

Maximizing performance and scalability using Intel performance libraries

Roger Philp

Intel HPC Software Workshop Series 2016

HPC Code Modernization for Intel® Xeon and Xeon Phi™

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Intel[®] Parallel Studio XE 2016 components

	Full Licensing (including Intel® Premier Support)			Free Licensing			
Component	Composer Edition	Professional Edition	Cluster Edition	<u>Student</u> / <u>Educator</u>	Open Source Contributor	Academic Researcher	<u>Community</u> (Everyone!)
Intel® C/C++ Compiler (including Intel® Cilk™ Plus)	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark		
Intel [®] Fortran Compiler	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark		
OpenMP 4.0	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark		
Intel [®] Threading Building Blocks (C++ only)	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark
Intel [®] IPP Library (C/C++ only)	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark
Intel [®] Math Kernel Library	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark
Intel [®] Data Analytics Acceleration Library	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark
Intel [®] MPI Library			\checkmark	\checkmark		\checkmark	
Rogue Wave IMSL Library (Fortran only)	Bundled and Add-on	Add-on	Add-on				
Intel [®] Advisor XE		\checkmark	\checkmark	\checkmark	\checkmark		
Intel [®] Inspector XE		\checkmark	\checkmark	\checkmark	\checkmark		
Intel® VTune™ Amplifier XE		\checkmark	\checkmark	\checkmark	\checkmark		
Intel [®] ITAC + MPI Performance Snapshot			\checkmark	\checkmark			

Intel[®] Parallel Studio XE: performance libraries

Intel Threading Building Blocks (Intel® TBB)	 C++ template library for task parallelism Rich set of components for scalable parallel applications
Intel [®] Integrated Performance Primitives (Intel [®] IPP)	 Collection of high performance routines Broad range of functionality on different domains
Intel [®] Math Kernel Library (Intel [®] MKL)	 Highly optimized C/Fortran computing math library Sequential/parallel/cluster implementations
Rogue Wave IMSL Fortran Numerical Library	 Mathematical and statistical library for HPC Available as a bundled or add-on package to Intel PSXE
Intel [®] Data Analytics Acceleration Library (Intel [®] DAAL)	 Optimized building blocks library for data analytics New in Intel Parallel Studio XE 2016





Intel[®] Threading Building Blocks Library

Intel[®] Parallel Studio XE Suite

Intel[®] System Studio Suite

Intel® Threading Building Blocks (TBB)

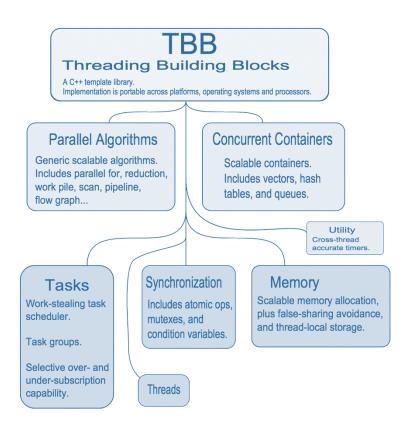
C++ template library for task parallelism

- Open specification, portable across platforms, OSs and processors
- Intel and open source versions available

Philosophy behind Intel[®] TBB

- Rich feature set for task based parallelism
 - Known parallel patterns easily mapped
- Logical tasks are transparently mapped to threads
 - Full support for nested parallelism
- Work-stealing scheduler to favour load balancing

Check <u>release notes</u> for news on latest 4.4 and earlier versions





tbb example

Standard C++ example

```
void SerialApplyFoo( float a[], size_t n ) {
    for( size_t i=0; i!=n; ++i )
        Foo(a[i]);
}
```

tbb version - with work stealing

```
#include "tbb/tbb.h"
using namespace tbb;
void ParallelApplyFoo( float a[], size_t n ) {
    parallel_for(0, n, [&](int i) {
        Foo(a[i]);
    });
}
```

Flow graph designer

(Alpha) Tool to assist developers in creating and tuning TBB applications

- As an analyzer, it provides capabilities to collect and visualize execution traces from TBB flow graph applications. Users can explore the topology of their graphs, interact with a timeline of node executions, and project statistics of their graphs
- As a designer, it provides the ability to visually create Intel TBB flow graph diagrams and generate C++ stubs for further development





