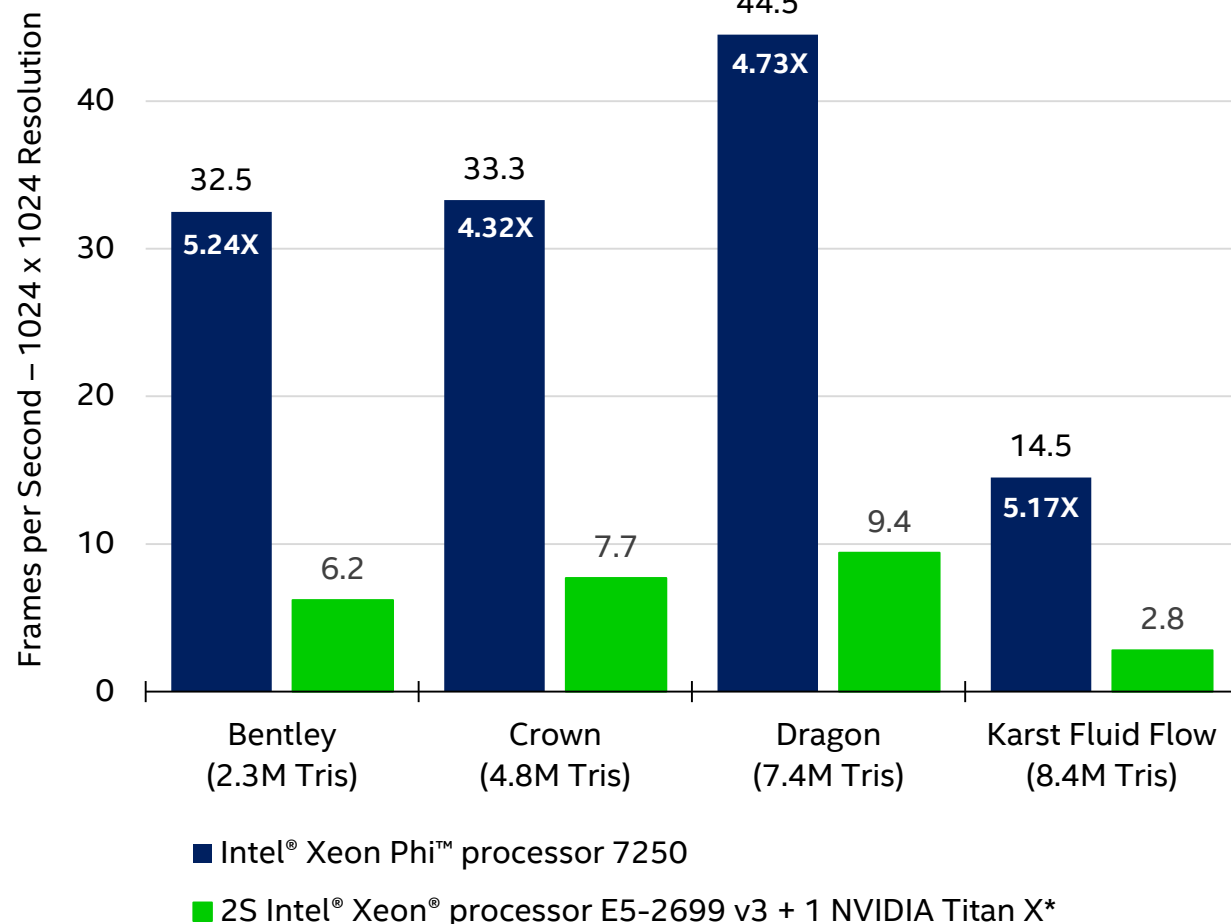
Images Source: L. Zhang, S. Chen, J. Ruan, J. Wu, A.B. Tong, Q. Yin, Y. Li, L. David, A. Lu, W.L. Wang, C. Marks, Q. Ouyang, X. Zhang, Y. Mao\*, H. Wu\*. Cryo-EM structure of the activated NAIP2-NLRC4 inflammasome reveals nucleated polymerization. Science 350, 404-409 (2015).

**Value Proposition:** Intel® Xeon Phi™ processor 7250 enables this application to significantly speed up the deep classification of cryo-EM images and subsequent reconstruction.

**Results:** The Intel® Xeon Phi™ processor 7250 improved performance by up to 2.36X compared to the Intel® Xeon® processor E5-2697 v4.



Embree Performance Improvement with the  
Intel® Xeon Phi™ Processor



*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. More at <http://embree.github.io/>.*

**Application:** Embree v2.9.0

**Code:** [Available here](#) **Recipe:** In development



Image Source: Intel

**Value Proposition:** The kernels are optimized for photo-realistic rendering on the latest Intel® processors with support for SSE, AVX, AVX2, and the 16-wide Xeon Phi™ vector instructions..

**Results:** Up to 5.17X improved compared to the NVIDIA Titan X\*.

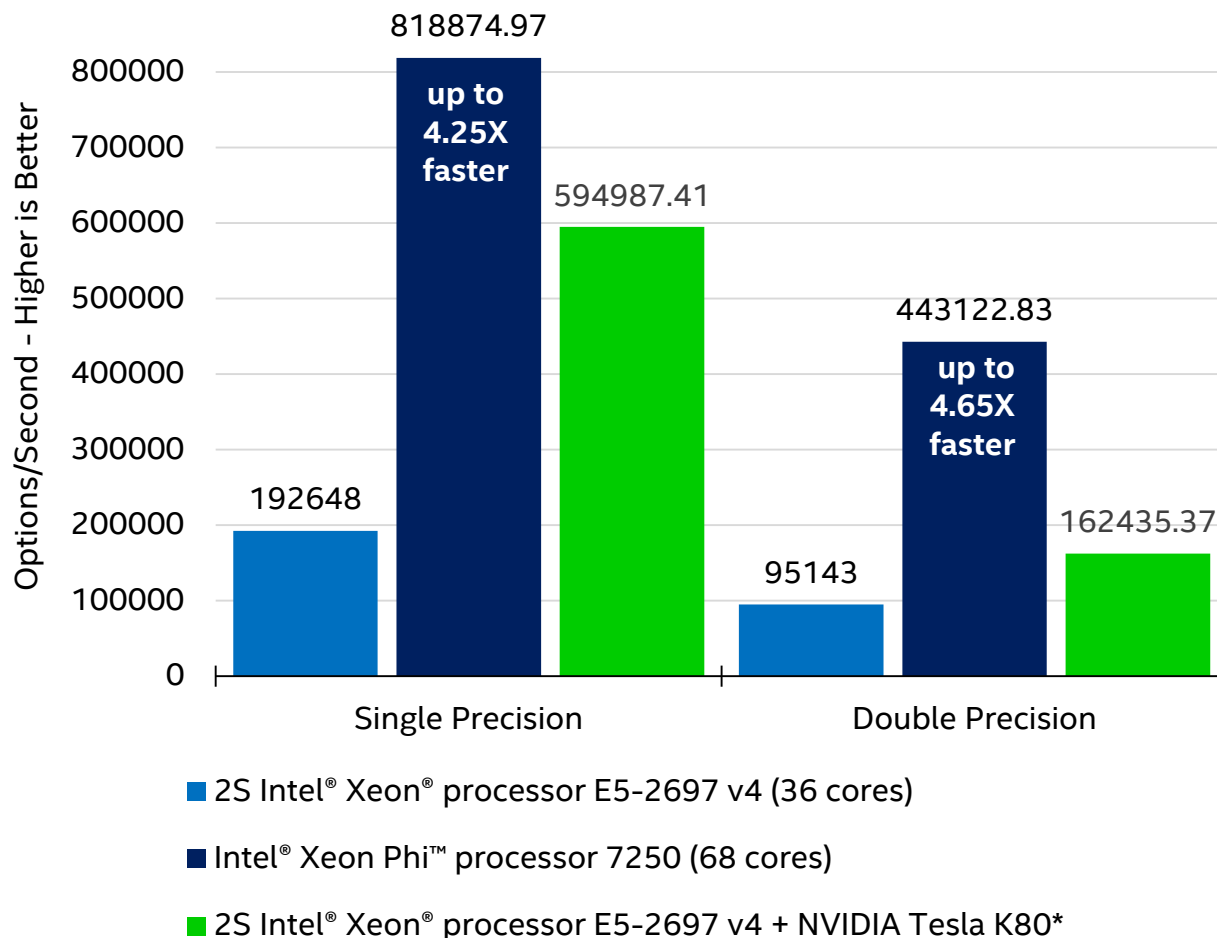
See next slide for configuration details.

SOURCE: INTEL MEASURED RESULTS AS OF JUNE, 2016



# MONTE CARLO EUROPEAN OPTIONS BENCHMARK\*

Monte Carlo European Options Performance Improvement with the Intel® Xeon Phi™ Processor



See slide 27 for configuration details.

SOURCE: INTEL MEASURED RESULTS AS OF MAY, 2016

*Industrial standard benchmark that uses Monte Carlo method for pricing European call options. It pre-generates random numbers then uses them in all options pricing processes. Used by all financial firms to price derivatives with multiple dimensions. Uses the stock price, strike price and time as input streams then creates a call output stream.*

**Application:** Monte Carlo European Options

**Code:** Currently not available **Recipe:** Currently not available

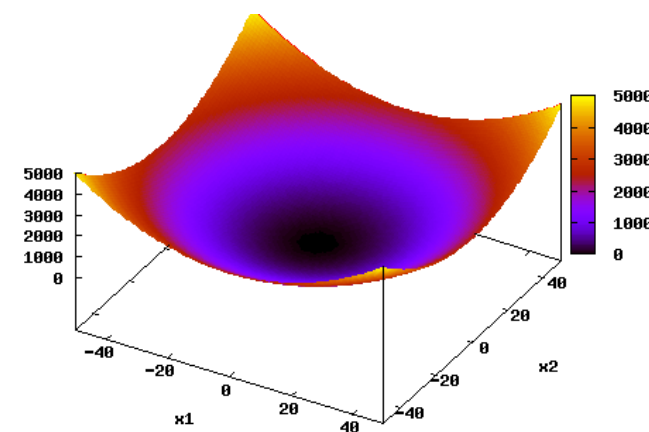


Image Source: US gov.

## Value Proposition:

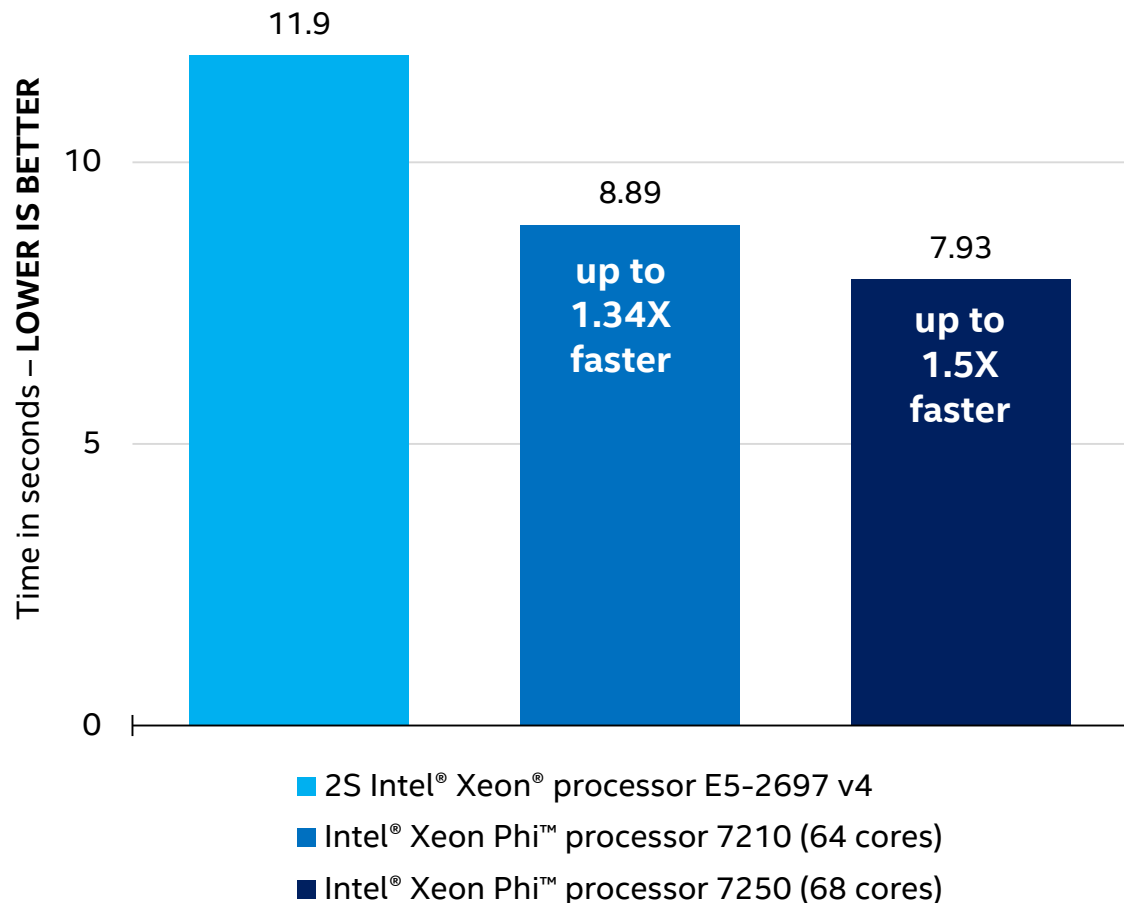
- Foundation of Financial derivatives pricing
- Widely used all over financial libraries
- EMU benefits transcendental functions

**Results:** Up to 4.65X improved Double Precision performance compared to the Intel® Xeon® processor E5-2697 v4 and up to 2.72X better than NVIDIA Tesla\*.



## OPENLB\*

OpenLB Performance Improvement with the Intel® Xeon Phi™ Processor



Testcase: OpenLB with Cylinder2D workload

*The OpenLB project provides a C++ package for the implementation of lattice Boltzmann simulations that is general enough to address a vast range of problems in computational fluid dynamics. The package is mainly intended as a programming support for researchers and engineers who simulate fluid flows by means of a Lattice Boltzmann method.*

**Application:** OpenLB

**Code:** [Available here](#) **Recipe:** [Available here](#)

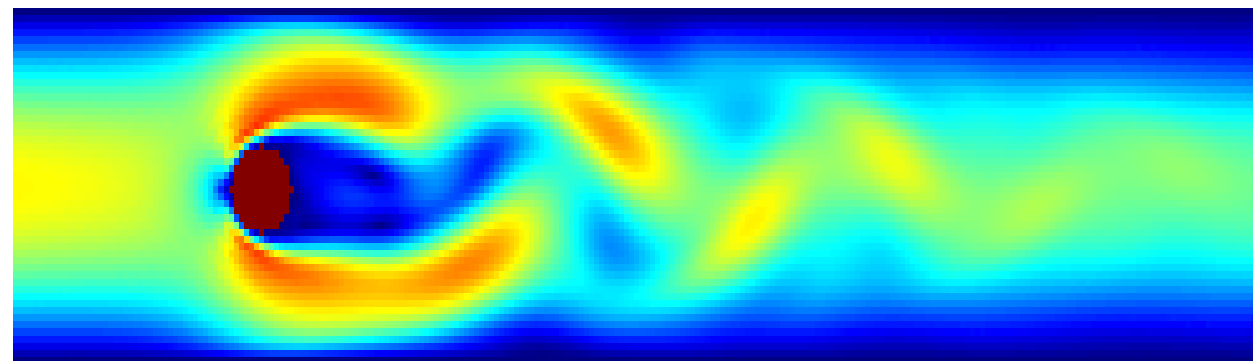


Image Source: [Used with permission](#)

**Value Proposition:** OpenLB is one of the most important simulation software for CFD with growing influence and widely used.

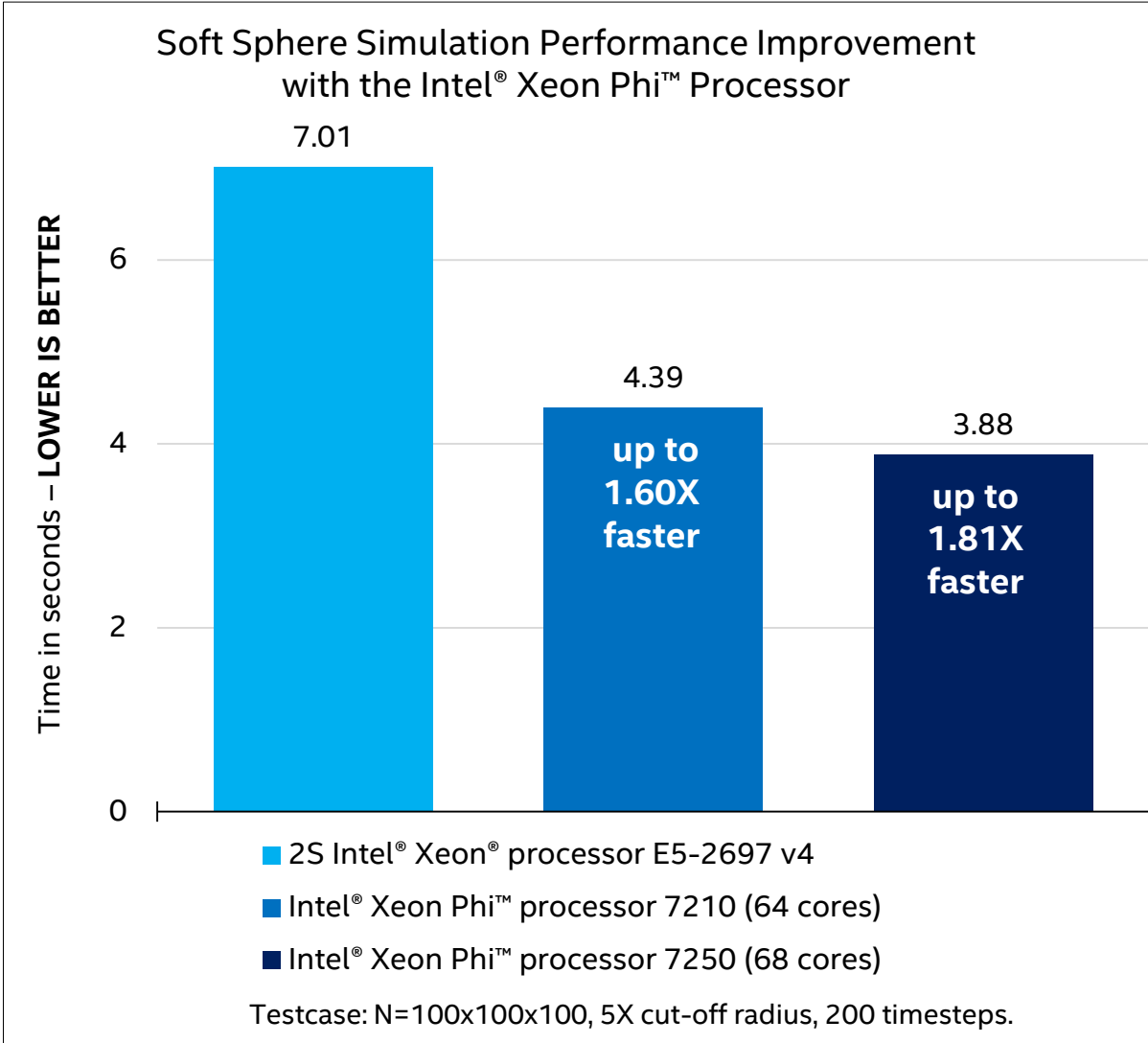
**Results:** Up to 1.5X improved performance by compared to the Intel® Xeon® processor E5-2697 v4.

See next slide for configuration details.

SOURCE: INTEL MEASURED RESULTS AS OF APRIL 2016



# SOFT SPHERE SIMULATION\*



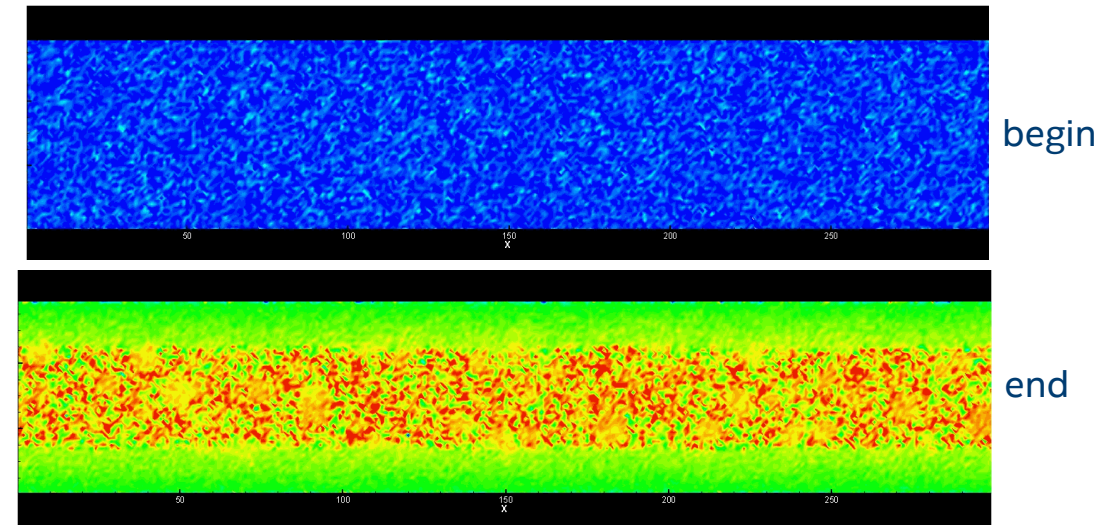
See next slide for configuration details. SOURCE: INTEL MEASURED RESULTS AS OF MARCH, 2016

*Soft Sphere is a 3D Molecular Dynamic simulation of IPE-CAS (Institute of Process Engineering), China. Using sphere particles to simulate structured molecules and calculation based on BKS(Beest-Kramers-Santen) Experience Potential Model allows scientists to fight epidemics like the 2014 Ebola virus.*

**Application:** Soft Sphere Simulation

**Code:** in-house code, contact Prof. Ge at [wge@ipe.ac.cn](mailto:wge@ipe.ac.cn) for code and workload

**Recipe:** Please contact Prof. Ge above.



The simulation of force-driven flow in the nano-scale channel  
Image Source: IPE-CAS, China

**Value Proposition:** Intel® Xeon Phi™ processor 7250 enables this application to significantly outperform (time-to-solution) alternative processing solutions.

**Results:** Up to 1.81X faster with the Intel® Xeon Phi™ processor 7250 compared to the Intel® Xeon® processor E5-2697 v4.

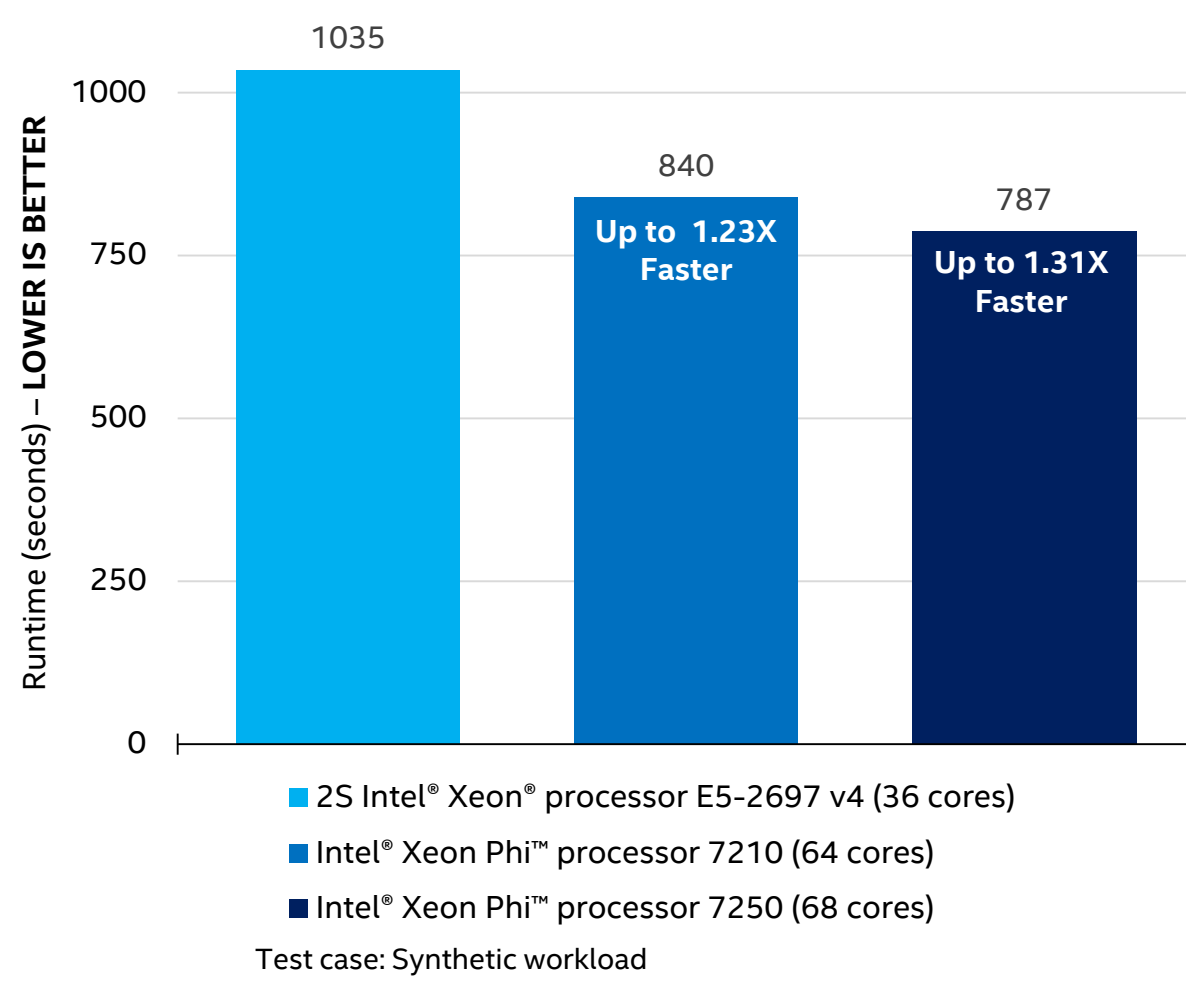






# RELION

RELION Performance Improvement with the Intel® Xeon Phi™ Processor



See next slide for configuration details.

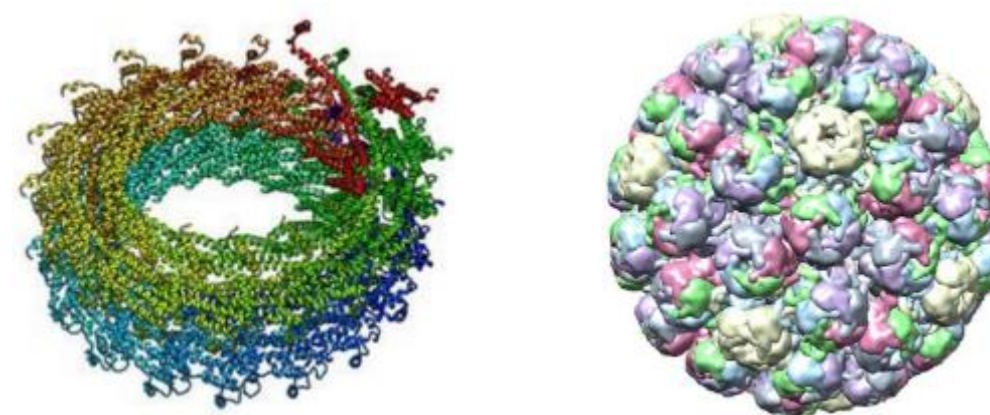
SOURCE: INTEL MEASURED RESULTS AS OF APRIL 2016

**RELION (REGularised Likelihood Optimisation)** is a stand-alone computer program that employs an empirical Bayesian approach to refinement of 3D reconstructions or 2D class averages in Cryo-EM.

