OpenMP®

SC’20 Booth Talk Series

OpenMP offload optimization guide: beyond kernels - Lessons learned in QMCPACK

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EXASCALE COMPUTING PROJECT

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QMCPACK

A real-world production application

- QMCPACK, is a modern high-performance open-source Quantum Monte Carlo (QMC) simulation code. QMCPACK is written in C++ and designed with the modularity afforded by object-oriented programming. It makes extensive use of template metaprogramming to achieve high computational efficiency. https://qmcpack.org/
- It is a real-world production application. All the examples in this presentation reflects OpenMP use patterns in QMCPACK. https://github.com/QMCPACK/qmcpack
- Most OpenMP explorations are done via miniQMC, a miniapp. https://github.com/QMCPACK/miniqmc

ACCELERATOR PORTING MYTH

Why my code runs even slower?

- The repeated story very similar to other GPU porting stories not just OpenMP.
  - Profiler shows GPU activity is low.
  - Host time and overall wall clock time go up.
- OpenMP is limited by the characteristics of accelerator in use.
- The goal is to minimize OpenMP overhead on top of vendor native programing model.
  - Within a kernel. Ensure source code efficient transformation into kernels.
  - Beyond kernel. Ensure OpenMP abstraction with minimal overhead.
    - Adopt best practice in user code.
    - Good OpenMP compiler/runtime implementation.

PORTABILITY AT THE SOURCE CODE

Choosing OpenMP programing style carefully

OPENMP DIRECTIVE

#pragma omp target enter data map(alloc: a[:100])

- Prons:
  - No side effect when turned off
  - Fall back to host for debugging OMP_TARGET_OFFLOAD=disabled
- Cons:
  - Less verbose

OPENMP API

int * a_dev = omp_target_alloc(omp_get_default_device(), 100);

- Prons:
  - Explicit device control
- Cons:
  - Need #ifdef _OPENMP
  - Complicated fallback logic

PRE-ARRANGE MEMORY ALLOCATION

Move beyond textbook example

- Accelerator memory resource allocation/deallocation is orders of magnitude slower than that on the host.
- These operations may also block asynchronous execution.

```
// simple case
#pragma omp target map(array[:100])
for(int i ...) { // operations on array }

// optimized case
// pre-arrange allocation
#pragma omp target enter data \
  map(alloc: array[:100])
…
// use always to enforce transfer
#pragma omp target map(always, array[:100])
for(int i ...) { // operations on array }
```

HIDE MEMORY ALLOCATION IN C++

Create customized allocator

- Used in container classes like std::vector
- HostAllocator can be further customized to satisfy
  - Alignment
  - Registration in the accelerator memory space for maximal transfer performance, for example cudaHostRegister.

```
template<typename T, class HostAllocator =
std::allocator<T>>
struct OMPallocator : public HostAllocator
{
  value_type* allocate(std::size_t n)
  {
    value_type* pt = HostAllocator::allocate(n);
    #pragma omp target enter data map(alloc:pt[0:n])
    return pt;
  }
  void deallocate(value_type* pt, std::size_t n)
  {
    #pragma omp target exit data map(delete:pt[0:n])
    HostAllocator::deallocate(pt, n);
  }
}
```

AVOID UNNECESSARY MAP

firstprivate scalars don’t need mapping

- Compilers implement explicit mapping as allocating the memory for each scalar and transferring data.
- Since OpenMP 4.5, scalars are firstprivate by default. Compilers pack them as kernel arguments and no allocation and explicit transfers involved.

```
// simple case
int a, b, c;
#pragma omp target map(to: a, b, c)
{ // use a,b,c parameters }

// optimized case, no need of map
int a, b, c;
#pragma omp target
{ // use a,b,c parameters }
```

