Intel[®] oneAPI Math Kernel Library (oneMKL)

HLRS oneAPI Workshop

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Introduction

What is "the" oneMKL?

Different meaning in different contexts, but one common theme:

A set of functions of commonly used mathematical operations, such as:

- Linear algebra (basic arithmetic, solvers & decompositions, etc.)
- Fast Fourier Transforms (FFT)
- Random number generators

Do not write these routines yourself, use oneMKL!

A "good" oneMKL implementation often outperforms naïvely written code by a factor of 100x and more. (Performance varies depending on implementation, machine, context, problem type and size, etc. pp.)

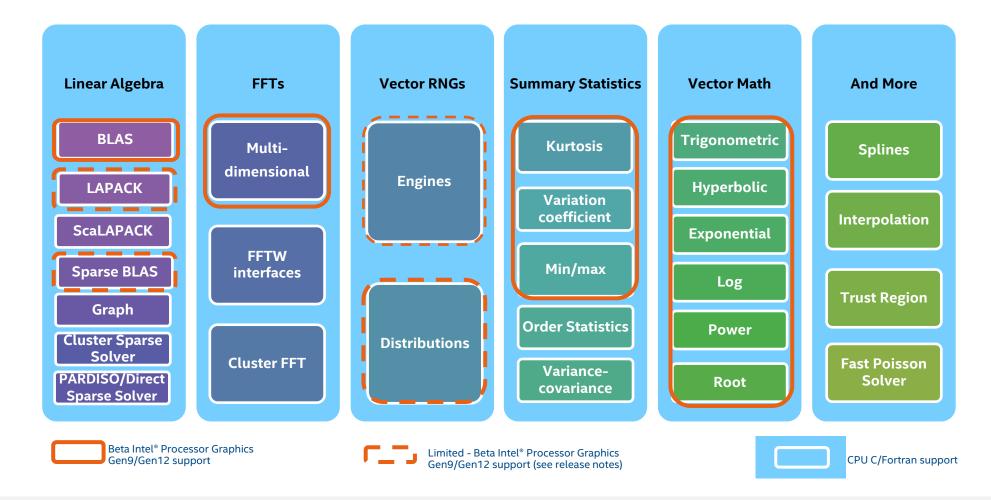
The different meanings of "oneMKL"

- 1. The SYCL* interface defined in the open oneAPI standard
- 2. Other vendors' (partial) implementations of the standard

The different meanings of "oneMKL"

- 1. The SYCL* interface defined in the open oneAPI standard
- 2. Other vendors' (partial) implementations of the standard
- 3. Intel's implementation of it: Intel[®] oneAPI Math Kernel Library
 - Origin of the standard and the most complete implementation of it
 - Extremely optimised for Intel[®] hardware
 - Apart from the SYCL* interface, also provides interfaces for:
 - C++ and plain C, Fortran
 - Other de facto standard APIs: BLAS, LAPACK, FFTW, etc.
 - Support for distributed and heterogeneous computing via OpenMP and MPI.

Overview of Intel® oneMKL Functionality



oneMKL is part of the Intel® oneAPI Base Toolkit

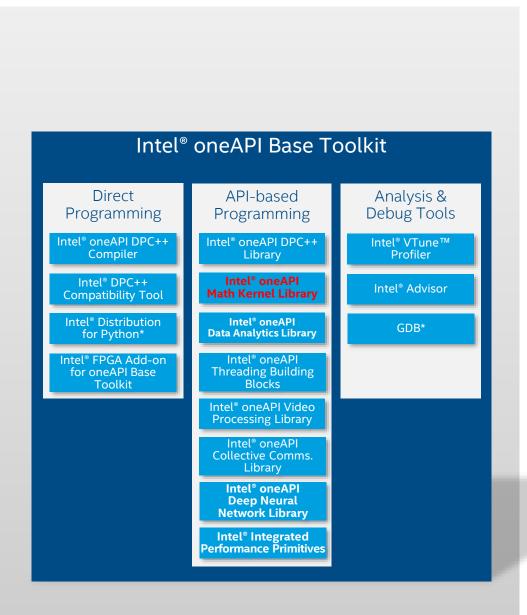
Core set of frequently used tools and libraries for developing high-performance applications across diverse architectures—CPU, GPU, FPGA.

