INTEL® MATH KERNEL LIBRARY 2018 (INTEL® MKL)

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Intel® Math Kernel Library

Intel® MKL

- Speeds computations for scientific, engineering, financial and machine learning applications
- Provides key functionality for dense and sparse linear algebra (BLAS, LAPACK, PARDISO), FFTs, vector math, summary statistics, deep learning, splines and more
- Included in Intel® Parallel Studio XE and Intel® System Studio Suites
- Available at no cost and royalty free

- Optimized for single core vectorization and cache utilization
- Automatic parallelism for multi-core and many-core
- Scales from cores to clusters
- Great performance with minimal effort

Optimization Notice

Intel® MKL Optimized Mathematical Building Blocks

Linear Algebra

- BLAS
- LAPACK and ScaLAPACK
- Sparse BLAS
- PARDISO* Direct Sparse Solver
- Parallel Direct Cluster Sparse Solver
- Iterative sparse solvers

Fast Fourier Transforms

- Multidimensional
- FFTW* interfaces
- Cluster FFT

Vector Math

- Trigonometric
- Hyperbolic
- Exponential
- Log
- Power
- Root
- Vector RNGs

Deep Neural Networks

- Convolution
- Pooling
- Normalization
- ReLU
- Inner Product

Summary Statistics

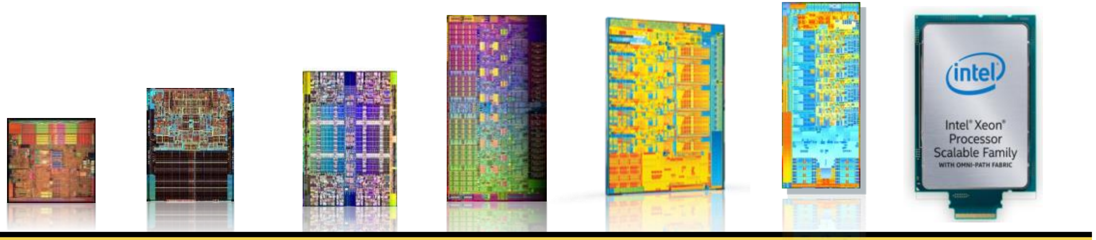
- Kurtosis
- Central moments
- Variation coefficient
- Order statistics and quantiles
- Min/max
- Variance-covariance
- Robust estimators

