Software

OPENMP® OFFLOAD CAPABILITIES IN ONEAPI HPC TOOLKIT

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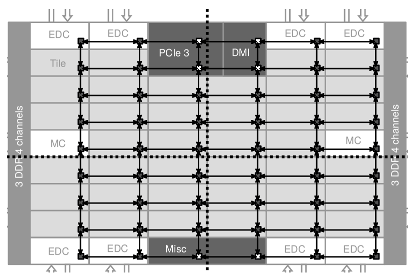
Agenda

- OpenMP® for accelators
- Managing data movement
- Expressing Parallelisms
  - Data parallelism
  - Hierarchical parallelism
  - CPU-GPU parallelism
- Coming-soon features
- Conclusions

OpenMP® for developing parallel applications
https://www.openmp.org/

a *portable*, *scalable* model that gives programmers a simple and *flexible* interface for developing *parallel* applications for a wide range of platforms – Wikipedia


SGI/Cray Origin 2000, NCSA, 1997

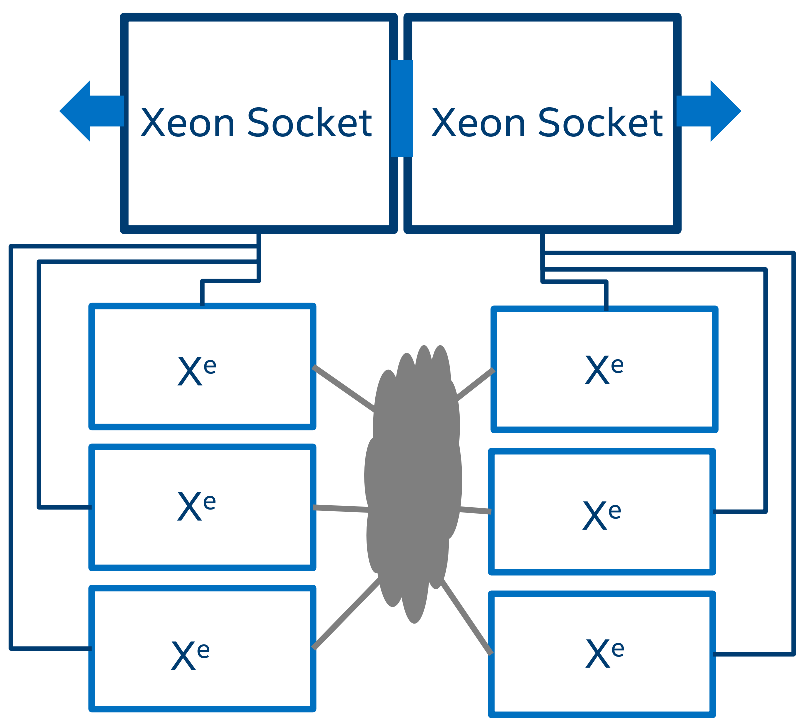


Intel KNL, Theta, ALCF

Intel® Xeon + Xe, 2021

Resources
- ALCF OpenMP training
- https://github.com/UoB-HPC/openmp-tutorial
- oneAPI webinar on OpenMP, Xinmin Tian, Intel

OpenMP® APIs for heterogeneous systems



Schematics of Aurora Supernode

Provide a set of directives to instruct the compiler and runtime to offload a block of code to the device.

Allow applications to exploit much increased compute density and BW of accelerators, such as X^e GPU.