Who Uses It?

- A broad range of developers across industries
- Add-on toolkit users because this is the base for all toolkits

Top Features/Benefits

- Data Parallel C++ (DPC++) compiler, library, and analysis tools
- DPC++ Compatibility tool helps migrate existing CUDA code
- Python distribution includes accelerated scikit-learn, NumPy, SciPy libraries
- Optimized performance libraries for threading, math, data analytics, deep learning, and video/image/signal processing



7

Also available as a standalone Download

https://www.intel.com/content/www/us/en/developer/tools/oneapi/onemkl-download.html

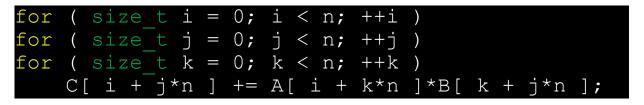


A Simple Example

Given two NxN matrices A and B, compute their product C = A*B.

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Naïve C code:



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Naïve C code:

for (size_t i = 0; i < n; ++i)
for (size_t j = 0; j < n; ++j)
for (size_t k = 0; k < n; ++k)
 C[i + j*n] += A[i + k*n]*B[k + j*n];</pre>

Performance on my Laptop: 1.01 GFLOPs

Given two NxN (N=1024) matrices A and B, compute their product C = A*B.

Naïve C code:

```
for ( size_t i = 0; i < n; ++i )
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```

Performance on my Laptop: 1.01 GFLOPs

Corresponding oneMKL Call:

cblas_dgemm(CblasColMajor, CblasNoTrans, CblasNoTrans, n, n, n, 1.0, A, n, B, n, 0.0, C, n);

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Corresponding oneMKL Call:

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193.3 GFLOPs

oneMKL, DGEMM, CAPI

int main() {

....

int64_t m = 10, n = 6, k = 8, lda = 12, ldb = 8, ldc = 10; int64_t sizea = lda * k, sizeb = ldb * n, sizec = ldc * n; double alpha = 1.0, beta = 0.0;

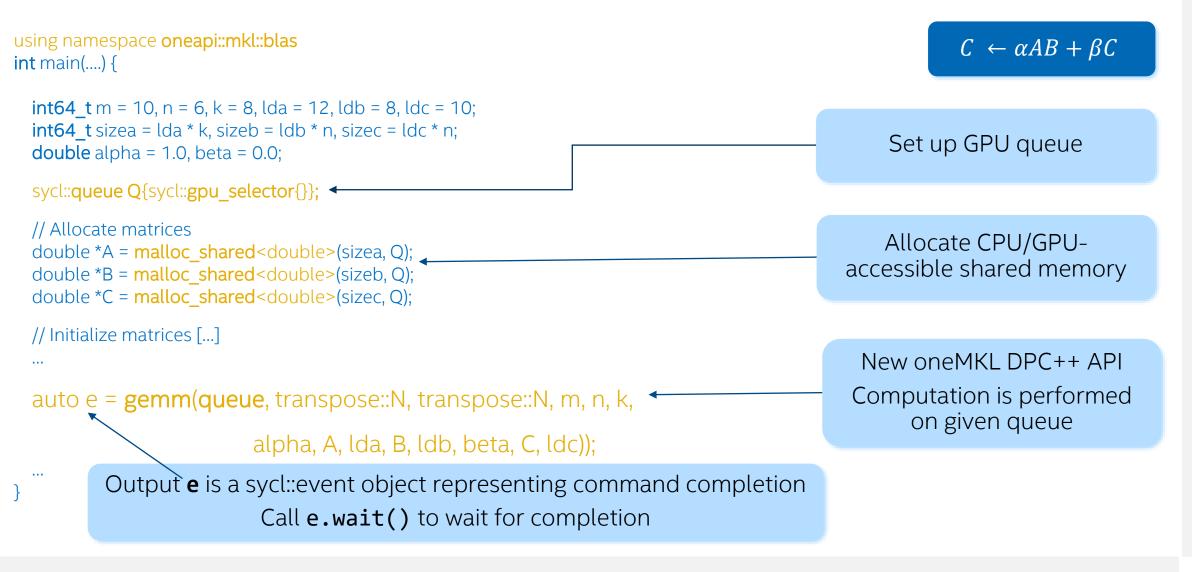
```
// Allocate matrices
double *A = (double *) mkl_malloc(sizeof(double) * sizea);
double *B = (double *) mkl_malloc(sizeof(double) * sizeb);
double *C = (double *) mkl_malloc(sizeof(double) * sizec);
```