**Application:** RELION 1.4

**Code:** [Available here](#)

**Recipe:** "mpiicpc -O3 -xMIC-AVX512 -fno-alias -align"



Images Source: <http://www.rcsb.org/>

## Value Proposition:

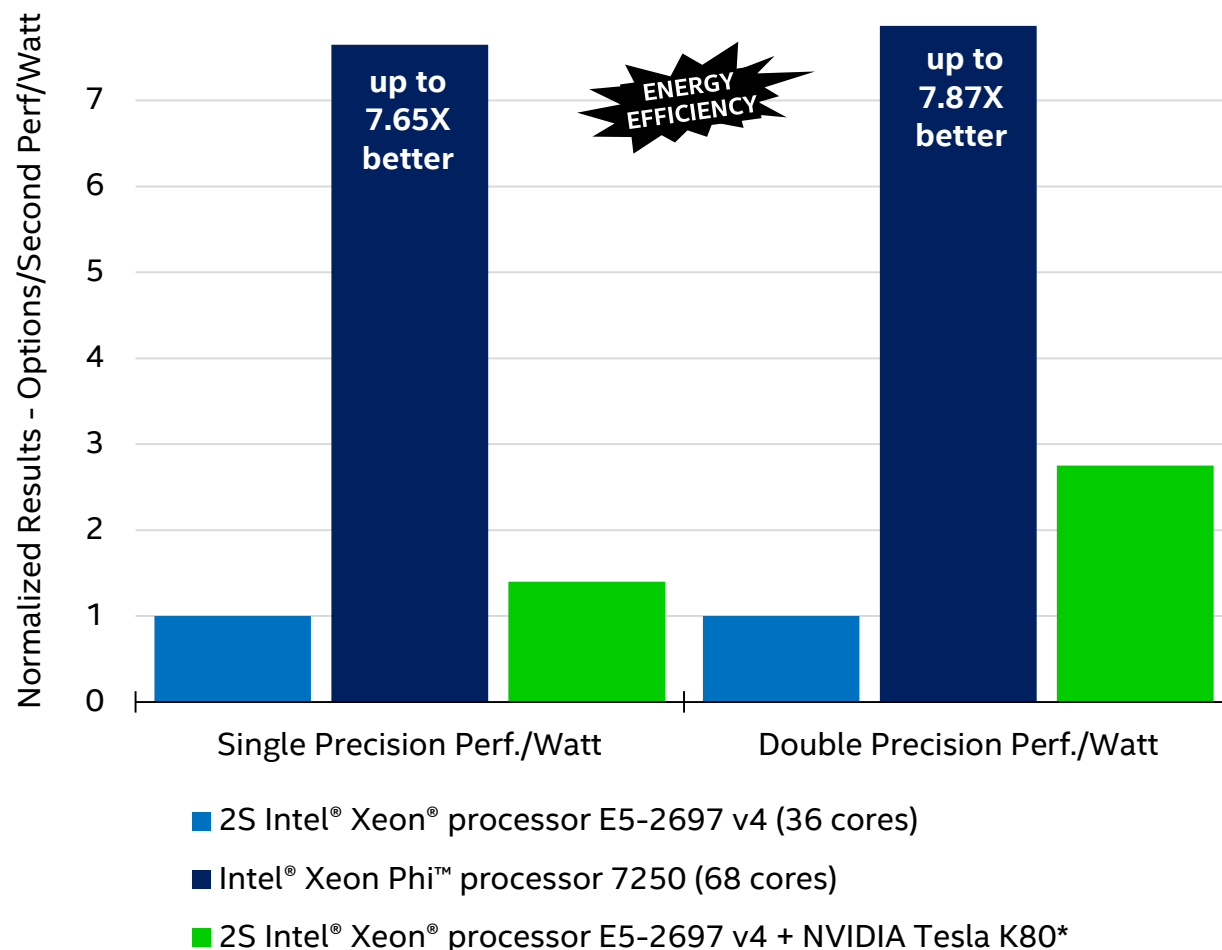
- This application is based on C++ and uses MPI and pthread for different level parallelisation
- Intel® Xeon Phi™ processor 7250 enables this application to significantly speed up image processing

**Results:** Up to 1.3X improved performance compared to the Intel® Xeon® processor E5-2697 v4.



# MONTE CARLO EUROPEAN OPTIONS BENCHMARK\*

Monte Carlo European Options Performance/Watt Improvement with the Intel® Xeon Phi™ Processor



See next slide for configuration details.

SOURCE: INTEL MEASURED RESULTS AS OF MAY, 2016

*Industrial standard benchmark that uses Monte Carlo method for pricing European call options. It pre-generates random numbers then uses them in all options pricing processes. Used by all financial firms to price derivatives with multiple dimensions. Uses the stock price, strike price and time as input streams then creates a call output stream.*

**Application:** Monte Carlo European Options

**Code:** Currently not available **Recipe:** Currently not available

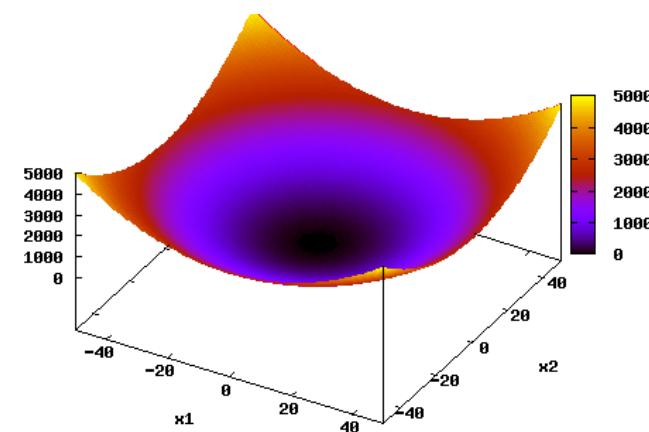


Image Source: US gov.

## Value Proposition:

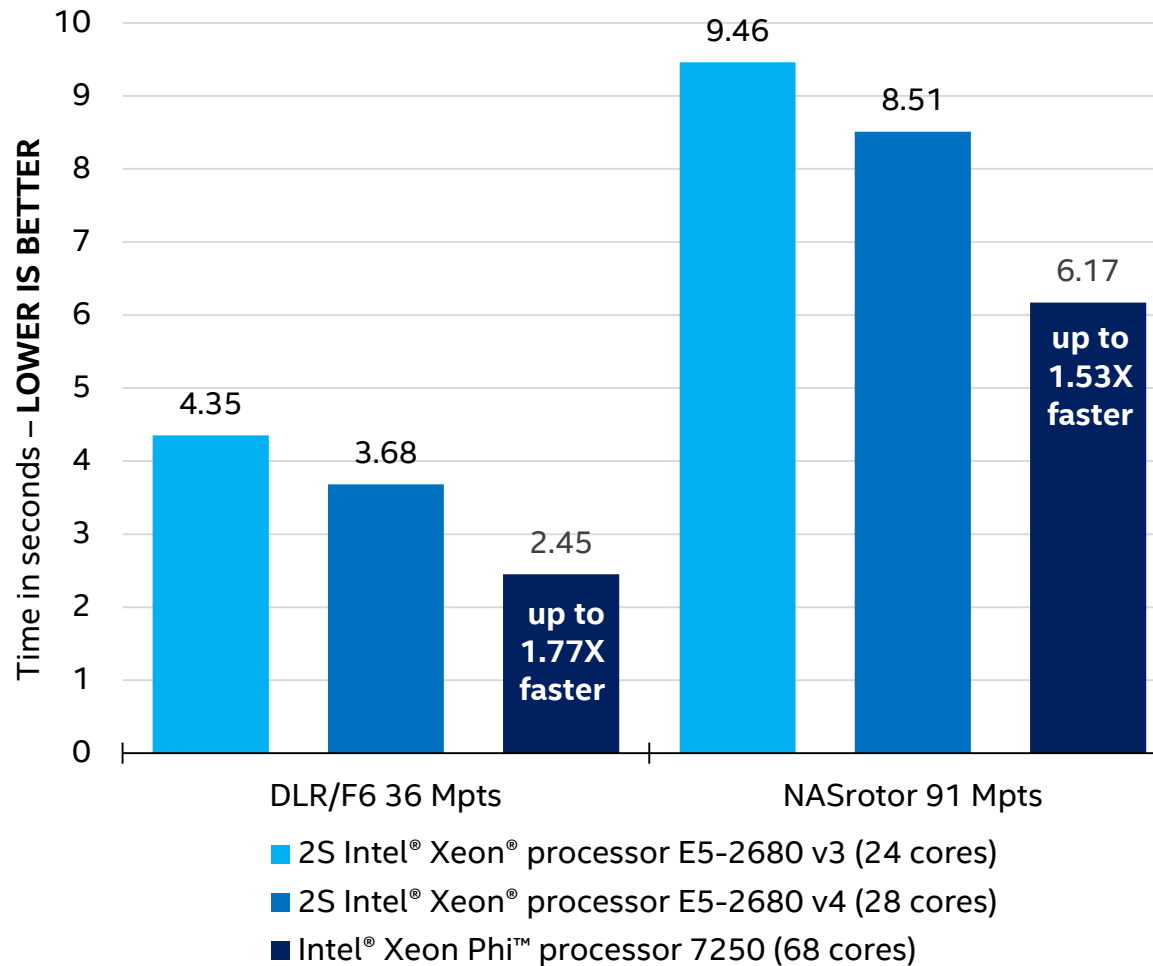
- Improved performance/watt for single and double precision
- Foundation of Financial derivatives pricing
- EMU benefits transcendental functions

**Results:** Up to 7.87X improved Double Precision performance/watt compared to the Intel® Xeon® processor E5-2697 v4 and up to 5.46X better than NVIDIA Tesla\* (single precision).



# NASA OVERFLOW\*

## NASA OVERFLOW CFD Performance



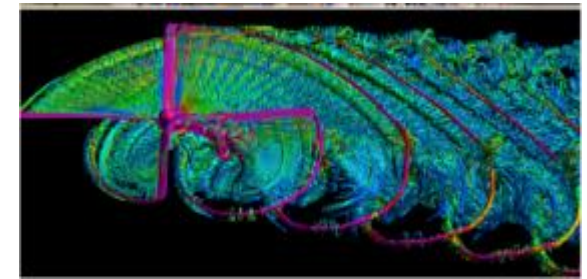
SOURCE: NASA/Ames (Dennis Jespersen) April 2016

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

**Application:** OVERFLOW 2.2L has an extensive feature set supporting collision detection and modelling with support for thin layer and full viscous terms.

**Code:** <http://overflow.larc.nasa.gov/>

**Recipe:** No code changes were required. Recompile with KNL AVX-512.



UH-60 Black Hawk helicopter and Navier-Stokes detached eddy simulation of a flexible UH-60 rotor using the OVERFLOW CFD code in forward flight.

Image Source: Neal Chaderjian and Tim Sandstrom, NASA/Ames

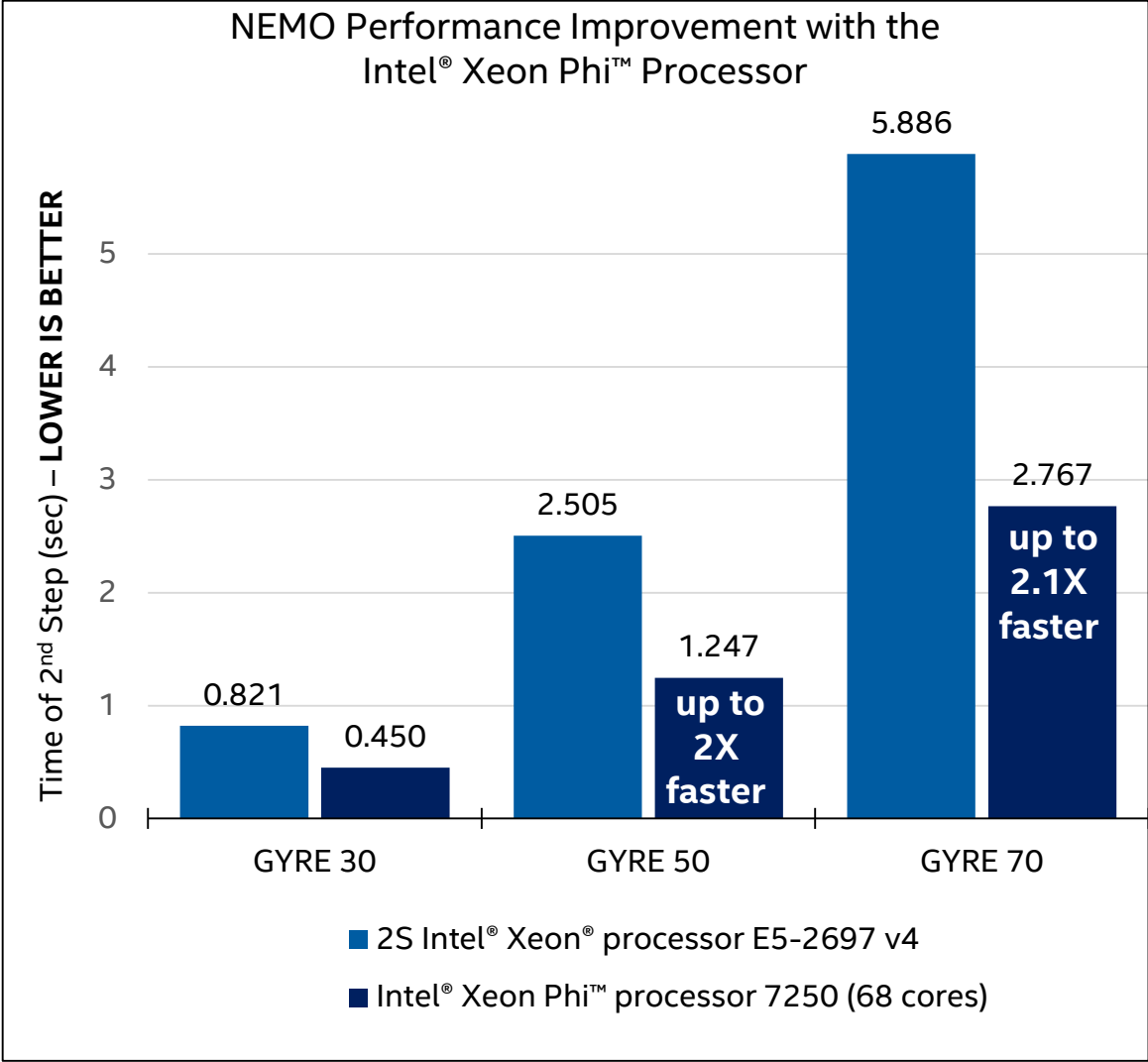
### Value Proposition:

Overflow performance on KNL beats contemporary Haswell and Broadwell Architecture 2S servers. This provides better performance, performance density and better energy efficiency than today's best Intel Xeon processor based systems.

**Results:** Up to 1.78X performance improvement compared to the Intel® Xeon® processor E5-2680v3.

# NUCLEUS FOR EUROPEAN MODELLING OF THE OCEAN\* (NEMO)

NEMO Performance Improvement with the Intel® Xeon Phi™ Processor



See slide 69 for configuration details. SOURCE: INTEL MEASURED RESULTS AS OF MARCH, 2016

*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. The "environment" consists of the pre- and post-processing tools, the interface to the other components of the Earth System, the user interface, the computer dependent functions and the documentation of the system. NEMO allows several ocean related components of the earth system to work together or separately.*

Application: NEMO 3.6

Code: <http://www.nemo-ocean.eu/>

Recipe: See next slide

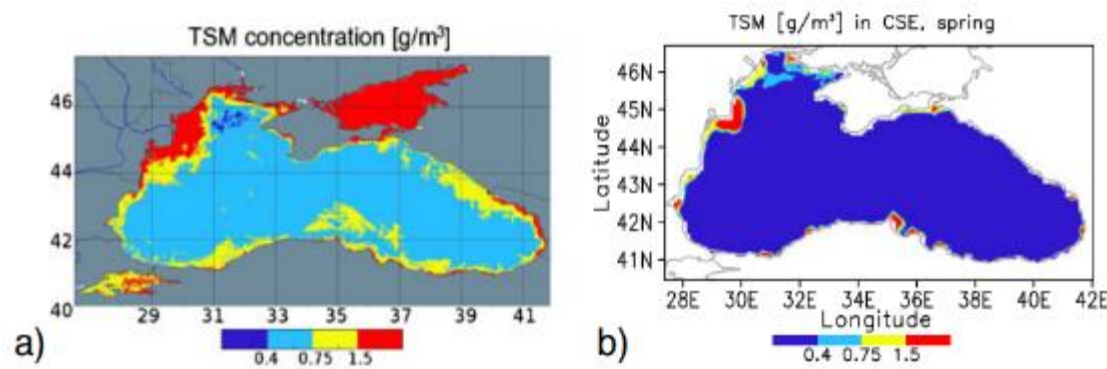


Image Source: [Sediment Dynamics in the Black Sea](#)

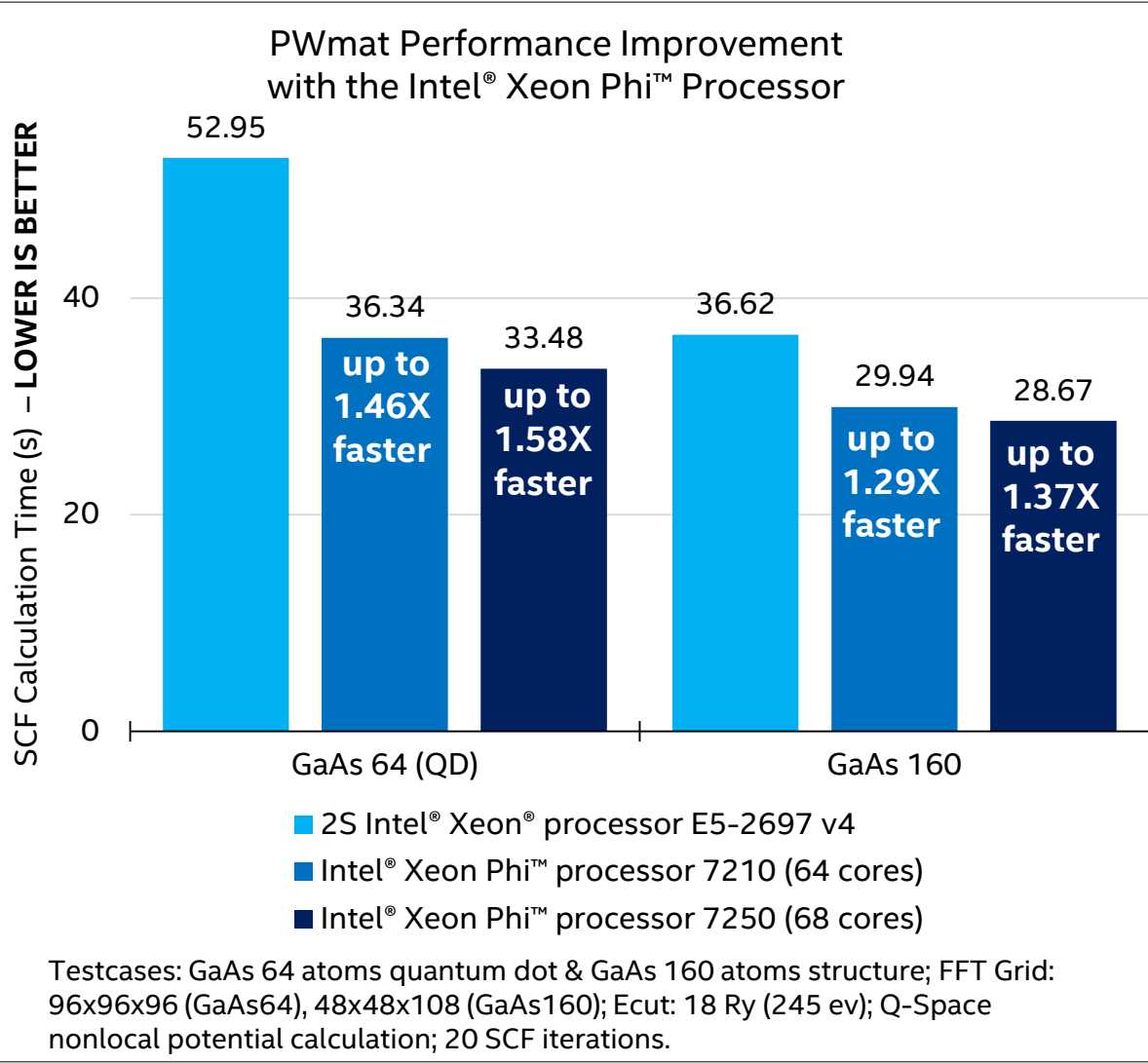
**Value Proposition:** Provides users with a tool for oceanographic research, operational oceanography seasonal forecast and climate studies, and it is used by various universities and meteorological services.

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





PWmat Performance Improvement with the Intel® Xeon Phi™ Processor



See next slide for configuration details.

SOURCE: INTEL MEASURED RESULTS AS OF MAY, 2016

*PWmat is a commercial software using plane wave pseudopotential method for density functional theory (DFT) material simulations. It is an ab initio code, meaning it uses initial atomic positions to predict the material properties. PWmat is developed and optimized by Beijing LongXun Inc. based on the open source code PETot (PETot has a BSD 3-Clause license).*

**Application:** PWmat

**Code:** Commercial software. Contact LongXun Inc. ([support@pwmatt.com](mailto:support@pwmatt.com)). PETot can be downloaded as a reference (<http://cmsn.lbl.gov/html/PETot/PETot.html>).

**Recipe:** Evaluation binaries: [http://www.pwmatt.com/pwmatt\\_performance](http://www.pwmatt.com/pwmatt_performance) (encrypted). Contact LongXun Inc. ([support@pwmatt.com](mailto:support@pwmatt.com)) for approval at first.

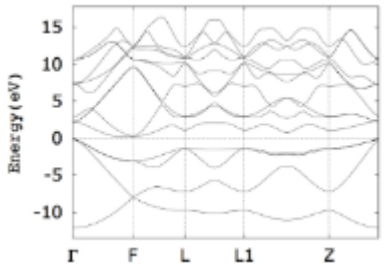
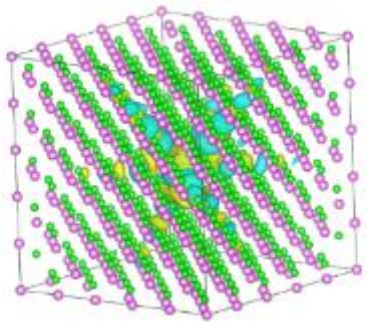
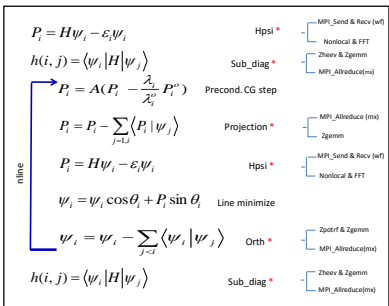
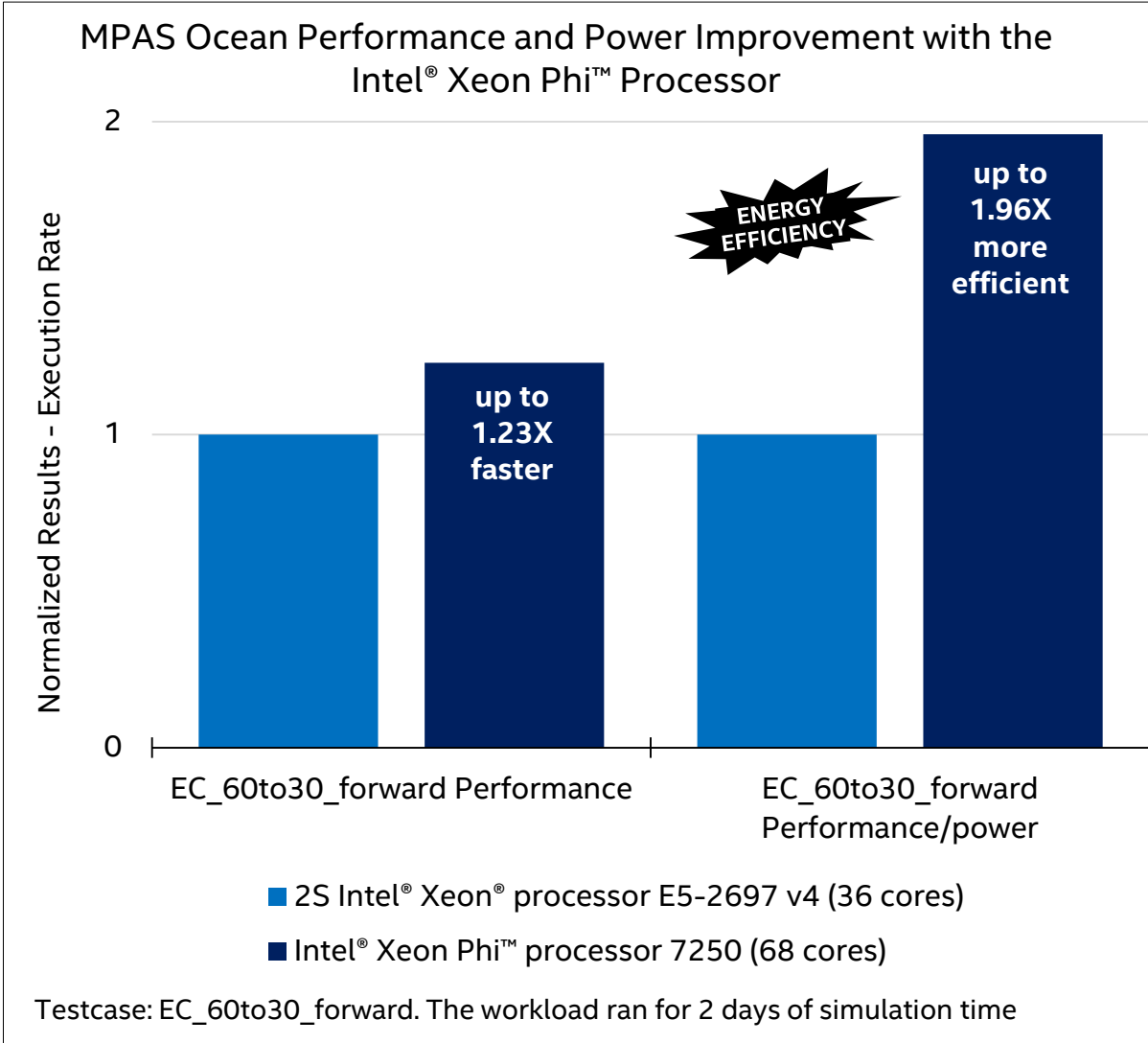


Image Source: LongXun Inc.

**Value Proposition:** PWmat is local developed state-of-art material simulation software with growing influence in China.

**Results:** Up to 1.58X faster with the Intel® Xeon Phi™ processor 7250 compared to the Intel® Xeon® processor E5-2697 v4.

# MPAS OCEAN 4.0\*



See next slide for configuration details.

SOURCE: INTEL MEASURED RESULTS AS OF MAY 2016

*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, [jacobsen.douglas@gmail.com](mailto:jacobsen.douglas@gmail.com))*

**Application:** MPAS-O

**Code:** [Available here](#)   **Recipe:** See the configuration details slide.

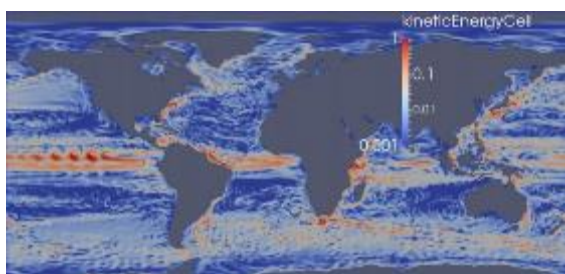


Image Source: [Los Alamos National Laboratory](#)

**Value Proposition:** Intel® Xeon Phi™ processor 7250 enables this application to outperform (time-to-solution) and performance/power of alternative processing solutions.

