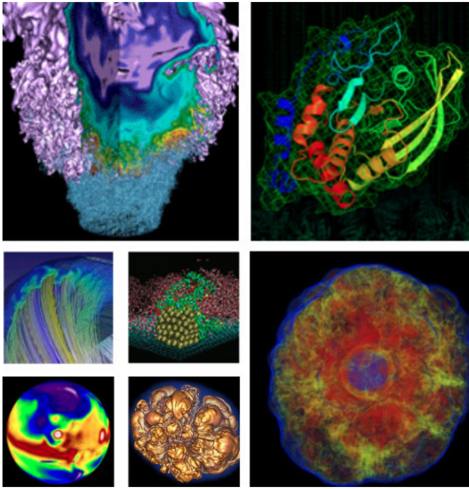
Optimizing Large Reductions in BerkeleyGW on GPUs

Using OpenMP and OpenACC



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March 8, 2019

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Why Attend this Talk

- 5 of the top 10 supercomputers are using NVIDIA GPUs
- Most of the codes optimized for CPUs have to now be rewritten for GPUs
- Compiler directive based approaches are attractive due to their ease of use
    - Port incrementally for big codes
- This talk would provide a detailed analysis of the current state of the directive based programming models
    - Their performance compared to optimized CUDA code
    - Supported compilers
    - Differences in compiler implementations

Outline of the Presentation

- BerkeleyGW, a material science code
    - General Plasmon Pole (GPP), a mini-app
- Baseline CPU implementation
- GPU programming models (OpenMP, OpenACC, CUDA)
- GPP on GPU
    - Naive implementation
    - Optimized implementation
    - Compare approaches and performance of each implementation
- Backport GPU implementation on CPU for performance portability

BerkeleyGW

- The GW method is an accurate approach to simulate the excited state properties of materials
  - What happens when you add or remove an electron from a system
  - How do electrons behave when you apply a voltage
  - How does the system respond to light or x-rays
- Extract stand alone kernels that could be run as mini-apps

General Plasmon Pole (GPP)

- Mini-app from BerkeleyGW
  - Computes the electron self-energy using the General Plasmon Pole approximation
- Characteristics of GPP
  - Reduction over a series of double complex arrays involving multiply, divide and add instructions (partial FMA)
  - For typical calculations, it evaluates to an arithmetic intensity (Flops/Byte) between 1-10, i.e., the kernel has to be optimized for memory locality and vectorization/SIMT efficiency

Complex Number Class

- BerkeleyGW consist of double-complex number calculation
- std::complex difficulties
  - Performance issues
  - Difficult to vectorize
  - Cannot offload operations onto the device using OpenMP 4.5
- Thrust::complex
  - Challenges in offloading complex operator routines on device
- Built an in-house complex class
  - 2-doubles on CPU
  - double2 vector type on GPU

GPP pseudo code - reduction in the innermost loop

Code

```
for(X){     // X = 512
  for(N){   // N = 1638
    for(M){ // M = 32768
      for(int iw = 0; iw < 3; ++iw){
        //Some computation
        output[iw] += ...
      }
    }
  }
}
```

- Memory O(2GBs)
- Typical single node problem size
- output - double complex

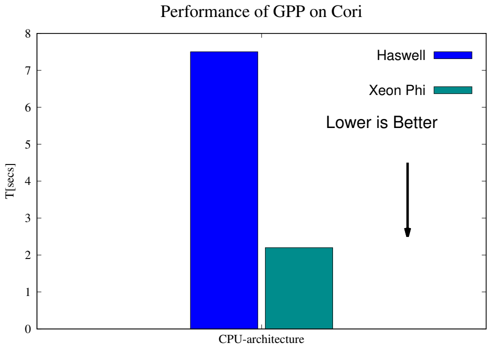
GPP On CPU

OpenMP 3.0 parallelization of GPP

```
#pragma omp parallel for
   reduction(output_re[0-2], output_im[0-2]
for(X){
  for(N){
    for(M){ //Vectorize
      for(int iw = 0; iw < 3; ++iw){ //Unroll
        //Store local
      }
    }
    for(int iw = 0; iw < 3; ++iw){
      output_re[iw] += ...
      output_im[iw] += ...
    }
  }
}
```

