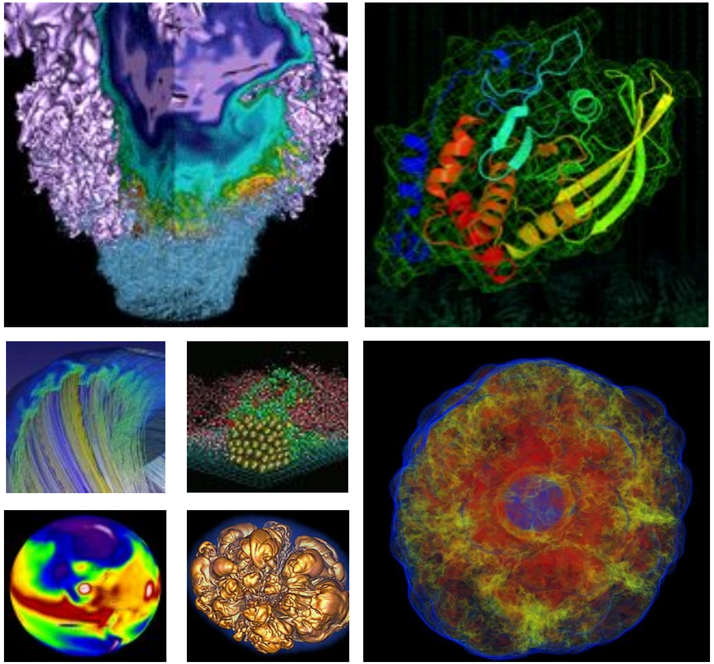
A case study of performance portability with OpenMP 4.5



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Outline

- General Plasmon Pole (GPP) application from BerkeleyGW
- Baseline CPU implementation using OpenMP 3.0
    - Reference Xeon Phi implementation
- GPU implementation
    - Naive implementation
    - Optimized implementation
    - Comparison with optimized OpenACC and CUDA implementation
- Backport OpenMP 4.5 on CPU

General Plasmon Pole (GPP)

- Mini-app from BerkeleyGW
    - Compute excited state properties of complex materials
- Characteristics of GPP
    - Reduction over a series of double complex arrays involving multiply, divide and add (FMA) instructions
    - For typical calculations, it evaluates to an arithmetic intensity between 1-10, i.e., the kernel has to be optimized for memory locality and vectorization efficiency

GPP- pseudo code

```
for(X){                    // X = 512
     for(N){               // Y = 32768/20 (1638)
          for(M){         // M = 32768
               for(iw){ //iw = 3
                    //Computation
                    output[iw] +=
               }
          }
     }
}
```

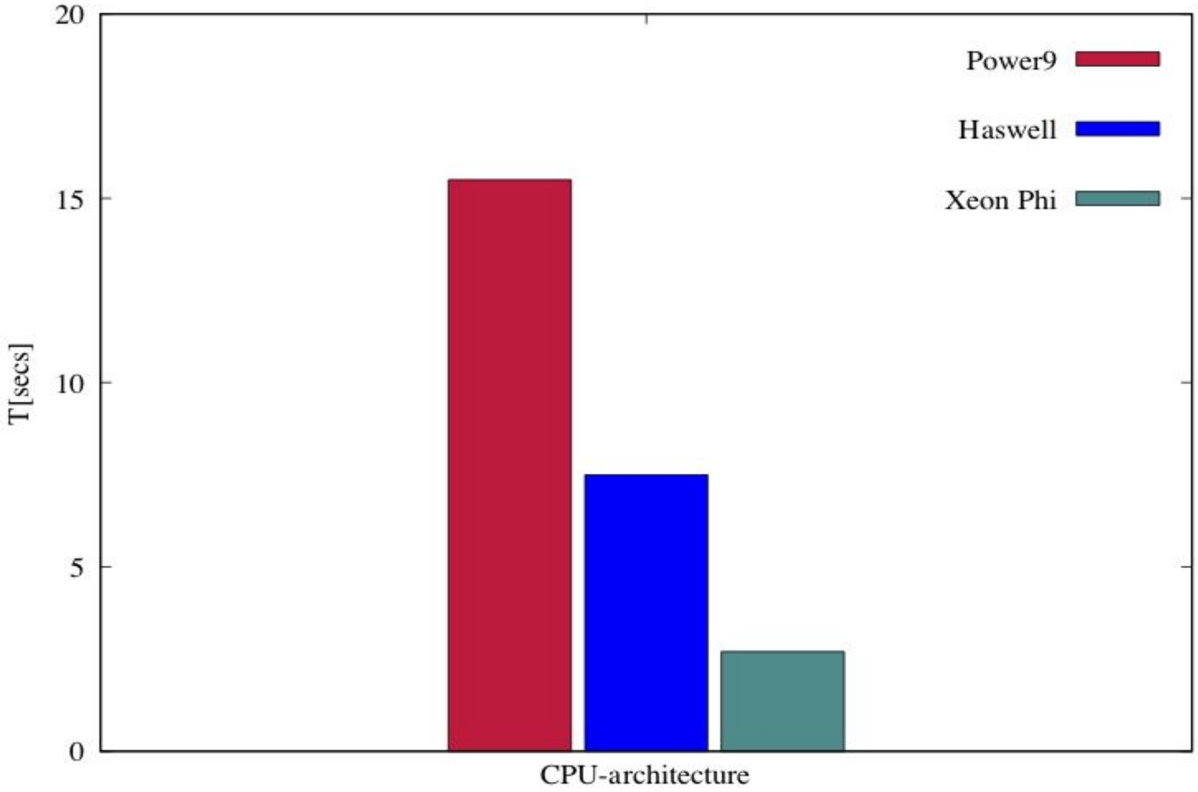
- Memory ~ 2GB
- Typical single-node problem size
- `output` - double complex

