Practical Usage of the Intel Math Kernel Library (MKL)

The Hands-On Tutorial (HOT) Series

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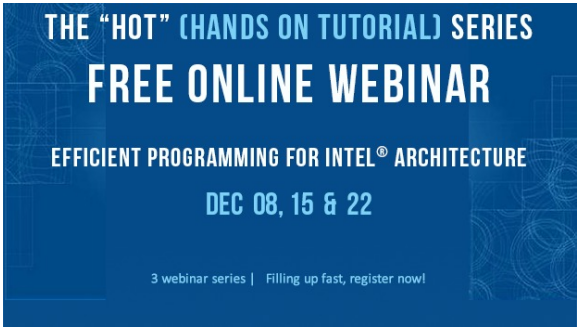
About the Series

Hands-On Tutorial (HOT) series: webinars on efficient programming for the Intel architecture. Select topics of parallel programming and performance optimization with detailed practical demonstrations.



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Slides, Code, Video

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§2. Intel Architecture

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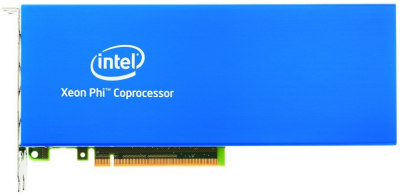
Intel Xeon Phi Coprocessors and the MIC Architecture

- C/C++/Fortran; OpenMP/MPI
- Standard Linux OS
- Up to 768 GB of DDR3 RAM
- ≤18 cores/socket ≈3 GHz
- 2-way hyper-threading
- 256-bit AVX vectors



- C/C++/Fortran; OpenMP/MPI
- Special Linux distribution
- 6–16 GB cached GDDR5 RAM
- 57 to 61 cores at ≈1 GHz
- 4 hardware threads per core
- 512-bit IMCI vectors

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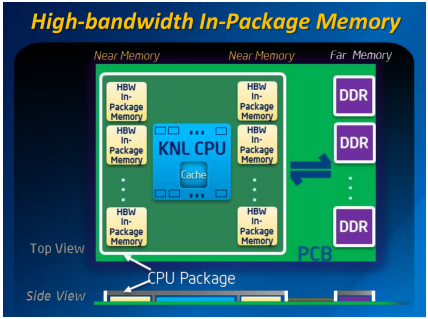
Next Generation of the MIC Architecture

- 2nd generation MIC product: code name Knights Landing (KNL)
- Intel's 14 nm manufacturing process
- A processor (running the OS) or a coprocessor (PCIe device)
- On-package high-bandwidth memory w/flexible memory models: flat, cache, & hybrid
- Intel Advanced Vector Extensions AVX-512 (public)



Source: Intel Newsroom

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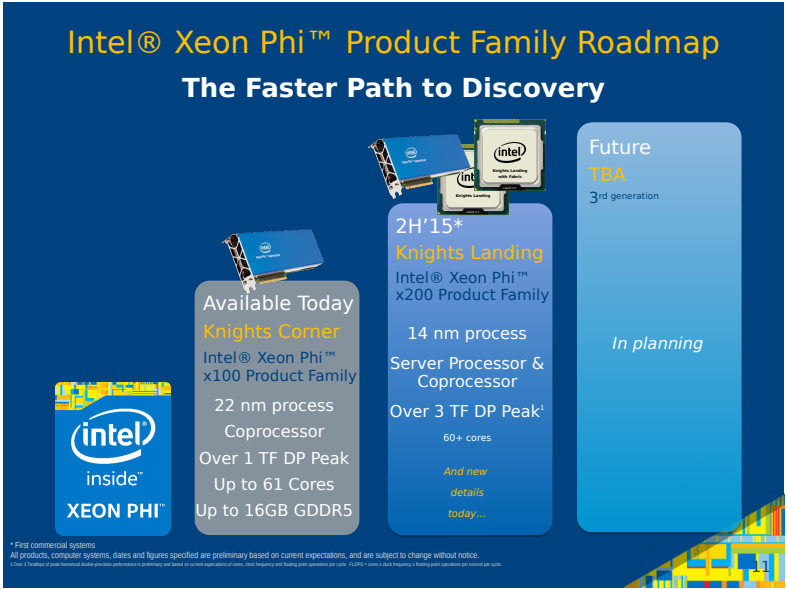

Source: https://www.brighttalk.com/webcast/10773/116329

§3. Intel Math Kernel Library

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Performance Tuning Methodology

- **Scalar optimization** (compiler-friendly practices)
- **Vectorization** (must use 16- or 8-wide vectors)
- **Multi-threading** (must scale to 100+ threads)
- **Memory access** (streaming access or tiling)
- **Communication** (offload, MPI traffic control)

Details in the HOW Series and our book.