- Unroll innermost iw-loop
- Vectorize M-loop
- Collapse increased the runtime by 10%
- Check compiler reports (intel/2018) to guarantee vectorization and unrolling
- Flatten arrays into scalars with compilers that do not support array reduction

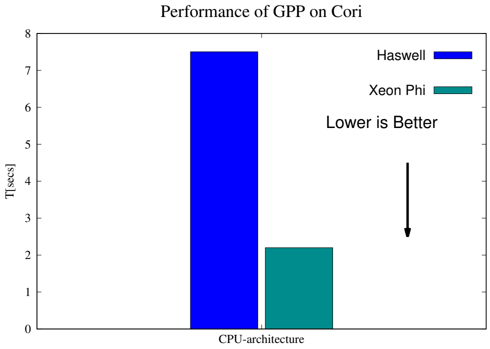
Runtime of GPP on Cori



- Performance numbers from Cori at NERSC,LBL
  - Haswell
  - Xeon Phi
- intel/2018 compilers
- A perfect scaling would allow a KNL execution to be 4$\times$ faster than Haswell
  - KNL implementation of GPP is approximately 3.5$\times$ faster than Haswell

Runtime of GPP on Cori

Xeon Phi - 2.2 seconds

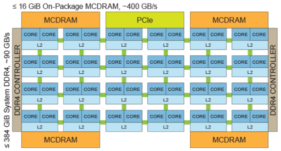


- Performance numbers from Cori at LBNL
  - Haswell
  - Xeon Phi
- intel/2018 compilers
- A perfect scaling would allow a KNL execution to be 4× faster than Haswell
  - KNL implementation of GPP is 3× faster than Haswell

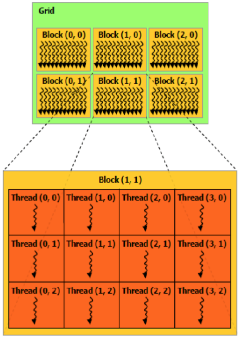
GPP On GPU

GPU Hardware

KNL


≤ 16 GiB On-Package MCDRAM, ~400 GB/s
MCDRAM
PCIe
CORE
L2
DDR4 CONTROLLER
≤ 384 GiB System DDR4, ~90 GB/s

GPU



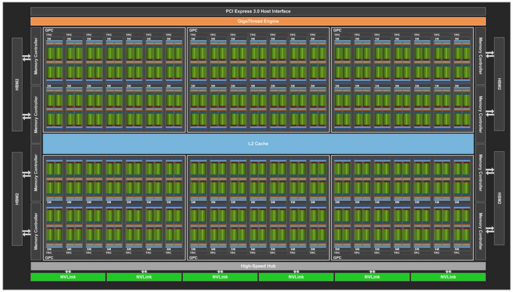
- Going from 272 to 164K threads
- 164k threads
  - 80 SMs
  - 2048 threads within a SM

Programming Models used to port GPP on GPU

- OpenMP 4.5
  - Cray
  - XL(IBM)
  - Clang
  - GCC
- OpenACC
  - PGI
  - Cray
- CUDA

Volta GPU available on Cori and Summit

Target architecture - Volta



OpenMP offloading to GPU

- **OpenMP 4.5**
  - **Cray**
  - **XL(IBM)**
  - **Clang**
  - **GCC**
- OpenACC
  - PGI
  - Cray
- CUDA

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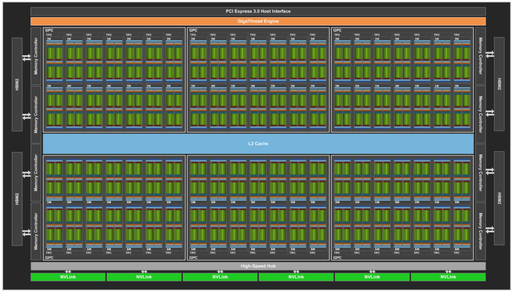