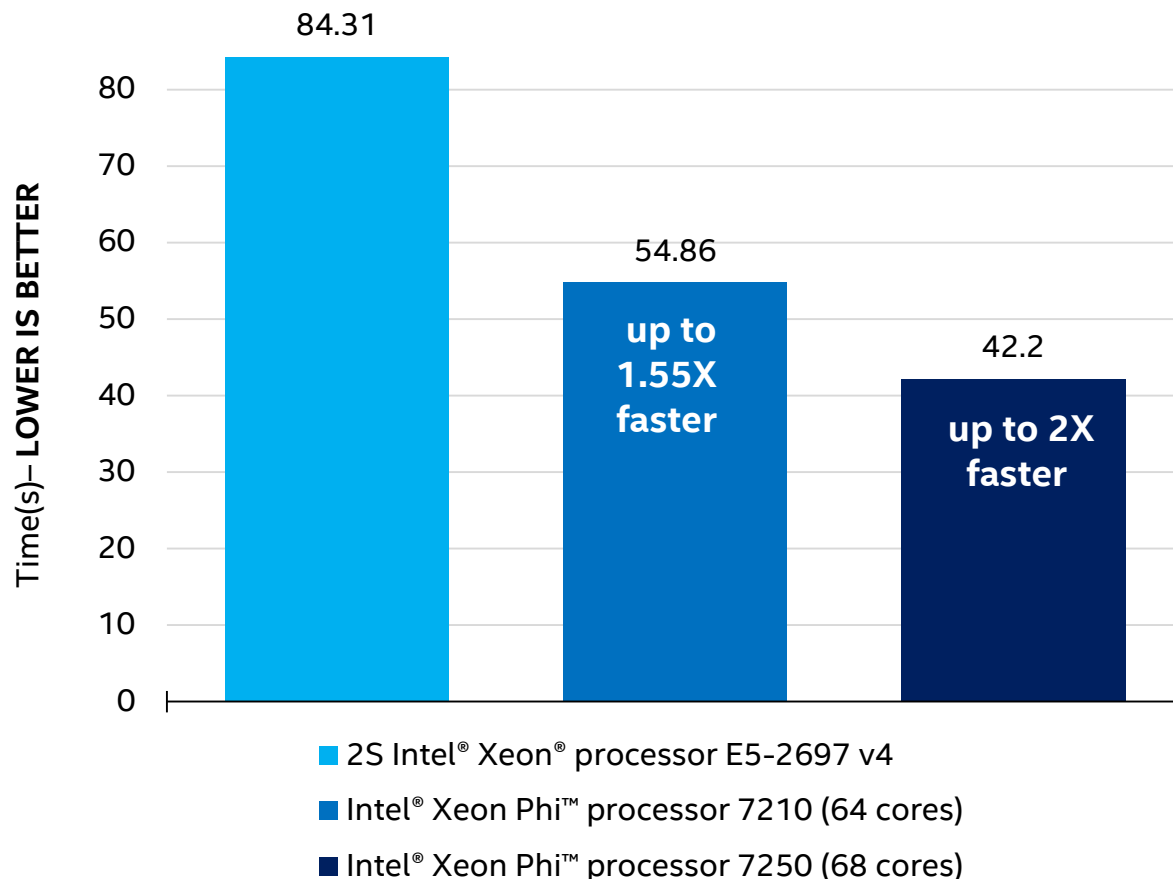
**Power Data:** Total system wall power is measured out-of-band over iPMI interface, polling the BMC chip every one tenth second. Energy usage is matched to internally timed code segment to arrive at performance per Watt estimate. Only power consumed during the time steps were used for efficiency calculations.

**Results:** up to 1.23X improved performance and up to 1.96X performance/power compared to the Intel® Xeon® processor E5-2697 v4 for EC\_60to30\_forward workload.





VLPL-S Performance Improvement with the Intel® Xeon Phi™ Processor



Test case: v2d-test3.ini 2D (1200<sup>2</sup>, Particles number in cell is 16, 20 time steps)

See next slide for configuration details.

SOURCE: INTEL MEASURED RESULTS AS OF APRIL, 2016

**VLPL-S** is the in-house code from Germany Heinrich-Heine University of Dusseldorf (HHUD) and PRC Shanghai Jiao Tong University (SJTU), paralleled with MPI and written in C++. The application is about Particle-in-Cell method for laser plasma simulation by solving the particles motion equation, current density distribution and Maxwell equations.

**Application:** VLPL-S.

**Code:** In-house code. To get access to the code and test cases, please contact [minchen@sjtu.edu.cn](mailto:minchen@sjtu.edu.cn)

**Recipe:** Please contact [minchen@sjtu.edu.cn](mailto:minchen@sjtu.edu.cn)

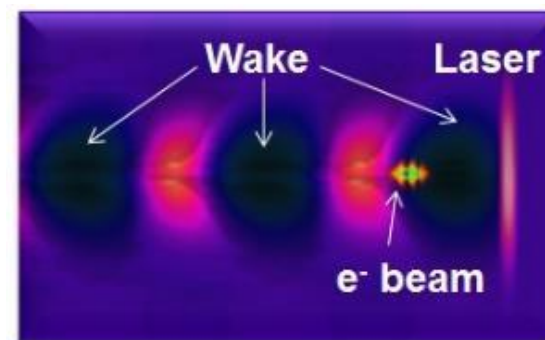
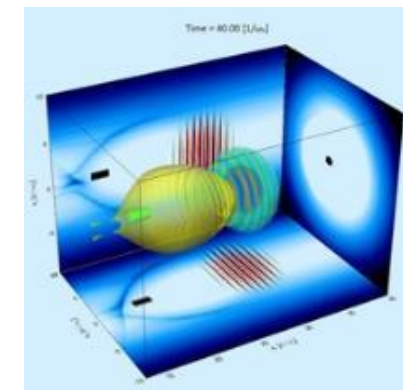


IMAGE SOURCE: PRC SJTU



### Value Proposition:

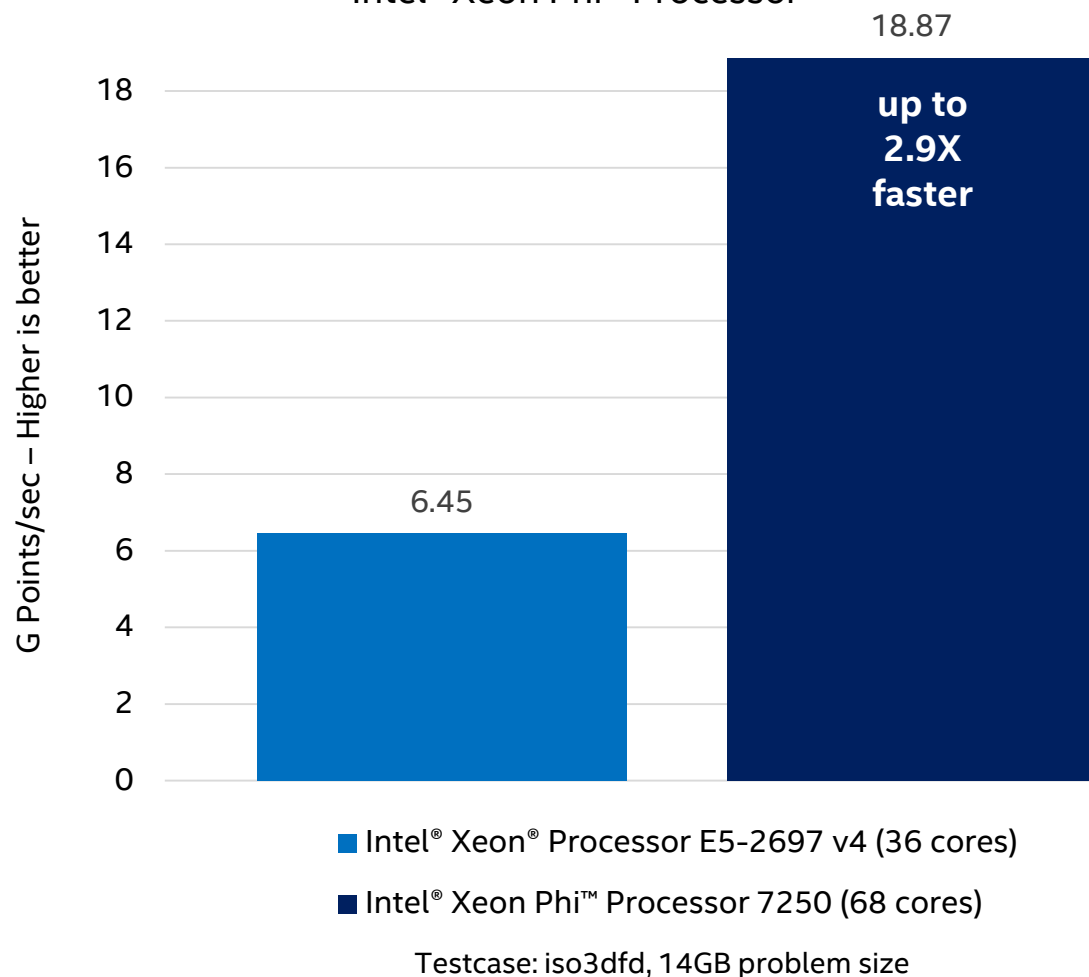
- Intel® Xeon Phi™ processor 7250 enables this application to significantly outperform (time-to-solution) alternative processing solutions.
- Performance is enhanced by Intel® AVX512.

**Results:** Up to 2X improved performance compared to the Intel® Xeon® processor E5-2697 v4.



# YASK HPC STENCILS, ISO3DFD KERNEL

YASK ISO3DFD Kernel Performance Improvement with the Intel® Xeon Phi™ Processor



See next slide for configuration details.

SOURCE: INTEL MEASURED RESULTS AS OF May, 2016

**YASK, Yet Another Stencil Kernel, is a framework to facilitate design exploration and tuning of HPC kernels. One of the stencils included in YASK is iso3dfd, a finite-difference code found in seismic imaging software used by energy-exploration companies to predict the location of oil and gas deposits.**

**Application:** YASK, iso3dfd stencil

**Code:** [Available here](#)

**Recipe:** 1536\*1024\*768 problem size (see command lines in next slide)



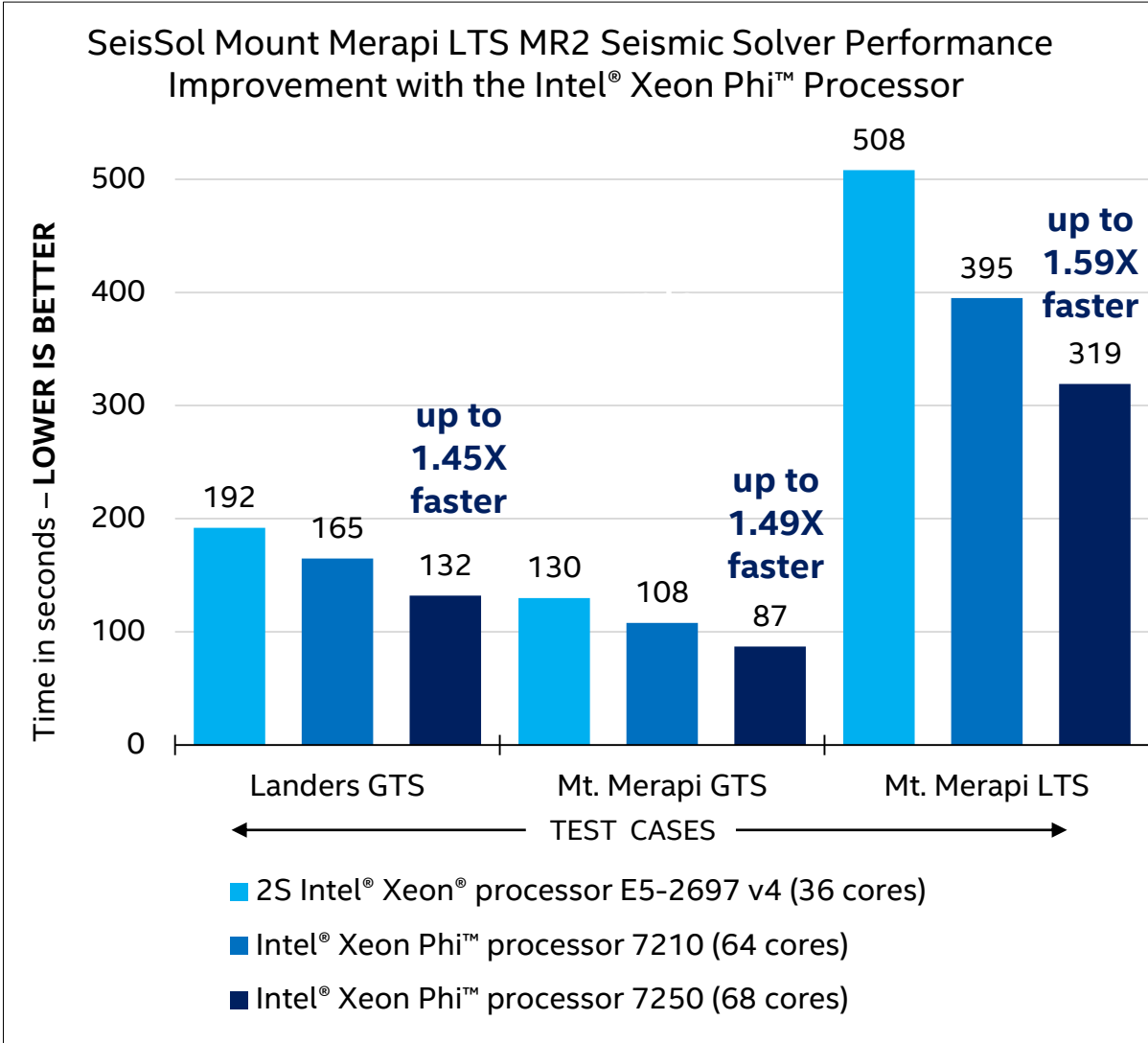
Image Source: US Dept. Energy

**Value Proposition:** Intel® Xeon Phi™ processor 7250 enables this application to leverage the high-bandwidth memory and 512-bit SIMD for higher performance.

**Results:** Up to 2.9X improved performance compared to the Intel® Xeon® processor E5-2697 v4.



# SEISSOL MOUNT MERAPI LTS MR2 SEISMIC SOLVER\*



See next slide for configuration details.

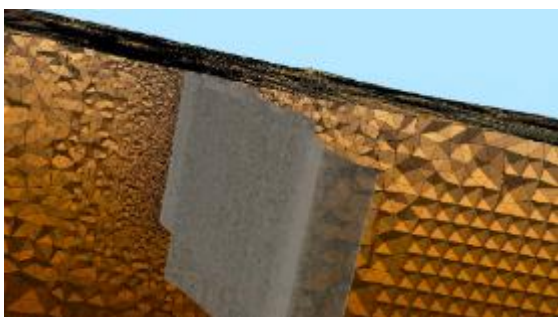
SOURCE: INTEL MEASURED RESULTS AS OF MARCH, 2016

*SeisSol software simulates wave propagation and dynamic rupture based on the arbitrary high-order accurate derivative discontinuous Galerkin method (ADER-DG). Characteristics include tetrahedral meshes to approximate complex 3D model geometries and rapid model generation use of elastic, viscoelastic and viscoplastic material to approximate realistic geological subsurface properties. The code is Open Source.*

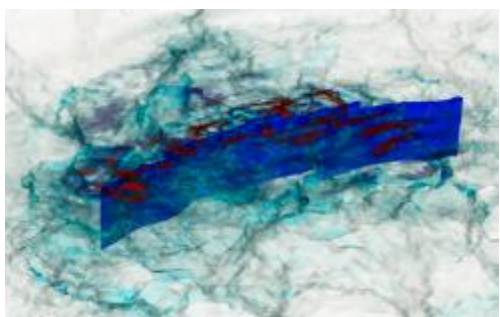
**Application:** SeisSol Mount Merapi LTS MR2 Seismic Solver.

**Code:** [Available here](#)

**Recipe:** Download code and follow instructions



Images Source: Intel Labs



**Value Proposition:** SeisSol relies on Intel's Open Source Library for small BLAS operations (matrix multiplications) [LIBXSMM](#), enabling BLAS extensions on drop-in basis and automatically targets Intel® AVX, Intel® AVX2 and Intel® AVX-512 through future-proof just-in-time compilation techniques. LIBXSMM is also used in other widely-used scientific Open Source packages such as [CP2K](#) and [Nek5000/NekBox](#).

**Results:** Up to 1.59X faster compared to the Intel® Xeon® processor E5-2697 v4.



# Technical, Enterprise & Cloud Development Tools



- C++ and Fortran Compilers
- Standards Driven Parallel Programming Models & Libraries
- Performance Profiling for Optimization and Tuning
- Threading & Vectorization Design & Analysis for Performance



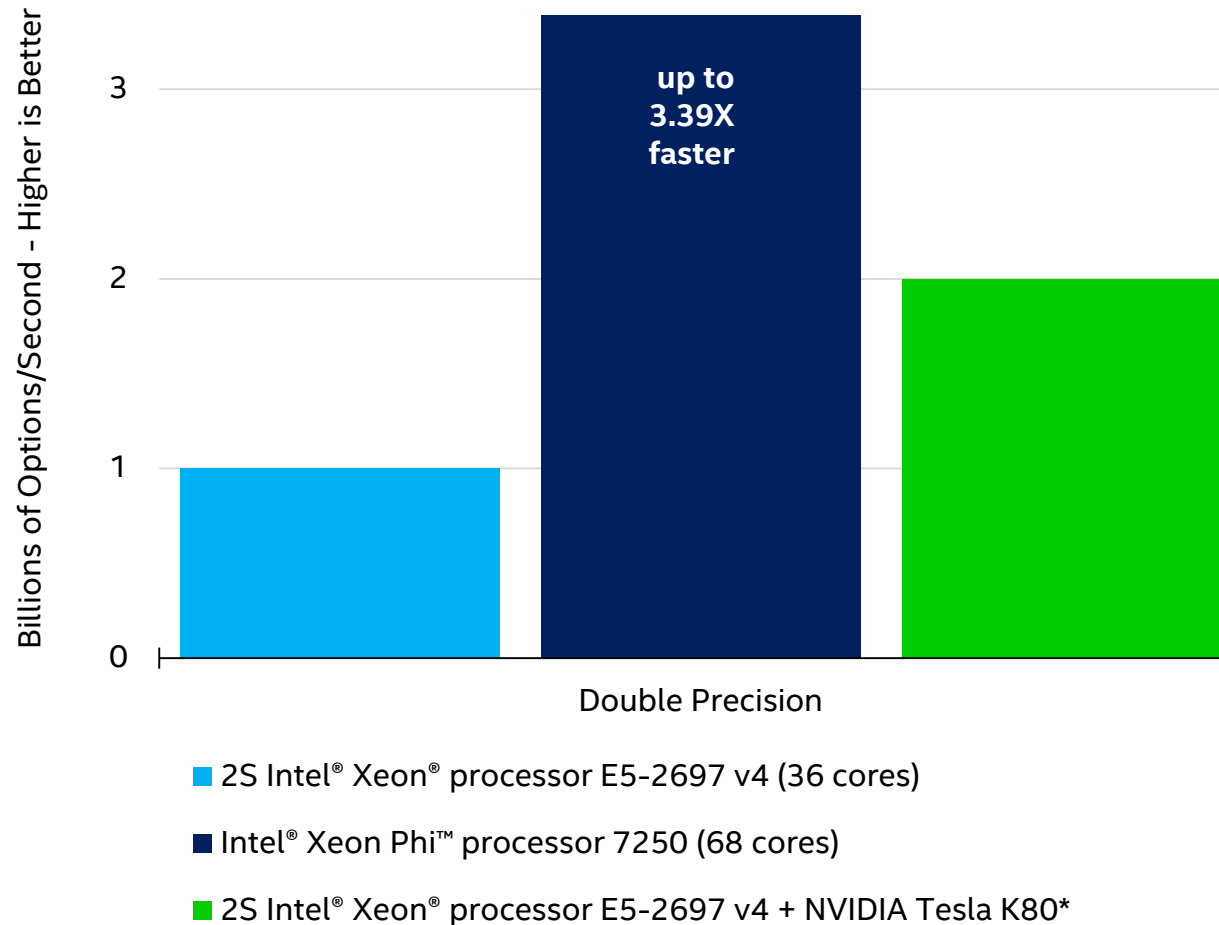
- Powerful Data Analytics, Machine Learning and Scientific Compute Libraries
- Coming Soon – High Performance Python Distribution

***Faster Code Faster***



# BLACK-SCHOLES BENCHMARK\*

Black-Scholes Formula Performance Improvement with the Intel® Xeon Phi™ Processor



See next slide for configuration details.

SOURCE: INTEL MEASURED RESULTS AS OF MAY, 2016

*Industrial standard benchmark that calculates call and put option price using the Black-Scholes-Merton Formula. Used by all financial firms to price derivatives with multiple dimensions. Stock price, strike price and time are input streams that create call and put as output streams.*

**Application:** Black-Scholes formula

▪ **Code:** Currently not available    **Recipe:** Currently not available

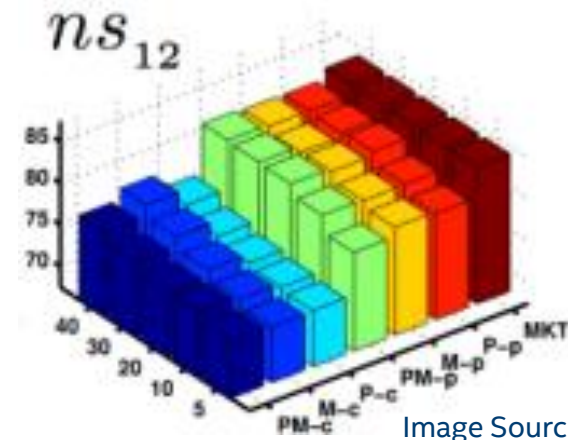


Image Source: US gov

$$C(S, t) = N(d_1)S - N(d_2)Ke^{-r(T-t)}$$

$$d_1 = \frac{1}{\sigma\sqrt{T-t}} \left[ \ln\left(\frac{S}{K}\right) + \left(r + \frac{\sigma^2}{2}\right)(T-t) \right]$$

$$d_2 = \frac{1}{\sigma\sqrt{T-t}} \left[ \ln\left(\frac{S}{K}\right) + \left(r - \frac{\sigma^2}{2}\right)(T-t) \right]$$

$$= d_1 - \sigma\sqrt{T-t}$$

**Value Proposition:**

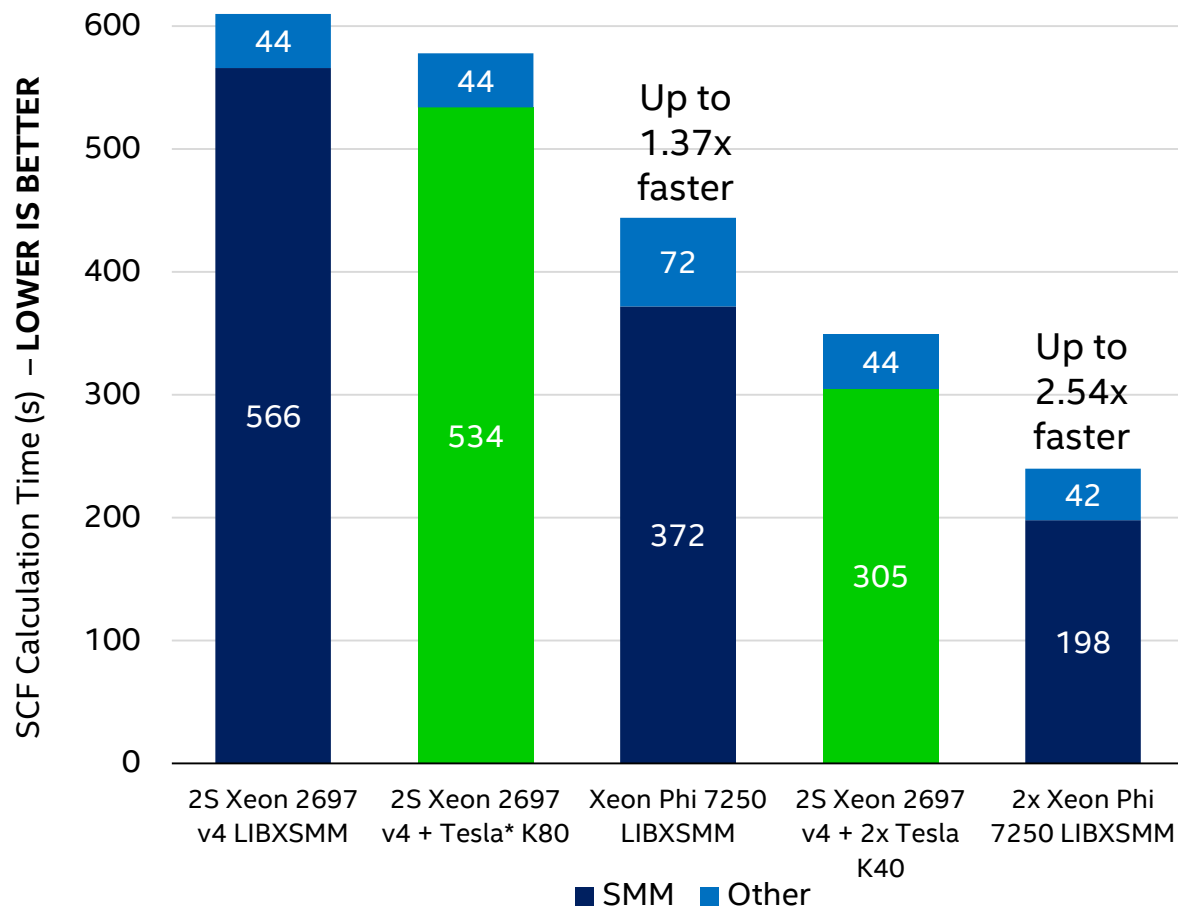
- Foundation of financial derivatives pricing
- Widely used all over financial libraries
- Performance enhanced by Intel® AVX512 and MCDRAM

**Results:** Up to 4.3X improved Double Precision compared to the Intel® Xeon® processor E5-2697 v4 and up to 2.5X better than NVIDIA Tesla\*.



# LINEAR SCALING (LS) DENSITY FUNCTION THEORY (DFT)

CP2K Linear Scaling (LS) Density Function Theory (DFT)



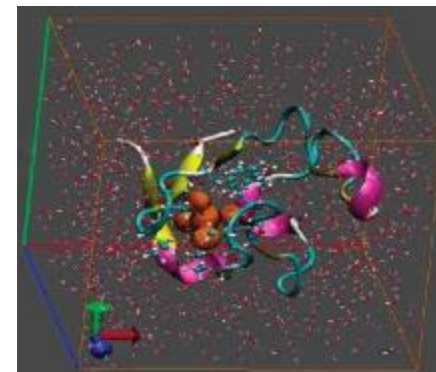
Workload: Electronic structure of 864 H<sub>2</sub>O molecules (2.5k atoms). Linear Scaling DFT (DFT LS) and 10 MD steps

*CP2K is a powerful and scalable program for atomistic simulations of a wide range of systems, including condensed phase, molecular systems and complex interfaces. CP2K features a wide range of atomistic interaction models including classical potentials, semi-empirical schemes, Density Functional Theory (DFT), Hartree-Fock (HF), and post-HF correlation methods such as MP2 and RPA. The program was a Gordon Bell Finalist in 2015. CP2K is freely available.*

**Application:** CP2K Quantum Chemistry & Solid State Physics Software Package

**Code:** [Available Here](#)

CP2K



Courtesy of ETH Zurich. ([url](#))

CP2K

**Value Proposition:** CP2K optionally uses Intel's Open Source Library for small BLAS operations (matrix multiplications) called [LIBXSMM](#), which enables BLAS extensions on a drop-in basis, and automatically targets Intel® AVX, Intel® AVX2 and Intel® AVX-512 through future-proof just-in-time compilation techniques. LIBXSMM is also used in other scientific Open Source packages such as [SeisSol](#) and [Nek5000/NekBox](#).

**Results:** Up to 1.37X faster with the Intel® Xeon Phi™ processor 7250 compared to the Intel® Xeon® processor E5-2697 v4.

See next slide for configuration details.