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Scope of MKL

Intel Math Kernel Library (MKL) — standard mathematical functions optimized for Intel architecture.

Linear Algebra	Fast Fourier Transform	Vector Math	Vector Random Number Generators	Summary Statistics	Data Fitting
BLAS LAPACK Sparse solvers ScaLAPACK	Multidimentional (up to 7D) FFTW interfaces Cluster FFT	Trigonometric Hyperbolic Exponential Logarithmic Power/Root Rounding	Congruential Recursive Wichmann-Hill Mersenne Twister Sobol Neiderreiter Non-deterministic	Kurtosis Variation coefficitent Quantiles, order statistics Min/max Variance-covariance	Splines Interpolation Cell search

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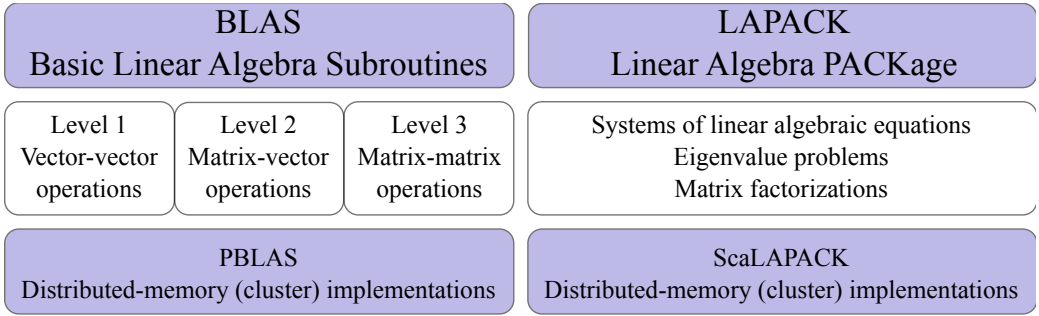
Linear Algebra Support



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Using MKL with Intel Xeon Phi Coprocessors

	Native	Compiler-Assisted Offload (CAO)	Automatic Offload (AO)
Programming:	Call MKL functions like from CPU code	Call MKL functions from #pragma offload	Call MKL functions from CPU code
Compilation:	With argument -mmic	Conventional for CPU	Conventional for CPUs
Running	On Xeon Phi	On host CPU	On host CPU; MKL_MIC_ENABLE=1
Data movement	Data already on coprocessor	Managed by programmer	Managed by MKL
Functions	All	All	Some; problem size > threshold
Multiple Copr.	Use cluster functions	DIY	Supported out-of-box

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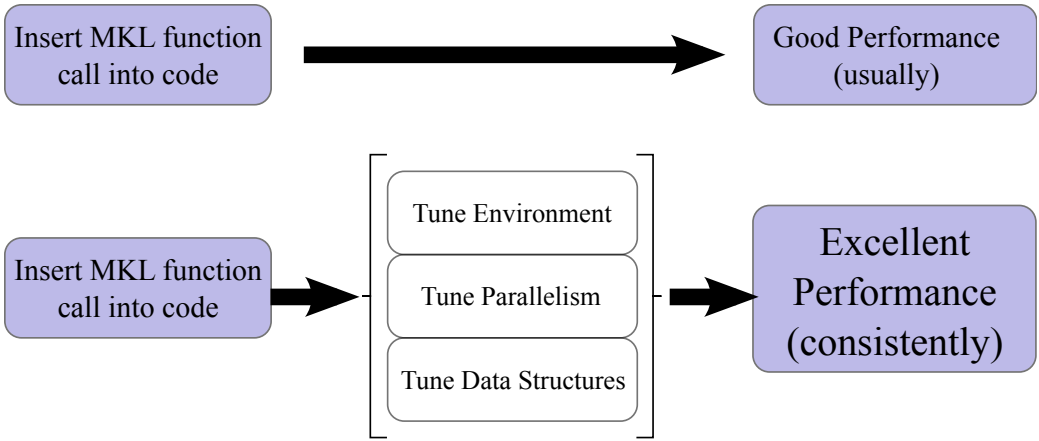
Performance Tuning with MKL



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§4. Hands-On Labs

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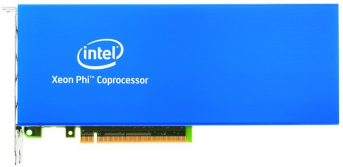
“Standard Candle” Testbench



vs.