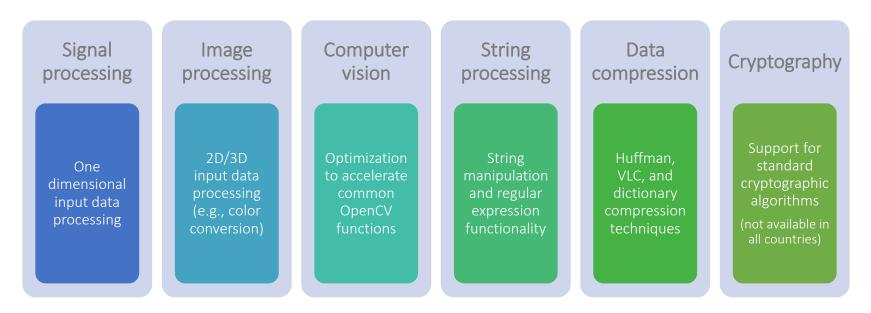


Intel[®] Integrated Performance Primitives

Intel[®] Parallel Studio XE Suite

Intel[®] System Studio Suite

Intel[®] Integrated Performance Primitives



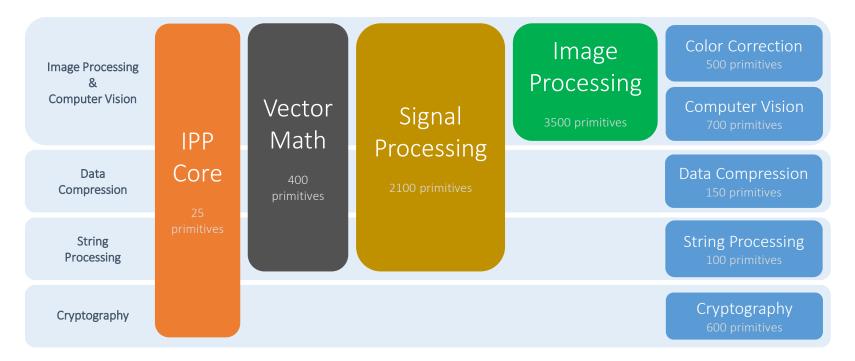
Intel[®] IPP: Extensive C/C++ performance library for multiple domains

• Multi-core-ready, computationally intensive optimized functions

Available on a wide variety of Intel platforms and OSs



Primitives and supporting domains



Function naming convention

• ipp<data-domain><name>_<datatype>[_<descriptor>] (<parameters>)

Intel[®] IPP and OpenCV 3.0

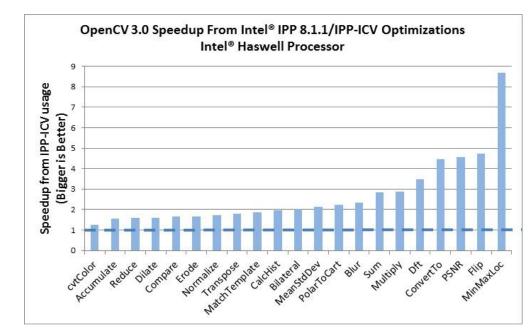
OpenCV 3.0 (Open Source Computer Vision)

- Computer vision and machine learning software library
- Supports optimization on Intel platforms with Intel® IPP

Intel[®] IPP for OpenCV (<u>ICV</u>)

- Subset of Intel[®] IPP, ~750 functions fully integrated into OpenCV 3.0
- Integration enabled by default on x86/intel64 configurations

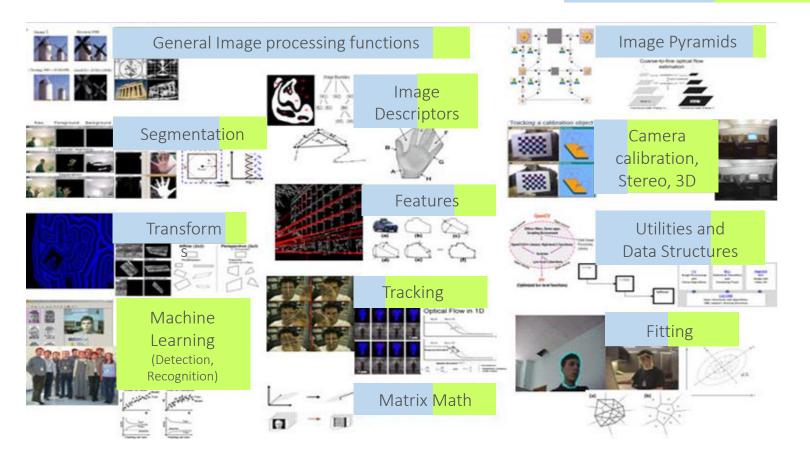
ICV provides ~40% performance gains



OpenCV 3.0 at glance

More than 500 algorithms (~60% benefit from Intel[®] IPP)