```
// Initialize matrices [...]
```

```
cblas_dgemm(CblasColMajor, CblasNoTrans, CblasNoTrans, m, n, k, alpha, A, Ida, B, Idb, beta, C, Idc);
```

$C \leftarrow \alpha AB + \beta C$

oneMKL, DGEMM, SYCL API



Different Ways of using oneMKL

Interfaces to the Intel® oneAPI Math Kernel Library

Operating Systems: Windows and various Linux flavours

Intel CPUs:

- C, C++, and Fortran interfaces
- Support for 32- and 64-bit integers
- Multi-threaded and single-threaded versions
- Controlled through linker flags and environment variables
- Static and dynamic linking possible
- Can be used with other compilers as well

Intel GPUs:

- SYCL interface
- OpenMP 5.0 support for GPU offloading, can be used from both C and Fortran

Interfaces to the Intel® oneAPI Math Kernel Library

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Many different combinations! Use the <u>link-line advisor</u> for help!



The oneMKL Interfaces Project

What is it?

- Implements (parts of) the oneMKL SYCL* API for Nvidia* and AMD* GPUs
- Wrapper around the vendor-supplied libraries (e.g., cuBLAS*, ...)
- Allows you to use the oneMKL APIs on all common GPUs and with a single source code. Only compiler and linker flags change!

Where do I get it?

<u>On GitHub</u>



oneAPI MKL Interfaces Project

		<i>.</i>	Туре	Compiler
BLAS	x86 CPU	Intel(R) oneAPI Math Kernel Library	Dynamic, Static	DPC++, LLVM*, hipSYCL
	Intel GPU		Dynamic, Static	DPC++
	NVIDIA GPU	NVIDIA CUBLAS	Dynamic, Static	LLVM*, hipSYCL
	x86 CPU	NETLIB LAPACK	Dynamic, Static	DPC++, LLVM*, hipSYCL
	AMD GPU	AMD rocBLAS	Dynamic, Static	LLVM*, hipSYCL
	x86 CPU, Intel GPU, NVIDIA GPU, AMD GPU	SYCL-BLAS	Dynamic, Static	DPC++, LLVM*
LAPACK	x86 CPU	Intel(R) oneAPI Math Kernel Library	Dynamic, Static	DPC++, LLVM*
	Intel GPU		Dynamic, Static	DPC++
	NVIDIA GPU	NVIDIA cuSOLVER	Dynamic, Static	LLVM*
	AMD GPU	AMD rocSOLVER	Dynamic, Static	LLVM*
RNG	x86 CPU	Intel(R) oneAPI Math	Dynamic, Static	DPC++, LLVM*, hipSYCL
	Intel GPU	Kernel Library	Dynamic, Static	DPC++
	NVIDIA GPU	NVIDIA cuRAND	Dynamic, Static	LLVM*, hipSYCL
	AMD GPU	AMD rocRAND	Dynamic, Static	LLVM*, hipSYCL
DFT	Intel GPU	Intel(R) oneAPI Math Kernel Library	Dynamic, Static	DPC++
	x86 CPU		Dynamic, Static	DPC++
	NVIDIA GPU	NVIDIA cuFFT	Dynamic, Static	DPC++

What's new in the Intel[®] oneAPI Math Kernel Library (oneMKL)

oneMKL on 4th Gen Intel[®] Xeon[®] Scalable processors

Maximize performance with oneMKL, unleashing the power of built-in accelerators



4th Gen Intel® Xeon® Scalable Processors with Intel® Advanced Matrix Extensions. Ouick assist Technology, Intel® AVX-512, bfloat16, and more built-in accelerators

INT8 data types.

(HBM).

intel

SIEVER

Xeon

oneMKL on Intel® Data Center GPU Max Series

Breakthrough Performance for HPC and AI

- The Intel[®] oneAPI Math Kernel Library (oneMKL) leverages Intel[®] Xe Matrix Extensions (Intel[®] XMX) to optimize matrix computations for TF32, FP16, BF16 and INT8 data types on Intel[®] Data Center GPU Max Series (codenamed Ponte Vecchio).