OpenMP directives to offload code-blocks onto GPUs

Directives to distribute work across GPU threads

target – offload the code–block on to the device

teams – spawn one or more thread team

distribute – distribute iterations of the loops onto master threads of the team

parallel for – distribute loop iterations among threads in a threadblock

simd – implementation dependent on compilers

```
#pragma omp target teams distribute
for() //Distribute the loop across threadblocks
#pragma omp parallel for
for() //Distribute the loop across threads within a threadblock
```

OpenMP 4.5 directives to move data from device to host

Allocate and delete data on the device

```
#pragma omp target enter data map(alloc: list−of−data−structures[:])
#pragma omp target exit data map(delete: list−of−data−structures[:])
```

Update data on device and host

```
#pragma omp target update to/from (list−of−data−structures[:])
to − HostToDevice
from − DeviceToHost
```

Clauses to use with **target** directives

```
map(to:...)     map(from:...)     map(tofrom:...)
```

OpenMP 4.5 directives to offload routines on the device

Routines

```
#pragma omp declare target
void foo();
#pragma omp end declare target
```

Not necessary if routines are inlined

Naive OpenMP 4.5 implementation of GPP

```
#pragma omp target teams distribute
    map(to:...)
    map(tofrom:output_re[0-2], output_im[0-2])
for(X){
#pragma omp parallel for
  for(N){
    for(M){
      for(int iw = 0; iw < 3; ++iw){
        //Store local
      }
    }
  for(int iw = 0; iw < 3; ++iw){
#pragma omp atomic
    output_re[iw] += ...
#pragma omp atomic
    output_im[iw] += ...
  }
}
```

- Distribute **M-loop** across threadblocks
- Distribute **N-loop** among threads in a threadblocks
- No array reduction with OpenMP 4.5 directives. Hence use atomic to maintain correctness
- Parallelizing **M-loop** increases overhead of synchronization

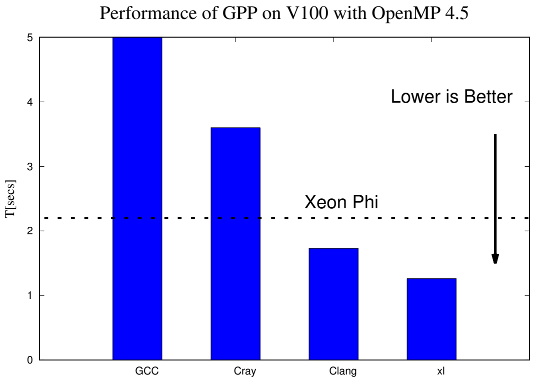
Optimized implementation with OpenMP 4.5

```
#pragma omp target enter data
map(alloc:input[0:X])
#pragma omp target update input[0:X])

#pragma omp target teams distribute  \
parallel for collapse(2) \
reduction(+:output_re(0,1,2), output_im(0,1,2))
for(X){
  for(N){
    for(M){
      for(int iw = 0; iw < 3; ++iw){
        //Store local
      }
    }
    output_re(0,1,2) += ...
    output_im(0,1,2) += ...
  }
}
#pragma omp target exit data map(delete:input)
```

- XL, Clang, Cray and GCC gave the best performance with the same parallelization technique
  - Collapse N and M loops and distribute them across threadblocks and threads within a block
- Memory allocation improved the performance of the kernel by 10%
  - **#pragma omp target enter/exit data**
- Reduction gave a 3× boost in the performance
  - Flatten arrays to scalars

Performance of GPP on V100 with OpenMP 4.5



- Cray is 3× slower than XL
- Clang is 30% slower than XL
- GCC implementation takes 26 seconds

OpenMP 4.5 directives map onto hardware

	Grid	**Thread**
GCC	teams distribute	parallel for
XL	teams distribute	parallel for
Clang	teams distribute	parallel for
Cray	teams distribute	simd