Covered by IPP OpenCV only



Intel[®] IPP 9.0 main features

Optimized for performance, throughput and power efficiency

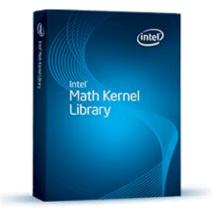
- Dynamic dispatching of best host-based function version (including SIMD capabilities)
- Extensive support of latest Intel[®] processors/coprocessors

Other feature highlights

- Integration of IPP subset (<u>ICV</u>) into <u>OpenCV 3.0</u>
- Static/dynamic, PIC/no-PIC library versions
- No internal memory allocation or threading

What's new in latest 9.0 release?

- New API for external threading
- Improved CPU dispatcher (including auto-initialization)
- Optimized cryptography functions to support SM2/SM3/SM4 algorithm
- Custom dynamic library building tool
- Additional optimizations for new Intel® processors/coprocessors



Intel[®] Math Kernel Library

Intel[®] Parallel Studio XE Suite

Intel[®] System Studio Suite

Intel[®] Math Kernel Library (Intel[®] MKL)



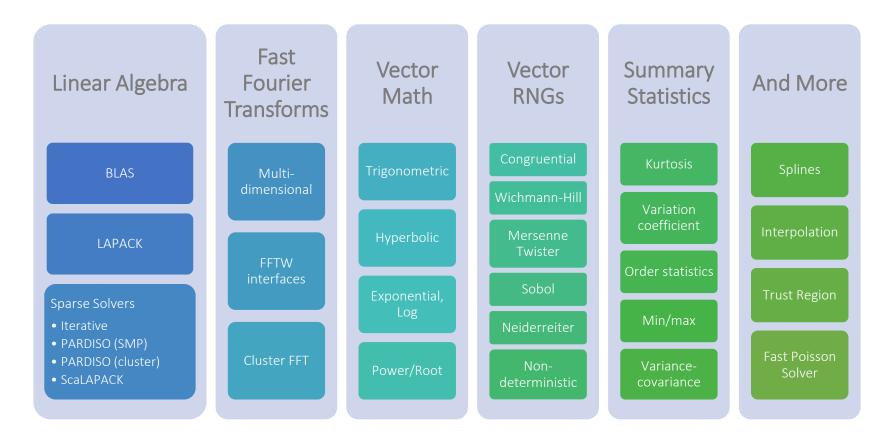
Intel[®] MKL: Collection of C/Fortran high-performance math routines for science, engineering and financial applications

- Extract great parallel performance with minimal effort
- De-facto industry standard APIs (C/Fortran)
- Additional API and environment variables for runtime configuration
- Support for Windows, Linux, and OS X

Optimized for performance on Intel[®] processors/coprocessors

- Dynamic dispatching of best host-based function version
 - Extensive use of SIMD extensions and optimal cache blocking factors
- Highly optimized sequential/parallel/cluster implementations

Mathematical building blocks on Intel[®] MKL



Intel[®] MKL on Intel[®] Xeon PhiTM

Automatic Offload	 No code changes required Automatically uses both host and target (MKL_MIC_ENABLE=1) Transparent data transfer and execution management
Compiler Assisted Offload	 Explicit control for data transfer and remote execution Invoked with compiler offload or OpenMP target pragmas Can be used together with Automatic Offload
Native Execution	 Uses the coprocessors as independent nodes Input data and binaries are copied to targets in advance