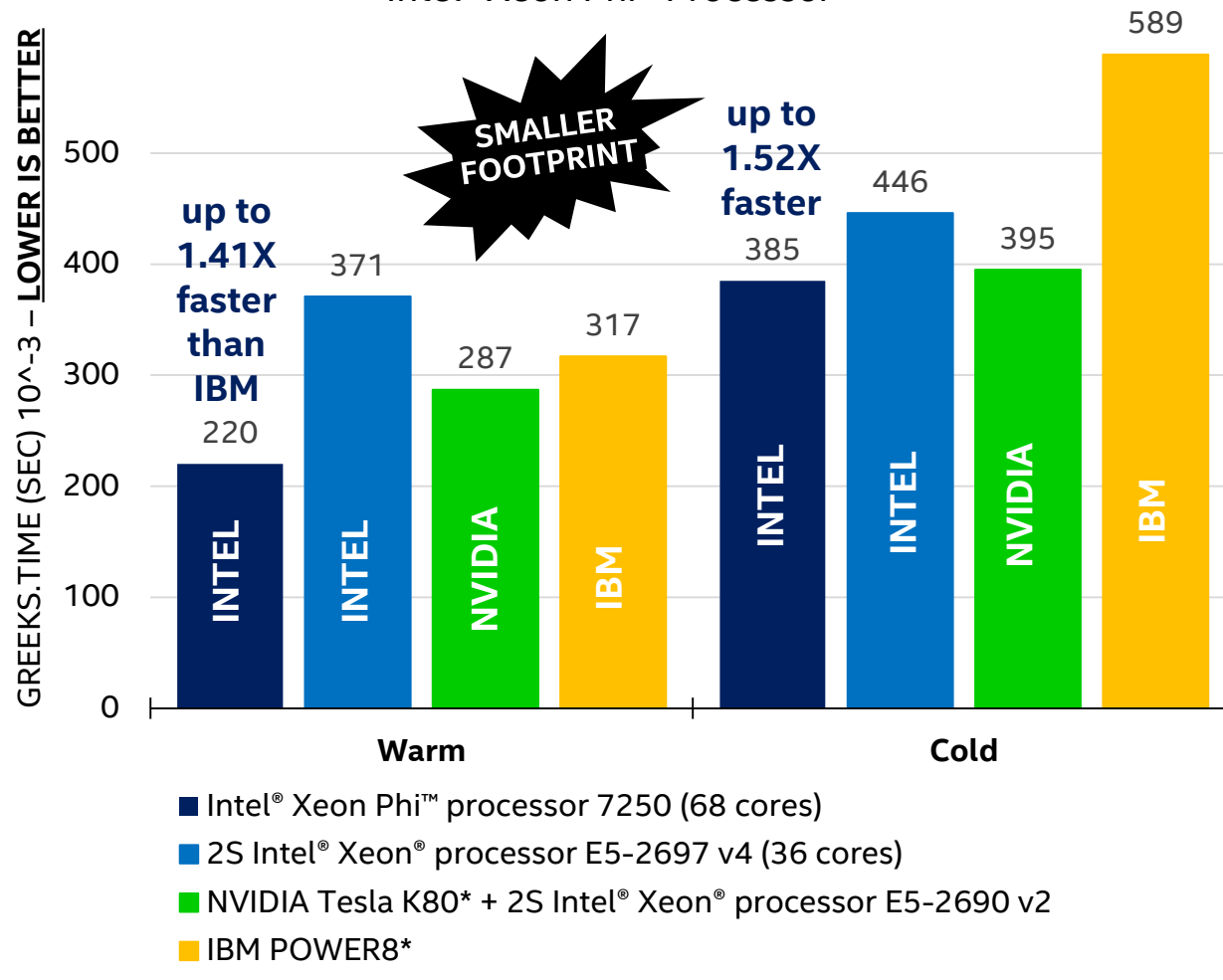
MEASUREMENT: CP2K (Intel), LIBCUSMM ([K40](#), [K80](#))





# STAC-A2\* BENCHMARK

STAC-A2 Benchmark Performance Improvement with the Intel® Xeon Phi™ Processor



*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*

**Application:** Intel Composer XE STAC Pack Rev. H

**Code:** [Available here](#)

**Recipe:** [Available here](#)



"STAC" and all STAC names are trademarks or registered trademarks of the Securities Technology Analysis Center LLC.



Image Source: Intel

## Value Proposition:

- The Intel Xeon Phi processor based-system takes up 1/8th the space (0.5U vs 4U) than the IBM Power8\* based-system
- Performance enhanced by Intel® AVX512 and MCDRAM

**Baseline problem size results:** The Intel® Xeon Phi™ 7250 processor system is up to 1.2X faster than next competitor (NVIDIA K80\* system) in warm runs, and is up to 2X more power efficient and is up to 5.7X more space efficient compared to the IBM Power8 system.

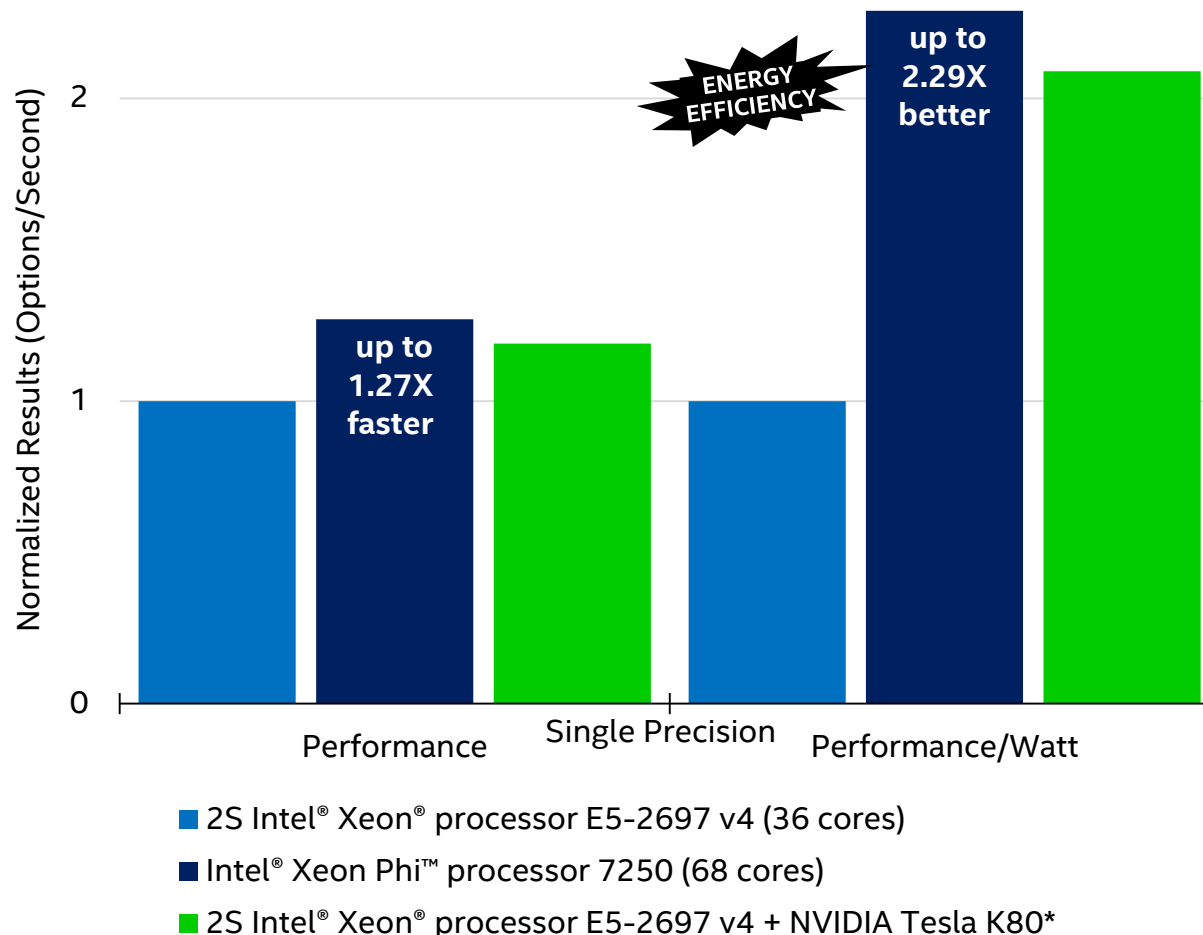
See next slide for configuration details.

SOURCE: STAC\* AUDITED RESULTS AS OF MAY 2016



# BINOMIAL TREE OPTION PRICING BENCHMARK\*

Monte Carlo European Options Single Precision Performance Improvement with the Intel® Xeon Phi™ Processor



See next slide for configuration details.

SOURCE: INTEL MEASURED RESULTS AS OF MAY, 2016

*Binomial Tree Option pricing method is an industrial standard benchmark that calculates call option prices. Used by financial firms especially for options that involve early exercise clause. Uses stock price, strike price and time as input streams, then creates a call output stream.*

**Application:** Binomial Tree Option Pricing

**Code:** Currently not available **Recipe:** Currently not available

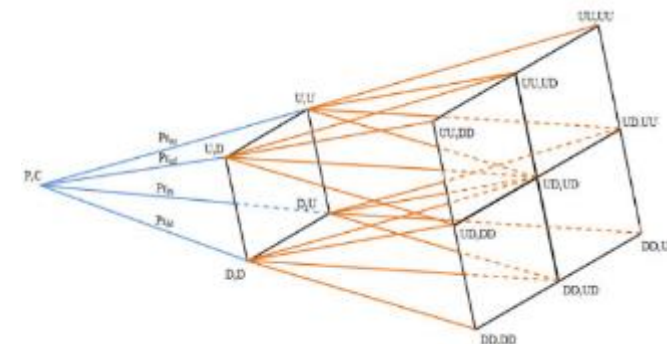
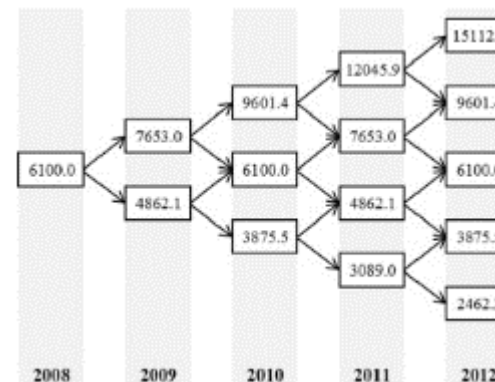


Image Source: [Science Direct](http://www.sciencedirect.com)

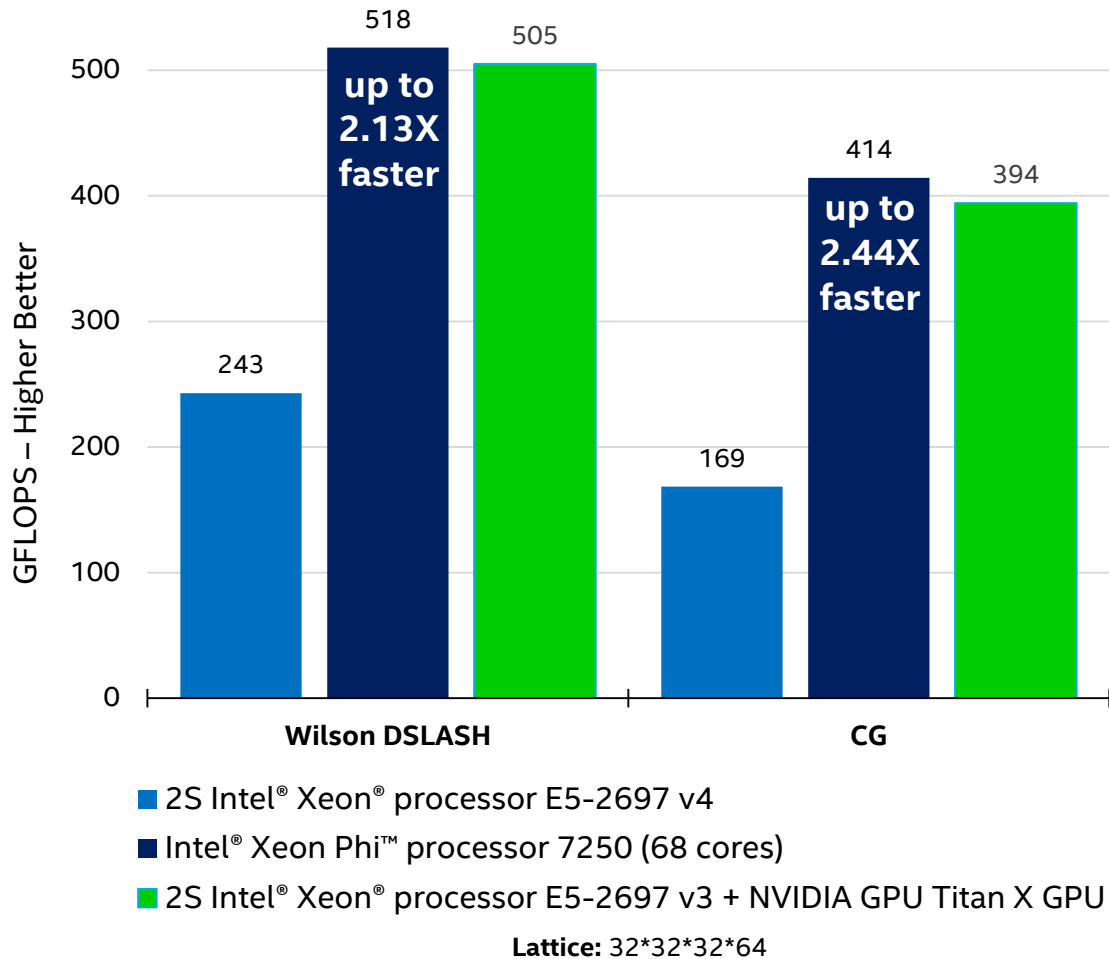
## Value Proposition:

- Foundation of Financial derivatives pricing
- Widely used by all financial libraries
- Unaligned penalty favors Intel® architecture

**Results:** Up to 1.27X improved Single Precision performance compared to Intel® Xeon® processor E5-2697 v4, and up to 1.09X better performance/watt compared to NVIDIA Tesla\*.



QPhiX : Performance Improvement with Intel® Xeon Phi™ Processor



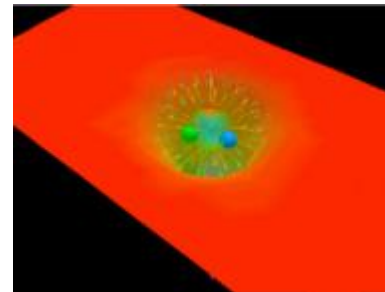
See next slide for configuration details.

SOURCE: INTEL MEASURED RESULTS AS OF MAY, 2016

**QPhiX is an optimized solver library for QCD on Intel® Xeon® and Intel® Xeon Phi™ processors and provides implementation for Dslash operator and CG, BICGStab and mixed precision solvers for Wilson and Clover improved Wilson Quarks.**

**Application:** QPhiX Test Benchmark (time\_dslash\_noqdp), QUDA\* (NVIDIA\*)

**Code:** <https://github.com/JeffersonLab/qphix> **Recipe:** Follow the instructions in the download package

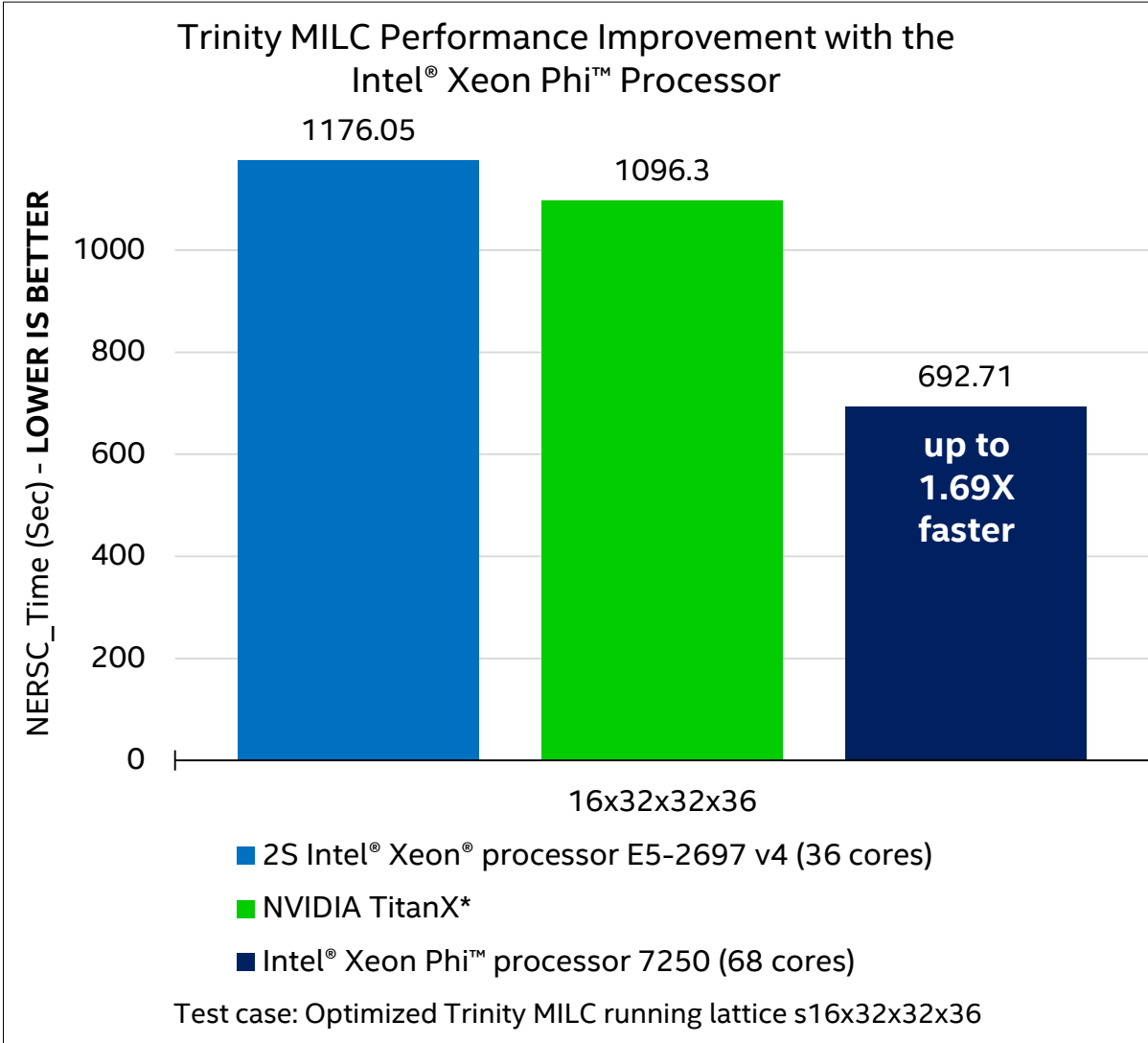


Flux tubes between 3 quarks.  
Credit: Dr Derek Leinweber, Centre for the Subatomic structure of Matter (CSSM) and Department of Physics, University of Adelaide, 5005 Australia

### Value Proposition:

- Lattice calculations are an important component of the nuclear physics research.
- QPhiX helps speed up the computation by multiple folds on Intel processors.
- Intel® Xeon Phi™ processor further improves performance with features such as high bandwidth memory (MCDRAM) and Intel® AVX-512 vector instruction set architecture.

**Results:** up to 2.44X improved performance compared to the Intel® Xeon® processor E5-2697 v4. CG performance is ~1.05x better vs. QUDA on a NVIDIA\* Titan X\* GPU.



See next slide for configuration details.

SOURCE: INTEL MEASURED RESULTS AS OF May 2016

*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.*

**Application:** Trinity MILC provided by NERSC as part of Trinity8 suite

**Code:** Original NERSC Benchmark code is [here](#), contact Intel for Optimized Code

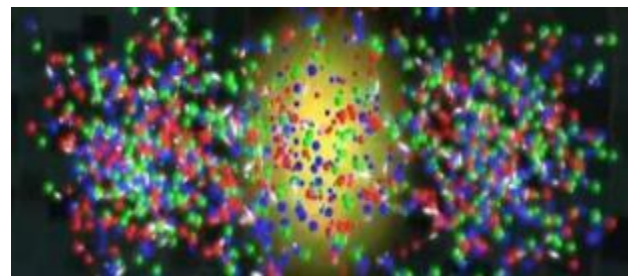
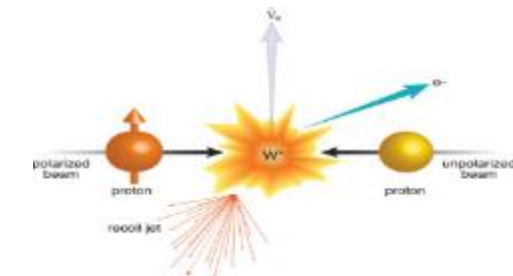


Image Credit: Brookhaven Lab (BNL)



**Value Proposition:**

- MILC is widely deployed on numerous supercomputers and 2<sup>nd</sup> most used application at US DOE's National Energy Research Scientific Computing Center (NERSC)
- Intel's optimizations are being incorporated into mainline by MILC collaboration
- Intel® Xeon Phi™ processor 7250 enables to run larger problem size per node

**Results:**

The Intel® Xeon Phi™ processor 7250 improved performance by up to 1.69X and 1.5Xx compared to the Intel® Xeon® processor E5-2697 v4 and NVIDIA TitanX respectively

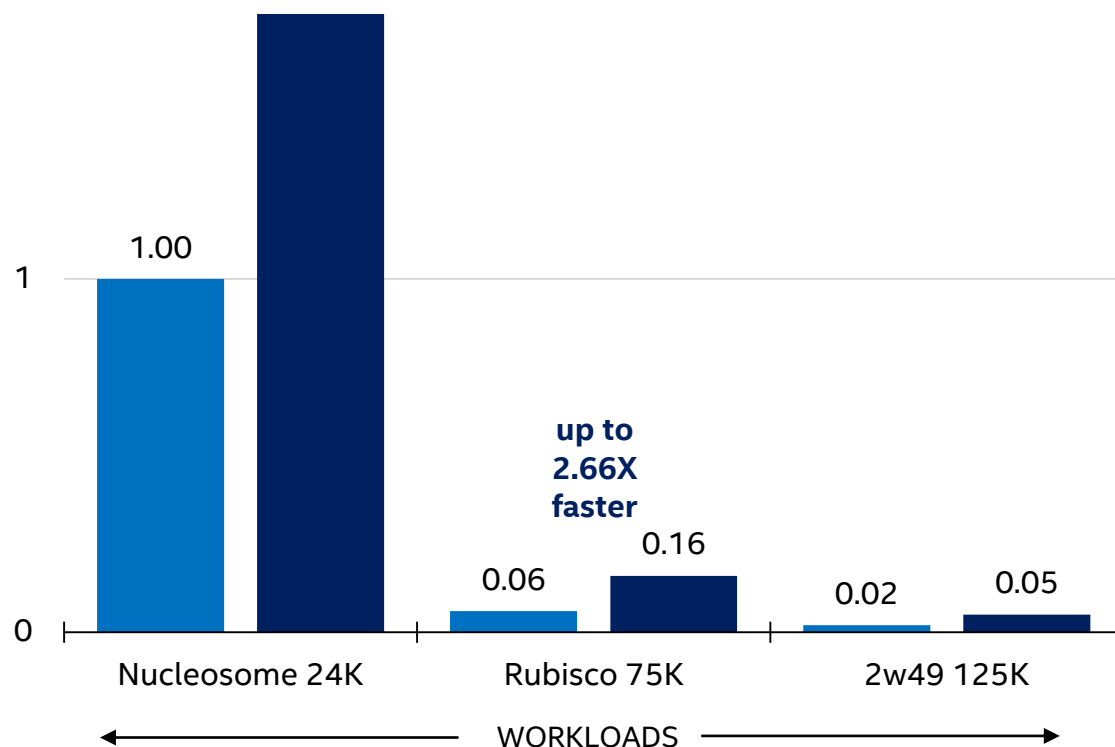


# AMBER 16 PMEMD IMPLICIT\*

Amber Implicit Performance Improvement with the Intel® Xeon Phi™ Processor

1.75

ns/day - Higher is Better



■ 2S Intel® Xeon® processor E5-2697 v4 (36 cores)

■ Intel® Xeon Phi™ processor 7250 (68 cores)

Test case: Cellulose NVE, Tobacco Virus and Poliovirus. All ran for more than 1000 steps

*Amber\* is a bio related simulation code for DNA, RNA, protein, and other bio-molecules. Particle Mesh Ewald Molecular Dynamics (PMEMD) is an Amber tool used for Molecular Dynamic Simulation. PMEMD includes two algorithms, Explicit and Implicit. PMEMD is written in Fortran 90 and is mainly MPI\*, OpenMP\* and Vectorization parallelized.*

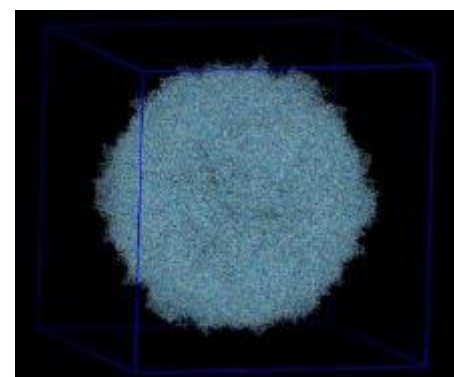
**Application:** Amber 16 PMEMD Implicit

**Code:** License required from <http://ambermd.org/>

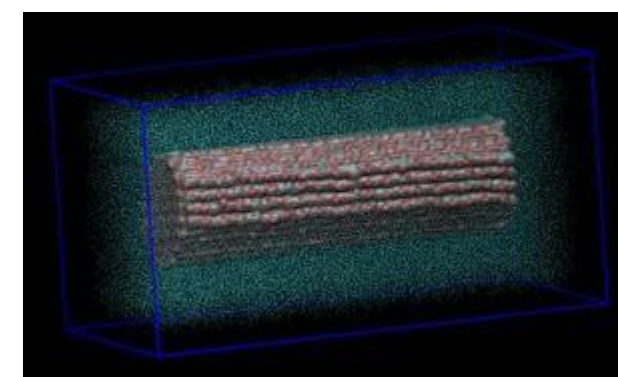
**Recipe:** ./configure -intelmpi -openmp -mic2 intel

On Intel® Xeon®: make install AMBERBUILD\_FLAGS="-xMIC-AVX512"

On Intel® Xeon Phi™: make install



Images Source: Intel



**Value Proposition:** This application provides users with a research tool for investigating code modernization approach for Bio-molecular dynamics applications.

**Results:** Up to 2.7X improved performance compared to the Intel® Xeon® processor E5-2697 v4 for the Rubisco workload.

See next slide for configuration details.

SOURCE: INTEL MEASURED RESULTS AS OF APRIL 2016



# AMBER 16 PMEMD EXPLICIT\*

*Amber\* is a bio related simulation code for DNA, RNA, protein, and other bio-molecules. Particle Mesh Ewald Molecular Dynamics (PMEMD) is an Amber tool used for Molecular Dynamic Simulation. PMEMD includes two algorithms, Explicit and Implicit. PMEMD is written in Fortran 90 and is mainly MPI\*, OpenMP\* and Vectorization parallelized.*

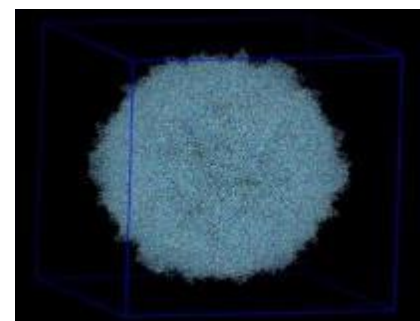
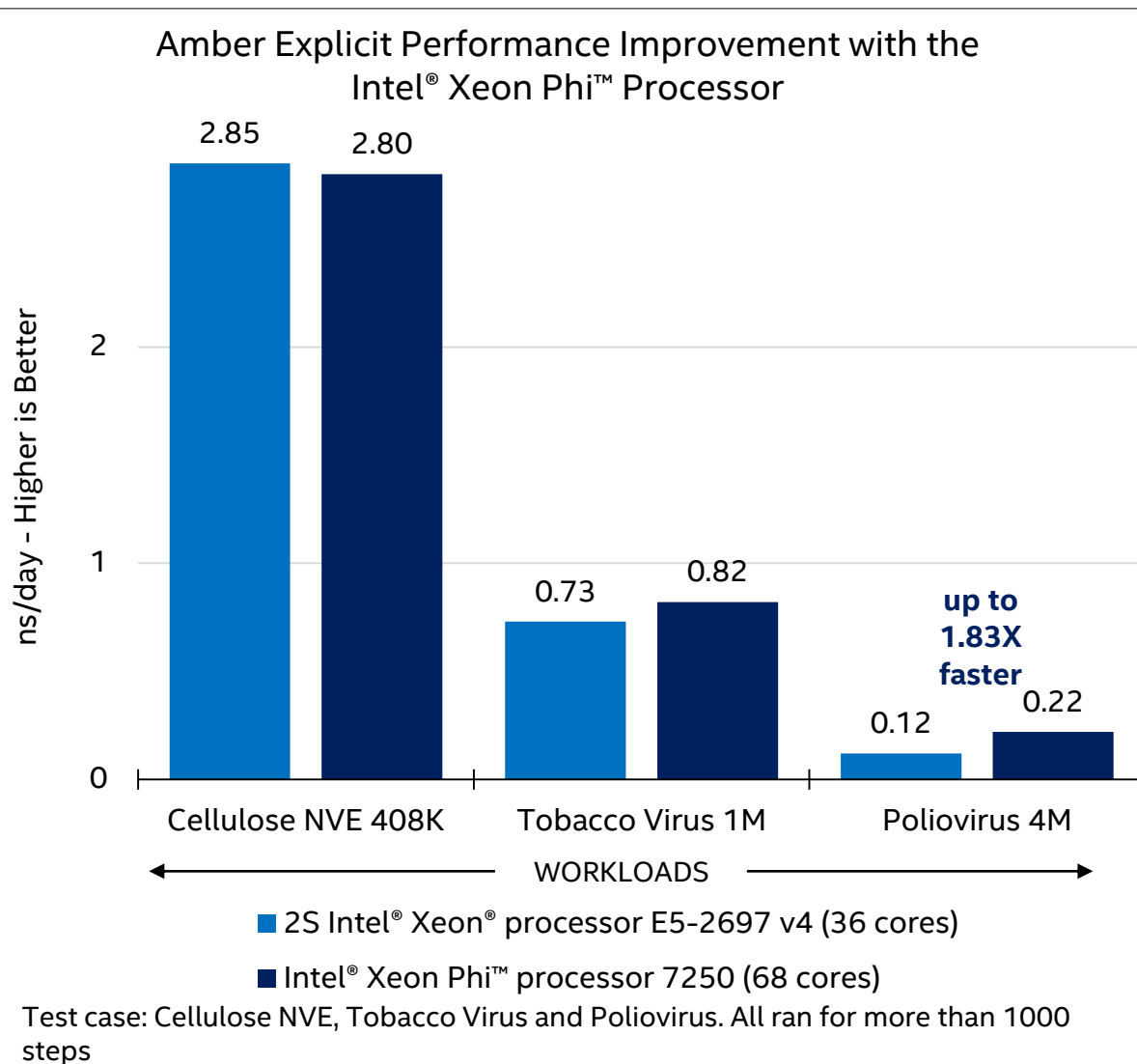
**Application:** Amber 16 PMEMD Explicit.

