Leibniz-Rechenzentrum
der Bayerischen Akademie der Wissenschaften

Intel MIC Programming Workshop: MKL

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GEFÖRDERT VOM
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Agenda

- A quick overview of Intel MKL
- Usage of MKL in Accelerator mode (KNC)
  - Compiler Assisted Offload
  - Automatic Offload
  - Native Execution
- Usage of MKL on KNL
- Hands-on & Performance
- Useful links where do we find more information ?

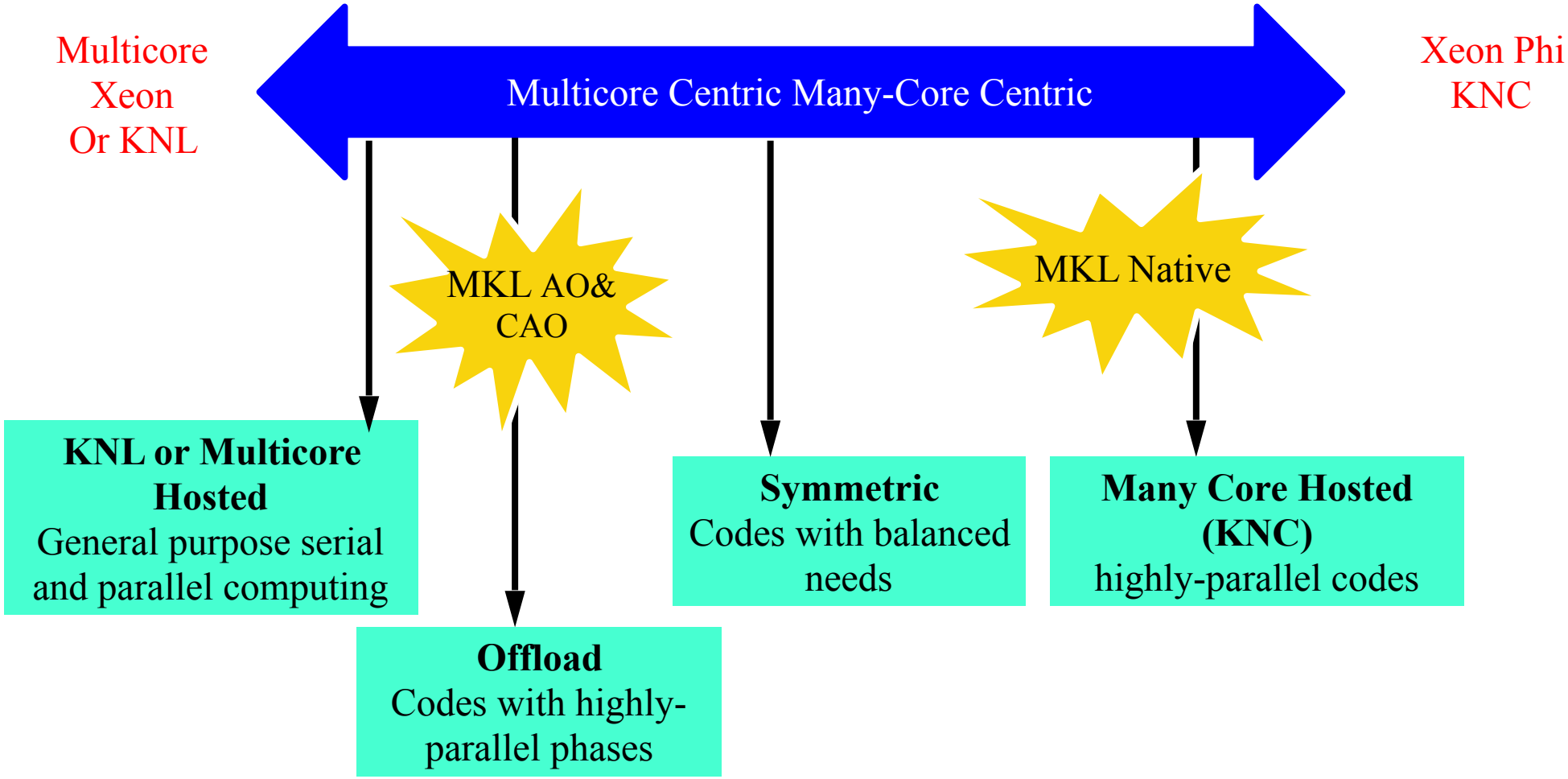
What is the Intel MKL ?