- oneMKL provides a variety of dense and sparse linear algebra (BLAS, LAPACK, sparse BLAS), FFT, vector math, vector RNG, summary statistics, and spline interfaces both for the SYCL and C/Fortran OpenMP* offload programming models to enable applications targeting Intel[®] Data Center GPUs.



Intel® Data Center GPUs with hardware AVI encode and Max with datatype flexibility, Intel® X^e Matrix Extensions, vector engine, XE-Link, and other features



oneMKL BLAS Compute Modes

- Core idea: use two or three FP16 numbers to obtain single precision (FP32)
 - "Concatenate" the mantissæ to achieve higher accuracy.
 - Warning: Not IEEE-754 conforming!

However:

- Can use hardware acceleration for FP16 to boost performance where high accuracy is not important (e.g., certain iterative algorithms)
- Mostly benefits dense linear algebra operations
- Supported in some BLAS routines

oneMKL, BLAS, GPU, the new compute modes

- The new MKL_BLAS_COMPUTE_MODE is intended for quickly evaluating whether alternate compute modes provide performance benefits and acceptable accuracy for an application. After initial testing, alternate mode settings can be permanently applied within the application using the per-call or per-source-file APIs.
- New alternate computation mode functionality for Level-3 routines
 - Better performance
 - Reduced accuracy
 - oneMKL does not enable any alternate compute modes by the default
 - The same or optional interfaces
 - Limitations: gemm, gemmt, syrk and syrk2 (MKL 2023)

oneMKL, BLAS, GPU, the new compute modes, cont.

from blas.hpp #define ONEMKL DECLARE GEMM(Ta, Tb, Tc, Ts) DLL EXPORT sycl::event gemm(sycl::queue &queue, transpose transa, transpose transb, \ std::int64 t m, std::int64 t n, std::int64 t k, \ Ts alpha, const Ta *a, std::int64 t Ida, \ const Tb *b, std::int64 t ldb, \ Ts beta, Tc *c, std::int64 t ldc, \ compute mode mode. const std::vector<sycl::event> &dependencies = {}); \ ONEMKL_INLINE_DECLARE sycl::event gemm(sycl::queue &queue, transpose transa, transpose transb, \ std::int64 t m, std::int64 t n, std::int64 t k, \ Ts alpha, const Ta *a, std::int64 t lda, \ const Tb *b, std::int64 t ldb, \ Ts beta, Tc *c, std::int64 t ldc, \ const std::vector<sycl::event> &dependencies = {})

{\

return gemm(queue, transa, transb, m, n, k, alpha, a, lda, b, ldb, beta, c, ldc, MKL_BLAS_COMPUTE_MODE, dependencies); \

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Intel[®] oneMKL Resources

Intel® oneMKL Product Page	https://www.intel.com/content/www/us/en/developer/tools/oneapi/onemkl.html			
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Intel® oneMKL Developer Guide	https://www.intel.com/content/www/us/en/develop/documentation/onemkl-windows-developer-guide/top.html			
Intel® oneMKL Specification	https://spec.oneapi.io/versions/latest/elements/oneMKL/source/index.html			
Intel® oneMKL Open-Source Interfa	https://github.com/oneapi-src/oneMKL			
Intel® oneMKL Release Notes	https://cqpreview.intel.com/content/www/us/en/developer/articles/release-notes/onemkl-release-notes.html			
Intel® oneMKL Forum	https://community.intel.com/t5/Intel-oneAPI-Math-Kernel-Library/bd-p/oneapi-math-kernel-library			