Intel[®] MKL provides full support for Intel[®] Xeon Phi[™] coprocessor

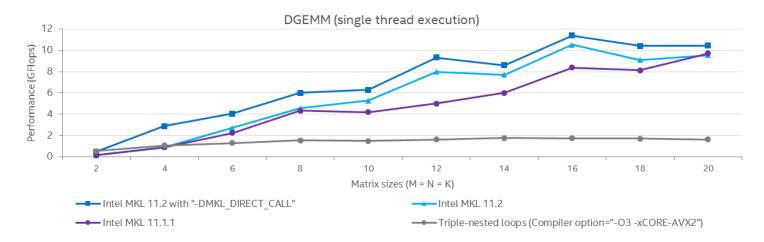
*GEMM improvements on small matrices

Significant performance improvements for square sizes smaller than 20

- Applicable to all small sizes and input parameters
- No errors reported when incorrect parameters are passed to the function call

How to enable small matrices optimization

- Include mkl_direct_call.fi/mkl_direct_call.h module
- Compile with the option MKL_DIRECT_CALL/MKL_DIRECT_CALL_SEQ symbol



What's new in Intel® MKL 11.3

Main new features an improvements

- Additional two-stage API for sparse BLAS2/3 routines
- MKL MPI wrappers
- Support for batched small *GEMM independent operations
- Support for Philox4x35 and ARS5 RNGs (2¹²⁸ period)
- Sparse solver SMP scalability improvements

Many other features and optimizations (check MKL 11.3 release notes)

- HBM support for 2nd generation of Intel[®] Xeon Phi[™]
- Improved MKL composability with Intel[®] TBB applications
- Cluster components now available for OS X
- Many BLAS/(Sca)LAPACK/PARDISO improvements
- Many improvements on latest AVX2/IMCI and future AVX-512 hardware

Intel[®] MKL Cookbook

Detailed recipes for solving complex problems with Intel® MKL

Using LAPACK symmetric Eigen solvers for Hermitian tri-diagonal matrices

Soal

Compute eigenvalues and eigenvectors for a Hermitian tridiagonal matrix using LAPACK symmetric eigensolvers.

LAPACK provides symmetric eigensolvers for real-valued tridiagonal matrices, but no corresponding eigensolvers for complex Hermitian matrices.

Solution

A simple matrix transformation to a Hermitian tridiagonal matrix allows you to use one of the LAPACK eigensolvers.

- Multiply the Hermitian tridiagonal matrix by a matrix calculated to eliminate the imaginary parts of the offdiagonal elements, which transforms it to a real-valued matrix.
- Choose the LAPACK eigensolver routine according to the task you wish to perform and the algorithm you wish to use:
 - o sstev, dstev: Compute all eigenvalues and, optionally, eigenvectors.
 - sstevd, dstevd: Compute all eigenvalues and, optionally, eigenvectors using a divide-and-conquer algorithm.
 - o sstevx, dstevx: Compute selected eigenvalues and eigenvectors.
 - sstevr: dstevr: Compute selected eigenvalues and, optionally, eigenvectors using Relatively Robust Representations.
- Reverse the transformation to the eigenvalues and eigenvectors returned by the LAPACK routine in order to get the eigenvalues and eigenvectors of the original matrix.

Calculating eigenvalues and eigenvectors for a Hermitian tridiagonal matrix using DSTEV

```
PROGRAM complex_tridiagonal_hev_solver
IMPLICIT NONE
INTEGER N, INFO,I,J
PARAMETER (N=5)
C Matrix
COMPLEX*16 EC(N-1)
REAL*8 D(N)
C Eigenvectors
```

Test the	vectors are eigenvectors
DO I=	1,N
D	0 J=1,N
	UZ(J) = -DCMPLX(D(I), 0D0) *VZ(J, I)
E	ND DO
υ	Z(1)=UZ(1) + DC(1)*VZ(1,I) + EC(1)*VZ(2,I)
D	0 J=2,N-1
	UZ(j)=UZ(j) + CONJG(EC(J-1))*VZ(J-1,I)+
8	DC(J) * VZ(J,I) + EC(J) * VZ(j+1,I)
E	ND DO
U	Z(N)=UZ(N) + CONJG(EC(N-1))*VZ(N-1,I) + DC(N)*VZ(N,I)
P	RINT *, "For ", I, "th eigenvalue S*U^j-lambda_j*U^j =",
8	DZNRM2 (N, UZ, 1)
END D	0
STOP	

Discussion

In this example, S is a complex-valued tridiagonal Hermitian matrix:

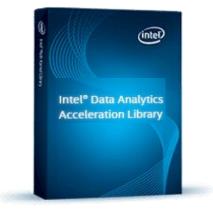
$$S = \begin{bmatrix} d_1 & e_1 & & \\ c_1 & d_2 & e_2 & & \\ & c_2 & d_3 & e_3 & & \\ & & \ddots & \ddots & \\ & & & c_{N-2} & d_{N-1} & e_{N-1} \\ & & & c_{j}, j = 1, 2, \dots N-1 \end{bmatrix}$$

Construct a diagonal matrix T, where $|t_i| = 1$ for i = 1, 2, ... N:



A new matrix $S_1 = T^H S T$ has the same eigenvalues as S.



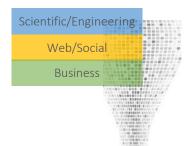


Intel[®] Data Analytics Acceleration Library

Intel[®] Parallel Studio XE Suite 2016

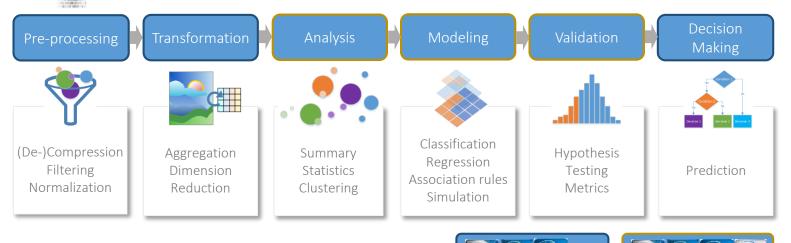


Intel[®] Data Analytics Acceleration Library



Intel[®] DAAL: An industry leading end-to-end IA-based data analytics acceleration library of fundamental algorithms covering all big data analysis stages

More information later in "Coding high performance big data analytics applications" session



Summary

Intel[®] Parallel Studio XE 2016 tool suite to boost performance of parallel applications on Intel[®] processors/coprocessors

Tool suite components

- High-performance C/C++ and Fortran compilers
- Performance and parallel libraries
- Design, tune, and verification tools

What's new in 16.0?

- Free licensing for selected communities
- Support for latest C/C++/Fortran standards
- Improved performance and compatibility with new/future Intel hardware
- Intel[®] DAAL: new library for big data analytics
- Intel® Vectorization Advisor: new design/analysis tool for vectorising your code

Online resources

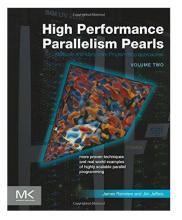
Intel[®] software development tools, performance tuning, etc.

- **Documentation library** All available documentation about Intel software
- HPC webinars
- <u>Modern code</u>
- Forums

- Free technical webinars about HPC on Intel platforms Intel resources about code modernization
 - Public discussions about Intel SIMD, threading, ISAs, etc.
- Intel[®] Xeon PhiTM resources
 - <u>Developer portal</u>
 - <u>Solutions catalog</u>
- Programming guides, tools, trainings, case studies, etc. Existing Intel[®] Xeon Phi[™] solutions for known codes
- Other resources (white papers, benchmarks, case studies, etc.)
 - <u>Go parallel</u>
 - Colfax research
 - <u>Bayncore labs</u>

BKMs for Intel multi- and many-core architectures Publications and material on parallel programming Research and development activities (WIP)

Recommended books



Optimizing HPC

exander Supploy Andrey Semin, Michael Klemn

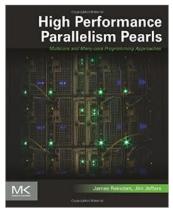
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Applications with Intel[®] Cluster Tools *High performance parallelism pearls: multi-core and many-core approaches (Vol. 2),* by James Reinders and Jim Jeffers, Morgan Kaufmann, 2015

High performance parallelism pearls: multi-core and many-core approaches, by James Reinders and Jim Jeffers, Morgan Kaufmann, 2014

Optimizing HPC applications with Intel® cluster tools, by Alexander Supalov et al, Apress, 2014

> Parallel programming with Intel® Parallel Studio XE, by Stephen Blair-Chappell and Andrew Stokes, Wrox press, 2012





Parallel Programming with Intel[®] Parallel Studio XE reverte Jone Road Found Found Stephen Blair-Chappell, Andrew Stokes