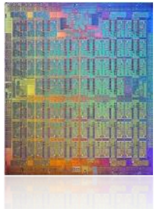
And More

- Splines
- Interpolation
- Trust Region
- Fast Poisson Solver

Automatic Dispatching to Tuned ISA-specific Code Paths

More cores → More Threads → Wider vectors



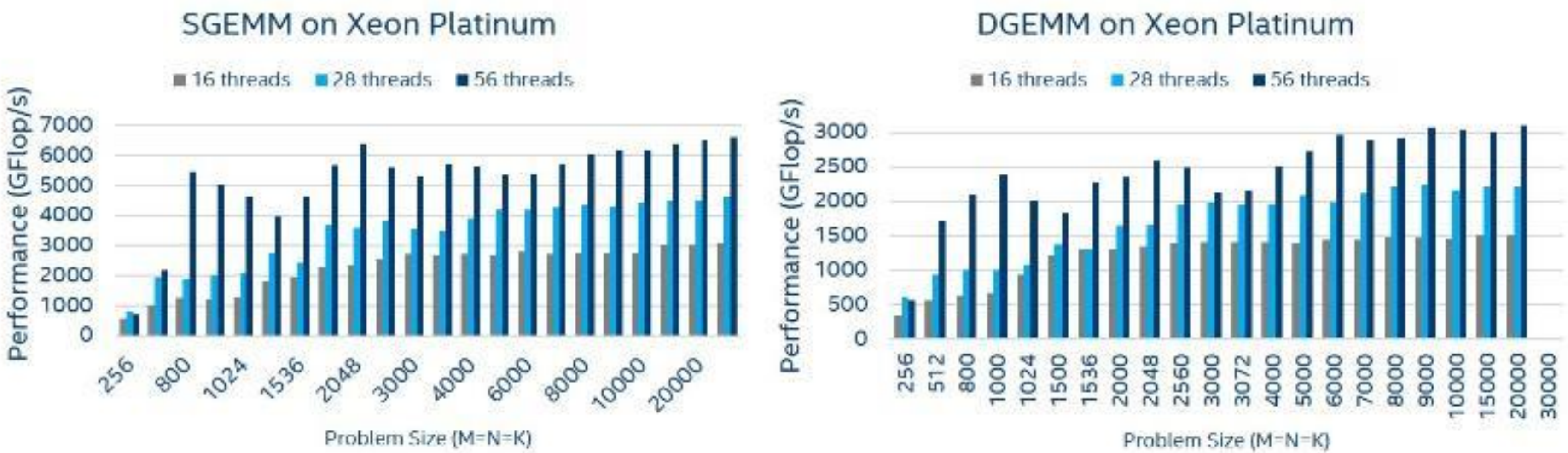


	Intel® Xeon® Processor 64-bit	Intel® Xeon® Processor 5100 series	Intel® Xeon® Processor 5500 series	Intel® Xeon® Processor 5600 series	Intel® Xeon® Processor E5-2600 v2 series	Intel® Xeon® Processor E5-2600 v3 series v4 series	Intel® Xeon® Scalable Processor[1]	Intel® Xeon Phi™ x200 Processor (KNL)
Up to Core(s)	1	2	4	6	12	18-22	28	72
Up to Threads	2	2	8	12	24	36-44	56	288
SIMD Width	128	128	128	128	256	256	512	512
Vector ISA	Intel® SSE3	Intel® SSE3	Intel® SSE4- 4.1	Intel® SSE 4.2	Intel® AVX	Intel® AVX2	Intel® AVX-512	Intel® AVX-512

[1] Product specification for launched and shipped products available on ark.intel.com.

Performance Benefits for the latest Intel Architectures

DGEMM, SGEMM Optimized by Intel® Math Kernel Library for Intel® Xeon® Platinum Processor
(formerly codenamed Skylake Server)



SGEMM on Xeon Platinum

DGEMM on Xeon Platinum

Configuration: Intel® Xeon® Platinum 8180, 2x28 cores, 2.5GHz, 38.5MB L3 cache, 376GB RAM, OS Ubuntu 16.04 LTS; Intel® Math Kernel Library (Intel® MKL) 2018. 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 consult other information 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 complete information visit www.intel.com/benchmarks. Benchmark Source: Intel Corporation. Optimization Notice: Intel's compilers may or may not optimize to the same degree for non-Intel microprocessors for optimizations that are not unique to Intel microprocessors. These optimizations include SSE2, SSE3, and SSSE3 instruction sets and other optimizations. Intel does not guarantee the availability, functionality, or effectiveness of any optimization on microprocessors not manufactured by Intel. Microprocessor-dependent optimizations in this product are intended for use with Intel microprocessors. Certain optimizations not specific to Intel microarchitecture are reserved for Intel microprocessors. Please refer to the applicable product User and Reference Guides for more information regarding the specific instruction sets covered by this notice. Notice revision #20110804.

Intel® MKL BLAS (Basic Linear Algebra Subprograms)

De-facto Standard APIs since the 1980s

100s of Basic Linear Algebra Functions	Level 1 – vector vector operations, O(N) Level 2 – matrix vector operations, $O(N^2)$ Level 3 – matrix matrix operations, $O(N^3)$
Precisions Available	Real – Single and Double Complex - Single and Double
BLAS-like Extensions	Direct Call, Batched, Packed and Compact
Reference Implementation	*http://netlib.org/blas/*

Intel® MKL LAPACK (Linear Algebra PACKage)

De-facto Standard APIs since the 1990s

1000s of Linear Algebra Functions	Matrix factorizations - LU, Cholesky, QR Solving systems of linear equations Condition number estimates Symmetric and non-symmetric eigenvalue problems Singular value decomposition and many more …
Precisions Available	Real – Single and Double, Complex – Single and Double
Reference Implementation	*http://netlib.org/lapack/*

Intel® MKL Fast Fourier Transforms (FFTs)

FFTW Interfaces support	C, C++ and FORTRAN source code wrappers provided for FFTW2 and FFTW3. FFTW3 wrappers are already built into the library
Cluster FFT	Perform Fast Fourier Transforms on a cluster Interface similar to DFTI Multiple MPIs supported
Parallelization	Thread safe with automatic thread selection
Storage Formats	Multiple storage formats such as CCS, PACK and Perm supported
Batch support	Perform multiple transforms in a single call
Additional Features	Perform FFTs on partial images Padding added for better performance Transform combined with transposition mixed-language usage supported

Intel® MKL DNN (Deep Neural Network) Functions

Highly optimized basic building blocks for DNNs	
Use cases	Inference and training Image recognition, semantic segmentation, object detection
Functions	Convolution, Inner Product Activation, Normalization, Pooling, Sum, Split/Concat, Data transformation
Applications	Supported in Tensorflow, MXNet, IntelCaffe and more
Open source version	*https://github.com/01org/mkl-dnn*

Intel® MKL Vector Math

Example:	$y(i) = e^{x(i)}$ for $i = 1$ *to* n
Broad Function Support	Basic Operations – add, sub, mult, div, sqrt Trigonometric– sin, cos, tan, asin, acos, atan Exponential – exp,, pow, log, log10, log2, Hyperbolic – sinh, cosh, tanh Rounding – ceil, floor, round And many more
Precisions Available	Real – Single and Double Complex - Single and Double
Accuracy Modes	High - almost correctly rounded Low - last 2 bits in error Enhanced Performance - 1/2 the bits correct