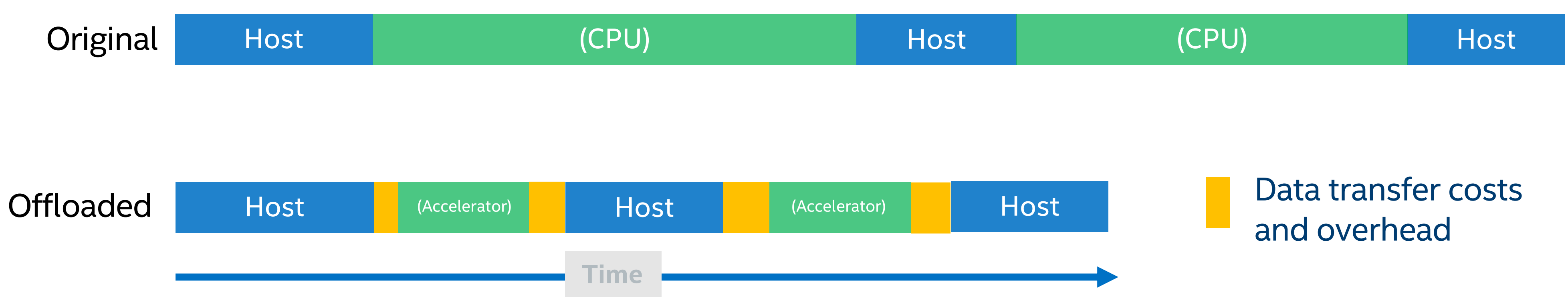
Reminders for the developers of parallel codes on heterogeneous platforms with discrete GPUs

- Massively parallel but simple compute engines
  - 72-EU Gen9: 72 EU *7 threads*32 SIMD= 16128
  - Expect big increases for future X^e
- Thread blocks, block of threads and SIMD (WARP, wavefront)
  - Memory model, forward progress guarantee, synchronization
- Distinct memory spaces of host and GPUs
  - Where the data are allocated and reside and how to move are critical
  - Unified Shared/Virtual Memory removes the need for the programmers to explicitly move data but does not remove data movement
- Heterogeneous and hierarchical memory
  - Memory BW: host-host, host-GPU, HBM/DDR on GPUs, Cache