Optimized CPU implementation (OpenMP 3.0)

```
#pragma omp parallel for \
    reduction(+:output_re[0:3], output_im[0:3])
for(X){
    for(N){
        for(M){ //vectorize
            for(iw){ //unroll
                //Compute and store in local variables
            }
        }
        for(iw){
            output_re[iw] += …
            output_im[iw] += ...
        }
    }
}
```

- Divide the complex number into real and imaginary parts
- Array reduction to maintain correctness
- Collapse was not optimal (runtime > 10%)
- Vectorize the `M-loop`
- Unroll the `iw-loop`

Performance on CPUs

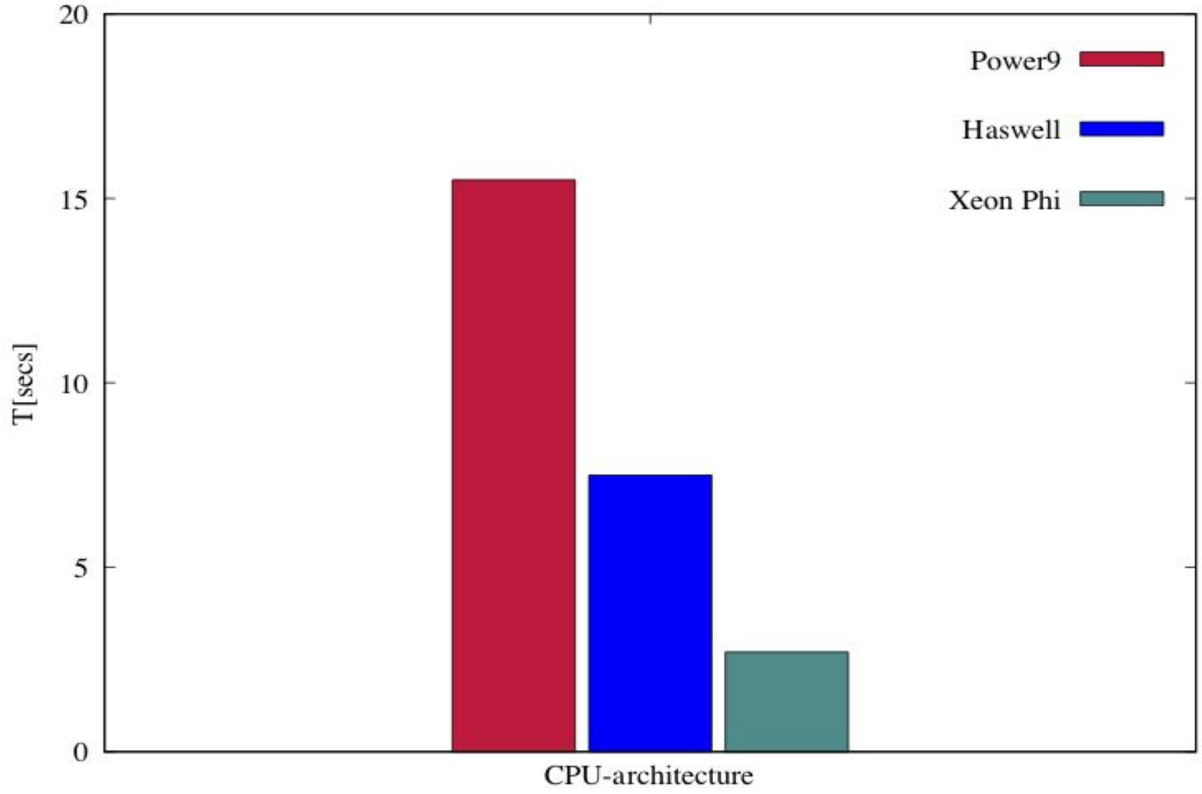


xl/2018 - Power processors (Summit)

intel/2018 - Haswell and Xeon Phi (Cori)

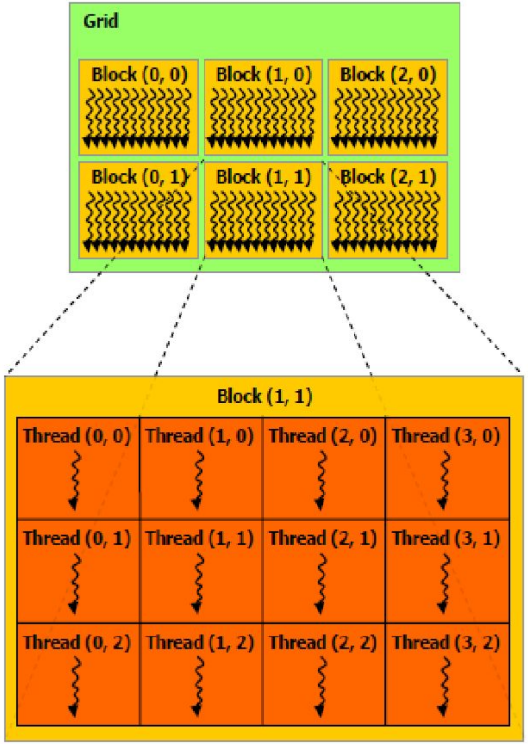
- Haswell is 2X faster than P9

Performance on CPUs



Xeon Phi - 2.5 seconds

GPU threads



1. Grid (threadblocks)
2. Block (threads)

Compilers used

- OpenMP 4.5
  - xl (IBM)
    - xl/2018 (latest version on Summit)
  - clang (coral)
    - llvm (latest version on Summit)
- OpenACC
  - pgi/18.4

OpenMP map directives

```
#pragma omp target teams distribute  →  Threadblocks

 #pragma omp parallel for  →  Threads in a threadblock

    #pragma omp target \
            map(to: input[0:X], …) \     //Copy-to-device
            map(tofrom: …) \             //Copy-to-from-device
            map(from: …) \               //Copy-from-device
```

Naive OpenMP 4.5 porting