**Code:** License required from <http://ambermd.org/>

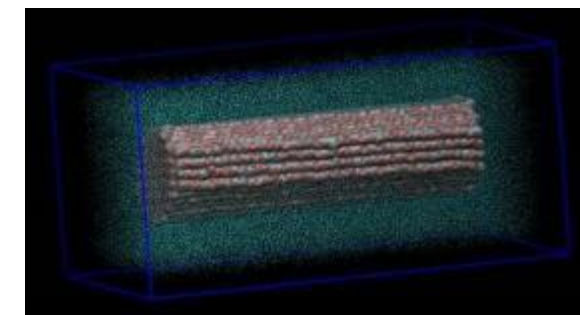
**Recipe:** ./configure -intelmpi -openmp -mic2 intel

On Intel® Xeon®: make install AMBERBUILDFLAGS="-xMIC-AVX512"

On Intel® Xeon Phi™: make install



Images Source: Intel



**Value Proposition:** This application provides users with a research tool for investigating code modernization approach for Bio-molecular dynamics applications. KNL is best suited for larger problem sizes.

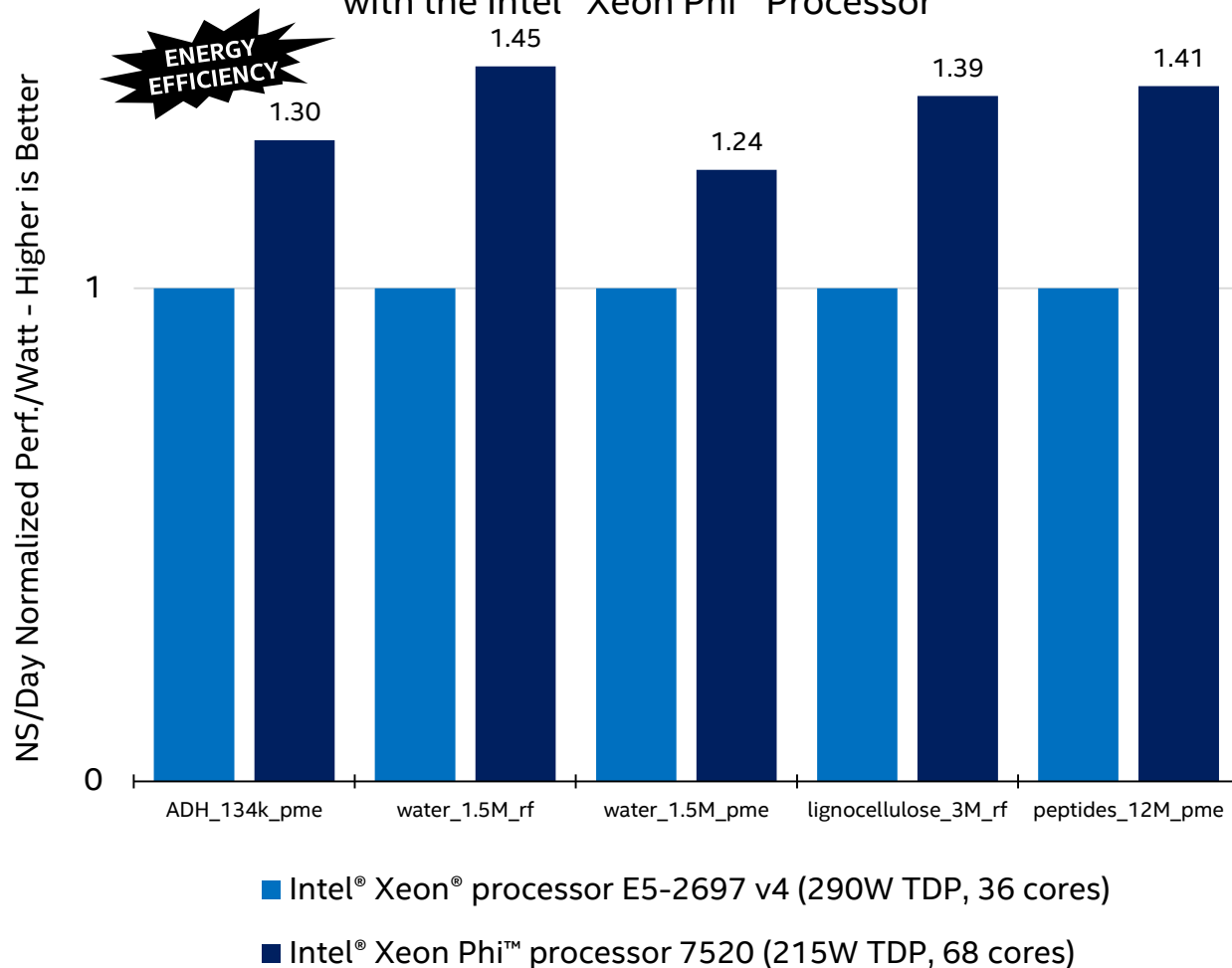
**Results:** Up to 1.83X improved performance compared to the Intel® Xeon® processor E5-2697 v4 for the Poliovirus workload.

See next slide for configuration details.

SOURCE: INTEL MEASURED RESULTS AS OF APRIL 2016



GROMACS Single Node NS/Day Performance/Watt Improvement with the Intel® Xeon Phi™ Processor

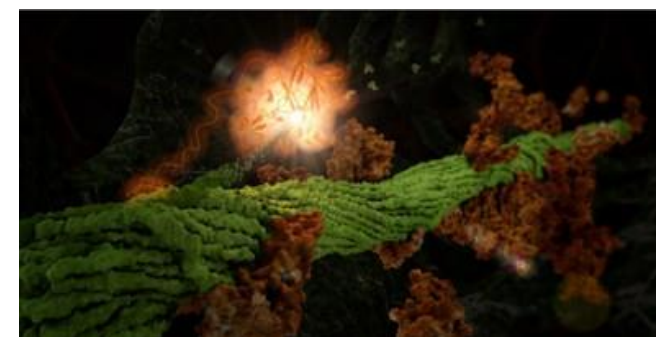


**GROMACS (GROningen MACHine for Chemical Simulations)** is a versatile package to perform classical Molecular Dynamics simulations. Heavily optimized for most modern platforms and provides extremely high performance compared to all other MD codes.

**Application:** GROMACS

**Code:** [Available here](#)

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



**Power Data:** Total system wall power is measured out-of-band over iPMI interface, polling the BMC chip every second. Energy usage is matched to internally timed code segment to arrive at performance per Watt estimate.

Images Source: Used with permission

**Value Proposition:** This application provides users with wide range of functionality for chemical simulations and highest out-of-the-box performance across all MD codes. GROMACS on the Intel® Xeon Phi™ processor outperforms Intel® Xeon® processors for simulating large biochemical systems due to enabling new Intel® AVX512 features and enabling enhanced parallelism and provides more performance simulations within the same energy envelope.

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

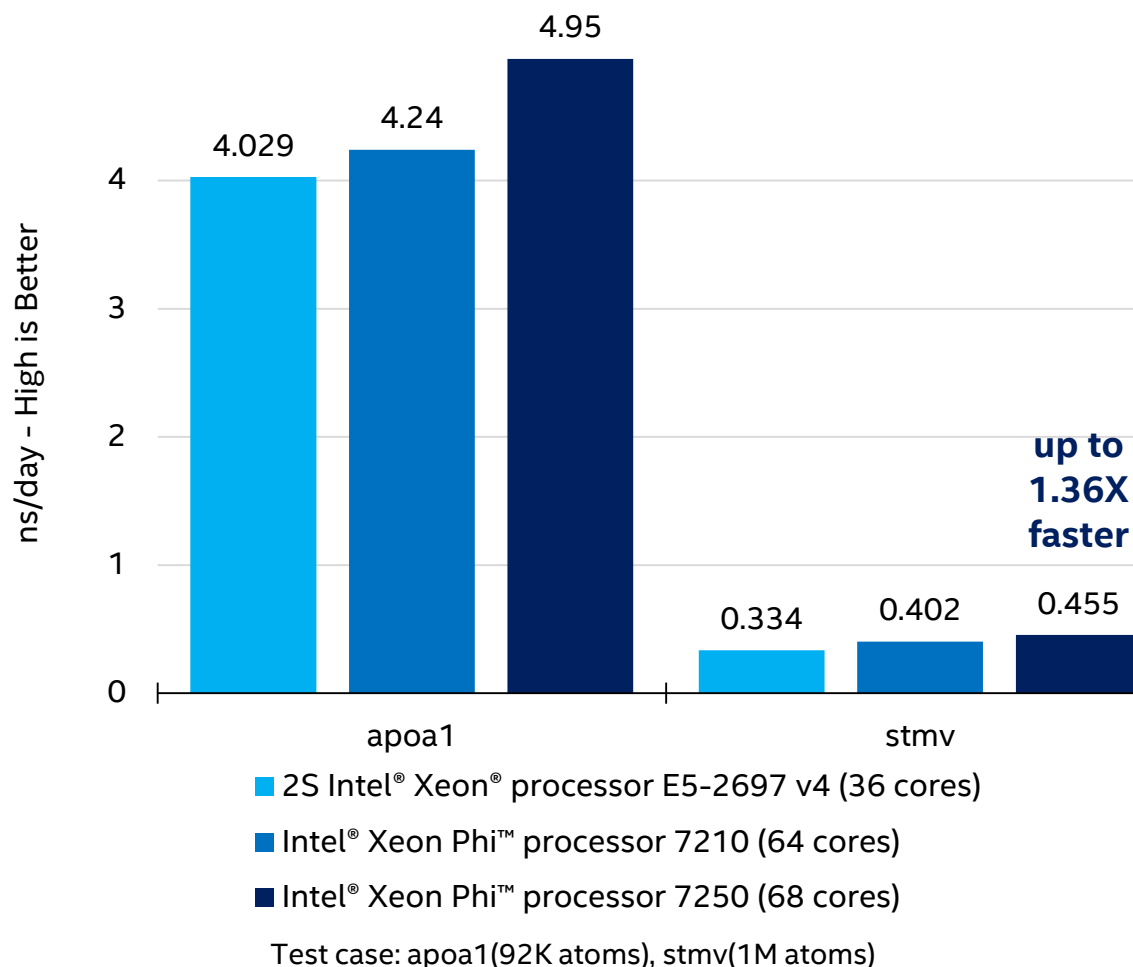
See next slide for configuration details.

SOURCE: INTEL MEASURED RESULTS AS OF JUNE 2016



# NANOSCALE MOLECULAR DYNAMICS PROGRAM\*

NAMD Performance Improvement with the Intel® Xeon Phi™ Processor



See next slide for configuration details.

SOURCE: INTEL MEASURED RESULTS AS OF APRIL 2016

*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.*

**Application:** NAMD 2.11

**Code:** <http://www.ks.uiuc.edu/Research/namd/>

**Recipe:** Under development for external release

NAMD  
Scalable Molecular Dynamics

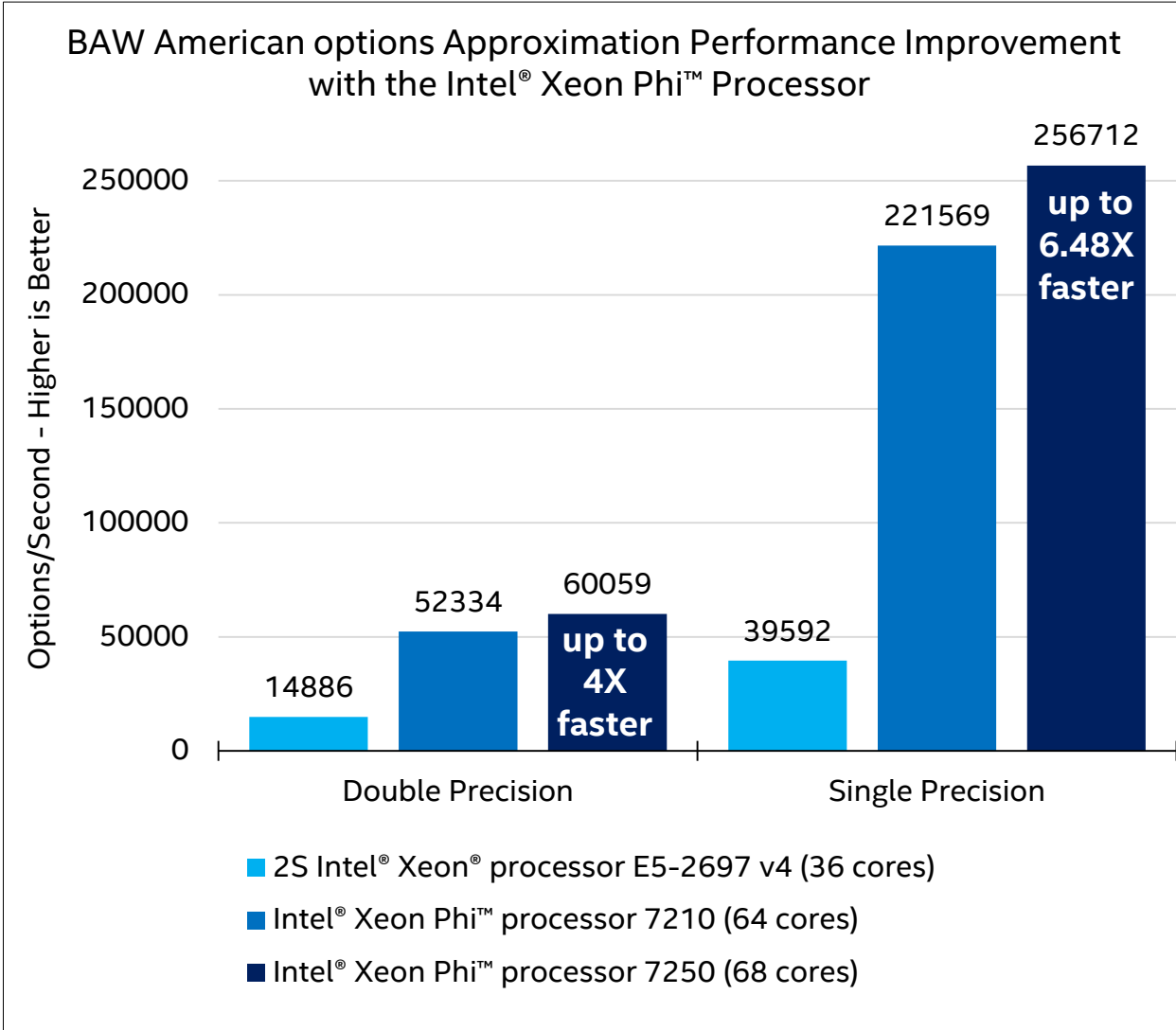


Image Source: Use approved by NAMD

**Value Proposition:** NAMD is the 2<sup>nd</sup> most popular MD code. Intel® AVX 512 instructions are used heavily by the Assembler code. Source code performance tuning with intrinsics demonstrates advantages of MCDRAM and SMT 4.

**Results:** Up to 1.36X improved performance compared to the Intel® Xeon® processor E5-2697 v4.

# BAW AMERICAN OPTIONS APPROXIMATION BENCHMARK\*



See next slide for configuration details. SOURCE: INTEL MEASURED RESULTS AS OF MAY, 2016

*Popular analytical method of pricing exchange-traded American options using quadratic approximation. Uses an underlying asset and carrying cost rate as key inputs and prices commodity options, futures and foreign exchange options, precious metals, long-terms debt and stock indexes with continuous dividend yields. Uses the stock price, strike price and time as input streams and creates a call output stream.*

**Application:** Barone-Adesi and Whaley (BAW) American Options Approximation  
**Code:** Currently not available **Recipe:** [Available here](#) (Original C/++, re-implemented on IA using parallel programming techniques)

Image Sources: [Parsiad.azimzadeh](#), [finance.bi.no](#)

$$C(S,T) = \begin{cases} c(S,T) + A_2 \left(\frac{S}{S^*}\right)^{q_2} & \text{if } S < S^* \\ S - X & \text{if } S \geq S^* \end{cases}$$

where

$$q_2 = \frac{1}{2} \left( -(N-1) + \sqrt{(N-1)^2 + \frac{4M}{K}} \right)$$
$$A_2 = \frac{S^*}{q_2} \left( 1 - e^{(b-r)(T-t)} N(d_1(S^*)) \right)$$
$$M = \frac{2r}{\sigma^2}, N = \frac{2b}{\sigma^2}, K(T) = 1 - e^{-r(T-t)}$$

and  $S^*$  solves

$$S^* - X = c(S^*, T) + \frac{S^*}{q_2} \left( 1 - e^{(b-r)(T-t)} N(d_1(S^*)) \right)$$

Formula 12.1: The functional form of the Barone Adesi Whaley approximation to the value of an American call

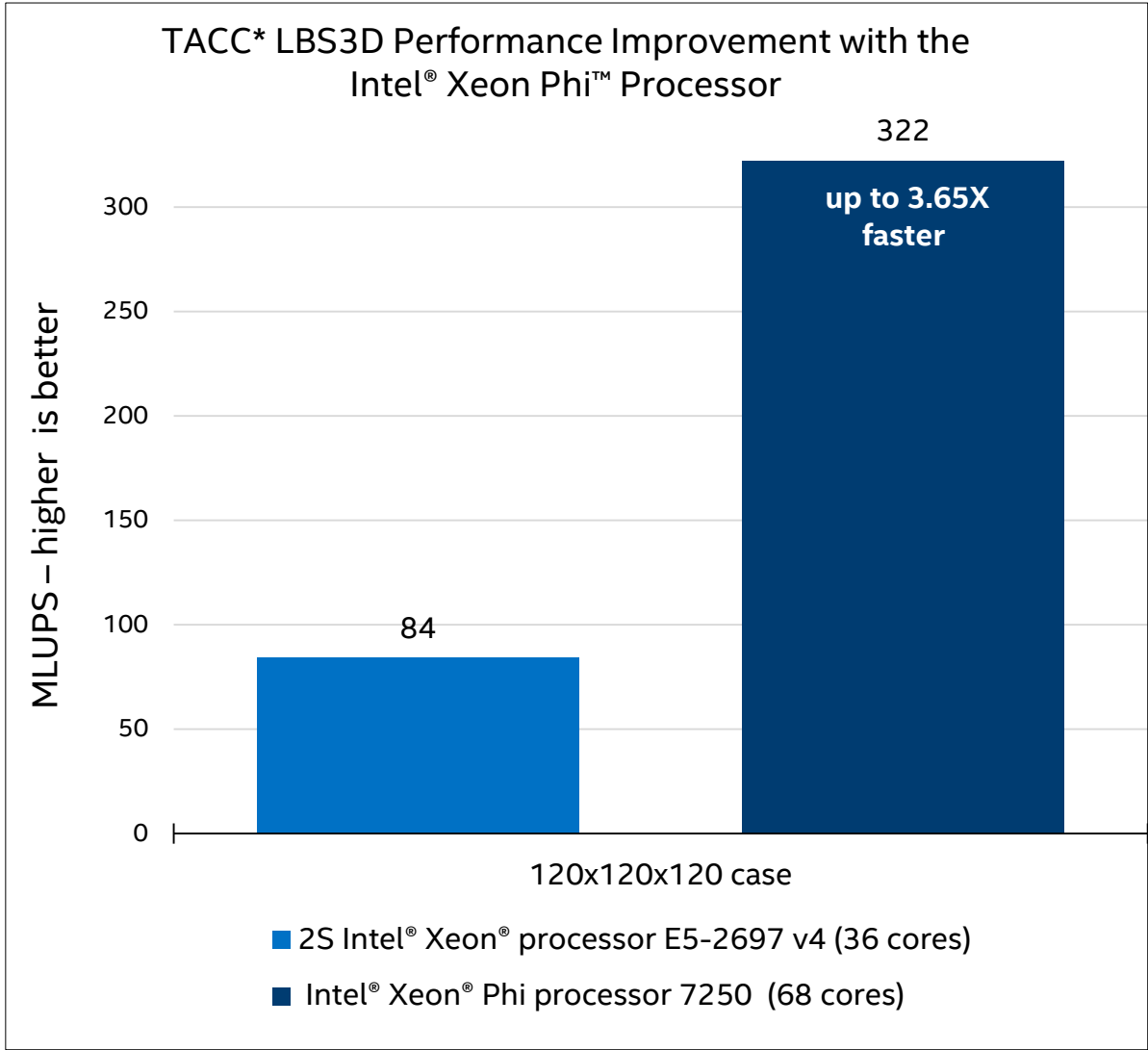
**Value Proposition:**

- Foundation of Financial derivatives pricing
- Widely used all over financial libraries
- EMU benefits transcendental functions

**Results:** Up to 6.48X improved Single Precision performance compared to the Intel® Xeon® processor E5-2697 v4.



# TEXAS ADVANCED COMPUTER CENTER LBS3D\*



See next slide for configuration details.

SOURCE: TACC (Carlos Rosales-Fernandez) April 2016

*LB3D is a 3D Lattice Boltzmann method kernel developed by Carlos Rosales of Texas Advanced Computer Center (TACC) and used in multiphase flows with applications in the multiphase reactors and separation systems.*

**Application:** LB3D (Advanced support for multiphase flows with large density and viscosity ratios)

**Code:** [Available here](#)

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

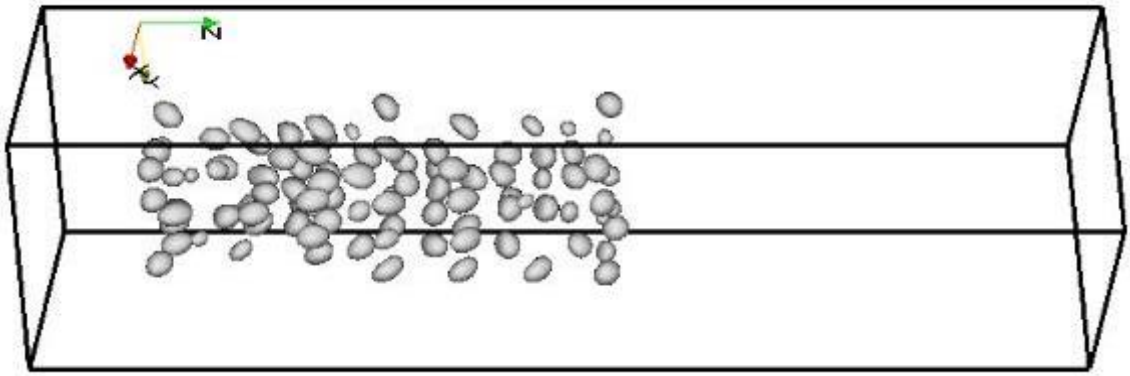


Image Source: Used with permission

**Value Proposition:** LB3D performance on the Intel® Xeon Phi™ Processor 7250 provides better performance, performance density and better energy efficiency than today's best Intel® Xeon® processor based systems.

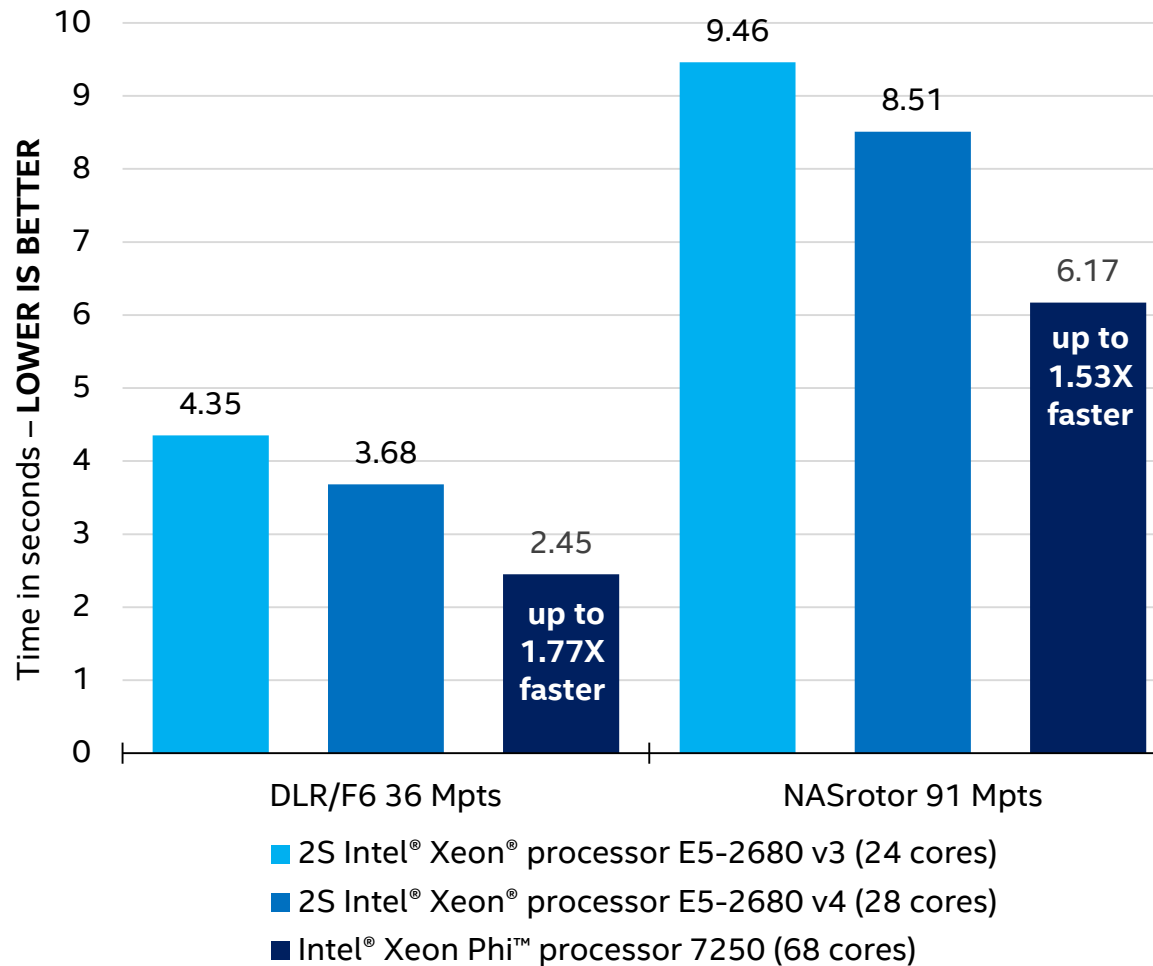
**Results:** Up to 3.65X performance improvement with the Intel® Xeon Phi™ processor 7250 compared to the Intel® Xeon® processor E5-2697v4.





# NASA OVERFLOW\*

## NASA OVERFLOW CFD Performance



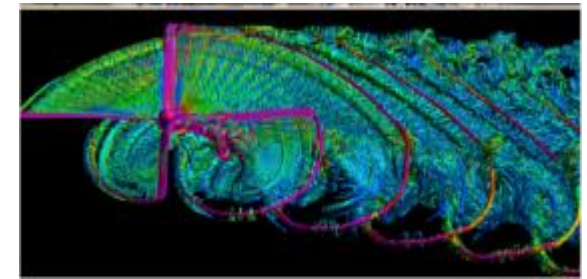
SOURCE: NASA/Ames (Dennis Jespersen) April 2016

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

**Application:** OVERFLOW 2.2L has an extensive feature set supporting collision detection and modelling with support for thin layer and full viscous terms.

**Code:** <http://overflow.larc.nasa.gov/>

**Recipe:** No code changes were required. Recompile with KNL AVX-512.



UH-60 Black Hawk helicopter and Navier-Stokes detached eddy simulation of a flexible UH-60 rotor using the OVERFLOW CFD code in forward flight.