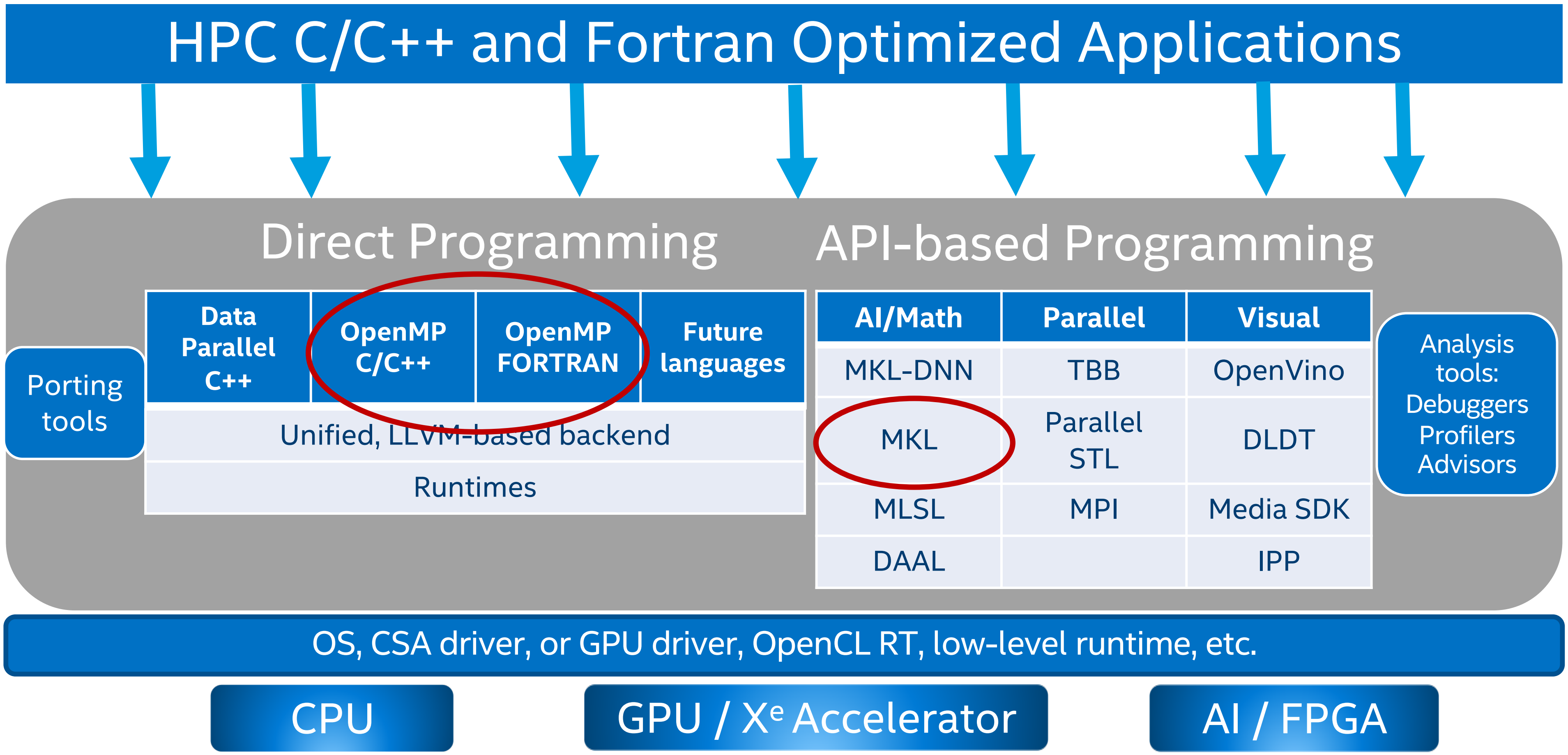
Offload Where it Pays Off the Most

Design your code to efficiently offload to accelerators

- Determine if your code would benefit from offload to accelerator – even before you have the hardware
- Identify the opportunities to offload
- Project performance on accelerators
- Estimate overhead from data transfers and kernel launch costs
- Pinpoint accelerator performance bottlenecks (memory, cache, compute and data transfer)
- Follow good SIMD guidelines (e.g. avoid branch divergence and gathers/scatters)



Intel® oneAPI HPC Toolkit (beta)



OpenMP® using oneAPI® compilers

Based on beta07 release http://www.oneapi.com

- Download and install oneAPI HPC Toolkit
- Setup oneAPI environment

```
$source /opt/intel/inteloneapi/setvars.sh
```

- Compile a C++ application OpenMP target (offload)

```
$icpx –fiopenmp –fopenmp-targets=spir64 test.cpp
```

```
$icpc –qnextgen –fiopenmp –fopenmp-targets=spir64 test.cpp
```

- Compile an application using oneMKL

```
$icx –I${MKLROOT}/include –DMKL_ILP64 –m64 –fiopenmp
–fopenmp-targets=spir64 –c <file>.c{pp} –o <file>.o
$icx <file>.o –fiopenmp –fopenmp-targets=spir64 –lOpenCL
-L${MKLROOT}/lib/intel64 -lmkl_intel_ilp64 -lmkl_intel_thread \
-lmkl_core -lpthread -ldl -lm -o <file>
```

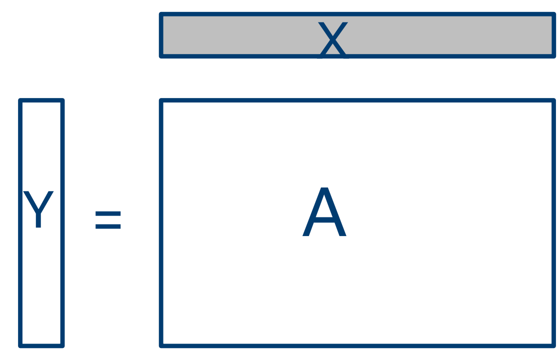
OpenMP® using oneAPI® compilers

- Useful environments for a run

```
LIBOMPTARGET_DEBUG=<int>
LIBOMPTARGET_PROFILE=T
OMP_TARGET_OFFLOAD=MANDATORY|DISABLED|DEFAULT
```