Table 1: **OpenMP 4.5 mapping onto GPU hardware**

Optimized implementation with XL

```
#pragma omp target enter data
    map(alloc:input[0:X])

#pragma omp target teams distribute  \
  parallel for collapse(2) \
  map(to:input[0:X]) \
  reduction(+:output_re(0,1,2), output_im(0,1,2))
for(X){
  for(N){
    for(M){
      for(int iw = 0; iw < 3; ++iw){
        //Store local
      }
    }
    output_re(0,1,2) += ...
    output_im(0,1,2) += ...
  }
}
#pragma omp target exit data map(delete:input)
```

- Did not support class operators in older versions.
- Variables passed to the **reduction** clause should not be passed to any other clause in the same directive
- All data accessed inside the **target** region has to be passed via a **map** clause
- **simd** has no effect

Optimized implementation with Clang

```
#pragma omp target enter data
    map(alloc:input[0:X])
#pragma omp target update input[0:X])

#pragma omp target teams distribute  \
  parallel for collapse(2) \
map(tofrom:output_re(0,1,2), output_im(0,1,2)) \
  reduction(+:output_re(0,1,2), output_im(0,1,2))
for(X){
  for(N){
    for(M){
      for(int iw = 0; iw < 3; ++iw){
        //Store local
      }
    }
    output_re(0,1,2) += ...
    output_im(0,1,2) += ...
  }
}
#pragma omp target exit data map(delete:input)
```

- Data allocated on the device using OpenMP 4.5 directives need not be passed via **map** clauses
- Variables passed to the **reduction** clause have to also be passed to **map** clauses

Optimized Cray implementation

```
#pragma omp target enter data
map(alloc:input[0:X])
#pragma omp target update input[0:X])

#pragma omp target teams distribute  \
    simd collapse(2) \
map(tofrom:output_re(0,1,2), output_im(0,1,2))
reduction(+:output_re(0,1,2), output_im(0,1,2))
for(X){
  for(N){
    for(M){
      for(int iw = 0; iw < 3; ++iw){
        //Store local
      }
    }
    output_re(0,1,2) += ...
    output_im(0,1,2) += ...
  }
}
#pragma omp target exit data map(delete:input)
```

- **parallel for** is executed sequentially inside the **target** region
- **simd** distributes loop across threads of a threadblock
- **reduction** variables have to be passed to the **map** clauses
- Previously allocated data allocated need not be passed via the **map** clauses
- **printf** is not supported inside routines annotated with **declare target**

Optimized GCC implementation

```
#pragma omp target enter data
map(alloc:input[0:X])

#pragma omp target teams distribute  \
    parallel for collapse(2) \
map(tofrom:output_re(0,1,2), output_im(0,1,2)) \
reduction(+:output_re(0,1,2), output_im(0,1,2))
for(X){
  for(N){
    for(M){
      for(int iw = 0; iw < 3; ++iw){
        //Store local
      }
    }
    output_re(0,1,2) += ...
    output_im(0,1,2) += ...
  }
}
#pragma omp target exit data map(delete:input)
```

- **simd** gives compiler error
- If data is allocated beforehand using **data map (alloc:...)** clauses, they need not be passed to **map** clauses again
- Variables passed to the **reduction** clause have to also be passed to **map** clauses

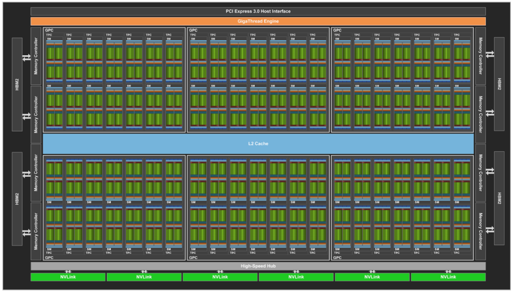
Cheat Sheet of Do's and Dont's

- **XL**
  - Everything accessed inside the **target** region has to be mapped explicitly via **map** clauses
    - Even if they are allocated on the device beforehand
  - Do not pass the same data to two different clauses in the same directive
    - Even if one of them is a **reduction** clause
- **Clang, GCC, Cray**
  - Always pass the directionality information to the **reduction** variables via **map** clauses
- **GCC** - Do not use **simd**

OpenACC offloading to GPU

- OpenMP
  - Cray
  - XL(IBM)
  - Clang
  - GCC
- **OpenACC**
  - **PGI**
  - **Cray**
- CUDA