- Math library for C and Fortran, Includes:
  - BLAS, BLAS95 and Square BLAS
  - LAPACK
  - ScaLAPACK with BLACS
  - FFT and FFTW
  - Vector Math, Vector Statistics Functions
  - …

- Containing optimised routines
  - For Intel CPUs and MIC architecture
- All MKL functions are supported on Xeon Phi

  But optimised at different levels

Execution Models on Intel Xeon Phi Architectures



MKL Usage In Accelerator Mode (KNC)

- Compiler Assisted Offload
  - Offloading is explicitly controlled by compiler pragmas or directives.
  - All MKL functions can be inserted inside offload region to run on the Xeon Phi (In comparison, only a subset of MKL is subject to AO).
  - More flexibility in data transfer and remote execution management.
- Automatic Offload Mode
  - MKL functions are automatically offloaded to the accelerator.
  - MKL decides:
    - When to offload
    - Work division between host and targets
  - Data is managed automatically
- Native Execution

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How to use CAO

- The same way you would offload any function call to MIC
- An example in C:

```
#pragma offload target(mic) \
  in(transa, transb, N, alpha, beta) \
  in(A:length(matrix_elements)) \
  in(B:length(matrix_elements)) \
  in(C:length(matrix_elements)) \
  out(C:length(matrix_elements) alloc_if(0))
 {
     sgemm(&transa, &transb, &N, &N, &N, &alpha, A, &N, B, &N,&beta, C, &N);
 }
```

How to use CAO

- An example in Fortran:

```
!DEC$ ATTRIBUTES OFFLOAD : TARGET( MIC ) :: SGEMM
!DEC$ OMP OFFLOAD TARGET( MIC ) &
!DEC$ IN( TRANSA, TRANSB, M, N, K, ALPHA, BETA, LDA, LDB, LDC ), &
!DEC$ IN( A: LENGTH( NCOLA * LDA )), &
!DEC$ IN( B: LENGTH( NCOLB * LDB )), &
!DEC$ INOUT( C: LENGTH( N * LDC ))

!$OMP PARALLEL SECTIONS
!$OMP SECTION
   CALL SGEMM( TRANSA, TRANSB, M, N, K, ALPHA, &A, LDA, B, LDB BETA, C, LDC )
!$OMP END PARALLEL SECTIONS
```

Tips for Using Compiler Automatic Offload

- Use larger (>2MB) pages for data transferring;

e.g: ~$export MIC_USE_2MB_BUFFERS=50M

- This means that for any array allocation larger than 50MB, uses huge pages

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How to Use Automatic Offload

- User does not have to change the code at all
- Either by calling the function mkl_mic_enable() or by setting the following environment variable

```
~$export MKL_MIC_ENABLE=1
```

- In Intel MKL 11.0.2 the following functions are enabled for automatic offload:

Level-3 BLAS functions

*GEMM (for M,N > 2048, k > 256)
*TRSM (for M,N > 3072)
*TRMM (for M,N > 3072)
*SYMM (for M,N > 2048)

LAPACK functions

LU (M,N > 8192)
QR
Cholesky

How to Use Automatic Offload

- Blas only: work can be divided between host and device using

```
mkl_mic_set_workdivision(TARGET_TYPE, TARGET_NUMBER, WORK_RATIO)
```

- What if there doesn't exist a MIC card in the system ?
  - Runs on the host as usual **without any penalty** !!

