Evaluation of OpenMP for Portable CPU and GPU Programming with GridMini

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Introduction

- Lattice QCD is a computational framework to simulate the strong interactions between quarks and gluons, and provides essential theoretical input to nuclear and high energy physics research.
- Computationally expensive. Need as many resources as we can get.
- Multi-prong approach to exascale performance portability
  - HIP, SyCL, Kokkos are all being investigated
- **OpenMP as another possible path to performance portability**

Grid and GridMini

- **Grid [1]** is a modern C++ library for lattice QCD
- Arranges the data layout as if the lattice is divided into virtual "sub-lattices", with one SIMD lane for each sublattice.
- Same data layout can be mapped to GPU architectures
- Extensive use of templates for high-level abstraction
- Custom expression template engine for performance
- **Header file with macros to encapsulate architecture-dependent implementations**

```
#ifdef GRID_NVCC
#define accelerator          __host__ __device__
#define accelerator_inline __host__ __device__ inline
#define accelerator_for (…) { //CUDA kernel}
#else
#define strong_inline      __attribute__((always_inline)) inline
#define accelerator
#define accelerator_inline strong_inline
#define accelerator_for(…)  thread_for(…) //for loop with
#pragma omp parallel for
```

- **Custom AlignedAlloctor for dynamic memory allocation on different architecture**

```
#ifdef GRID_NVCC
    if ( ptr == (_Tp *) NULL ) auto err =
cudaMallocManaged((void **)&ptr,bytes);
#else
  #ifdef HAVE_MM_MALLOC_H
    if ( ptr == (_Tp *) NULL ) ptr = (_Tp *)
_mm_malloc(bytes,GRID_ALLOC_ALIGN);
  #else
    …
```

- **GridMini [2]:** A substantially reduced version of Grid for experimentation with different programming models.
- Retains same Grid structure: data structures/types, data layout, aligned allocators, macros, …
- Only keeps the high-level components necessary for the benchmarks.

[1] https://github.com/paboyle/Grid
[2] https://github.com/meifeng/GridMini

OpenMP Offloading w/ UVM

- SU(3)×SU(3) benchmark: STREAM-like memory bandwidth test
- Important as LQCD is bandwidth bound.

```
double start=usecond();
for(int64_t i=0;i<Nloop;i++){
    z=x*y; //x,y,z are all arrays of 3x3 matrices
}
double stop=usecond();
double time=(stop-start)/Nloop*1000.0;

double bytes=3*vol*Nc*Nc*sizeof(Complex);
double flops=Nc*Nc*(6+8+8)*vol;
double bandwidth=bytes/time; //GB/s
double Gflops=flops/time;    //0.9 flops/byte SP
```

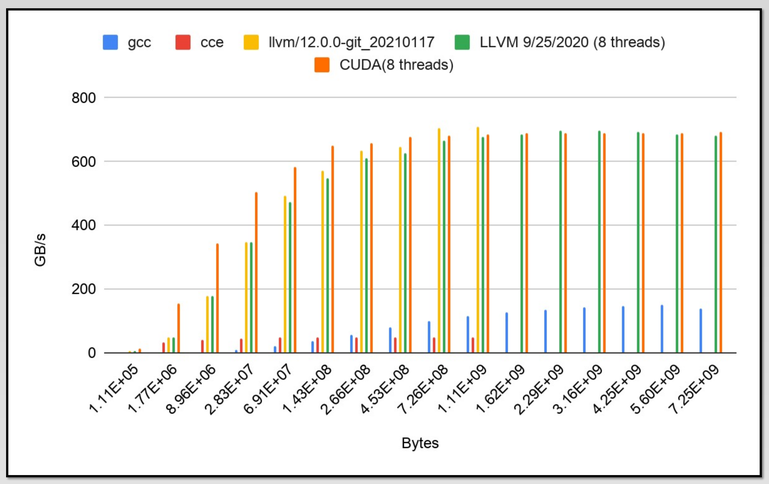
- To enable OpenMP offloading requires **two considerations**
  - **New macros** for OpenMP target offloading

```
#elif defined (OMPTARGET)
#define accelerator_inline strong_inline
#define accelerator_for(iterator,num,nsimd, ... )  \
{                                                  \
    _Pragma("omp target teams distribute parallel for") \
     naked_for(iterator, num, { __VA_ARGS__ }); \
}
```

  - Optionally can add `num_teams` and `thread_limit` to the omp target pragma.
  - **Memory management:** CUDA UVM for simplicity

```
#if defindded (GRID_NVCC) || defined (OMPTARGET_MANAGED)
    if ( ptr == (_Tp *) NULL ) auto err =
cudaMallocManaged((void **)&ptr,bytes);
```

- **Results on Cori-GPU with NVIDIA V100**
  - CUDA implementation as comparison (compiled with nvcc, cuda 11)
  - LLVM/Clang compiler two versions tested (mainline 9/25/2020 and 01/17/2021)
  - **gcc:** gcc/10-devel-omp_20201218
  - **cce:** Cray cce/11.0.1



OpenMP Offloading w/ Map

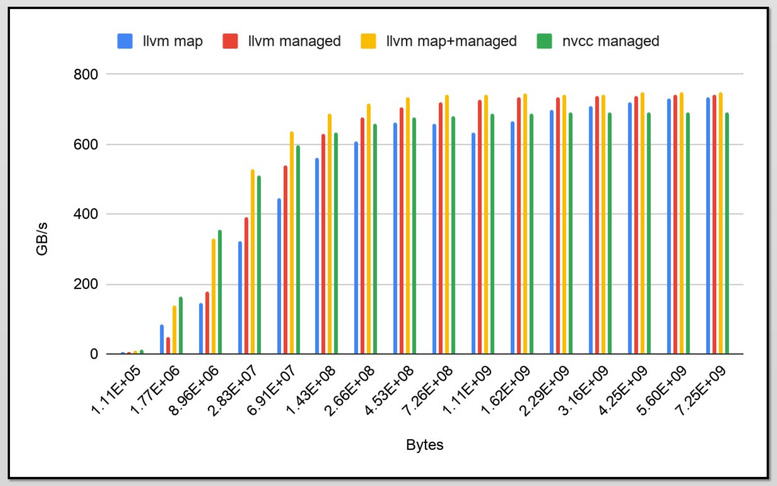
- Using `cudaMallocManaged` is not portable to other GPUs.
- Best to replace it with OpenMP pragmas or APIs for portability.
- Use **`declare mapper`** to simplify data mapping of complex objects

```
#pragma omp declare mapper(decltype(xv) x)
map(x._odata[0:x.size()]) map(x)
```

- Use **`omp target enter/exit data`** for data movement

```
#pragma omp target enter data map(alloc:zv) map(to:xv)
map(to:yv)
```

- So far only works with mainline LLVM (last tested with llvm/12.0.0-git_20210117): `_odata` is still a composite object.
- **Results on Cori-GPU with NVIDIA V100**
  - **llvm map**: compiled with LLVM with the above data mapping
  - **llvm managed**: use cudaMallocManaged without explicit data mapping
  - **llvm map+managed**: use cudaMallocManaged with data mapping
  - **nvcc managed:** CUDA version with cudaMallocManaged compiled with nvcc



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