One Intel Xeon Phi 7120P coprocessor (2012)
TDP: 300 W, RCP: $4129

Two Intel Xeon E5-2697 v3 CPUs (2014)
TDP: 290 W, RCP: $5404

See also “Intel Xeon Product Family: Performance Brief”

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Batch Processing

- Feed multiple signals to MKL
- Let the library decide on the parallel strategy.

```
MKL_Complex16* data =
                (MKL_Complex16*) malloc(sizeof(MKL_Complex16)*fft_size*num_fft);

DFTI_DESCRIPTOR_HANDLE handle;
DftiCreateDescriptor(&handle, DFTI_DOUBLE, DFTI_COMPLEX, 1, (MKL_LONG)fft_size);
DftiSetValue(handle, DFTI_NUMBER_OF_TRANSFORMS, num_fft);
DftiSetValue(handle, DFTI_INPUT_DISTANCE, fft_size);
DftiSetValue(handle, DFTI_OUTPUT_DISTANCE, fft_size);
DftiSetValue(handle, DFTI_PLACEMENT, DFTI_INPLACE);
DftiCommitDescriptor(handle);
```


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Thread Affinity Tuning

Xeon	**Xeon Phi**
MKL uses 1 thread/core	MKL uses 4 threads/core
`OMP_NUM_THREADS`=#phys. cores	`OMP_NUM_THREADS`=4×#cores
`KMP_AFFINITY`=scatter	`KMP_AFFINITY`=scatter
`KMP_AFFINITY`=compact (HT off)	`KMP_AFFINITY`=compact
`KMP_AFFINITY`=compact,1 (HT on)	

See also HOW series Episode 3.4.

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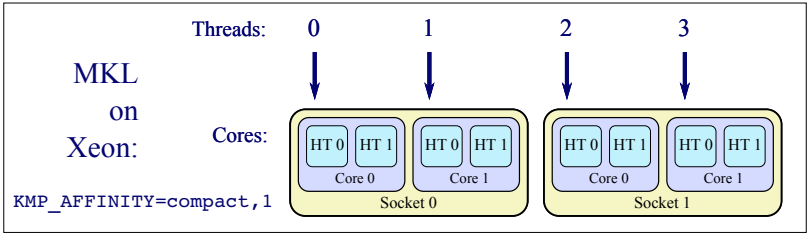
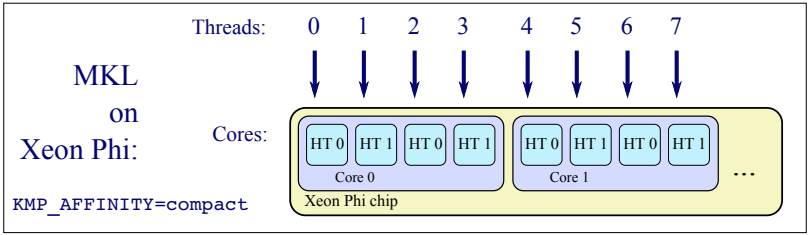
Thread Affinity: Compact Pattern

Generally beneficial for compute-bound applications.





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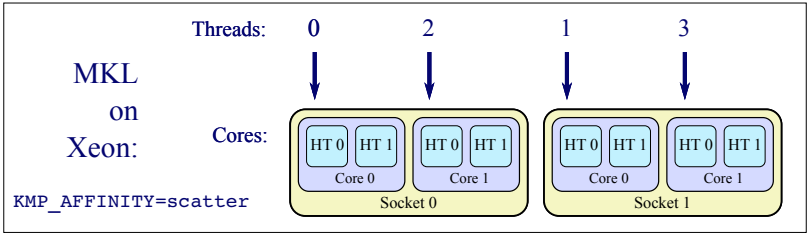
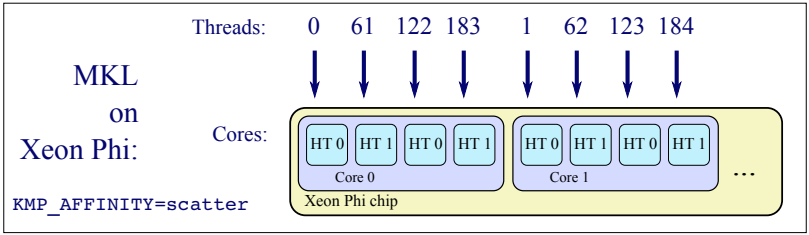
Thread Affinity: Scatter Pattern

Generally beneficial for bandwidth-bound applications.