Demo, MKL

MKL Verbose mode, cont.

Examples:

MKL_VERBOSE oneMKL 2023.0 Product build 20221128 for Intel(R) 64 architecture Intel(R) Advanced Vector Extensions 512 (Intel(R) AVX-512) with Intel(R) DL Boost, bfloat16 support, Intel(R) AMX with bfloat16 and 8-bit integer support, and FP16 instructions, Lnx 3.00GHz ilp64 intel_threadMKL_VERBOSE

GEMM_BF16BF16F32(N,N,1024,1024,1024,0x7ffeb4e10028,0x7ff21d2b5080,1024,0x7ff21d4b6080,102 4,0x7ffeb4e10030,0x7ff21ceb4080,1024) 69.71ms CNR:OFF Dyn:1 FastMM:1 TID:0

NThr:112**FFT(dcbi</mark>5x13x7</mark>,tLim:22,desc:0xeb6d80) 93.11us CNR:OFF Dyn:1 FastMM:1 TID:0 NThr:44**

MKL GPU Verbose mode, cont.

GPU Verbosing – extension of the existing env variable and run time functions

To change the verbose mode, do one of the following:

• set the environment variable *MKL_VERBOSE*

	CPU Targets	GPU Targets			
(default) Set MKL_VERBOSE to 0	to disable verbose	to disable verbose			
Set MKL_VERBOSE to 1	to enable verbose	to enable verbose without timing			
Set MKL_VERBOSE to 2	to enable verbose	to enable verbose with synchronous timir			

• Or call the support function mkl_verbose(int mode)

	CPU Targets	GPU Targets
(default) Call mkl_verbose(0)	to disable verbose	to disable verbose
<i>Call</i> mkl_verbose(1)	to enable verbose	to enable verbose without timing
<i>Call</i> mkl_verbose(2)	to enable verbose	to enable verbose with synchronous timir

MKL GPU Verbose mode, cont. export MKL_VERBOSE=2

Running tests on GPU. Running with double precision complex-to-complex 1-D FFT: Using SYCL buffers MKL VERBOSE oneMKL 2022.0 Product build 20211022 for Intel(R) 64 architecture Intel(R) MKL VERBOSE Detected GPU0 Intel(R) Gen9 Backend:Level Zero VE:72 Stack:1 maxWGsize:256 MKL VERBOSE FFT (dcfil6, bScale: 0.0625) 88.88ms GPU0 Verify the result, errthr = 4.44089e-15 Verified, maximum error was 1.9405e-16 MKL VERBOSE FFT (dcbi16, bScale:0.0625) 179.05ms GPU0 Verify the result, errthr = 4.44089e-15 Verified, maximum error was 6.93889e-18 Using USM MKL VERBOSE FFT (dcfil6, bScale: 0.0625) 191.91us GPU0 Verify the result, errthr = 4.44089e-15 Verified, maximum error was 1.9405e-16 MKL VERBOSE FFT (dcbil6, bScale:0.0625) 204.91us GPU0 Verify the result, errthr = 4.44089e-15 Verified, maximum error was 6.93889e-18 Test Passed



DEMO, BLAS

..\2023\ww23_LRZ\DEMO:

PART I

- Reviewing the examples.
- Reviewing the makefiles. : -lmkl_sycl -lmkl_intel_ilp64 -lmkl_tbb_thread lmkl_core -lsycl -lOpenCL -lpthread -lm -ldl

PART II

- make usm comp <-- Compilation
- Verbosing -- clarification

DEMO, BLAS, cont.

- 3. Small sizes, Conclusion
- 4. C/Fortran vs DPCPP performance
- 5. sequential Code: make seq
- 6. ZE_AFFINITY_MASK=0.0, 0.1
- 6.1 → BLAS, 2 sub-slises.
- 6.2 BLAS example 2 slices....
- 6.3 BLAS. Splitting works. 2 tiles case.
- 7. Backends, comparisons
- 8. BLAS. New Compute Mode

DEMO, BLAS, newCompute mode.

./a.out 3000 0

size == 3000, GFlops == $4003.065 \rightarrow host$ (SPR), default call

./a.out 3000 1

size == 3000, GFlops == 14863.280 -> PVC, default call, no Compute Mode