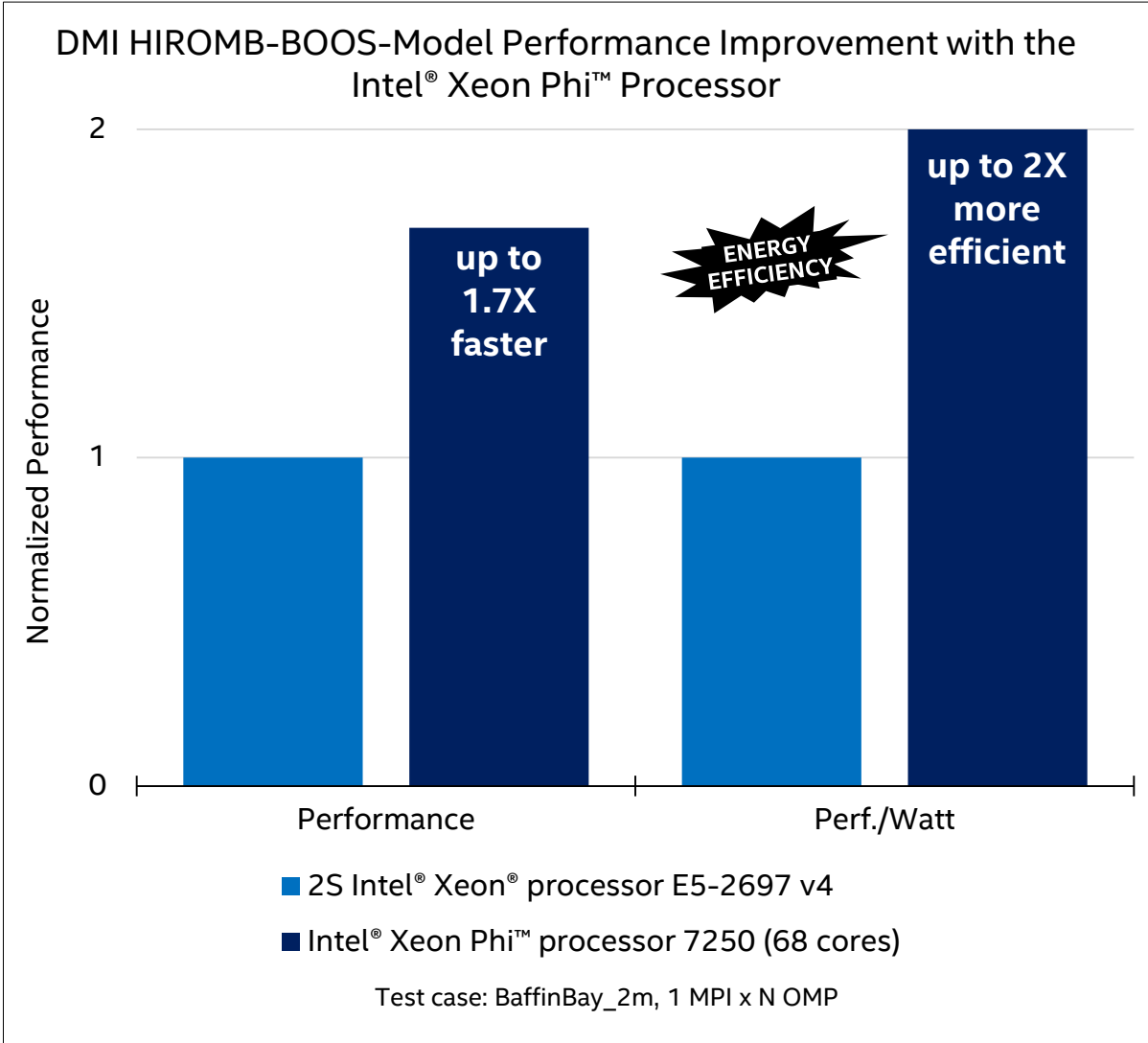
Image Source: Neal Chaderjian and Tim Sandstrom, NASA/Ames

### Value Proposition:

Overflow performance on KNL beats contemporary Haswell and Broadwell Architecture 2S servers. This provides better performance, performance density and better energy efficiency than today's best Intel Xeon processor based systems.

**Results:** Up to 1.78X performance improvement compared to the Intel® Xeon® processor E5-2680v3.

# DANISH METEOROLOGICAL INSTITUTE HIROMB-BOOS-MODEL\*



See next slide for configuration details. SOURCE: INTEL MEASURED RESULTS AS OF MARCH, 2016

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

**Application:** DMI HIROMB-BOOS-Model is a 3D ocean circulation model code forced by atmospheric meteo-fields from a weather model.  
**Code:** To get access to the code and test cases, [please contact DMI](#)  
**Recipe:** TBD

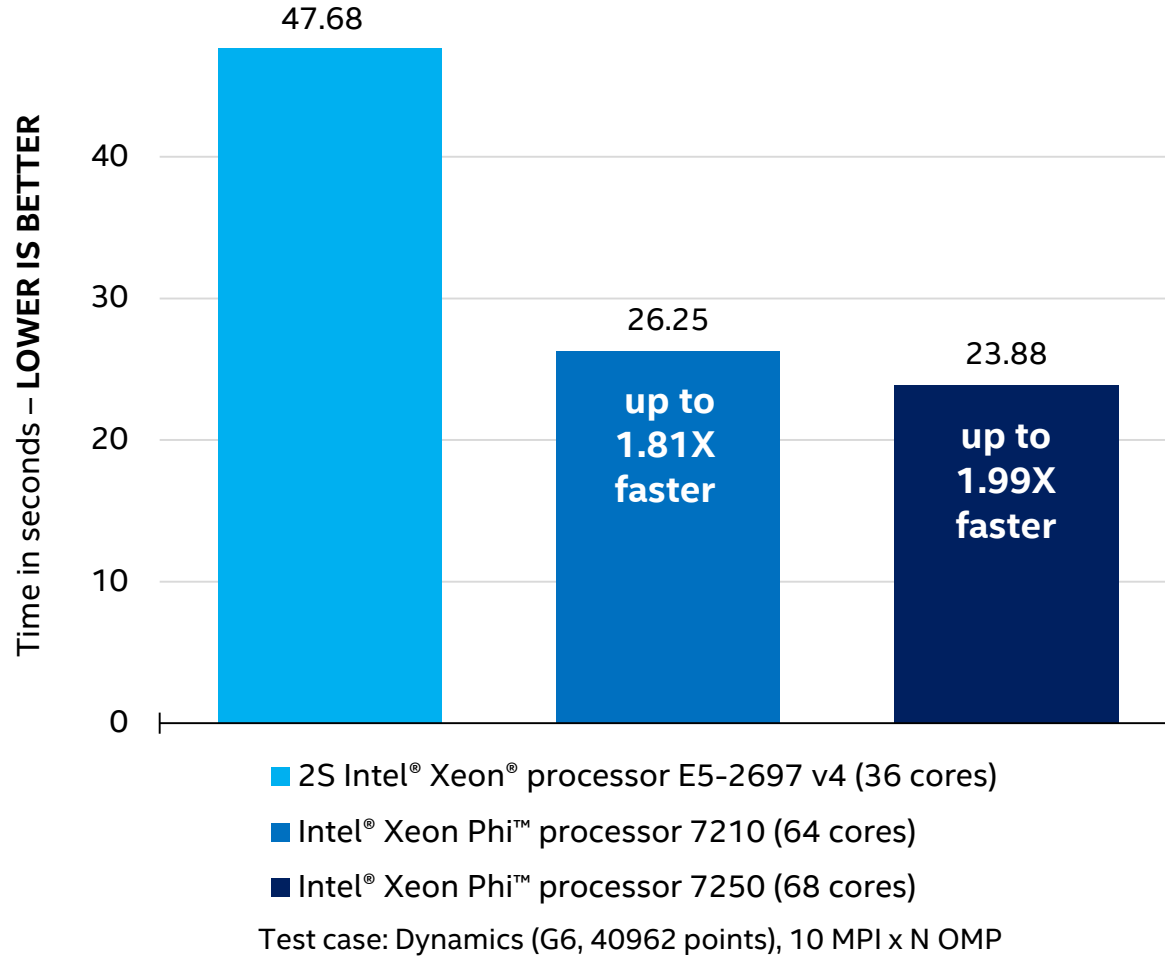
Image Source: [DMI](#)



**Value Proposition:** The improved performance from the Intel® Xeon Phi™ processor helps deliver improved forecasting of hazardous meteorological phenomena allowing for improved weather forecasting which impacts critical infrastructure affecting human activity.  
**Results:** Up to 1.7X performance improvement compared to the Intel® Xeon® processor E5-2697 v4.

# NON-HYDROSTATIC ICOSAHERDRAI MODEL \* (NIM)

NIM Dynamics (G6) Performance Improvement with the Intel® Xeon Phi™ Processor



*Non-hydrostatic Icosahedral Model (NIM) is developed by NOAA's Earth System Research Laboratory. NIM is used for earth system modeling and weather and climate prediction. NIM is a multi-scale model designed to improve tropical convective clouds and to extend weather forecasts into intra-seasonal predictions.*

**Application:** Non-hydrostatic Icosahedral Model

**Code:** To get access to the code and test cases, [please contact NOAA](#)

**Recipe:** Build and run instructions are similar to those for Intel® Xeon® processor E5-2697 v4, except build with `-xMIC-AVX512` flag and run with `"numactl -m 1"` prepended to the command-line.

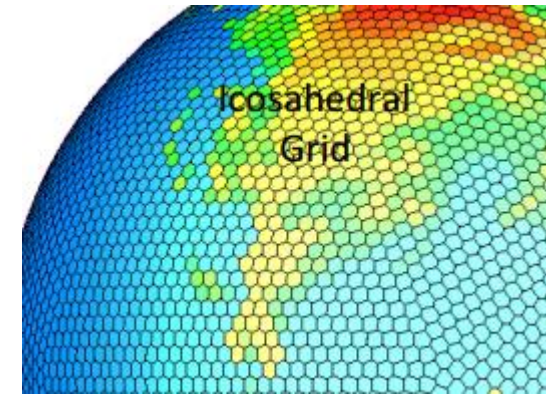


Image Source: NOAA

**Value Proposition:** The improved performance from the Intel® Xeon Phi™ processor helps deliver improved weather and climate forecasting.

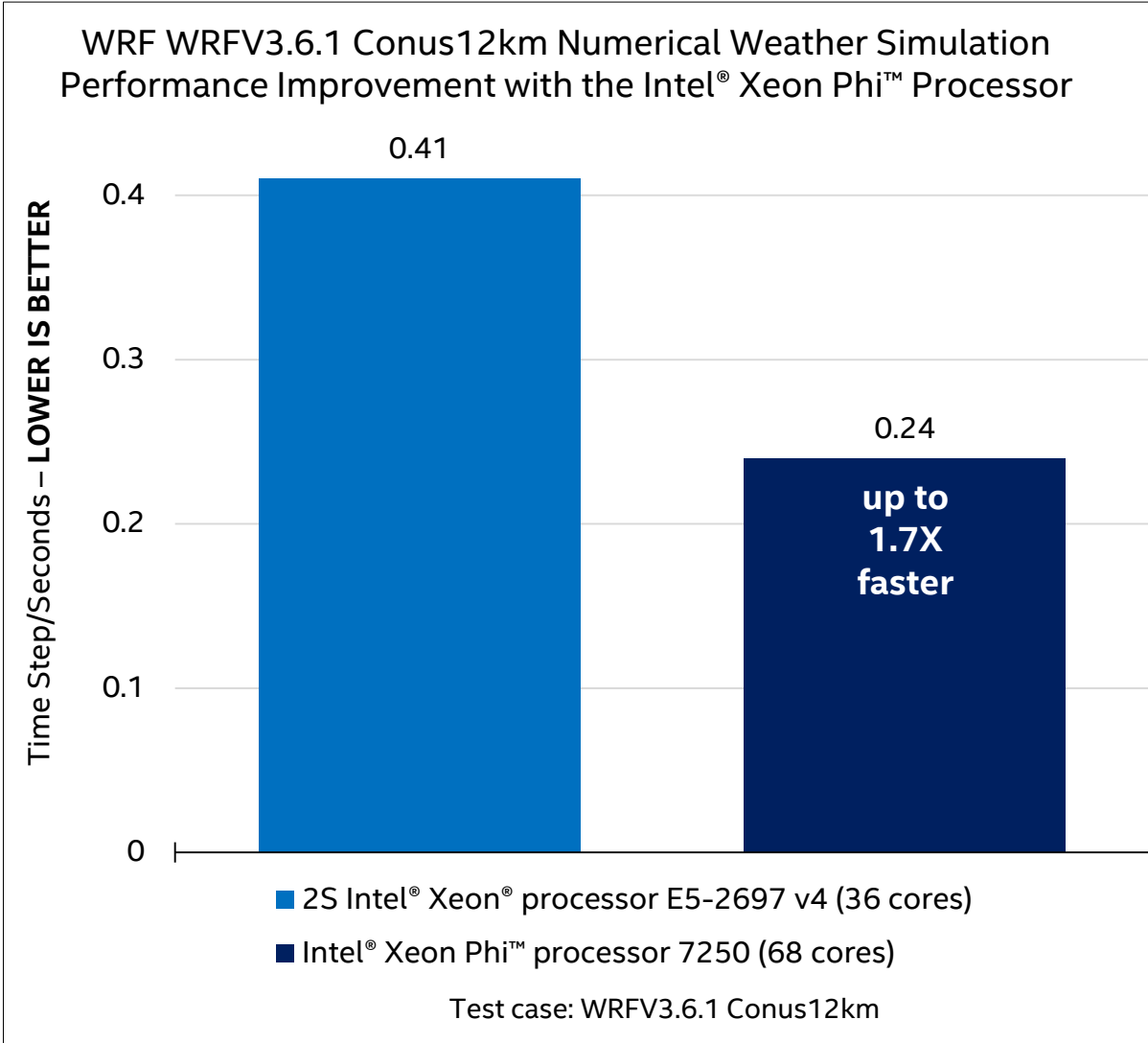
**Results:** Up to 1.99X performance improvement compared to the Intel® Xeon® processor E5-2697 v4.

See next slide for configuration details.

SOURCE: INTEL MEASURED RESULTS AS OF MARCH, 2016



# WEATHER & RESEARCH FORECAST MODEL\* NUMERICAL WEATHER SIMULATION



See next slide for configuration details. SOURCE: INTEL MEASURED RESULTS AS OF FEBRUARY, 2016

*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.*

**Application:** The Weather & Research Forecast Model\* (WRF) WRFV3.6.1 Conus12km. Community code is managed by NCAR. CONUS12KM benchmark is an adhoc industry standard workload and is widely cited.

**Code:** [Available here](#). (WRF 3.6 & 3.6.1) **Recipe:** Not available.

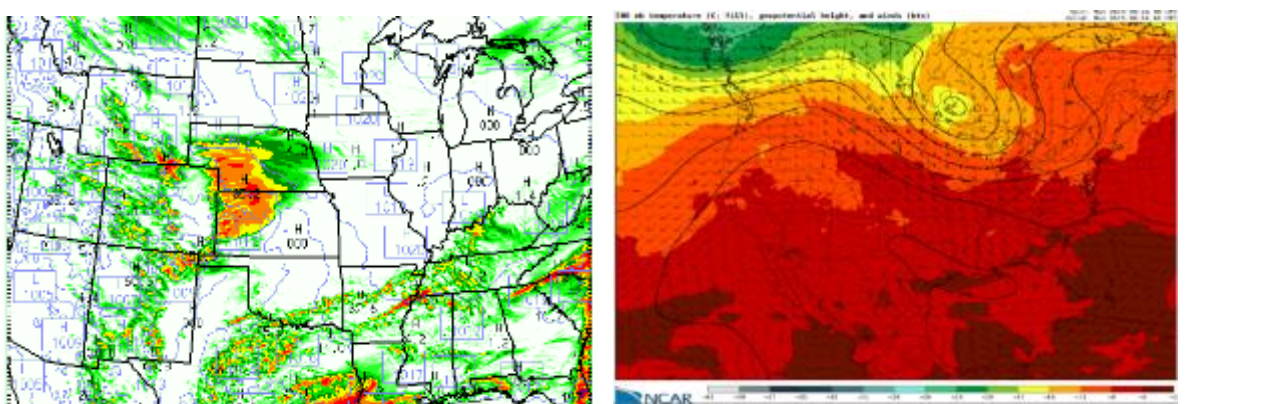


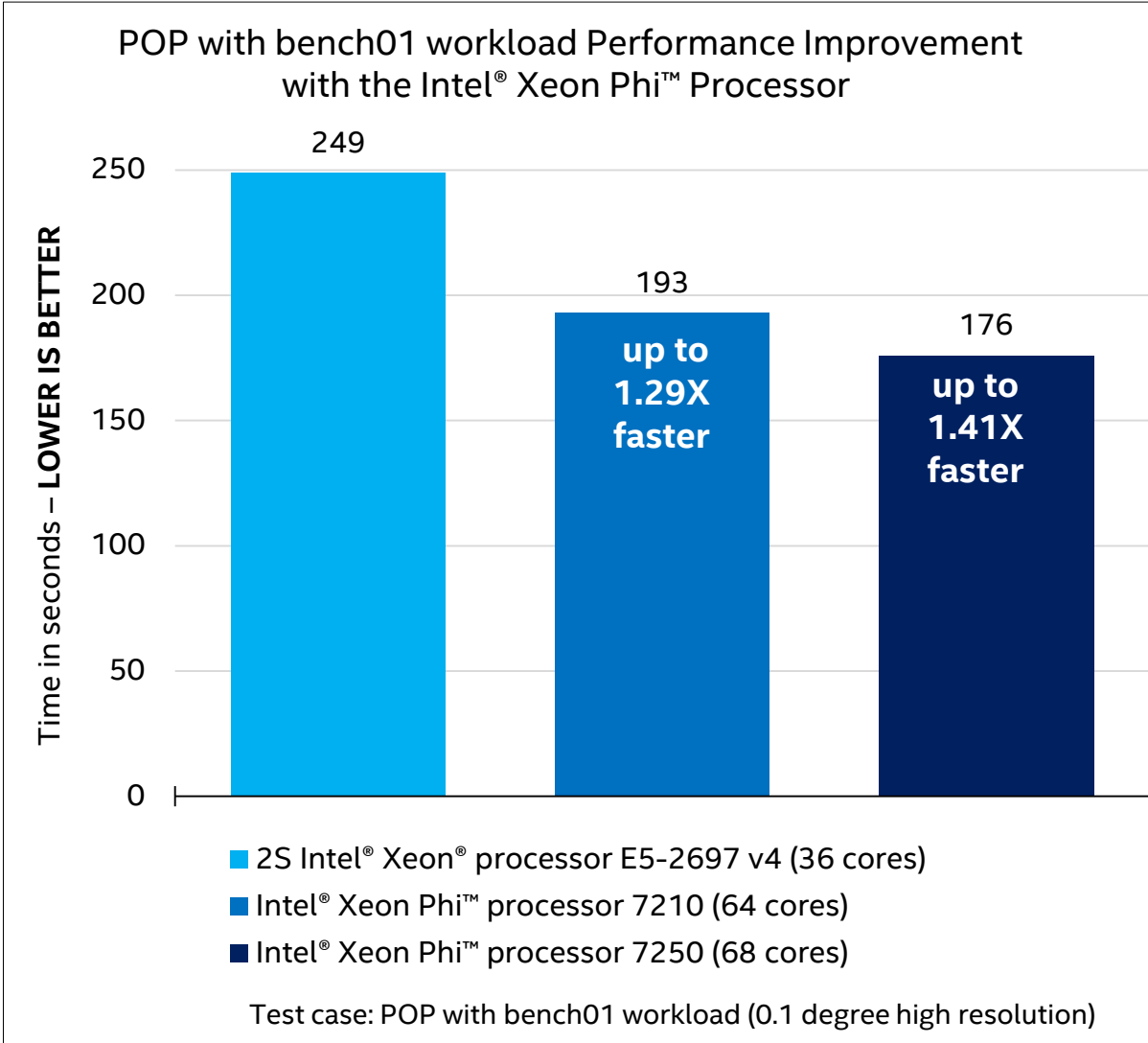
Image Source: NOAA

**Value Proposition:** The most widely-used weather forecasting code runs in its entirety on the Intel platform only. Speed up the WRF weather simulation code and results with Intel® architecture.

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



# PARALLEL OCEAN PROGRAM\*



See next slide for configuration details. SOURCE: INTEL MEASURED RESULTS AS OF MARCH, 2016

*Parallel Ocean Program (POP) is an ocean circulation model that solves the three-dimensional primitive equations for ocean dynamics. It consists of the baroclinic and barotropic solvers that solve 3-D equations explicitly and 2-D surface pressure implicitly, respectively. It is widely used for oceanography. The code is Open Source.*

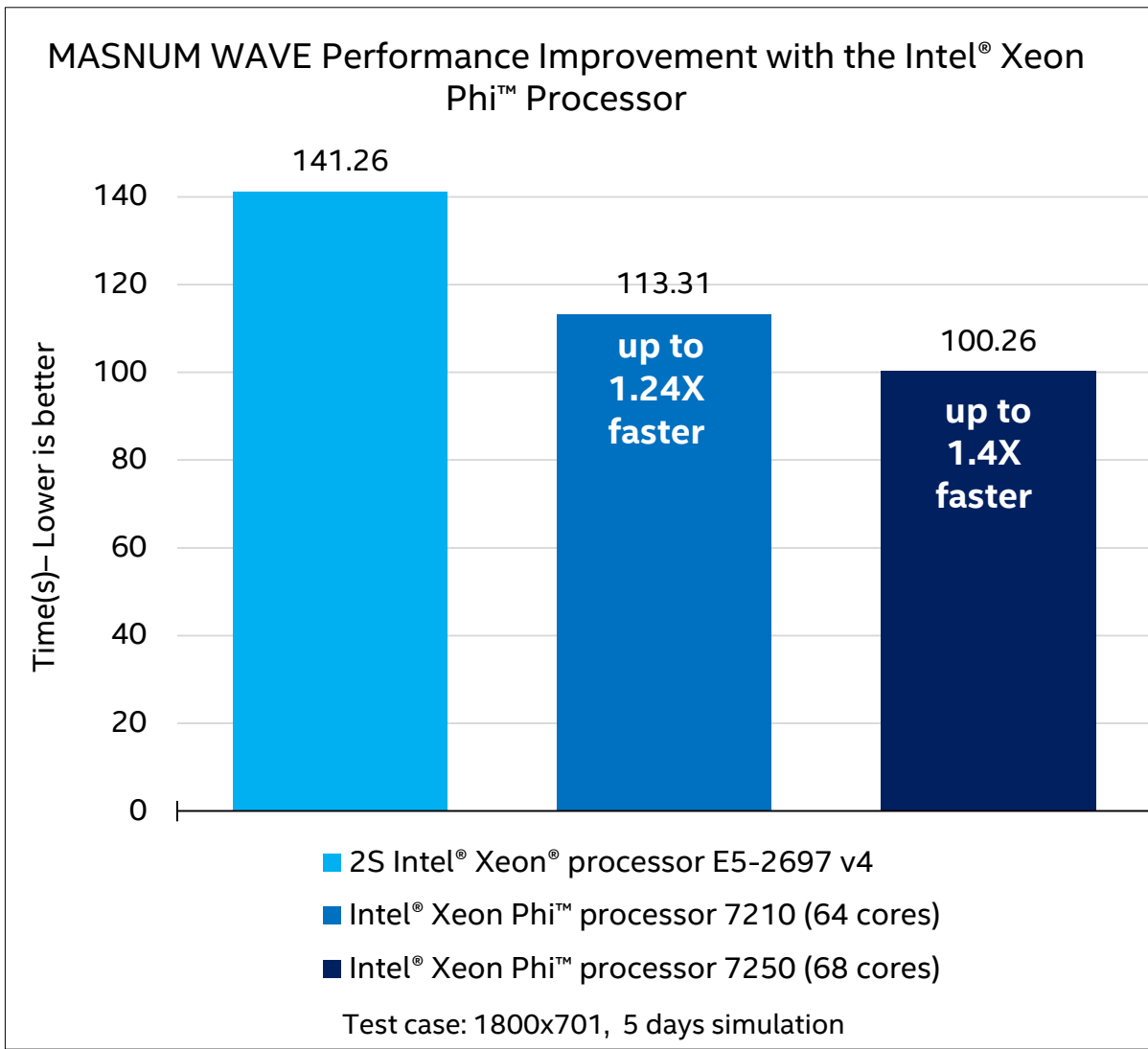
**Application:** POP (Parallel Ocean Program).  
**Code:** <http://www2.cesm.ucar.edu/>  
**Recipe:** -mcmmodel=medium -O3 -ipo -xMIC-AVX512 -fp-model fast=2



Image Source: FIO, China

- Value Proposition:**
- POP is developed by LANL USA and widely used in ocean and climate research. It is also incorporated into FIO-ESM (First Institute of Oceanography-Earth System Model) as the ocean component.
  - Intel® Xeon Phi™ processor 7250 enables this application to significantly outperform (time-to-solution) alternative processing solutions.
- Results:** Up to 1.41X faster with the Intel® Xeon Phi™ processor 7250 compared to the Intel® Xeon® processor E5-2697 v4.

# MASNUM WAVE\*



See next slide for configuration details. SOURCE: INTEL MEASURED RESULTS AS OF April,2016

*MASNUM WAVE model is the 3rd generation surface wave model proposed early in 1990s in LAGFD (Laboratory of Geophysical Fluid Dynamics) from FIO. The application is used to simulate and predict the wave process by solving the wave energy spectrum balance equation and its complicated characteristic equations in wave-number space, which is written in Fortran and parallelized with MPI+OMP.*

**Application:** MASNUM WAVE.  
**Code:** In-house code. To get access to the code and test cases, please contact [songroy@fio.org.cn](mailto:songroy@fio.org.cn), [yinxq@fio.org.cn](mailto:yinxq@fio.org.cn)  
**Recipe:** Please contact [songroy@fio.org.cn](mailto:songroy@fio.org.cn), [yinxq@fio.org.cn](mailto:yinxq@fio.org.cn)

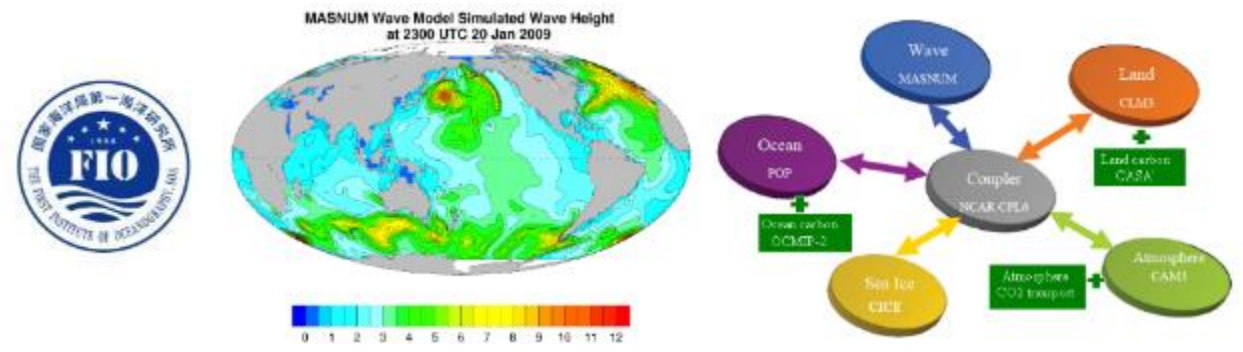
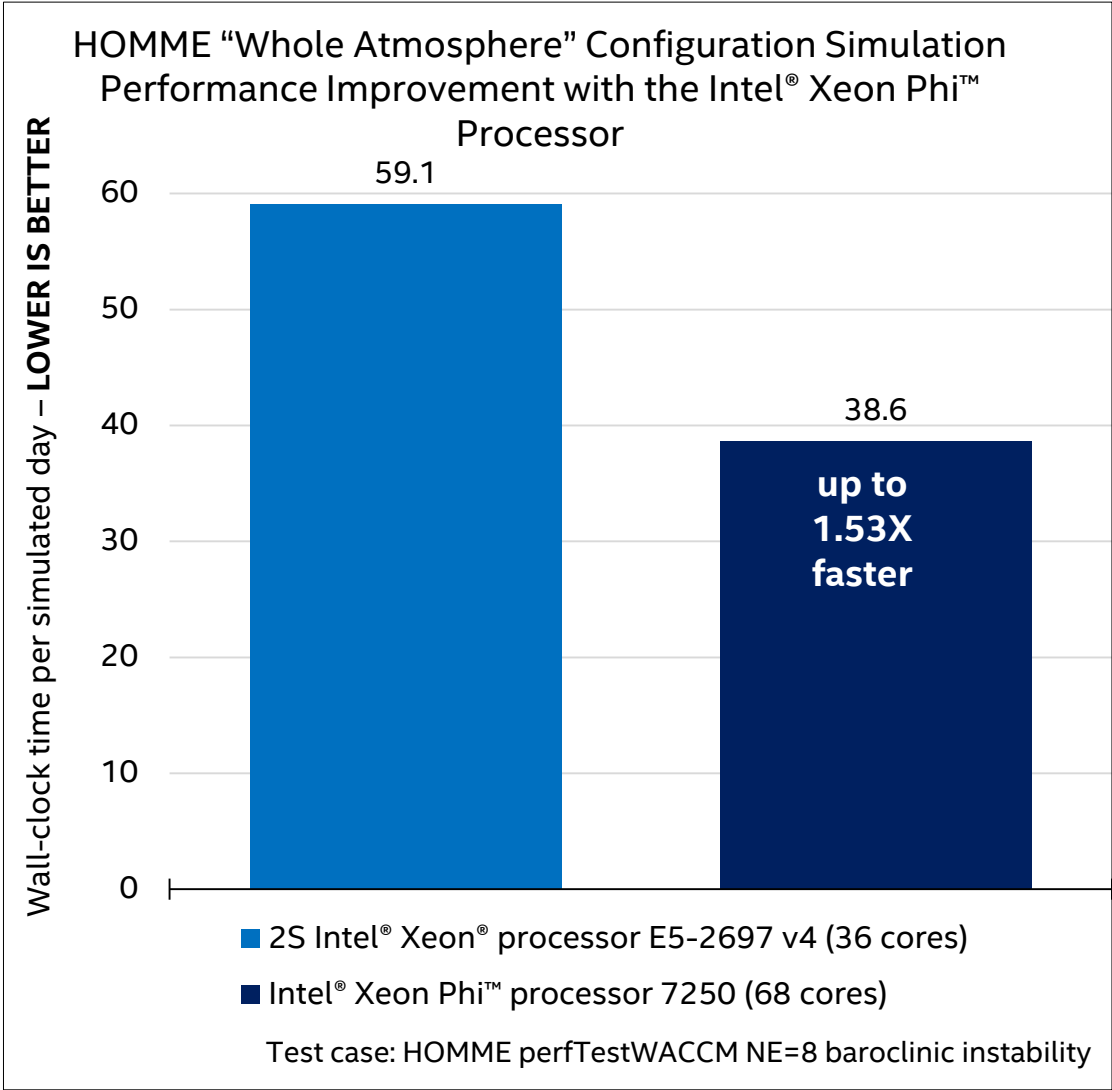


Image Source: FIO, China

**Value Proposition:** Performance is enhanced by Intel® AVX512.  
**Results:** Up to 1.41X improved performance compared to the Intel® Xeon® processor E5-2697 v4.