```
#pragma omp target teams distribute \
     map(to:...) \
     map(tofrom:output_re[0:3], output_im[0:3])
for(X){
#pragma omp parallel for
     for(N){
          for(M){
               for(iw){
                    //Compute and store in local variables
               }
          }
          for(iw){
#pragma omp atomic
               output_re[iw] += …
#pragma omp atomic
               output_im[iw] += ...
          }
     }
}
```

- Distribute X among threadblocks
- Distribute N among threads in a threadblock
- No array-reduction with OpenMP offload directives hence use atomic to maintain correctness
  - Hence pass output_re and output_im into map(tofrom:) clause
- Parallelizing `M-loop` increases the overhead of synchronization

Optimized OpenMP 4.5

```
#pragma omp target enter data map(alloc:input[0:X], …) //Allocate data on device
#pragma omp target update to(input[0:X], …) //Update the data
#pragma omp target teams distribute collapse(2) map(to:...) \
    map(tofrom:...) \
    reduction(+:output_re{0,1,2}, output_im{0,1,2})
for(X){
    for(N){
#pragma omp parallel for \
    reduction(+:output_re{0,1,2}, output_im{0,1,2})
        for(M){
            for(iw){
                //Compute and store in local variables
            }
            output_re{0,1,2} += …;
            output_im{0,1,2} += …;
        }
    }
}
#pragma omp target exit data map(delete:input[0:X], …) //Delete allocated data
```