Target architecture - Volta



OpenACC directive map on GPU

OpenACC

gang – threadblock

vector – Threads in a threadblock

worker – y dimension inside a threadblock (PGI compiler)

OpenMP

teams distribute

parallel for

simd

```
#pragma acc parallel loop gang

#pragma acc loop vector

#pragma acc loop worker
```

OpenACC directives for memory movement

```
#pragma acc enter data copyin

#pragma acc enter data copyout

#pragma acc enter data copy
```

```
#pragma acc enter data create(...)

#pragma acc exit data delete(...)
```

Optimized GPP implementation with PGI OpenACC

```
#pragma acc enter data create
  copyin(input[0:X])
#pragma acc enter data update
  device(input[0:X]

#pragma acc parallel loop gang collapse(2)
  present(input) \
  reduction(+:output_re(0,1,2), output_im(0,1,2))
for(X){
  for(N){
#pragma acc loop vector\
  reduction(+:output_re(0,1,2), output_im(0,1,2))
    for(M){
      for(int iw = 0; iw < 3; ++iw){
        //Store local
      }
    }
    output_re{0,1,2} += ...
    output_im{0,1,2} += ...
  }
}
```

- Collapse X and N loops to distribute across threadblocks
- Distribute M loops across threads of a threadblock
- **reduction** required at **gang** and **vector** level since the output variables are updated by every thread.

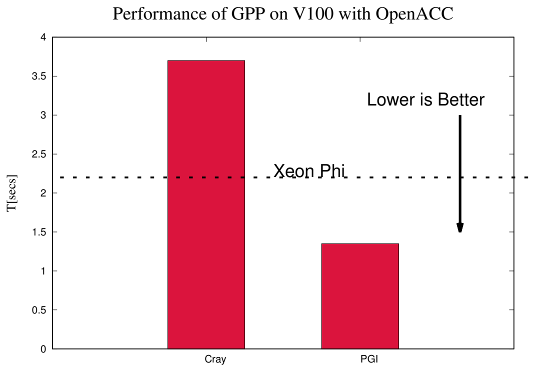
Optimized GPP implementation with Cray OpenACC

```
#pragma acc enter data create copyin(input[0:X])
#pragma acc enter data update device(input[0:X]

#pragma acc parallel loop gang vector collapse(2)
  present(input[0:X]) \
  reduction(+:output_re(0,1,2), output_im(0,1,2))
for(X){
  for(N){
    for(M){
      for(int iw = 0; iw < 3; ++iw){
        //Store local
      }
    }
    output_re{0,1,2} += ...
    output_im{0,1,2} += ...
  }
}
```

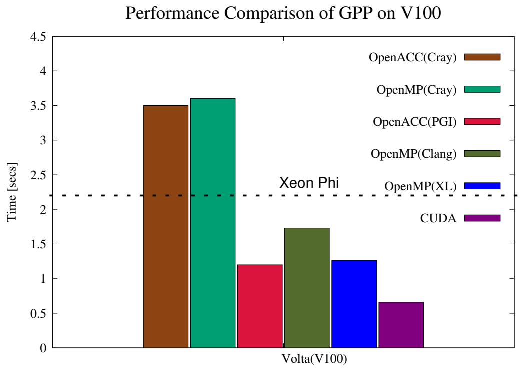
- Collapse Distribute X and N loops to distribute across threadblocks and threads within a block
- Dimensions of the data structures have to be passed to the **present** clause

Cray and PGI implementations of GPP using OpenACC



- Cray is 3× slower than PGI
- Cray is 50% slower than optimized Xeon Phi runtime

Performance comparison of all GPU implementations



- Dashed line is Xeon Phi reference time
- Cray OpenMP and OpenACC give similar performance and is slower than Xeon Phi
- CUDA is 2$\times$ faster than the 2nd best implementation

CUDA Implementation of GPP

CUDA

```
for(X){     // blockIdx.x
  for(N){   // blockIdx.y
    for(M){ // threadIdx.x
      for(int iw = 0; iw < 3; ++iw){
        //Store local
      }
    }
    output_re{0,1,2} += ... //Atomic
     Add
    output_im{0,1,2} += ... //Atomic
     Add
  }
}
```