# HOMME ATMOSPHERIC DYNAMICAL CORE \* NUMERICAL CLIMATE SIMULATION



See next slide for configuration details. SOURCE: INTEL MEASURED RESULTS AS OF APRIL, 2016

*HOMME is the spectral element dynamical core that solves the equations of motion in the CAM5 atmospheric model, part of the Community Earth System Model (CESM) jointly developed by NSF and DOE.*

**Application:** Baroclinic instability simulation in a “whole atmosphere” (extending to lower thermosphere) configuration.

**Code:** Request access to development branches [here](#).

**Recipe:** `cmake -DADD_Fortran_FLAGS="-O3 -xMIC-AVX512 -fp-model fast" \`

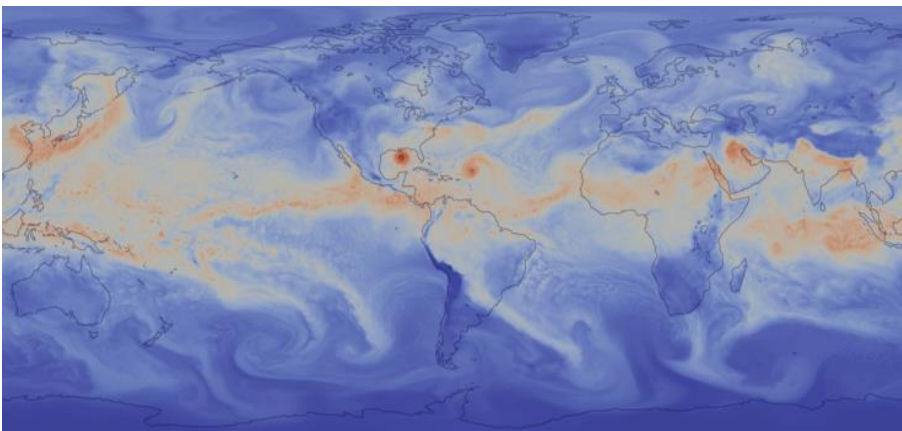


Image source: Used by permission.  
Global 1/8 degree simulation run using CAM5 with the HOMME spectral element dynamical core.  
Visualization from <http://www.sdav-scidac.org/29-highlights/visualization/64-precipitable-water-vis.html>.

**Value Proposition:**

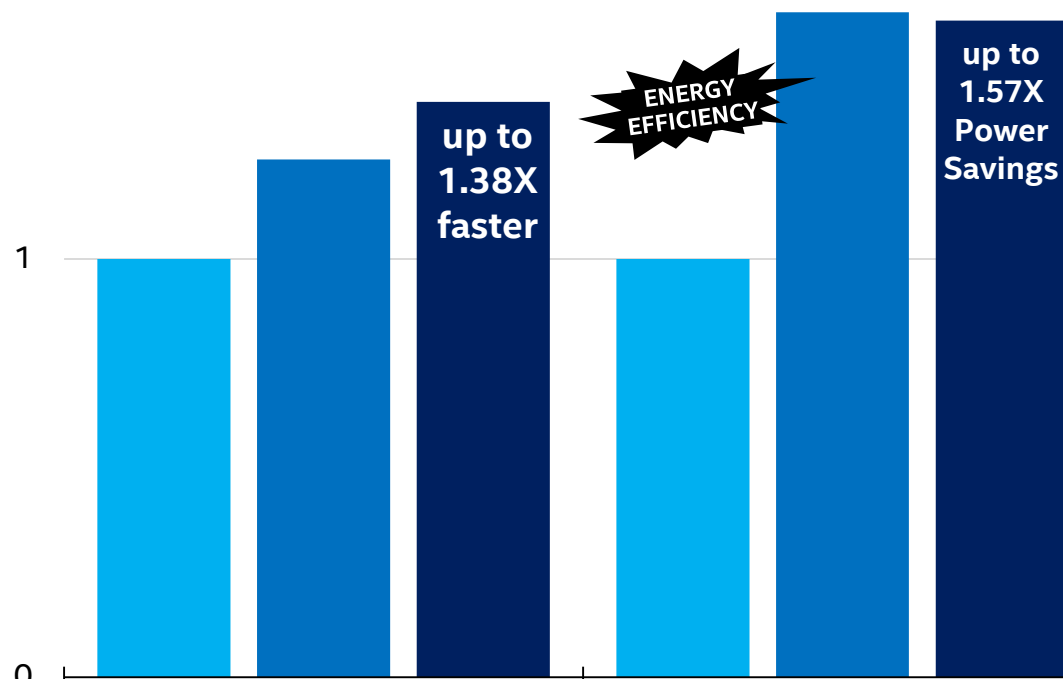
- CESM is a widely-used Earth system model and an important source of simulations used by the Intergovernmental Panel on Climate Change. Intel® Xeon Phi™ processors provide the high memory bandwidth required to advect many chemical tracers through the atmosphere.

**Results:** Up to 1.53X faster compared to the Intel® Xeon® processor E5-2697 v4.



BerkeleyGW Performance Improvement with the Intel® Xeon Phi™ Processor

Execution Rate – Higher is Better



Benzene Sigma  
phase

Perf/Watt

- 2S Intel® Xeon® processor E5-2697 v4
- Intel® Xeon Phi™ processor 7210 (64 cores)
- Intel® Xeon Phi™ processor 7250 (68 cores)

ENERGY  
EFFICIENCY

**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 that is based on many-body perturbation theory employing the *ab initio* GW and GW plus Bethe-Salpeter equation methodology. Sigma is the second half of the GW code. It gives the quasiparticle self-energies and dispersion relation for quasidelectron and quasihole states.**

**Application:** BerkeleyGW Sigma phase of Benzene analysis

**Source:** <http://www.berkeleygw.org>

Deslippe, Jack, Georgy Samsonidze, David A. Strubbe, Manish Jain, Marvin L. Cohen, and Steven G. Louie. "BerkeleyGW: A massively parallel computer package for the calculation of the quasiparticle and optical properties of materials and nanostructures." *Computer Physics Communications* 183, no. 6 (2012): 1269-1289.

**Recipe:** -xMIC-AVX512 -Ofast -qopenmp



# BerkeleyGW

Image Source: Used with permission

**Value Proposition:** Xeon™ Phi enables broader scaling, larger problem sizes and reduced runtimes within the same energy use envelope. Uses Intel® MKL, MPI and OpenMP for massive scaling.

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

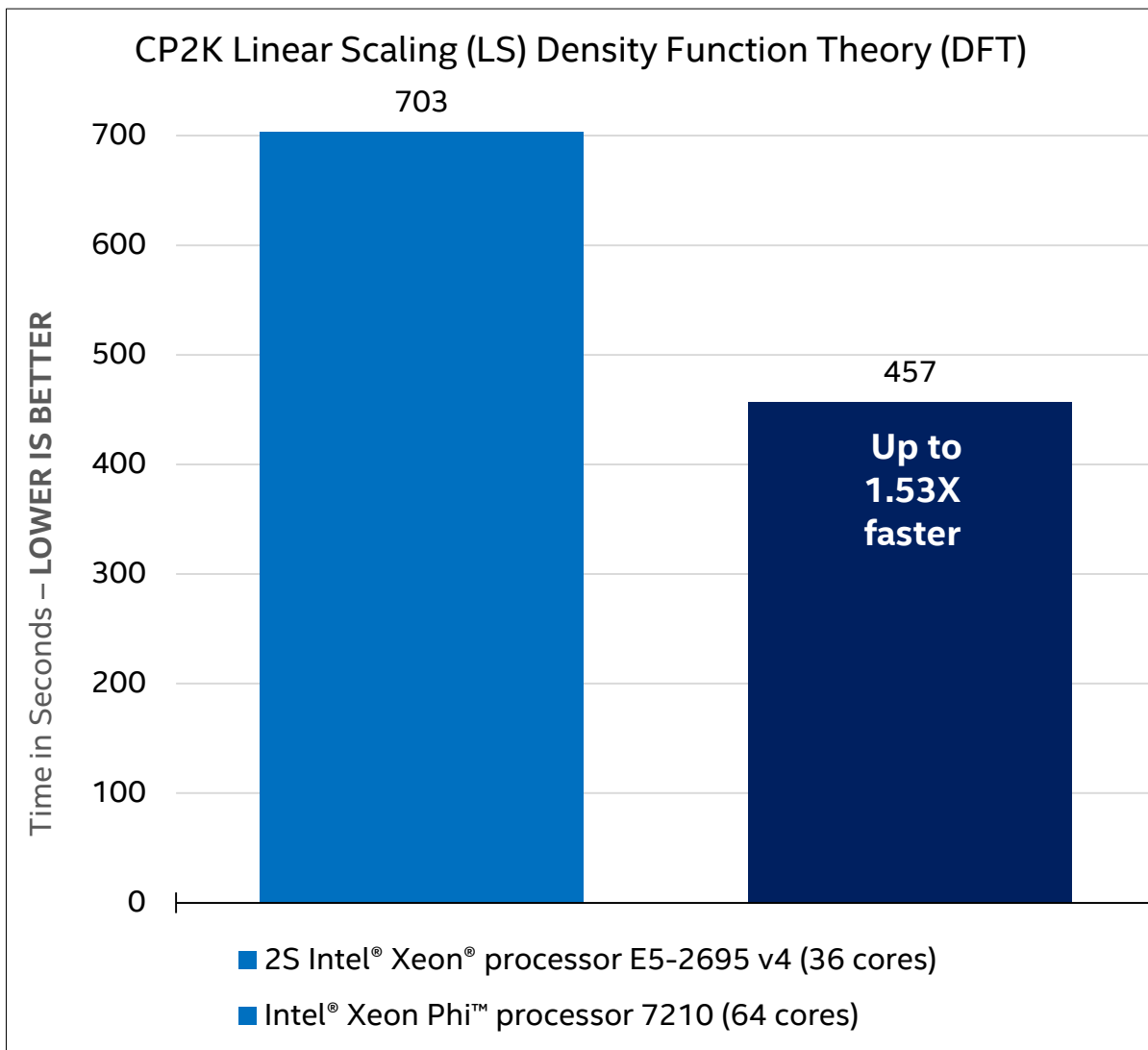
See next slide for configuration details.

SOURCE: INTEL MEASURED RESULTS AS OF APRIL, 2016





# LINEAR SCALING (LS) DENSITY FUNCTION THEORY (DFT)



See next slide for configuration details.

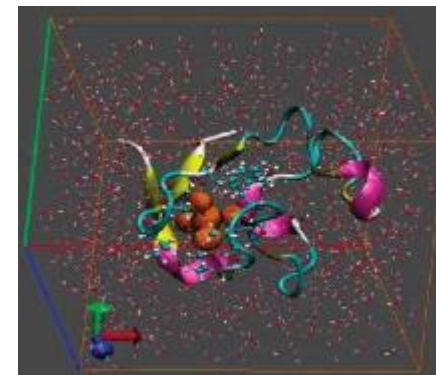
MEASUREMENT: University of Zurich / Intel, May 2016

*CP2K is a powerful and scalable program for atomistic simulations of a wide range of systems, including condensed phase, molecular systems and complex interfaces. CP2K features a wide range of atomistic interaction models including classical potentials, semi-empirical schemes, Density Functional Theory (DFT), Hartree-Fock (HF), and post-HF correlation methods such as MP2 and RPA. The program was a Gordon Bell Finalist in 2015. CP2K is freely available.*

**Application:** CP2K Quantum Chemistry & Solid State Physics Software Package

**Code:** [Available here](#)

CP2K



Courtesy of ETH Zurich.

CP2K

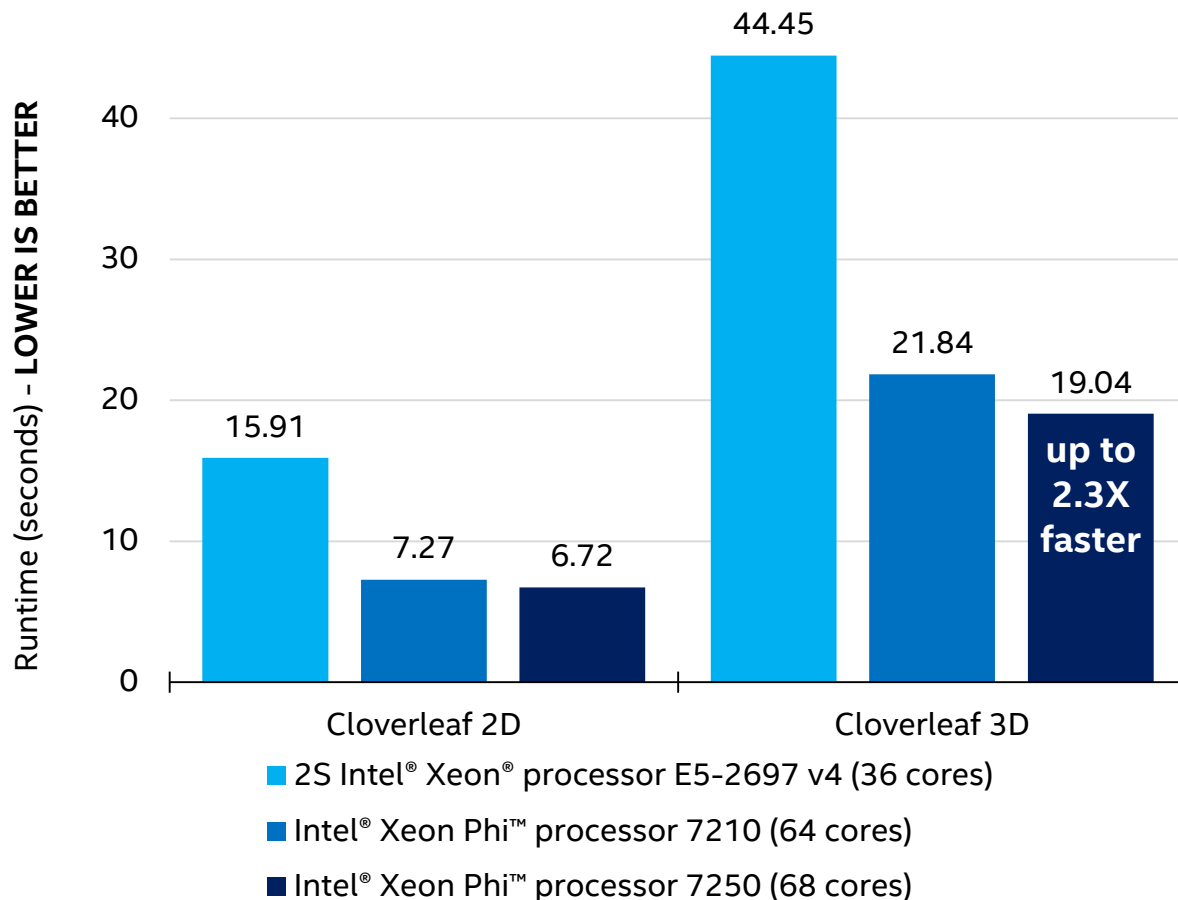
**Value Proposition:** CP2K optionally uses Intel's Open Source Library for small BLAS operations (matrix multiplications) called [LIBXSMM](#), which enables BLAS extensions on a drop-in basis, and automatically targets Intel® AVX, Intel® AVX2 and Intel® AVX-512 through future-proof just-in-time compilation techniques. LIBXSMM is also used in other scientific Open Source packages such as [SeisSol](#) and [Nek5000/NekBox](#).

**Results:** Up to 1.53X faster with the Intel® Xeon Phi™ processor 7210 when compared to the Intel® Xeon® processor E5-2695 v4.



# CLOVERLEAF\*

Cloverleaf Performance Improvement with the Intel® Xeon Phi™ Processor



Test case: Cloverleaf 2D (3840<sup>2</sup>, 87 time steps, Cloverleaf 3D (256<sup>3</sup>, 87 time steps)

See next slide for configuration details.

SOURCE: INTEL MEASURED RESULTS AS OF April 2016

*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.*

**Application:** Cloverleaf.

**Code:** <https://github.com/UK-MAC/CloverLeaf>

**Recipe:** make COMPILER=INTEL MPI\_COMPILER=mpiifort C\_MPI\_COMPILER=mpiicc OPTIONS="-xMIC-AVX512" C\_OPTIONS="-xMIC-AVX512"

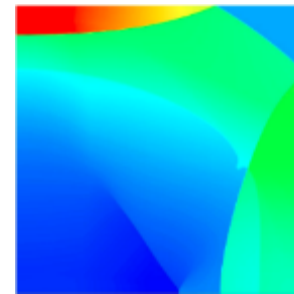


Image Source: Intel



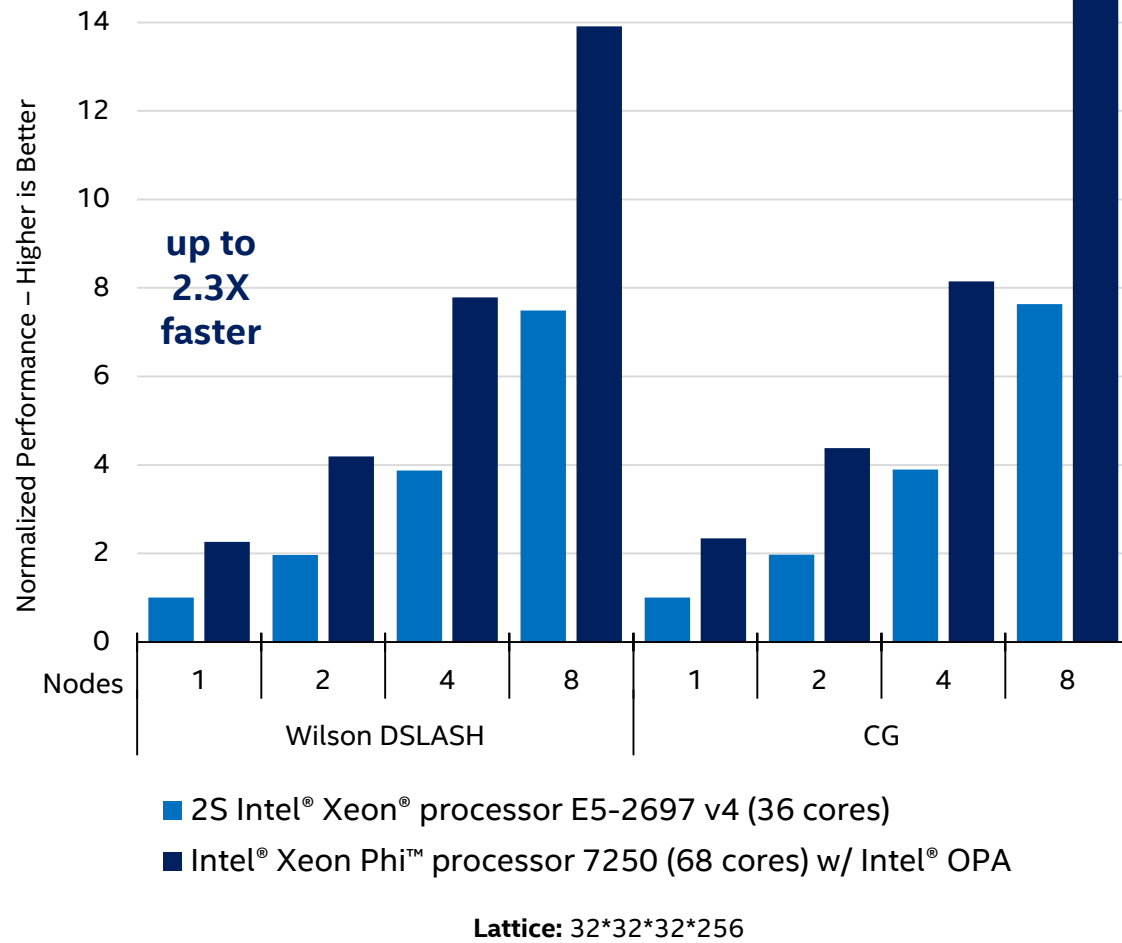
## Value Proposition:

- This application provides users with a research tool for investigating code modernization approaches for larger shock hydrodynamics applications.
- This application now significantly outperforms (time-to-solution) alternative processing solutions with the Intel® Xeon Phi™ processor 7250.

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



QPhiX Performance Improvement on an Intel® Xeon Phi™ Processor Cluster – Strong Scaling



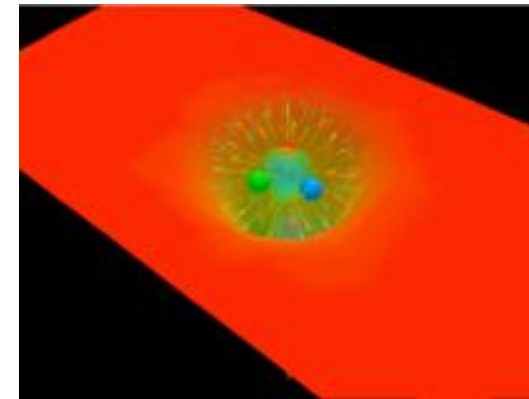
See next slide for configuration details.

SOURCE: INTEL MEASURED RESULTS AS OF MAY, 2016

**QPhiX is an optimized solver library for QCD on Intel® Xeon® processors and Intel® Xeon Phi™ processors and provides implementation for Dslash operator and CG, BICGStab and mixed precision solvers for Wilson and Clover improved Wilson Quarks.**

**Application:** QPhiX Test Benchmark (time\_dslash\_noqdp)

**Code:** [Available here](#) **Recipe:** Follow the instructions in the download package



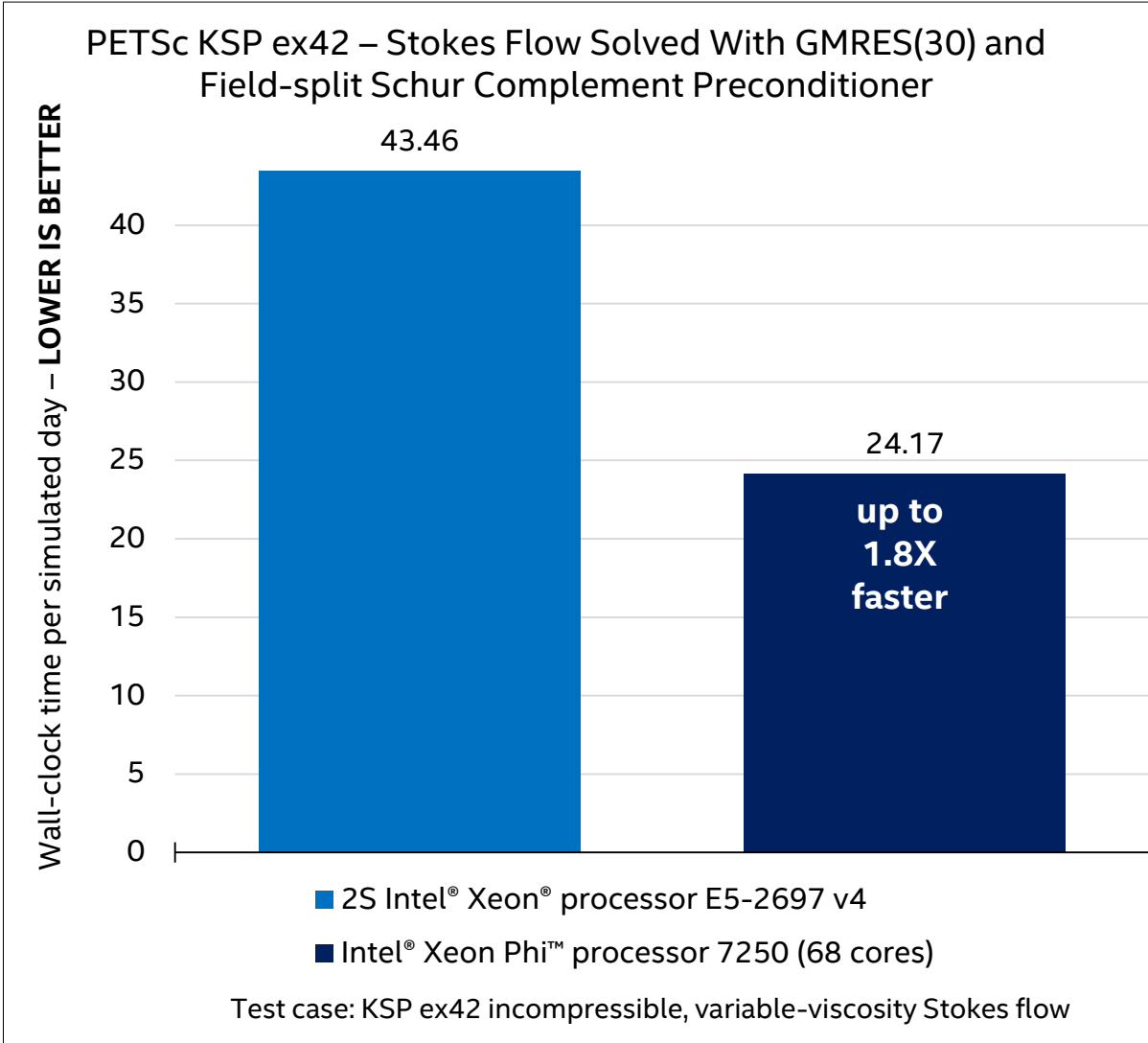
Flux tubes between 3 quarks.  
Credit: Dr Derek Leinweber,  
Centre for the Subatomic  
structure of Matter (CSSM) and  
Department of Physics,  
University of Adelaide, 5005  
Australia

### Value Proposition:

- Lattice calculations are an important component of the nuclear physics research.
- QPhiX helps speed up the computation by multiple folds on Intel processors.
- Intel® Xeon Phi™ processor further improves performance with features such as high bandwidth memory (MCDRAM) and Intel® AVX-512 vector instruction set architecture.

**Results:** Up to 2.3X one node improved performance compared to the Intel® Xeon® processor E5-2697 v4. Over 77% parallel efficiency with Intel® Omni-Path Architecture (8 nodes).