Optimized OpenMP 4.5

```
#pragma omp target enter data map(alloc:input[0:X]
#pragma omp target update to(input[0:X], …) //Upda
#pragma omp target teams distribute collapse(2) map(to
     map(tofrom:...) \
     reduction(+:output_re{0,1,2}, output_im{0,1,2})
for(X){
     for(N){
#pragma omp parallel for \
     reduction(+:output_re{0,1,2}, output_im{0,1,2})
          for(M){
               for(iw){
                    //Compute and store in local variab
               }
               output_re{0,1,2} += …;
               output_re{0,1,2} += …;
          }
     }
}
#pragma omp target exit data map(delete:input[0:X], …) //Delete allocated data
```

- Reduction required at threadblocks and thread level
- Reduction variables should not be added to the map clauses in the same construct
- Memory allocation improved the performance of the kernel by 10%
- Reduction gave a 3X performance boost

Optimized OpenACC

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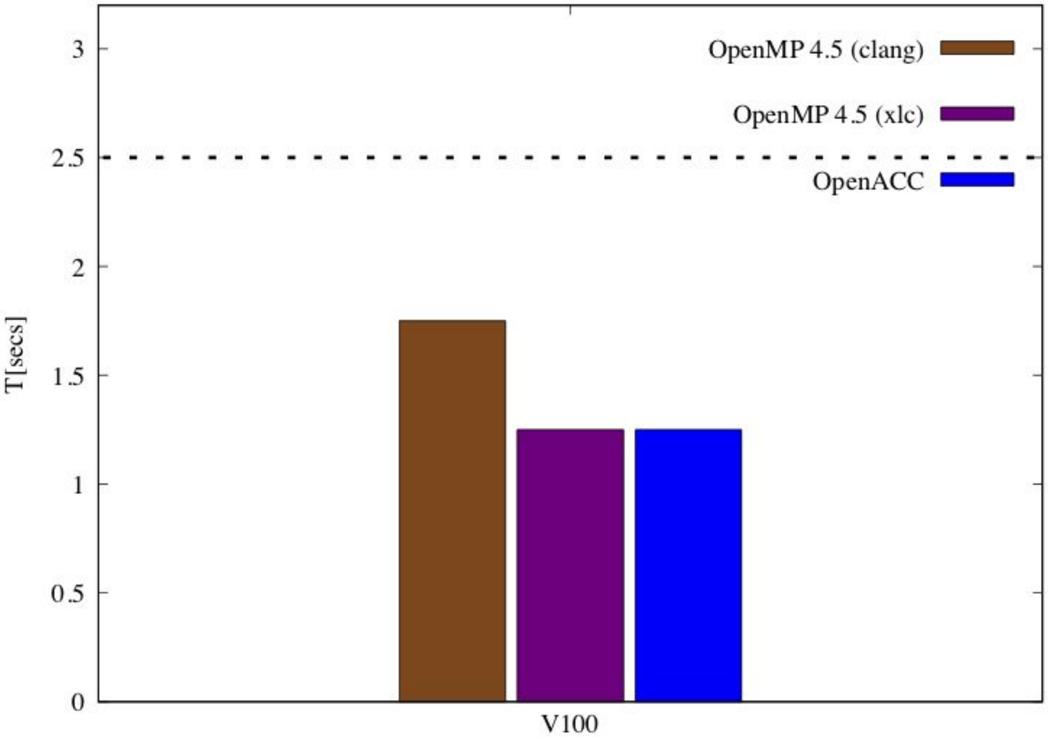
OpenACC

```
#pragma enter data create (input[0:X])
#pragma acc parallel loop gang collapse(2)\
present(input[0:X]) \
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(iw){
      //Compute and store in local variables
      }
     output_re{0,1,2} += …;
     output_re{0,1,2} += …;
    }
  }
#pragma exit data delete (input[0:X])
}
```

OpenMP

```
#pragma omp target enter data map(alloc:input[0:X])
#pragma omp target update to(input[0:X], …)
#pragma omp target teams distribute collapse(2)\
map(to:...) \
reduction(+:output_re{0,1,2}, output_im{0,1,2})
for(X){
 for(N){
#pragma omp parallel for \
      reduction(+:output_re{0,1,2}, output_im{0,1,2})
   for(M){
    for(iw){
      //Compute and store in local variables
      }
     output_re{0,1,2} += …;
     output_re{0,1,2} += …;
   }
 }
}
#pragma omp target exit data map(delete:input[0:X])
```