- Users can use AO for some MKL calls and use CAO for others in the same program
  - Only supported by Intel compilers
  - Work division must be set explicitly for AO, otherwise, all MKL AO calls are executed on the host

Automatic Offload Mode Example

```
#include “mkl.h”
err = mkl_mic_enable();

//Offload all work on the Xeon Phi
err = mkl_mic_set_workdivsion (MKL_TARGET_HOST, MIC_HOST_DEVICE, 0, 0);

//Let MKL decide of the amount of work to offload on coprocessor 0
err = mkl_mic_set_workdivision(MKL_TARGET_MIC, 0, MIC_AUTO_WORKDIVISION);

//Offload 50% of work on coprocessor 0
err = mkl_mic_set_workdivision(MKL_TARGET_MIC, 0, 0.5);

//Get amount of work on coprocessor 0
err = mkl_mic_get_workdivision(MKL_TARGET_MIC, 0, &wd);
```

Tips for Using Automatic Offload

- AO works only when matrix sizes are right
  - SGEMM: Offloading only when M, N > 2048
  - Square matrices give much better performance
- These settings may produce better results for SGEMM calculation for 60-core coprocessor:

```
export MIC_USE_2MB_BUFFERS=16K
export MIC_OMP_NUM_THREADS=240
export MIC_ENV_PREFIX=MIC
export MIC_KMP_AFFINITY=compact,granularity=fine
export MIC_PLACE_THREADS=60C,4t
```

- Work division settings are just hints to MKL runtime

Threading control tips:

Prevent thread migration on the host using:

```
export KMP_AFFINITY=granularity=fine, compact, 1,0
```

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Native Execution

- In order to use Intel MKL in a native application, an additional argument -mkl is required with the compiler option -mmic.

- Native applications with Intel MKL functions operate just like native applications with user-defined functions.

```
$ icc -O3 -mmic -mkl sgemm.c -o sgemm.exe
```

Compile to use the Intel MKL

- Compile using –mkl flag
  - -mkl=parallel(default) for parallel execution
  - -mkl=sequential for sequential execution

- AO: The same way of building code on Xeon:
  - user@host $ icc -O3 -mkl sgemm.c -o sgemm.exe

- Native using -mmic
  - user@host $ ifort –mmic –mkl myProgram.c –o myExec.mic

- MKL can also be used in native mode if compiled with -mmic

Involving different MKL versions

MKL Version	Link flag
Single thread, sequential	-mkl=sequential
Single thread MPI, Sequential	-mkl=cluster
Multi thread	-mkl=parallel or -mkl

More code examples:

- module show mkl
- $MKLROOT/examples/examples_mic.tgz
  - sgemm SGEMM example
  - sgemm_f SGEMM example (Fortran 90)
  - fft complex-to-complex 1D FFT
  - solverc Pardiso examples
  - sgaussian single precision Gaussian RNG
  - dgaussian double precision Gaussian RNG
  - . ..

Which Model to Choose:

- native execution for
  - Highly parallel code
  - Using MIC as independency compute nodes
- AO if
  - Sufficient Byte/FLOP ratio makes offload beneficial
  - Using Level-3 BLAS functions: GEMM, TRMM, TRSM
- CAO if
  - There is enough computations to offset data transfer overhead
  - Transferred data can be reused by multiple operations

https://software.intel.com/en-us/articles/recommendations-to-choose-the-right-mkl-usage-model-for-xeon-phi

Usage of MKL on KNL

- up to version 2017 MKL automatically try to use MCDRAM
  - with unlimited access to MCDRAM

- In order to restrict how much MCDRAM MKL uses is possible
  - ✦ Environment variable (in MB)

    MKL_FAST_MEMORY_LIMIT=40

  - ✦ Function call (in MB):

mkl_set_memory_limit(MKL_MEM_MCDRAM, 40)

MKL 2018

- Use the “intel64” MKL version
- “mic” version is for KNC only
- Usage:
- $host: icpc -O3 **-xMIC-AVX512** -lmemkind -qopenmp **-mkl** -qopt-report=0 ...