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Data Container Tweaks

Parallel first-touch (see also HOW series Episode 3.5):

```
#pragma omp parallel for
  for(int i = 0; i < num_fft; i++)
    for(int j = 0; j < fft_size; j++) {
      data[i*fft_size+j].real = cos(k*j);
      data[i*fft_size+j].imag = sin(k*j);
    }
```

Data alignment (see also HOW series Episode 3.2)

```
MKL_Complex16* data =
        (MKL_Complex16*) mkl_malloc(sizeof(MKL_Complex16)*fft_size*num_fft, 64);
```


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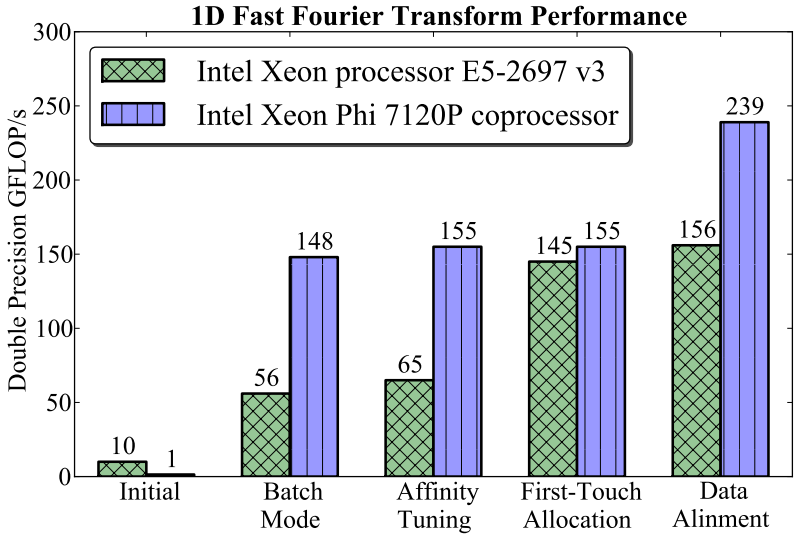
Complex-to-Complex 1D FFT Performance



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Problem Size Tuning

- Some functions require “good” problem sizes
- Good practice #1: array length a multiple of vector length
- Good practice #2: array length a multiple of number of threads
- Good practice #3: array length a multiple of a power of 2
- BLAS and LAPACK have “leading array dimension” for padding rows

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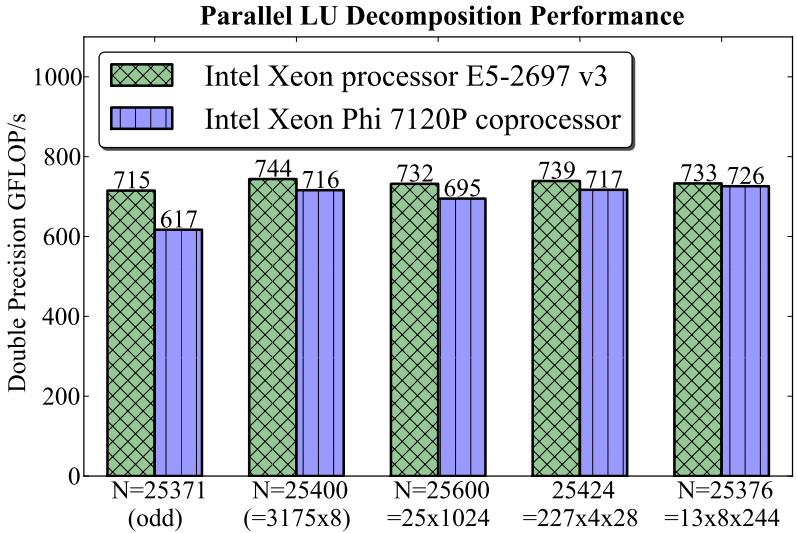
LU Decomposition Size Tuning