# PETSc – PORTABLE, EXTENSIBLE TOOLKIT FOR SCIENTIFIC COMPUTATION



See next slide for configuration details. SOURCE: INTEL MEASURED RESULTS AS OF MAY 2016

*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.*

**Application:** Solution of the incompressible, variable viscosity Stokes equation in 3d using Q1Q1 elements, using a state-of-the art Schur complement-based approach robust to large viscosity jumps.

**Code:** PETSc development code is completely open and [available here](#).

**Recipe:** “-g -O3 -fp-model fast” and “-xMIC-AVX512” or “-xCORE-AVX2

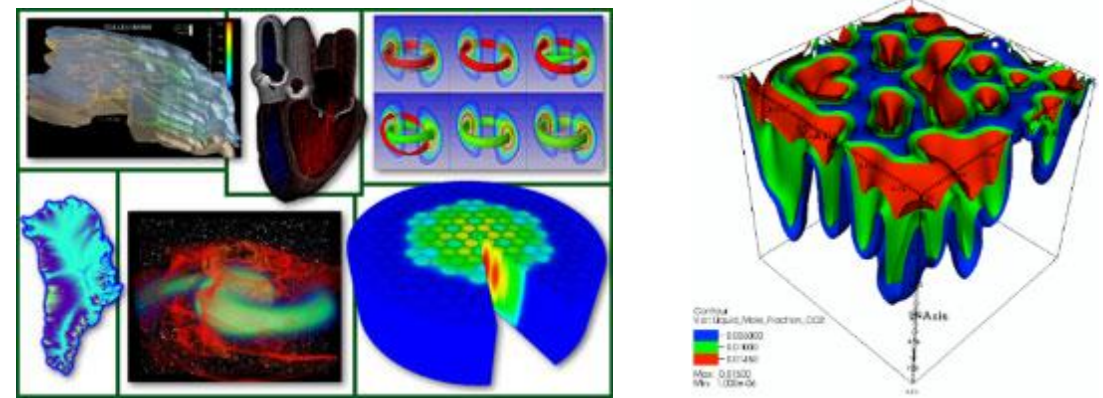


Image Source: Peter Lichtner, OFM Research

**Value Proposition:** PETSc is one of the world’s most widely-used software libraries in high-performance computing. Many PETSc solvers are limited by memory-bandwidth in practice, and the Intel® Xeon Phi™ processor can deliver the needed bandwidth for excellent performance.

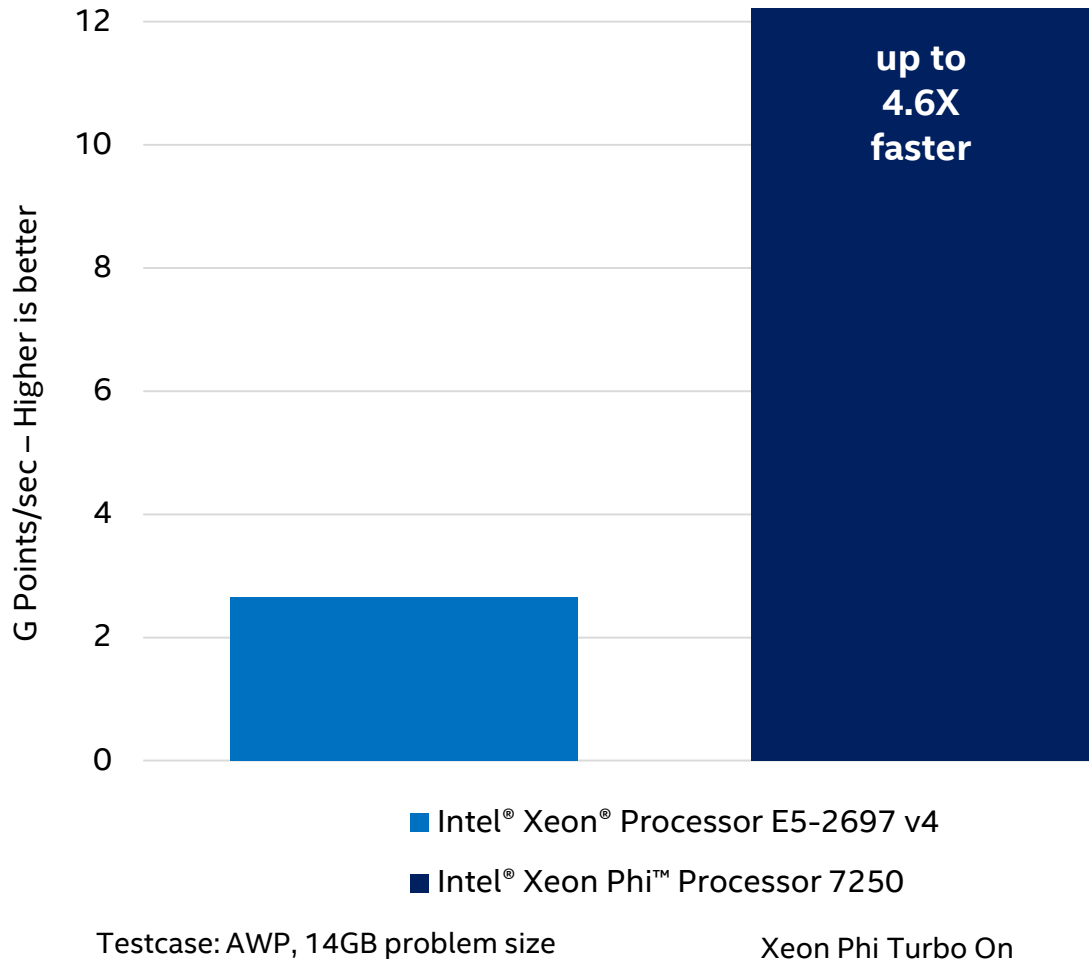
**Results:** Up to 1.8X faster with the Intel® Xeon Phi™ processor 7250 compared to the Intel® Xeon® processor E5-2697 v4.





# YASK HPC STENCILS, AWP-ODC KERNEL

YASK AWP-ODC Kernel Performance Improvement with the Intel® Xeon Phi™ Processor



See next slide for configuration details.

SOURCE: INTEL MEASURED RESULTS AS OF MAY, 2016

**YASK, Yet Another Stencil Kernel, is a framework to facilitate design exploration and tuning of HPC kernels. One of the stencils included in YASK is awp-odc, a staggered-grid finite difference scheme used to approximate the 3D velocity-stress elastodynamic equations:** <http://hpgeoc.sdsc.edu/AWPODC>. **Applications using this stencil simulate the effect of earthquakes to help evaluate designs for buildings and other at-risk structures.**

**Application:** YASK, AWP stencil (a single-node proxy for the compute kernel in the Anelastic Wave Propagation application)

**Code:** [Available here](#)

**Recipe:** 640\*640\*640 problem size (see command lines in next slide)

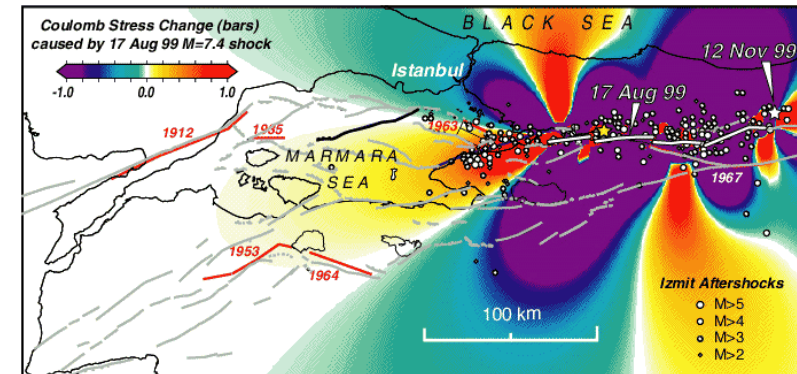


Image Source: USGS

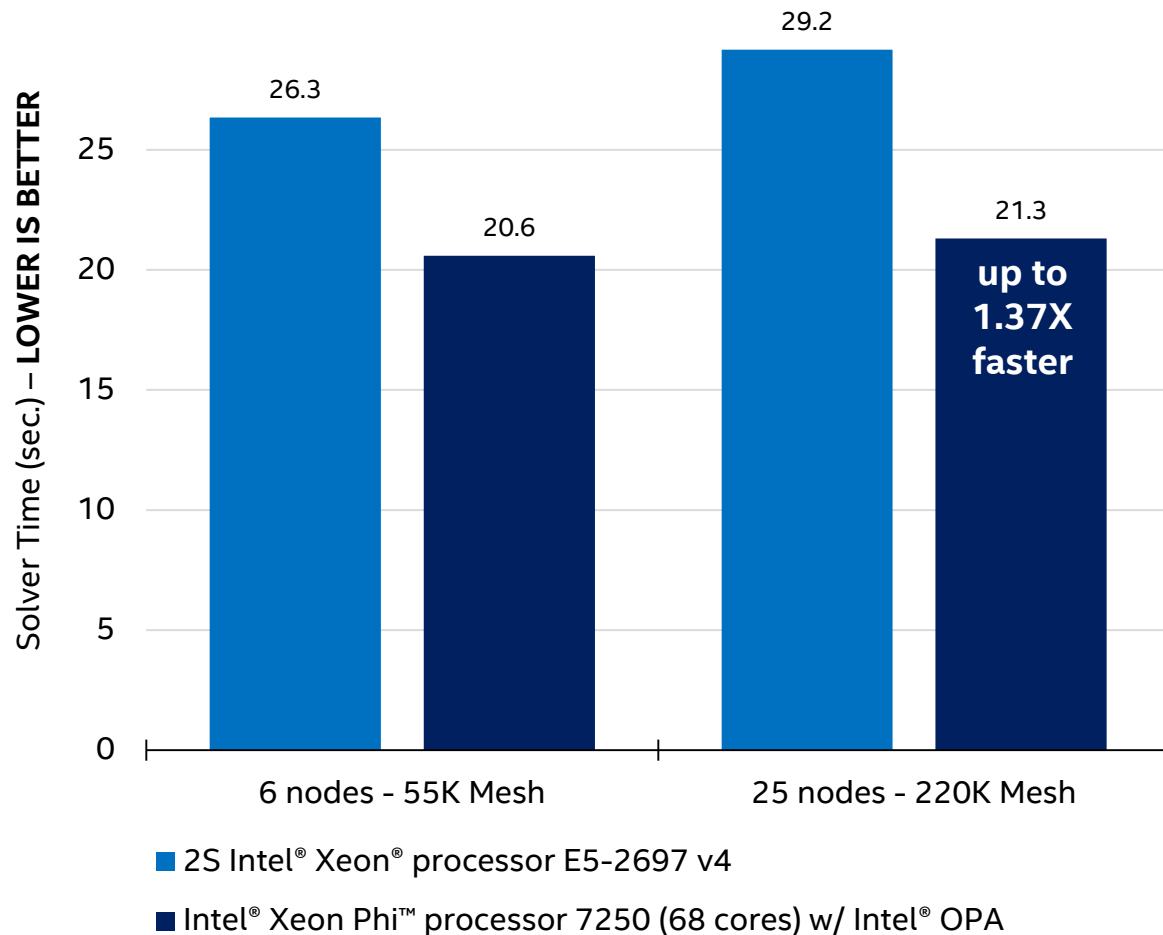
**Value Proposition:** Intel® Xeon Phi™ processor 7250 enables this application to leverage the high-bandwidth memory and 512-bit SIMD for higher performance.

**Results:** Up to 4.6X improved performance compared to the Intel® Xeon® processor E5-2697 v4.



# SPECFEM3D\_GLOBE\*

SPECFEM3D\_GLOBE : Performance Improvement on a cluster of Intel® Xeon Phi™ Processor – Weak Scaling



See slide 119 for configuration details.

SOURCE: INTEL MEASURED RESULTS AS OF MAY, 2016

***SPECFEM3D\_GLOBE simulates the three-dimensional global and regional seismic wave propagation based upon the spectral-element method (SEM). It is a time-step algorithm which simulates the propagation of earth waves given the initial conditions, mesh coordinates/ details of the earth crust.***

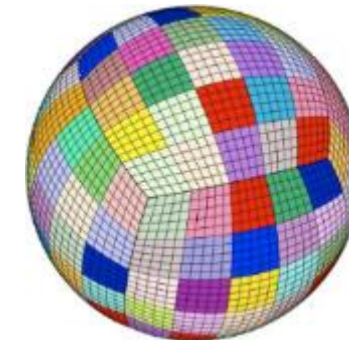
**Application:** specfem3D\_globe

**Baseline Code:** [https://geodynamics.org/cig/software/specfem3d\\_globe/](https://geodynamics.org/cig/software/specfem3d_globe/)

**Optimized Code:** Pending check-in. **Recipe:** Runs out-of-the-box.

Image Source:

[https://geodynamics.org/cig/software/specfem3d\\_globe/](https://geodynamics.org/cig/software/specfem3d_globe/)



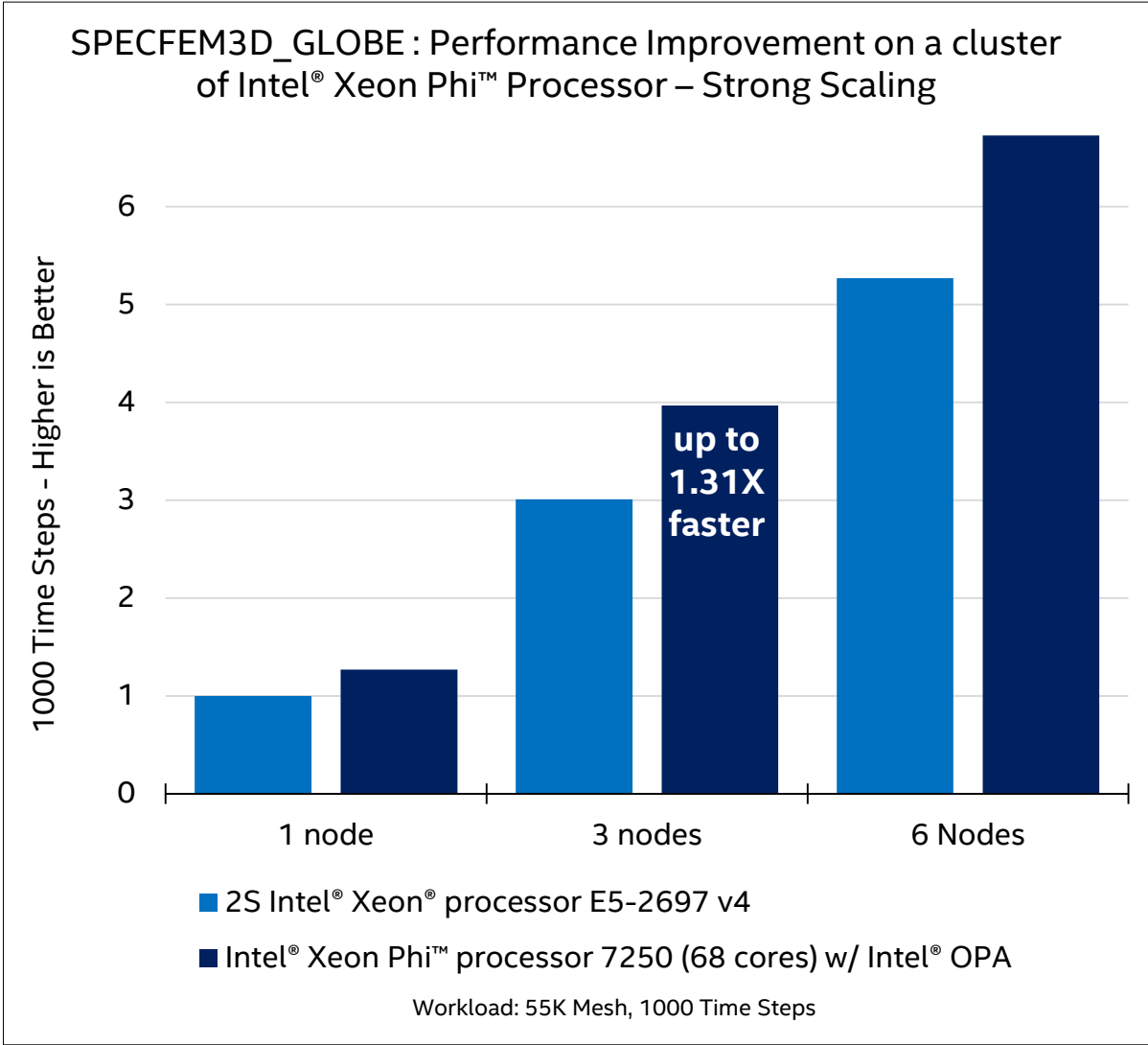
## Value Proposition:

- The Intel® Xeon Phi™ processor improves performance for scalable workloads.
- SPECFEM3D\_GLOBE benefits from AVX-512 and high-bandwidth memory available on the Intel® Xeon Phi™ processor.

**Results:** The Intel® Xeon Phi™ processor 7250 improved the simulation rate by up to 1.37X when compared to the Intel® Xeon® E5-2697v4 processors. **Over 90% parallel efficiency with Intel® Omni-Path Architecture (for 6 and 25 node runs of 55K and 220K mesh size workloads respectively).**



# SPECFEM3D\_GLOBE\*



See next slide for configuration details. SOURCE: INTEL MEASURED RESULTS AS OF MAY, 2016

*SPECFEM3D\_GLOBE simulates the three-dimensional global and regional seismic wave propagation based upon the spectral-element method (SEM). It is a time-step algorithm which simulates the propagation of earth waves given the initial conditions, mesh coordinates/ details of the earth crust.*

Application: specfem3D\_globe  
Baseline Code: [https://geodynamics.org/cig/software/specfem3d\\_globe/](https://geodynamics.org/cig/software/specfem3d_globe/)  
Optimized Code: Pending check-in. Recipe: Runs out-of-the-box.

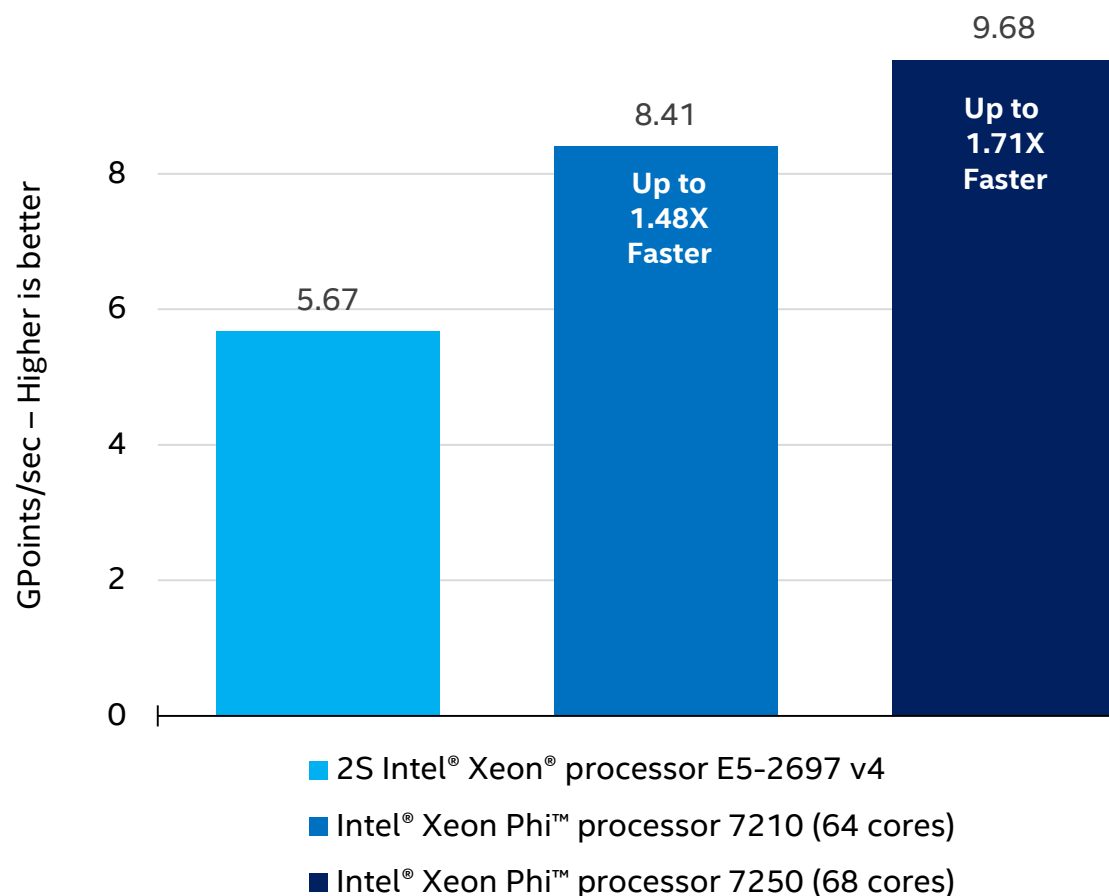
Image Source:  
[https://geodynamics.org/cig/software/specfem3d\\_globe/](https://geodynamics.org/cig/software/specfem3d_globe/)



- Value Proposition:**
- The Intel® Xeon Phi™ processor improves performance for scalable workloads.
  - SPECFEM3D\_GLOBE benefits from Intel® AVX-512 and high-bandwidth memory available on the Intel® Xeon Phi™ processor.
- Results:** Up to 1.31X improved 3-node simulation rate compared to the Intel® Xeon® E5-2697v4 processors. **Over 88% parallel efficiency with Intel® Omni-Path Architecture (6 nodes).**

# ISO3DFD (3D ACOUSTIC ISOTROPIC FINITE DIFFERENCE)\*

Iso3DFD Performance Improvement with the Intel® Xeon Phi™ Processor



Test case: Grid dimensions - (dimX, dimY, dimZ) => (224, 2125, 2100)

See next slide for configuration details.

SOURCE: INTEL MEASURED RESULTS AS OF MAY, 2016

*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.*

**Application:** Iso3DFD (3D Acoustic Isotropic Finite Difference)

**Code:** Posted to Intel Developer Zone (IDZ)

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

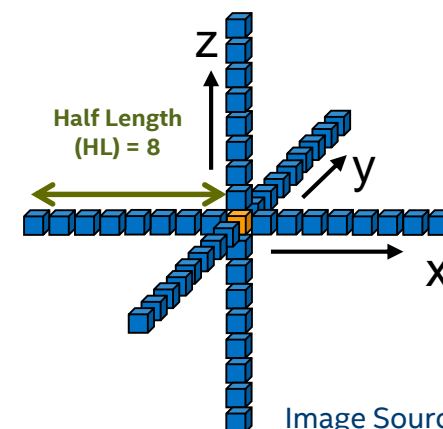


Image Source: Intel

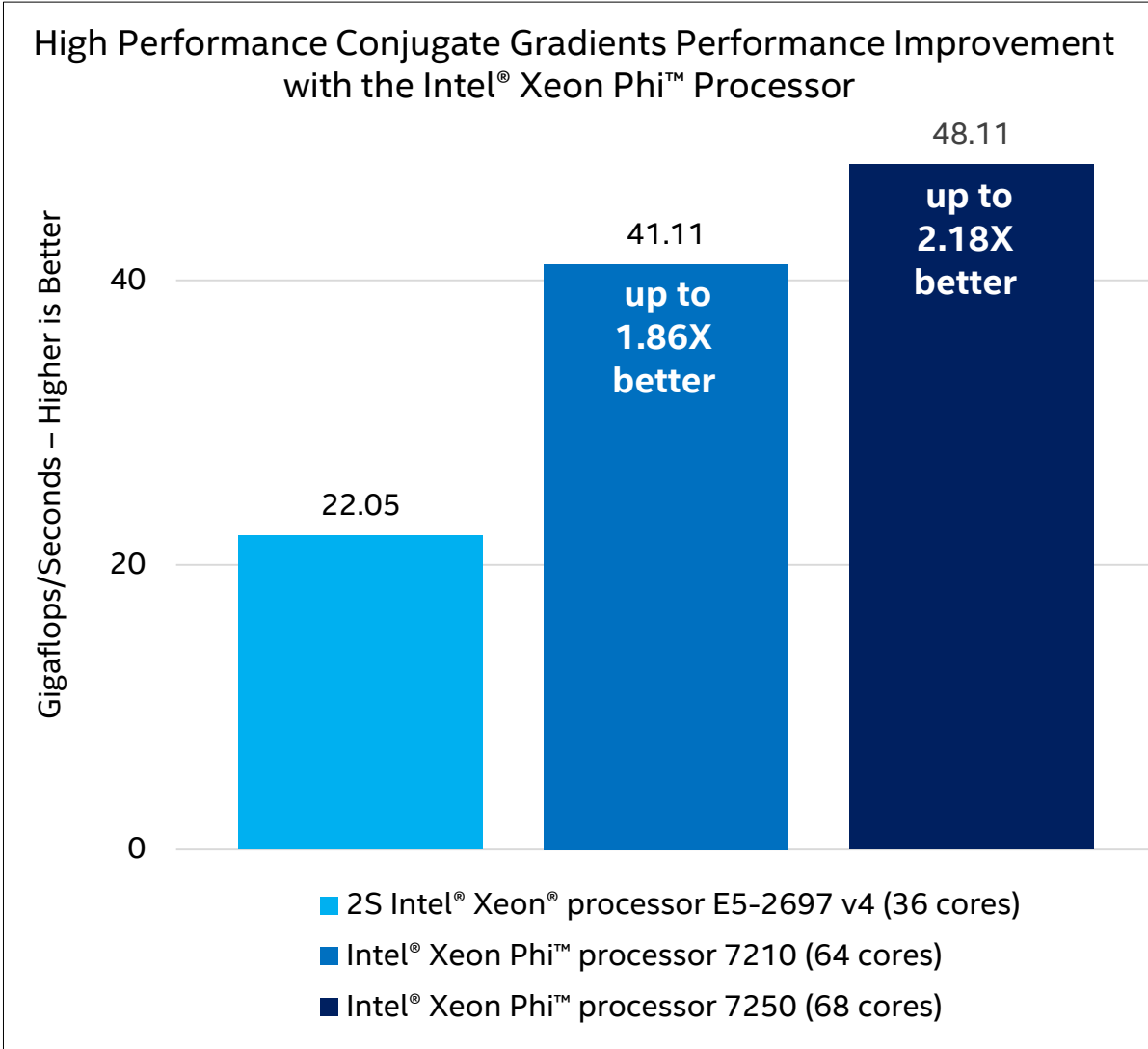
## Value Proposition:

- Iso3DFD kernel makes use of Intel® AVX512 instructions and MCDRAM High Bandwidth Memory.
- Intel® Xeon Phi™ processor 7250 enables this application to significantly speedup the computation of seismic wave propagation.

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



# HIGH PERFORMANCE CONJUGATE GRADIENTS



See next slide for configuration details.

SOURCE: INTEL MEASURED RESULTS AS OF APRIL, 2016

*The High Performance Conjugate Gradients (HPCG) Benchmark project is an effort to create a new metric for ranking HPC systems. HPCG is intended as a complement to the High Performance LINPACK (HPL) benchmark, currently used to rank the TOP500 computing systems.*

**Application:** High Performance Conjugate Gradients  
**Code:** [Available here](#). **Recipe:** In development

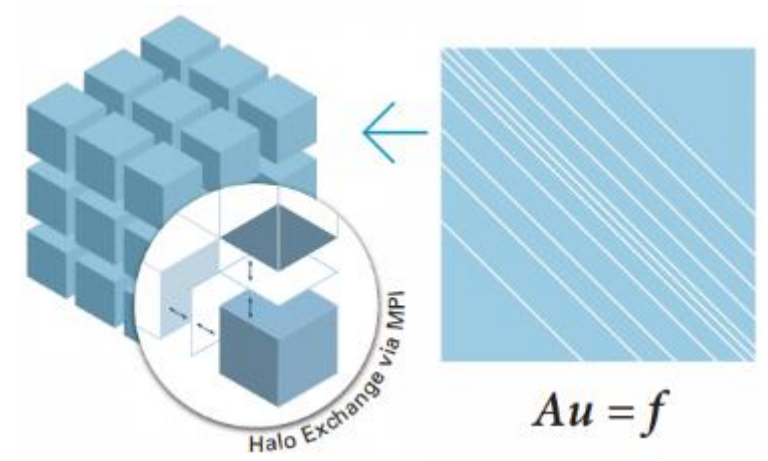


Image Source: [Univ. Maryland, Baltimore Co.](#)

**Value Proposition:** The HPCG benchmark, and is the more accurate portrayal of HPC App behavior vs. LINPACK and is thought to be the replacement to the top Top500 potentially. and validates the Intel Xeon Phi Processor's generational performance improvement.

**Results:** Up to 2.18X faster compared to the Intel® Xeon® processor E5-2697 v4.