Intel[®] oneAPI Math Kernel Library (oneMKL) INTEL / LRZ oneAPI Workshop, June 5th-7th, 2023



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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



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oneMKL, 32 bit - Your Feedback Matters

| 1 | Are you currently using Intel® oneAPI Math Kernel Library (Intel® oneMKL) 32-bit library? | Yes / No | |
|---|---|---------------------------------------|--|
| 2 | If you answered yes, what are some of the applications you're using Intel® oneMKL 32-bit library for? | Please enter use cases / applications | |
| 3 | When do you plan to move to 64-bit library? | 0 - 6 months | |
| | | 6 months – 1 year | |
| | | 1–2 years | |
| | | No current plans to move | |

https://community.intel.com/t5/Intel-oneAPI-Math-Kernel-Library/Your-Feedback-Matters/m-

p/1484337/emcs_t/S2h8ZW1haWx8Ym9hcmRfc3Vic2NyaXB0aW9ufExIRko5M1U3QTAyTklLfDE0ODQzMzd8U1VCU0NSSVBUSU9O

U3xoSw#M34561

Intel® oneAPI Math Kernel Library (oneMKL)

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Intel® oneAPI Math Kernel Library (oneMKL)



Intel® oneAPI Math Kernel Library (oneMKL), cont.



Intel[®] oneAPI MKL, BLAS, update

- BLAS, Netlib interfaces
 - USM and Buffer API ALL
 - C/Fortran Offloading ALL
 - BLAS Extensions

BLAS Level 1 Routines and Functions

- cblas ?asum
- cblas_?axpy
- cblas ?copy
- cblas_?dot
- cblas_?sdot
- cblas_?dotc
- cblas_?dotu
- cblas_?nrm2
- cblas_?rot
- cblas ?rotg
- cblas_?rotm
- cblas_?rotmg
- cblas_?scal
- cblas_?swap
- i?amax
- i?amin
- cblas ?cabs1

BLAS Level 2 Routines

- cblas_?gemv
- cblas ?ger
- cblas_?gerc
- cblas_?geru
- cblas_?hbmv
- cblas ?hemv
- cblas_?her
- cblas_?her2
- cblas_?hpmv
- cblas_?hpr
- cblas_?hpr2
- cblas_?sbmv
- cblas_?spmv
- cblas_?spr
- cblas_?spr2
- cblas ?symv
- cblas_?syr
- cblas_?syr2
- cblas_?tbmv
- cblas_?tbsv
- cblas_?tpsv
- cblas_?trmv
- cblas ?trsv

- cblas_?tpmv

OpenMP offload to support the OpenMP* 5.1 specification

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cblas_?gbmv

BLAS Level 3 Routines

cblas_?gemm

cblas_?hemm

cblas_?herk

cblas ?her2k

cblas ?symm

cblas_?syrk

cblas_?syr2k

cblas_?trmm

cblas_?trsm

Intel[®] oneAPI MKL, BLAS, update, cont.

BLAS, Netlib interfaces

- USM and Buffer API ALL
- C/Fortran Offloading ALL
- BLAS Extensions

| CPU | OpenMP Offload Intel GPU |
|--|--|
| {AXPY,GEMM,TRSM}_BATCH (group and strided) | {AXPY,GEMM,TRSM}_BATCH (group and strided) |
| GEMMT, AXPBY, GEMM3M | GEMMT |
| Integer GEMM (s8u8) | N/A |
| Bfloat16 GEMM | N/A |
| JIT GEMM API | N/A |
| PACK GEMM API | N/A |
| COMPACT GEMM API | N/A |