OpenMP 4.5 vs OpenACC



- Dashed line - Xeon Phi timing
- xlc-OpenMP and pgi-OpenACC give similar performance on V100
  - 2X faster than Xeon Phi
- clang-OpenMP is 20% slower compared to xlc-OpenMP

OpenMP 4.5 vs OpenACC on V100

Kernel Generated

	Grid	Thread	Registers
OpenMP (xl)	(1280,1,1)	(512, 1,1)	114
OpenACC (pgi)	(65535, 1,1)	(128,1,1)	136

- OpenACC generates ~50X more threadblocks, whereas OpenMP has 4X more threads per threadblock
- Volta has only 80 SM

CUDA kernels

Version 1

```
for(X){   blockIDx.x
   for(N){ threadId.x
     for(M){
       for(iw){
          //Compute and store
       }
     }
    for(iw){
     output_re[iw] += …; atomicAdd
     output_re[iw] += …; atomicAdd
    }
```

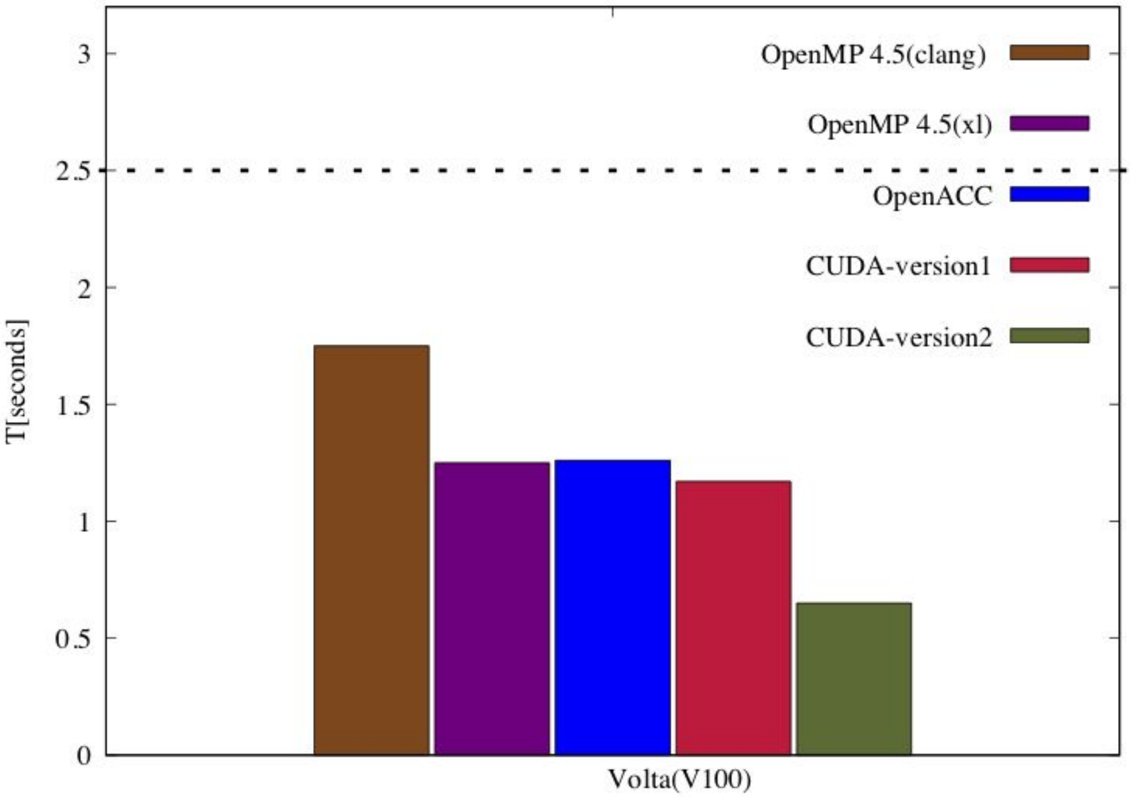
dim3 numblocks(X,1,1)
dim3 (32,1,1)