MKL_BLAS_COMPUTE_MODE=FLOAT_TO_BF16 ./a.out 3000 1 size == 3000, GFlops_== 53650.547 -> PVC, Compute mode enabled by Env. Variables.

\$./a1.out 3000 1 1

size == 3000, GFlops == 53881.142 -> PVC, compute mode is enabled explicitly by dgemm(...oneapi::mkl::blas::compute_mode::float_to_bf16)

DEMO, BLAS, cont.

9. Offloading

Demo, tips, ZE AFFINITY MASK

- sycl specification.
- sdp4451 1 device, 2 tiles.

- 0, 1: all devices and sub-devices are reported (same as default)
- 0: only device 0 is reported; with all its sub-devices
- 1: only device 1 is reported as device 0; with all its sub-devices
- 0.0: only device 0, sub-device 0 is reported as device 0
- 1.1, 1.2: only device 1 is reported as device 0; with its sub-devices 1 and 2 reported as sub-devices respectively
- 0.2, 1.3, 1.0, 0.3: both device 0 and 1 are reported; device 0 reports sub-devices 2 and 3 as sub-devices 0 and 1, respectively; device 1 reports sub-devices 0 and 3 as sub-devices 0 and 1, respectively; the order is unchanged.

ZE AFFINITY MASK. Level Zero

Environment Variables

The following table documents the supported knobs for overriding default functional behavior.

Category	Name	2	Values	Description
Device		Forces driver to only report devices (and sub- devices) as specified by values		
		ABLE_PCI_ID_DEVICE_ORDER	{ 0 , 1}	Forces driver to report devices from lowest to highest PCI bus ID
es 0 and 1,		ARED_FORCE_DEVICE_ALLOC	{ 0 , 1}	Forces all shared allocations into device memory

https://spec.oneapi.io/level-zero/latest/core/PROG.html

Demo, BLAS, multi-stack, explicit method

// #1 -- Create sub devices for multi-stack device
std::vector<sycl::device> subdev = {};
cl::sycl::queue subdev_queue0;
cl::sycl::queue subdev_queue1;

// # 2 -- Create context, execution queue, and buffers of matrix data subdev_queue0 = cl::sycl::queue(cxt, subdev[0], exception_handler); subdev_queue1 = cl::sycl::queue(cxt, subdev[1], exception_handler);

try
<pre>if (multistack mode == 1 && nb device > 1) {</pre>
// Split B and C for subdevices
n subdev = $n/2$;
sizeb subdev = ldB * n subdev;
sizec subdev = $1dC * n/2;$
gemm_done0 = gemm(subdev_queue0, transA, transB, m, n_subdev, k, a gemm_done1 = gemm(subdev_queue1, transA, transB, m, n_subdev, k, a
A[1], ldA, B[1] + sizeb subdev, ldB, beta, C[1] +
} else {
<pre>gemm_done0 = oneapi::mkl::blas::gemm(subdev_queue0, transA, transB</pre>
A[0], ldA, B[0], ldB, beta, C[0], ldC, gemm depend
}
}
Source as an an an ann

Demo, BLAS, multi-stack, explicit method. cont.

./usm2stacks.x 4000 1

gfedorov@sdp4451:~/5temp/ww22 2023\$ MKL VERBOSE=2 ./usm2stacks.x 4000 1

#of divices == 2
4KL_VERBOSE oneMKL 2023.0 Update 1 Product build 20230303 for Intel(R) 64 architecture Intel(R) Advanced Vector
Extensions 512 (Intel(R) AVX-512) with Intel(R) DL Boost, bfloat16 support, and FP16 instructions, Lnx 1.80GHz
ilp64 tbb_thread
4KL VERBOSE Detected GPU0 Intel(R) Xe HPC Backend:Level Zero VE:1024 Stack:2 maxWGsize:1024

4KL_VERBOSE oneapi::mkl::blas::column_major::gemm[double](0x7ffd64614010,NonTranspose,NonTranspose,4000,2000,40
00,2,0x14c053400000,4000,0x14c04b600000,4000,3,0x14c043800000,4000,unset,Vector<sycl::_V1::event>OfSize:0) mode