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, lda, B, ldb, beta, C, ldc);
```

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

oneMKL, DGEMM, DPCPP API



What's New for Intel[®] oneAPI Math Kernel Library (oneMKL) 2023.0

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, Quick assist Technology, Intel® AVX-512, bfloat16, and more built-in accelerators

The Intel[®] oneAPI Math Kernel Library (oneMKL) leverages Intel[®] AMX-Advanced Matrix eXtensions to optimize matrix computations for the BF16 and INT8 data types.

oneMKL also leverages Intel [®] AVX-512 - Advanced Vector Extensions for the FP16 data type on 4th Gen Intel[®] Xeon[®] Scalable processors.

Most oneMKL memory- bound dense and sparse linear algebra (BLAS, LAPACK, sparse direct solvers), FFT, vector math, vector RNG, summary statistics, or spline computations, directly benefit from the onboard High Bandwidth Memory (HBM).



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

oneAPI Math Kernel Library (oneMKL) Interfaces

•oneAPI specification

https://spec.oneapi.io/versions/latest/introduction.html

- oneMKL specification
 <u>https://spec.oneapi.io/versions/latest/elements/oneMKL/source/ind</u>
 <u>ex.html</u>
- One MKL Open-Source interface

https://github.com/oneapi-src/oneMKL

oneAPI MKL Interfaces Project

| | | | Туре | Compiler |
|--------|--|--|-----------------|--------------------------|
| | x86 CPU | Intel(R) oneAPI Math | Dynamic, Static | DPC++, LLVM*, hipSYCL |
| | Intel GPU | Remer Library | Dynamic, Static | DPC++ |
| | NVIDIA GPU | NVIDIA cuBLAS | Dynamic, Static | LLVM*, hipSYCL |
| BLAS | 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* |
| | x86 CPU | Intel(R) oneAPI Math | Dynamic, Static | DPC++, LLVM* |
| LADACK | Intel GPU | Kernel Library | Dynamic, Static | DPC++ |
| LAPACK | NVIDIA GPU | NVIDIA cuSOLVER | Dynamic, Static | LLVM* |
| | AMD GPU | AMD rocSOLVER | Dynamic, Static | LLVM* |
| | x86 CPU | Intel(R) oneAPI Math | Dynamic, Static | DPC++, LLVM*, hipSYCL |
| RNG | Intel GPU | Remer Library | Dynamic, Static | DPC++ |
| | NVIDIA GPU | NVIDIA cuRAND | Dynamic, Static | LLVM*, hipSYCL |
| | AMD GPU | AMD rocRAND | Dynamic, Static | LLVM*, hipSYCL |
| | Intel GPU | Intel(R) oneAPI Math Kernel Library | Dynamic, Static | DPC++ |
| DFT | x86 CPU | | Dynamic, Static | DPC++ |
| | NVIDIA GPU | NVIDIA cuFFT | Dynamic, Static | DPC++ |

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(gueue, transa, transb, m, n, k, alpha, a, lda, b, ldb, beta, c, ldc, MKL BLAS COMPUTE MODE, dependencies); \

BLAS_64/Lapack_64 API Extensions

- Using BLAS and LAPACK with the 32-bit and 64-bit interface (lp64 / ilp64) at the same time
- BLAS_64 and LAPACK_64 NetLib interfaces
- Declaration: mkl_blas_64.h, mkl_lapack.h
- Limitations :
 - Intel64 only.
 - no Fortran API at this moment
 - no mkl_lapacke.h (LAPACKE_cgetrf(*....))
 - CPU only

BLAS_64/Lapack_64 API Extensions, cont.

BLAS:

- void Sgemm(const char *transa, const char *transb, const MKL_INT *m, const MKL_INT *n, const MKL_INT *k, const float *alpha, const float *a, const MKL_INT *lda, const float *b, const MKL_INT *ldb, const float *beta, float *c, const MKL_INT *ldc)
- void Sgemm_64(const char *trans, const MKL_INT64 *m, const MKL_INT64 *n, const float *alpha, const float *a, const MKL_INT64 *lda, const float *x, const MKL_INT64 *incx, const float *beta, float *y, const MKL_INT64 *incy)

LAPACK:

- void sgetrf(const MKL_INT* m, const MKL_INT* n, float* a, const MKL_INT* lda, MKL_INT* ipiv, MKL_INT* info)
- void sgetrf_64(const MKL_INT64* m, const MKL_INT64* n, float* a, const MKL_INT64* lda, MKL_INT64* ipiv, MKL_INT64* info)

Demo, MKL

Intel[®] oneMKL Resources

| Intel® oneMKL Product Page | https://www.intel.com/content/www/us/en/developer/tools/oneapi/onemkl.html |
|------------------------------------|--|
| Get Started with Intel® oneMKL | https://www.intel.com/content/www/us/en/develop/documentation/get-started-with-mkl-for-dpcpp/top.html |
| Intel® oneMKL Developer Reference | https://www.intel.com/content/www/us/en/develop/documentation/onemkl-developer-reference-c/top.html |
| 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 Interfac | 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 |

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