- 2-dimensional grid for X and N loops
- Distribute M-loop across threads in a threadblock
- CUDA atomics to maintain correctness

```
dim3 numBlocks(X,N,1);
dim3 numThreads(64,1,1);
gpp_kernel<<<numBlocks, nunThreads>>>;
```

OpenMP loop re-reordering to match CUDA implementation

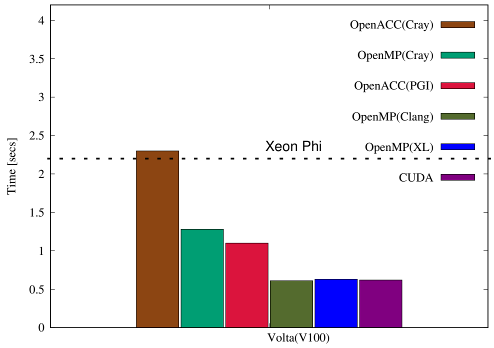
CUDA

```
for(X){     // blockIdx.x
  for(N){   // blockIdx.y
    for(M){ // threadIdx.x
      for(int iw = 0; iw < 3; ++iw){
        //Store local
      }
    }
    output_re{0,1,2} += ... //Atomic
    output_im{0,1,2} += ... //Atomic
  }
}
```

OpenMP

```
#pragma omp target teams distribute  \
parallel for collapse(2) \
map(to:...) \
reduction(+:output_re0,1,2, output_im0,1,2)
for(N){
  for(X){
    for(M){
      for(int iw = 0; iw < 3; ++iw){
        //Store local
      }
    }
    output_re{0,1,2} += ...
    output_im{0,1,2} += ...
  }
}
```

Performance of GPP implementations after loop reordering



- OpenMP(XL and Clang) are 2× faster after loop re-ordering
- OpenACC(PGI) is 30% faster
- OpenACC(Cray) is 3× faster
- XL and Clang OpenMP similar to optimized CUDA

Performance Portability

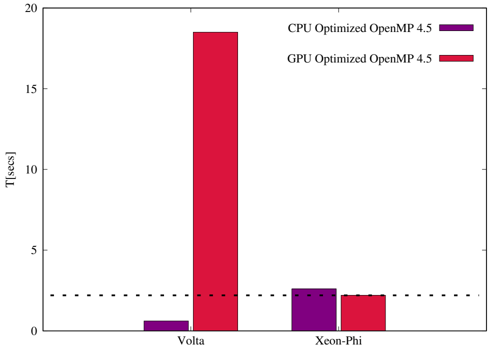
Interpretation of OpenMP 4.5 dierctives on CPU

```
#pragma omp target enter data
    map(alloc:input[0:X])
#pragma omp target update input[0:X])

#pragma omp target teams distribute  \
  parallel for collapse(2) \
map(tofrom:output_re(0,1,2), output_im(0,1,2)) \
  reduction(+:output_re(0,1,2), output_im(0,1,2))
for(N){
  for(X){
    for(M){
      for(int iw = 0; iw < 3; ++iw){
        //Store local
      }
    }
    output_re(0,1,2) += ...
    output_im(0,1,2) += ...
  }
}
#pragma omp target exit data map(delete:input)
```

- intel/2018 compilers
- **teams** - creates a single team and associates all threads to that team
  - Reverse the order of X and N loops and distribute them across threads
- Ignores other OpenMP 4.5 related directives, for example device memory allocation directives

Performance of GPU implementations on CPU



GPU - clang compiler

CPU - intel/2018 compilers

- GPU optimized OpenMP is 10% slower than optimized Xeon Phi
- CPU optimized OpenMP is 30× slower on Volta

Summary of the Presentation

- Multiple implementations of OpenMP offloading gave us close to optimized CUDA performance
  - Differences in Compiler interpretations of OpenMP 4.5 offload directives
- Loop reordering might provide benefits due to change in data access patterns
- OpenACC had difficulty in CPU-vectorization
- Portable code but not performance portable