MKL 2018

Intel® MKL 2018 Beta (18 April 2017)

DPD200576142	Improved the performance of functions DORCSD2BY1 routine
DPD200418144	Fixed the wrong result issue when calling zgetrf by MKL_DIRECT_CALL
DPD200592232	Fixed the scaling improvement of 3D r2c and c2r Cluster FFT, for some specific problems size
DPD200592231	Improved general performance on Intel® Xeon Phi™ product family x200
DPD200592229	MKL FFT : When 3D FFT scale is not 1, performance drops on KNL but not HSX for the c2r backward transform
DPD200591316	Fixed the problem with MKL Libraries mkl _ *. Dll have to load their dependence on the absolute path of the folder where the DLL itself is located
DPD200592227	Fixed the problem when MKL FFT selects 1 thread per core on KNL regardless how many threads are requested by environment

Lab: MKL

Memory Allocation: Data Alignment

- Compiler-assisted offload
  - Memory alignment is inherited from host!

- General memory alignment (SIMD vectorisation)
  - Align buffers (leading dimension) to a multiple of vector width (64 Byte)
  - `mkl_malloc`, `_mm_malloc` (`_aligned_malloc`), `tbb::scalable_aligned_malloc`, ...

Memory Allocation: Data Alignment

```
void * darray;
int    workspace;
int    alignment = 64;
...
darray = mkl_malloc(sizeof(double) * workspace,
                    alignment);
...
mkl_free(darray);
```

Memory Allocation: Page Size

Performance of many Intel MKL routines improves when input and output data reside in memory allocated with 2 MB pages

—>Address more memory with less pages,
reduce overhead of translating between host- and MIC address spaces

```
# Allocate all pointer-based variables with run-time
# length > 64 KB in 2 MB pages:
$ export MIC_USE_2MB_BUFFERS=64K
```

Memory Allocation: Page Size

Native:

KMP_AFFINITY=balanced
OMP_NUM_THREADS=244

Compiler-Assisted Offload:

MIC_ENV_PREFIX=MIC
MIC_KMP_AFFINITY=balanced
MIC_OMP_NUM_THREADS=240
MIC_USE_2MB_BUFFERS=64K

Automatic Offload:

MKL_MIC_ENABLE=1
OFFLOAD_DEVICES=<list>
MKL_MIC_MAX_MEMORY=2GB
MIC_ENV_PREFIX=MIC
MIC_OMP_NUM_THREADS=240
MIC_KMP_AFFINITY=balanced
+ Compiler-Assisted Offload:
OFFLOAD_ENABLE_ORSL=1

https://software.intel.com/en-us/articles/performance-tips-of-using-intel-mkl-on-intel-xeon-phi-coprocessor

Memory Allocation: Page Size

`KMP_AFFINITY=`

- Host: e.g., `compact,1`
- Coprocessor: `balanced`

`MIC_ENV_PREFIX=MIC; MIC_KMP_AFFINITY=`

- Coprocessor (CAO): `balanced`

`KMP_PLACE_THREADS`

- Note: does not replace `KMP_AFFINITY`
- Helps to set/achieve pinning on e.g., 60 cores with 3 threads each

`kmp_*` (or `mkl_*`) functions take precedence over corresponding env. variables

More MKL documentation

- Intel Many Integrated Core Community website:

  https://software.intel.com/en-us/mic-developer

- Performance charts online:

http://software.intel.com/en-us/intel-mkl#pid12768-1295

- Intel MKL forum

https://software.intel.com/en-us/forums/intel-math-kernel-library

- https://software.intel.com/en-us/node/528430
- https://www.nersc.gov/assets/MKL_for_MIC.pdf
- https://software.intel.com/en-us/articles/intel-mkl-on-the-intel-xeon-phi-coprocessors

Thank you.