Matrix-vector multiplication (GEMV)

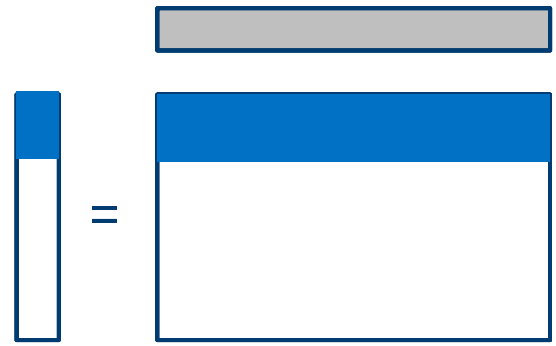
```
size_t N=1024;
size_t M=1048576;
Matrix<float> A(N,M);
Vector<float> X(M), Y(N);

// initialization

for(int i=0; i<N; ++i) {
  float sum{};
  for(int j=0; j<M; ++j) {
    sum += A[i][j]*X[j];
  }
  Y[i]=sum;
}
```

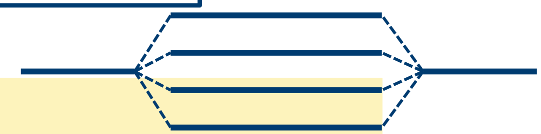


Using pseduo codes inspired and based on miniapps, Ye Luo (ANL), QMPCACK ECP
https://github.com/QMCPACK/miniqmc/

Parallel Matrix-vector multiplication

```
size_t N=1024;
size_t M=1048576;
Matrix<float> A(N,M);
Vector<float> X(M), Y(N);

// initialization

for(int i=0; i<N; ++i) {
  float sum{};
  for(int j=0; j<M; ++j) {
    sum += A[i][j]*X[j];
  }
  Y[i]=sum;
}
```



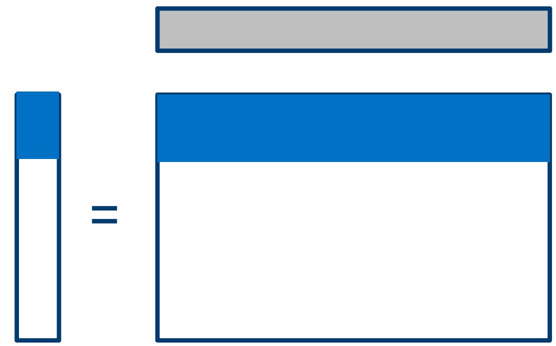


```
#pragma omp parallel for
  for(int i=0; i<N; ++i) {
    float sum{};

    for(int j=0; j<M; ++j) {
      sum += A[i][j]*X[j];
    }
    Y[i]=sum;
  }
```

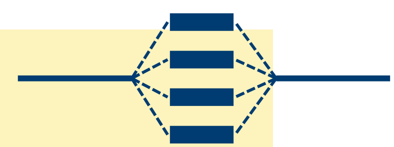
Parallel-SIMD Matrix-vector multiplication

```
size_t N=1024;
size_t M=1048576;
Matrix<float> A(N,M);
Vector<float> X(M), Y(N);

// initialization
```

```
for(int i=0; i<N; ++i) {
  float sum{};
  for(int j=0; j<M; ++j) {
    sum += A[i][j]*X[j];
  }
  Y[i]=sum;
}
```



```
#pragma omp parallel for
  for(int i=0; i<N; ++i) {
    float sum{};
#pragma omp simd reduction(+:sum)
    for(int j=0; j<M; ++j) {
      sum += A[i][j]*X[j];
    }
    Y[i]=sum;
  }
```