IMPLICIT ASYNCHRONOUS DISPATCH

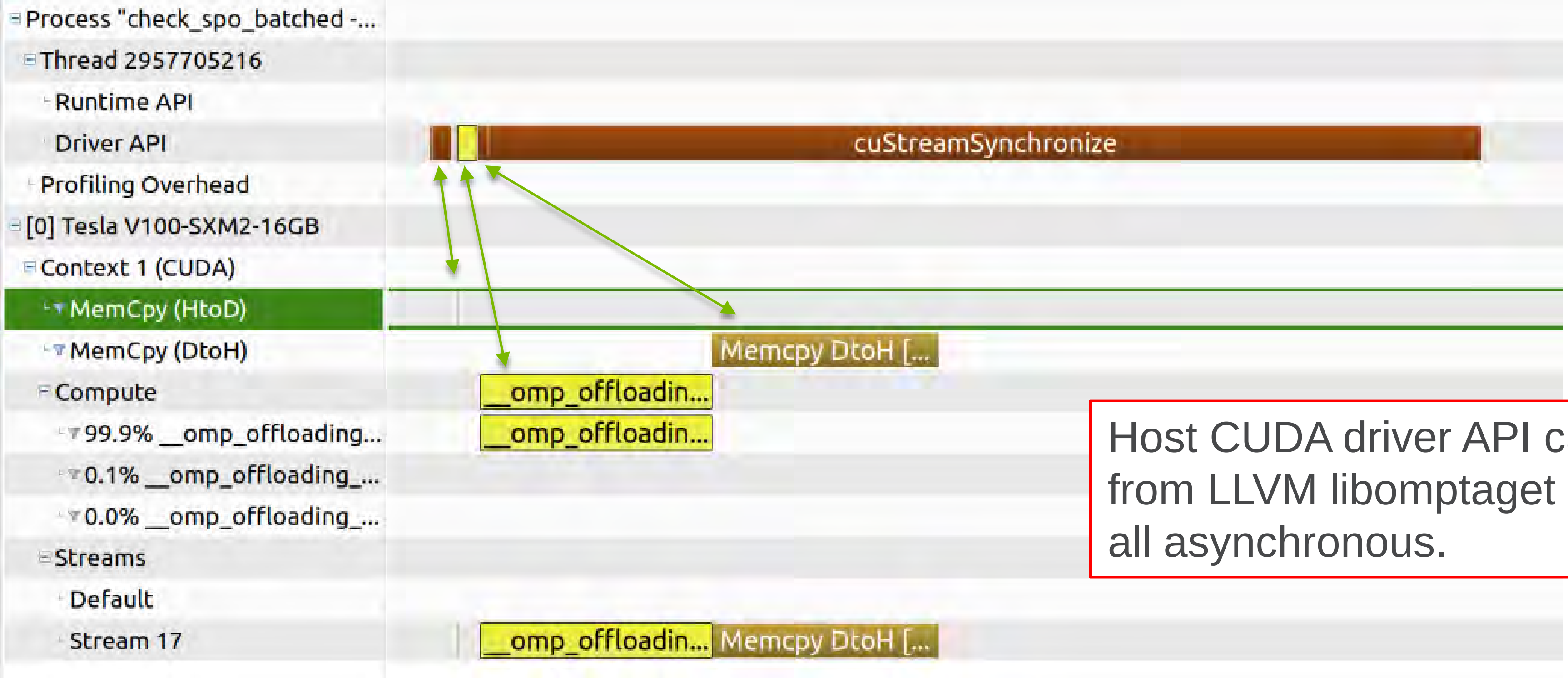
Using queues/streams

- NVIDIA CUDA supports streams for asynchronous computing
- IBM XL and LLVM Clang OpenMP runtime enqueue non-blocking H2D, kernel, D2H with only one synchronization in the end.
- Other vendors support similar features.

```
// simple case
#pragma omp target \
   map(always, tofrom: array[:100])
for(int i ...)
{ // operations on array }
```

IMPLICIT ASYNCHRONOUS DISPATCH (CONT)

Maximize asynchronous calls within one target region



Host CUDA driver API calls from LLVM libomptaget are all asynchronous.