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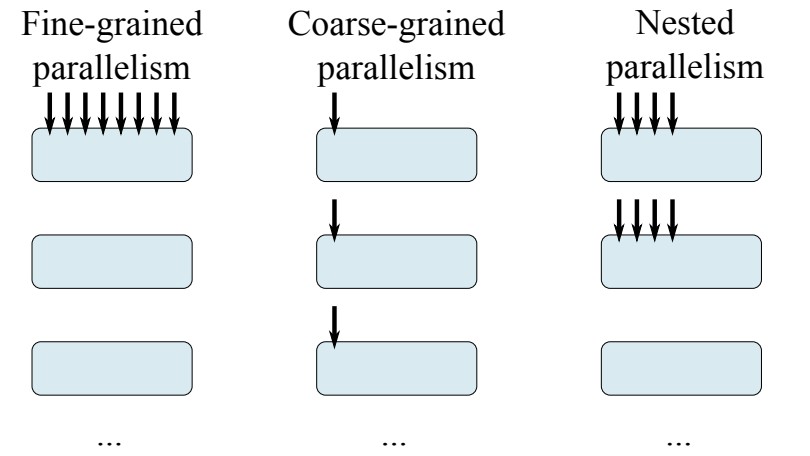
Nested Parallelism



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OpenMP Hot Teams

Xeon	Xeon Phi
`OMP_NUM_THREADS=2,14`	`OMP_NUM_THREADS=60,4`

`OMP_NESTED=1`
`OMP_PROC_BIND=spread,close`
`OMP_PLACES=cores`
	`OMP_NESTED=1`
	`OMP_PROC_BIND=spread,close`
	`OMP_PLACES=threads`

`KMP_HOT_TEAMS_MODE=1`
`KMP_HOT_TEAMS_MAX_LEVEL=2`
`OMP_MAX_ACTIVE_LEVELS=2`
	`KMP_HOT_TEAMS_MODE=1`
	`KMP_HOT_TEAMS_MAX_LEVEL=2`
	`OMP_MAX_ACTIVE_LEVELS=2`

`MKL_DYNAMIC=false`	`MKL_DYNAMIC=false`

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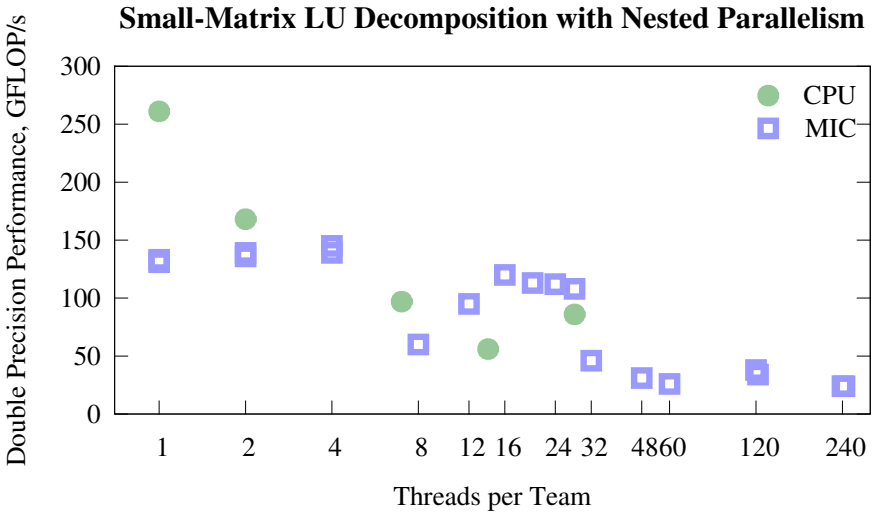
Small Matrix LU Decomposition with Nested Parallelism



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Automatic Offload

```
MKL_MIC_ENABLE=1

OMP_NUM_THREADS=... # CPU thread setting
KMP_AFFINITY=... # CPU affinity setting

MIC_KMP_PLACE_THREADS=4t # MIC thread setting
MIC_KMP_AFFINITY=... # MIC affinity setting
```


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Compilation of R with MKL

```
./configure \
   --with-blas="-L/opt/intel/mkl/lib/intel64 \
                -lmkl_intel_lp64 -lmkl_core -lmkl_intel_thread -lpthread -lm" \
   --with-lapack \
   CC=icc CFLAGS="-O2 -qopenmp -I/opt/intel/mkl/include" \
   CXX=icpc CXXFLAGS="-O2 -qopenmp -I/opt/intel/mkl/include" \
   F77=ifort FFLAGS="-O2 -qopenmp -I/opt/intel/mkl/include" \
   FC=ifort FCFLAGS="-O2 -qopenmp -I/opt/intel/mkl/include" \
   --prefix=/opt/R

user@host% make

user@host% su

root@host% make install
```