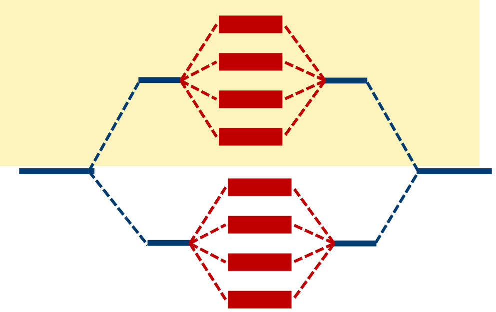


Compose your parallel problem

```
#pragma omp parallel
{
#pragma omp for nowait
  for(int i=0; i<N; ++i) {
    float sum{};
#pragma omp simd reduction(+:sum)
    for(int j=0; j<M; ++j) {
      sum += A[i][j]*X[j];
    }
    Y[i]=sum;
  }

  // do many more

}
```

OMP_NESTED=TRUE

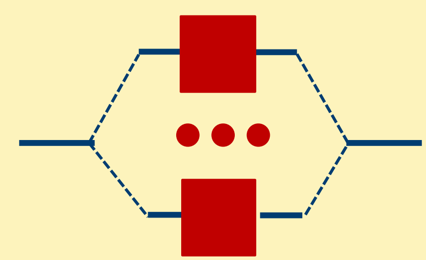
```
#pragma omp parallel
{
#pragma omp for nowait
  for(int i=0; i<N; ++i) {
    float sum{};
#pragma omp parallel for simd reduction(+:sum)
    for(int j=0; j<M; ++j) {
      sum += A[i][j]*X[j];
    }
    Y[i]=sum;
  }

  // do many more

}
```



GEMV with OpenMP® 4.5

```cpp
size_t N=1024;
size_t M=1048576;
Matrix<float> A(N,M);
Vector<float> X(M), Y(N);

// initialization

for(int i=0; i<N; ++i) {
  float sum{};
  for(int j=0; j<M; ++j) {
    sum += A[i][j]*X[j];
  }
  Y[i]=sum;
}
```

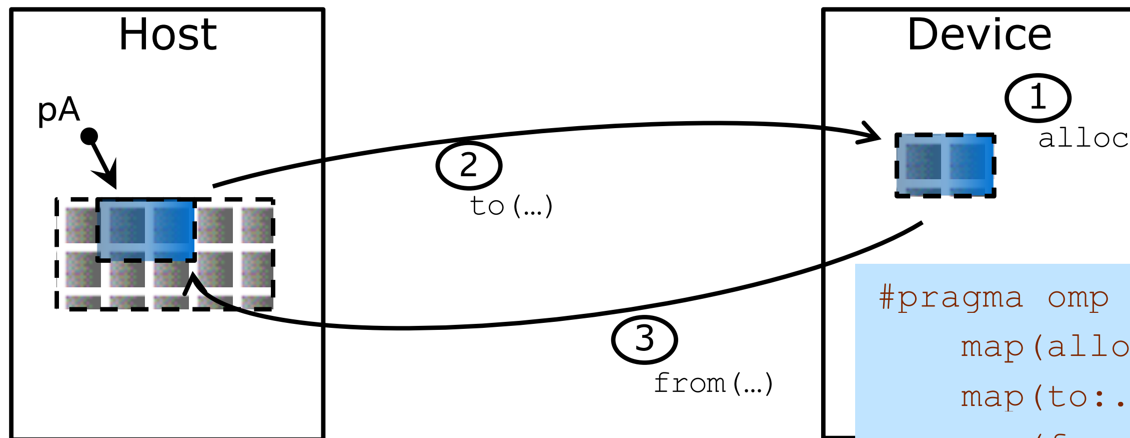
```cpp
Matrix<float> A(N,M);
Vector<float> X(M), Y(N);


float *pA=A.data(), *pX=X.data(), *pY=Y.data();
#pragma omp target map(to:pA[0:N*M],pX[0:M]) map(from:pY[0:N])
{
#pragma omp teams distribute
  for(int i=0; i<N; ++i) {
    float sum{};
#pragma omp parallel for simd reduction(+:sum)
    for(int j=0; j<M; ++j) {
      sum += pA[i*M+j]*pX[j];
    }
    pY[i]=sum;
  }
}
```