CONCURRENT EXECUTION AND TRANSFER

Overlapping computation and data transfer

- IBM XL and LLVM Clang OpenMP runtime select independent CUDA streams for each offload region.
- Target region executed by different threads happens concurrently.
- Kernel execution from one target region may overlap with kernel execution or data transfer dispatched by another thread

```
#pragma omp parallel for
for (int iw …)
{
    int* array = all_arrays[iw].data();
    #pragma omp target \
      map(always, tofrom: array[:100])
    for(int i ...)
    { // operations on array }
}
```

CONCURRENT EXECUTION (CONT)

From multiple OpenMP threads, in miniQMC

Overlapping kernel and transfer

Concurrent kernel execution

ASYNCHRONOUS TASKING

Coordinating host and offload computation

- Providing a feature complete application enables smoothing user experience when gradually enabling acceleration.
- Not all the features are worth the effort porting to accelerators
- Using tasking to leverage idle host resource for non-blocking host computation
- * performance heavily depends on compiler runtime implementation.

```
#pragma omp parallel for
for (int iw …) {
    int* array = all_arrays[iw].data();
    // offload task
    #pragma omp target nowait depend(out:a) \
       map(always, tofrom: array[:100])
    for(int i ...) { // operations on array }
    // host task 1
    #pragma omp task
    { // operations on array }
    // host task 2 depend on the offload task
    #pragma omp task depend(in:a)
    { // operations on array }
    #pragma omp taskwait
}
```

OPENMP 5.0 AND BEYOND

Many promising features

- Meta directives and declare variant functions
  - Help better organized source code and less duplication
- Detached task
  - For composability with other asynchronous runtime.
- Interop object
  - For exposing vendor native queue/streams
- OMPT, OMPD support for profiling and debugging tools.

DETACHED TASK

For better composability

- Desired code example asynchronously calling cuBLAS without explicit waiting.
- Listed 5.0 feature.
- Waiting for actual compiler implementation.

```
#omp task detach(cuda_event1) depend(out:p)
{
  cublas::gemm // first call
  cudaStreamAddCallback(stream, callback,
cuda_event1, 0);
}
#omp target nowait depend(inout:p)
{
   // applyW_batched body
}
#omp task detach(cuda_event2) depend(in:p)
{
  cublas::gemm // second call
  cudaStreamAddCallback(stream, callback,
cuda_event2, 0);
}
#omp taskwait
```

ESSENTIAL FEATURES FOR APPLICATIONS

Struggled in 2019. A lot of exciting improvements in 2020

- 2020 Aug 30th. https://github.com/QMCPACK/miniqmc/wiki/OpenMP-offload

Compiler	Clang 11	AOMP 11.8-0	XL 16.1.1-5	OneAPI beta08	Cray 9.0
device	NVIDIA	AMD	NVIDIA	Intel	NVIDIA
math functions	Pass	Pass	Pass	Pass	Pass
complex arithmetics	Pass	Pass	Pass	Pass	Fail
declare target static data	Pass	Pass	Pass	Pass	Pass
static linking	Fail	Pass	Pass	Pass	Pass
multiple streams	Pass	Pass	Pass	Functioning	Functioning
check_spo	Pass	Pass	Pass	Pass	Pass
check_spo_batched	Pass	Pass	Pass	Pass	Pass
miniqmc_sync_move	Pass	Pass	Pass	Pass	Pass

Workaround in CMake

SUMMARY

- Application developers needs to pay attention to application performance beyond kernels.
- Many simple patterns may be adopted to have significant performance gain.
- OpenMP offload runtime overhead and be minimized to negligible.
- Task level parallelism becomes essential for accelerators.
- Improved compilers and OpenMP runtimes in 2020 enable production use of OpenMP .

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