Intel® MKL Vector Statistics

Random Number Generators (RNGs)

Pseudorandom, quasi-random and non-deterministic random number generators with continuous and discrete distribution

Summary Statistics

Parallelized algorithms to compute basic statistical estimates for single and double precision multi-dimensional datasets

Convolution and Correlation

Linear convolution and correlation transforms for single and double precision real and complex data

Intel® MKL Sparse Solvers

PARDISO - Parallel Direct Sparse Solver	Factor and solve Ax = b using a parallel shared memory *LU*, *LDL*, or LL^T factorization Supports a wide variety of matrix types including real, complex, symmetric, indefinite, … Includes out-of-core support for very large matrix sizes
Parallel Direct Sparse Solver for Clusters	Factor and solve Ax = b using a parallel distributed memory *LU*, *LDL*, or LL^T factorization Supports a wide variety of matrix types (real, complex, symmetric, indefinite, …) Supports A stored in 3-array CSR3 or BCSR3 formats
DSS – Simplified PARDISO Interface	An alternative, simplified interface to PARDISO
ISS – Iterative Sparse Solvers	Conjugate Gradient (CG) solver for symmetric positive definite systems Generalized Minimal Residual (GMRes) for non-symmetric indefinite systems Rely on Reverse Communication Interface (RCI) for matrix vector multiply

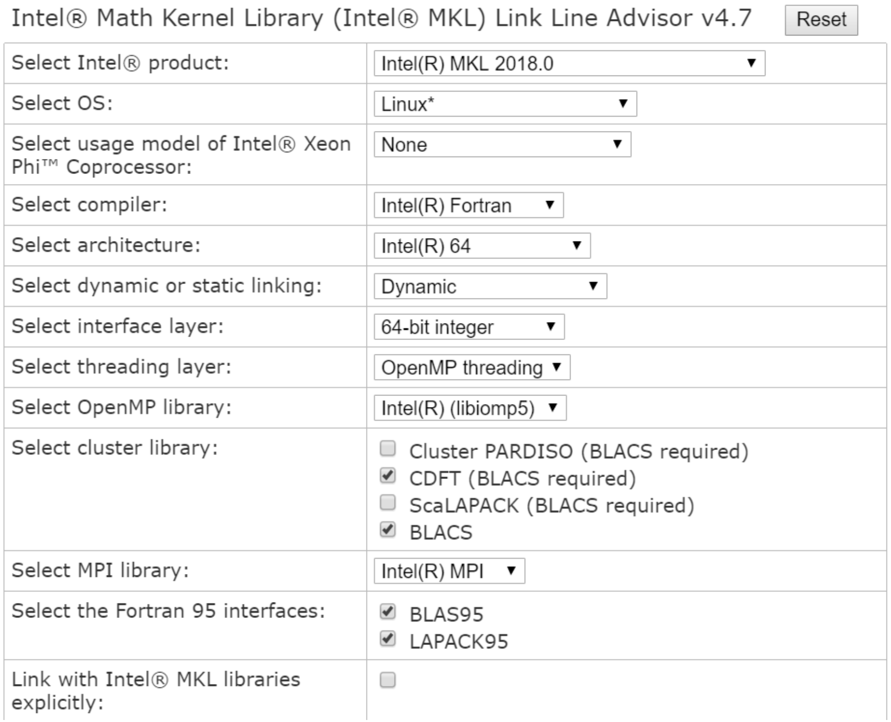
Some other Intel® MKL Components

Sparse BLAS	NIST-like and inspector execute interfaces
Data Fitting	1D linear, quadratic, cubic, step-wise and user-defined splines, spline-based interpolation and extrapolation
Partial Differential Equations	Helmholtz, Poisson, and Laplace equations
Optimization	Trust-region solvers for nonlinear least square problems with and without constraints
Service Functions	Threading controls (MKL_NUM_THREADS, for example) Memory management (mkl_allocate, for example) Numerical reproducibility (MKL_CBWR for example)

Compiling & Linking with Intel® MKL

- Intel® MKL is supported with gcc
  - Include “mkl.h”
- On Intel® systems, with icc & ifort, use the –mkl switch (for compiling and linking)
  - -mkl=sequential for sequential function execution in a parallel (or serial) program
  - -mkl=parallel for threaded Intel® MKL in a parallel (or serial) program
  - -mkl=cluster for Scalapack for example
- On Theta similar principles apply within the PrgEnv-intel environment
  - The Cray cc, CC, or ftn wrappers accept –mkl
    - Can be as simple as: **ftn –mkl code.f**
  - For Scalapack use the Intel® MKL Link Line Advisor for guidance