1. Transfer control of execution to a device
2. Map A and X **to** a device
3. Map Y **from** a device to host
4. Create teams of threads
5. Distribute the loop
6. Execution the loop in parallel
7. Reduce sum within a team
8. Assign the sum to Y

Offloading and Device Data Mapping

- Use *target* construct to
  - Transfer control from the host to the target device
  - Map variables between the host and target device data environments




```
#pragma omp target \
    map(alloc:...) \
    map(to:...) \
    map(from:...)
{ ... }
```

- Host thread waits until offloaded region is completed
  - Use other OpenMP tasks for asynchronous execution
- The **`map`** clauses determine how an *original variable* in a data environment is mapped to a *corresponding variable* in a device data environment

Data management

- Device allocator for the data exclusive accessed by a device

```
int deviceId= … ; // query device id
int *a = (int *)omp_target_alloc(1024, deviceId);
<use a>
omp_target_free(a, deviceId);
```

- Target data enter/exit and update

```
int A[N], B[N];
#pragma omp target enter data map(alloc:B)  map(to:A)
// do a lot of work with A & B
#pragma omp target update(A)
// do more on a device and host with new A
#pragma omp exit data map(from:A)
```

- Allocator specializations to reduce clutter and optimize data transfers

Maximizing data parallelism

- Same tasks/computations performed on subsets of the same data
- Synchronous computations with no or minimal branches
- Increasing gain with larger data sets

```
#pragma omp teams distribute
  for(int i=0; i<N; ++i) {
    float sum{};
#pragma omp parallel for simd reduction(+:sum)
    for(int j=0; j<M; ++j) {
      sum += pA[i*M+j]*pX[j];
    }
    pY[i]=sum;
  }
```

```
#pragma omp teams distribute parallel for simd collapse(2)
for(int i=0; i<N; ++i)
  for(int j=0; j<N; ++j)
    for(int k=0; k<N; ++k) {

       Body(i,j,k);

    }
```

Hierarchical parallelism on a GPU

```
#pragma omp target is_device_ptr(pA,pX,pZ) map(from:pY)
{
#pragma omp teams distribute
  for(int i=0; i<N; ++i) {
    float sum{};
#pragma omp parallel for simd reduction(+:sum)
    for(int j=0; j<M; ++j) {
      sum += pA[i*M+j]*pX[j];
    }
    pY[i]=sum;
#pragma omp parallel for simd
    for(int j=0; j<M; ++j) {
      pZ[j]+=sum*pX[j];
    }
  }
}
```

- Nested loops with shared variables
- Limited parallelism
- Data dependencies within a team
- Potential data reuse
- But, use with care!

Mixing host and GPU parallelism

```
#pragma omp parallel
{
  //per thread allocations

  #pragma omp target is_device_ptr(pA,pX,pZ) map(from:pY)
  {
  #pragma omp teams distribute
    for(int i=0; i<N; ++i) {
      float sum{};
  #pragma omp parallel for simd reduction(+:sum)
      for(int j=0; j<M; ++j) {
        sum += pA[i*M+j]*pX[j];
      }
      pY[i]=sum;
  #pragma omp parallel for simd
      for(int j=0; j<M; ++j) {
        pZ[j]+=sum*pX[j];
      }
    }
  }

}
```

```
#pragma omp target nowait
{


}

do_other_things();

#pragma omp taskwait
```

Unified Shared Memory Support

```
#include <stdio.h>
#include <stdlib.h>
#include <omp.h>
#define SIZE 1024
#pragma omp requires unified_shared_memory
int main() {
  int deviceId = (omp_get_num_devices() > 0) ? omp_get_default_device() : omp_get_initial_device();
  int *a = (int *)omp_target_alloc(SIZE, deviceId);
  int *b = (int *)omp_target_alloc(SIZE, deviceId);
  for (int i = 0; i < SIZE; i++) {
    a[i] = i;     b[i] = SIZE - i;
  }
#pragma omp target parallel for
  for (int i = 0; i < SIZE; i++) {
    a[i] += b[i];
  }

  for (int i = 0; i < SIZE; i++) {
    if (a[i] != SIZE) {
      printf("%s failed\n", __func__);  return EXIT_FAILURE;
    }
  }
  omp_target_free(a, deviceId);
  omp_target_free(b, deviceId);
  printf("%s passed\n", __func__);
  return EXIT_SUCCESS;
}
```