standard host:545.88ms device:nan GPU0
4KL_VERBOSE oneapi::mkl::blas::column_major::gemm[double](0x7ffd64614040,NonTranspose,NonTranspose,4000,2000,40
00,2,0x14c03ba00000,4000,0x14c037909000,4000,3,0x14c02fb09000,4000,unset,Vector<sycl::_V1::event>OfSize:0) mode
00,2,0x14c03ba00000,4000,0x14c037909000,4000,3,0x14c02fb09000,4000,unset,Vector<sycl::_V1::event>OfSize:0) mode

standard host:490.54ms device:nan GPU0

#of devices == 2 GPU Explicit, perf = 36252.8 GFlops

DEMO, tips, BACKEND

- SYCL_DEVICE_FILTER=level_zero MKL_VERBOSE=2 ./usm.x 4000 1
- MKL_VERBOSE Detected GPU0 Intel(R)_Xe_HPC Backend:Level_Zero VE:1024 Stack:2 maxWGsize:1024

- SYCL_DEVICE_FILTER=opencl MKL_VERBOSE=2 ./usm.x 4000 1
- MKL_VERBOSE Detected GPU0 Intel(R)_Xe_HPC Backend:OpenCL VE:10
- size == 4000, GFlops == 9634.553

Demo, BLAS, GPU, the new compute modes

Compute mode enum value	Environment variable	Description
		Convert single-precision inputs to bfloat16 format internally; Output is
		accumulated in single precision.
compute_mode::float_to_bf16	FLOAT_TO_BF16	Accuracy will be reduced, with possibly much higher performance.
		Convert each single-precision input value to a sum of two bfloat16 values
		internally; Output is accumulated in single precision.
		Expected accuracy is between that of standard single precision arithmetic and
compute_mode::float_to_bf16x2	FLOAT_TO_BF16X2	bfloat16 arithmetic.
		Convert each single-precision input value to a sum of three bfloat16 values
		internally; Output is accumulated in single precision.
		Expected accuracy is comparable to standard single precision arithmetic in most
compute_mode::float_to_bf16x3	FLOAT_TO_BF16X3	cases.
		Reduce the four real multiplications in a standard complex multiplication to three
		real multiplications.
compute_mode::complex_3m	COMPLEX_3M	Expected accuracy is comparable to standard arithmetic in most cases.
compute_mode::standard	STANDARD	Do not allow any alternate compute modes

Demo, BLAS, GPU, the new compute modes, cont.

Usage :

• Environment Variables:

set/export MKL_BLAS_COMPUTE_MODE=FLOAT_TO_BF16X2

• Per-call or per-source-file mode:

using oneapi::mkl::blas; auto mode_settings = compute_mode::float_to_bf16x2 | compute_mode::float_to_tf32; /* allow either of these two modes */

// USM API, with dependencies : syrk(my_queue, n, k, uplo, trans, alpha, a_ptr, lda, beta, c_ptr, ldc, compute_mode::float_to_bf16, event); // USM API, dependencies but no special compute_mode settings syrk(my_queue, n, k, uplo, trans, alpha, a_ptr, lda, beta, c_ptr, ldc, event);

• Checking Which Mode Is Used:

MKL_VERBOSE oneapi::mkl::blas::column_major::gemm[float](0x7ffd39046350,...,float_to_bf16) mode:float_to_bf16 host:nan device:nan GPU0

https://www.intel.com/content/www/us/en/develop/documentation/oneapi-mkl-dpcpp-developer-reference/top/blas-routines/blas-compute-modes.html

Demo, BLAS, Compute mode, cont

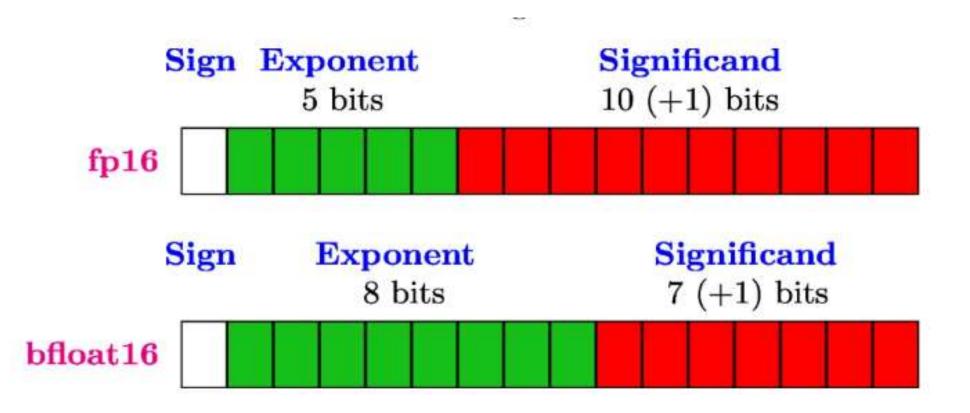
- Check sgemm_newcomputemode.cpp, makefile, run_newcompmode.sh
 - The same code
 - The same compiling
 - run_newcompmode.sh