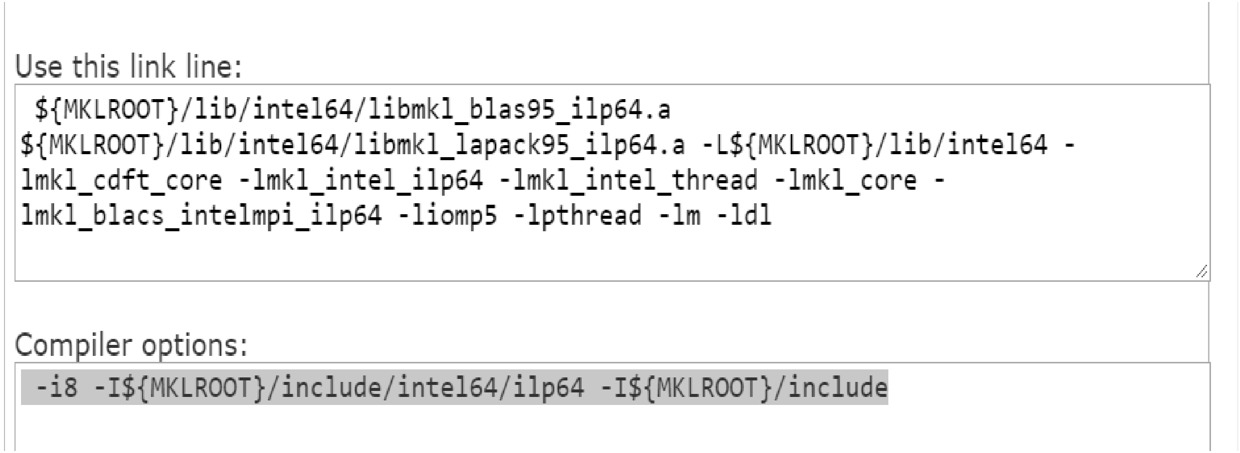
Compiling & Linking with Intel® MKL



Intel® Math Kernel Library (Intel® MKL) Link Line Advisor v4.7

Select Intel® product:	Intel(R) MKL 2018.0 ▼
Select OS:	Linux* ▼
Select usage model of Intel® Xeon Phi™ Coprocessor:	None ▼
Select compiler:	Intel(R) Fortran ▼
Select architecture:	Intel(R) 64 ▼
Select dynamic or static linking:	Dynamic ▼
Select interface layer:	64-bit integer ▼
Select threading layer:	OpenMP threading ▼
Select OpenMP library:	Intel(R) (libiomp5) ▼
Select cluster library:	□ Cluster PARDISO (BLACS required) ☑ CDFT (BLACS required) □ ScaLAPACK (BLACS required) ☑ BLACS
Select MPI library:	Intel(R) MPI ▼
Select the Fortran 95 interfaces:	☑ BLAS95 ☑ LAPACK95
Link with Intel® MKL libraries explicitly:	□

Compiling & Linking with Intel® MKL



Use this link line:

```
 ${MKLROOT}/lib/intel64/libmkl_blas95_ilp64.a
${MKLROOT}/lib/intel64/libmkl_lapack95_ilp64.a -L${MKLROOT}/lib/intel64 -
lmkl_cdft_core -lmkl_intel_ilp64 -lmkl_intel_thread -lmkl_core -
lmkl_blacs_intelmpi_ilp64 -liomp5 -lpthread -lm -ldl
```

Compiler options:

```
 -i8 -I${MKLROOT}/include/intel64/ilp64 -I${MKLROOT}/include
```

Memory related considerations

- Use mkl_malloc and mkl_free for allocating and freeing aligned memory
- For Apps that require high memory BW, allocate memory in MCDRAM
  - numactl
  - Install memkind library
- More details can be found in the developer guide for Intel® MKL

Intel® MKL Resources

Intel® MKL Website	https://software.intel.com/en-us/intel-mkl
Intel® MKL Forum	https://software.intel.com/en-us/forums/intel-math-kernel-library
Intel® MKL Benchmarks	https://software.intel.com/en-us/intel-mkl/benchmarks#
Intel®MKL Link Line Advisor	http://software.intel.com/en-us/articles/intel-mkl-link-line-advisor/

Intel® MKL Summary

Boosts application performance with minimal effort	feature set is robust and growing provides scaling from the core, to multicore, to manycore, and to clusters automatic dispatching matches the executed code to the underlying processor future processor optimizations included well before processors ship
Showcases the world's fastest supercomputers[1]	Intel® Distribution for LINPACK* Benchmark Intel® Optimized High Performance Conjugate Gradient Benchmark

[1] http://www.top500.org

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