Adding USM support via managed memory allocator

OpenMP* and DPC++ Composability

```
#include <CL/sycl.hpp>
#include <array>
#include <iostream>
float computePi(unsigned N) {
float Pi;
#pragma omp target map(from : Pi)
#pragma omp parallel for reduction(+ : Pi)
  for (unsigned I = 0; I < N; ++I) {
    float T = (I + 0.5f) / N;
    Pi += 4.0f / (1.0 + T * T);
  }
  return Pi / N;
}
// DPC++ Code
void iota(float *A, unsigned N) {
  cl::sycl::range<1> R(N);
  cl::sycl::buffer<int,1> X(A, R);
  cl::sycl::queue().submit([&](cl::sycl::handler &cgh) {
    auto Y = X.template get_access<cl::sycl::access::mode::write>(cgh);
    cgh.parallel_for<class Iota>(R, [=](cl::sycl::id<1> idx) {
       Y[idx] = idx;
    });
  });
}
```

OpenMP offloading code

DPC++ code

```
int main() {
  std::array<int, 1024u> V;
  float Pi;
#pragma omp parallel sections
  {
#pragma omp section
    iota(V.data(), V.size());
#pragma omp section
    Pi = computePi(8192u);
  }

  std::cout << "V[512] = " << V[512] << std::endl;
  std::cout << "Pi = " << Pi << std::endl;
  return 0;
}
```

```
xtian@scsel-cfl-02:~/temp$ icpx -fiopenmp -fopenmp-targets=spir64 -fsycl  compos.cpp -o run.y
xtian@scsel-cfl-02:~/temp$ OMP_TARGET_OFFLOAD=mandatory ./run.y
V[512] = 512
Pi = 3.14159
```

oneMKL C OpenMP offload Example (GEMM)

```
#include "mkl.h"
#include "mkl_omp_offload.h"
int main() {
    MKL_INT m = 10, n = 6, k = 8, lda = 12, ldb = 8, ldc = 10;
    MKL_INT 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, 64);
    double *B = (double *)mkl_malloc(sizeof(double) * sizeb, 64);
    double *C = (double *)mkl_malloc(sizeof(double) * sizec, 64);
    // initialize matrices
    …
#pragma omp target data map(to:A[0:sizea],B[0:sizeb]) map(tofrom:C[0:siz
    {
#pragma omp target variant dispatch use_device_ptr(A, B, C) [nowait]
        {
            // Compute C = A * B on GPU
            cblas_dgemm(CblasColMajor, CblasNoTrans, CblasNoTrans, m, n
                        alpha, A, lda, B, ldb, beta, C, ldc);
        }
    }
    …
}
```

Specific header file for oneMKL OpenMP offload

Use target variant dispatch to notify GPU computation is requested

List all device memory pointer in the use_device_ptr clause

Optional nowait clause for asynchronous execution, use omp taskwait for synchronization

Get Started with oneAPI Today!

Resources

Intel® DevCloud	**Start in the Cloud** - No Download, No Installation, No Setup – Sign up here - software.intel.com/devcloud/oneAPI
oneAPI Toolkits	**Develop On-Prem –** Download & Develop - Get them here - software.intel.com/oneAPI
Industry Support	**Break Free Now –** CodePlay* Contributes Data Parallel C++ Support for NVIDIA* GPU github.com/intel/llvm
oneAPI Specification	**Join the Initiative** - Cross-industry, open, standards-based unified programming model across architectures – Learn more here - oneapi.com

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