```
size=$1
mode=$2
#echo " std :"
./a.out $size $mode
#echo " BF : "
MKL_BLAS_COMPUTE_MODE=FLOAT_TO_BF16 ./a.out $size $mode
#echo " BFX2 :"
MKL_BLAS_COMPUTE_MODE=FLOAT_TO_BF16X2 ./a.out $size $mode
#echo " BFX3 : "
MKL_BLAS_COMPUTE_MODE=FLOAT_TO_BF16X3 ./a.out $size $mode
```

Demo, BLAS, Compute mode, cont

gfedorov@sdp4451:~/5temp/ww22 2023/Compute mode\$./run newcompmode.sh 2000 1 size == 2000, GFlops == 26092.908 size == 2000, GFlops == 30878.479 size == 2000, GFlops == 29908.475 size == 2000, GFlops == 27725.575 gfedorov@sdp4451:~/5temp/ww22 2023/Compute mode\$./run newcompmode.sh 3000 1 size == 3000, GFlops == 14988.770 size == 3000, GFlops == 55078.302 size == 3000, GFlops == 28512.450 size == 3000, GFlops == 12226.104

Bfloat16 Arithmetic



Bfloat16 Arithmetic, cont.

	Bits (significand,	Unit	Min positive	Min positive	Max
	exponent)	roundoff	subnormal	normalized	finite
bfloat16	(8, 8)	3.91×10^{-3}	9.18×10^{-41}	$\begin{array}{c} 1.18 \times 10^{-38} \\ 6.10 \times 10^{-5} \\ 1.18 \times 10^{-38} \\ 2.22 \times 10^{-308} \end{array}$	3.39×10^{38}
fp16	(11, 5)	4.88×10^{-4}	5.96×10^{-8}		6.55×10^4
fp32	(24, 8)	5.96×10^{-8}	1.40×10^{-45}		3.40×10^{38}
fp64	(53, 11)	1.11×10^{-16}	4.94×10^{-324}		1.80×10^{308}

Bfloat16 Arithmetic, cont.

Dynamic range

- fp32
- fp16
- bf16