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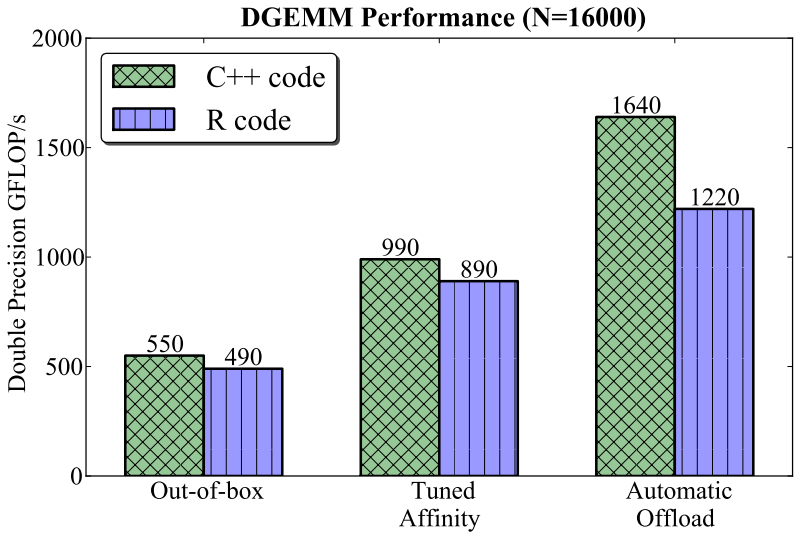
Performance with C++ Code and in R



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§5. Additional Information

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Acquiring MKL

	Community License	Commercial License
Cost	Free	Per developer
Support	Intel Premier Support	Community forum
Use in products	Yes	Yes
Royalty-free	Yes	Yes

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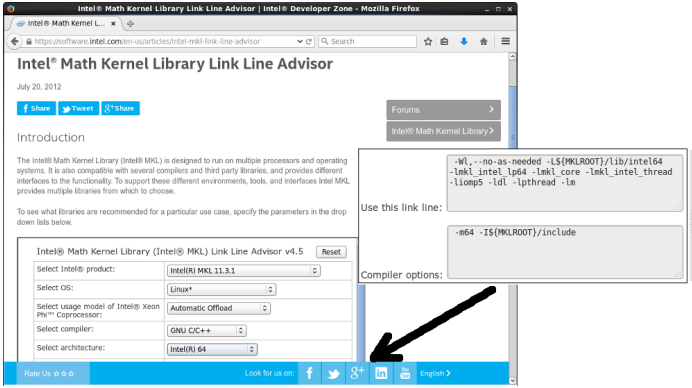
Compilation with MKL



https://software.intel.com/en-us/articles/intel-mkl-link-line-advisor

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§6. Resources

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Supplementary Materials: Textbook

ISBN: 978-0-9885234-0-1 (2nd edition, 508 pages, Electronic or Print)

Parallel Programming
and Optimization with
Intel® Xeon Phi™
Coprocessors

Handbook on the Development and
Optimization of Parallel Applications
for Intel® Xeon® Processors
and Intel® Xeon Phi™ Coprocessors

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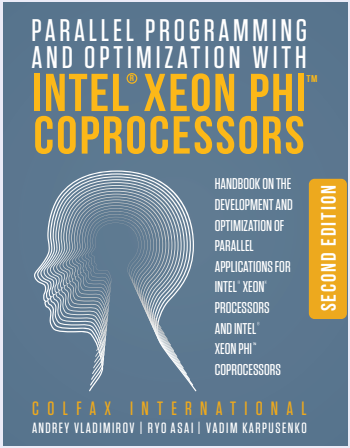

http://xeonphi.com/book

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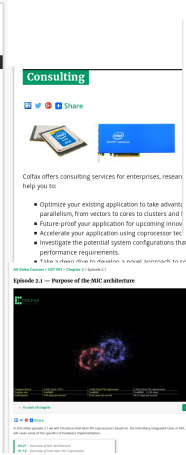

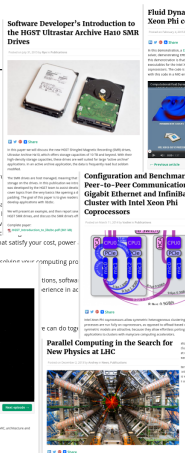

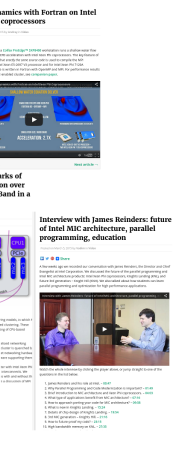

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