Version 2

```
for(X){   blockIDx.x
   for(N){ blockIDx.y
     for(M){threadId.x
       for(iw){
          //Compute and store
       }
     }
    for(iw){
     output_re[iw] += …; atomicAdd
     output_re[iw] += …; atomicAdd
     }
```

dim3 numblocks(X,N,1)
dim3 (32,1,1)

OpenMP 4.5 vs OpenACC Vs CUDA (1)



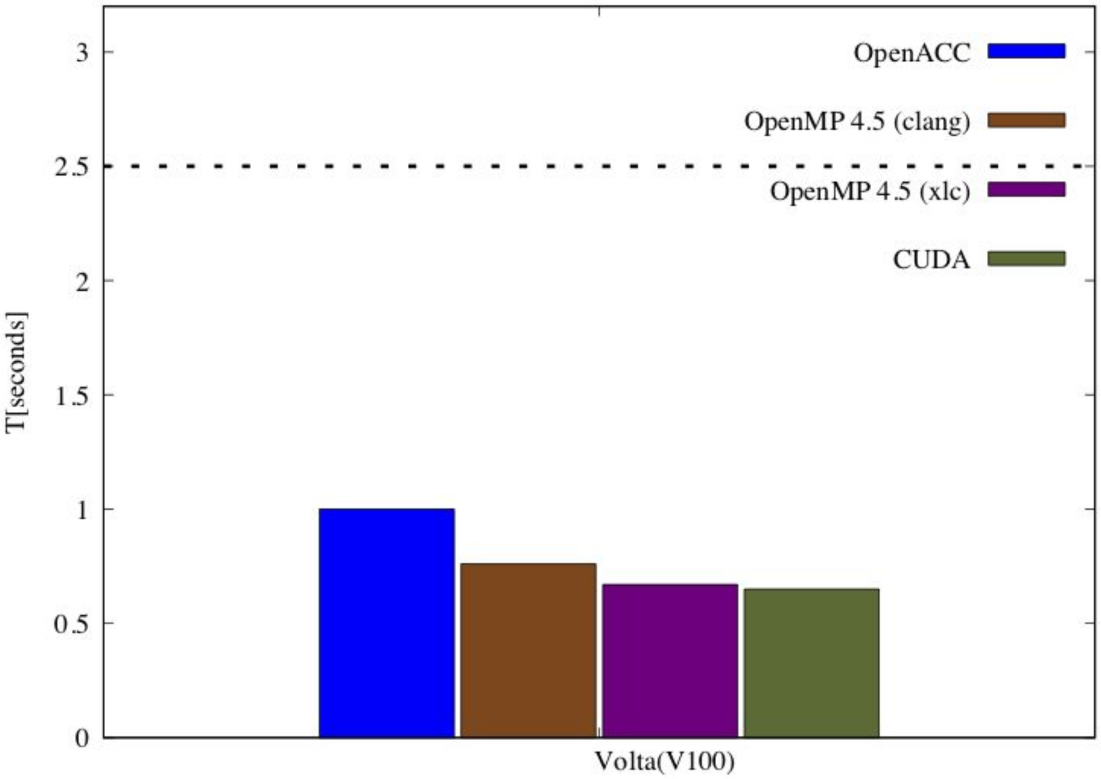
- OpenACC and CUDA-V1 have similar runtime
- OpenMP, OpenACC and CUDA-V1 have similar performance on V100
- CUDA-V2 is 2x faster than the closest counterpart

CUDA kernel V2 (best) vs OpenMP

```
for(X){ //blockIDx.x
 for(N){  // blockIdx.y
  for(M){// threadIdx.x
   for(iw){
     //Compute and store
     }
   }
   for(iw){
     output_re[iw] += …; atomicAdd
     output_re[iw] += …; atomicAdd
    }
  }
}
```

```
#pragma omp target enter data map(alloc:input[0:X])
#pragma omp target update to(input[0:X], …)
#pragma omp target teams distribute collapse(2)\
map(to:...) \
reduction(+:output_re{0,1,2}, output_im{0,1,2})
for(N){
 for(X){
#pragma omp parallel for \
      reduction(+:output_re{0,1,2}, output_im{0,1,2})
   for(M){
    for(iw){
      //Compute and store in local variables
      }
     output_re{0,1,2} += …;
     output_re{0,1,2} += …;
   }
 }
}
#pragma omp target exit data map(delete:input[0:X])
```

OpenMP 4.5 vs OpenACC vs CUDA (2)



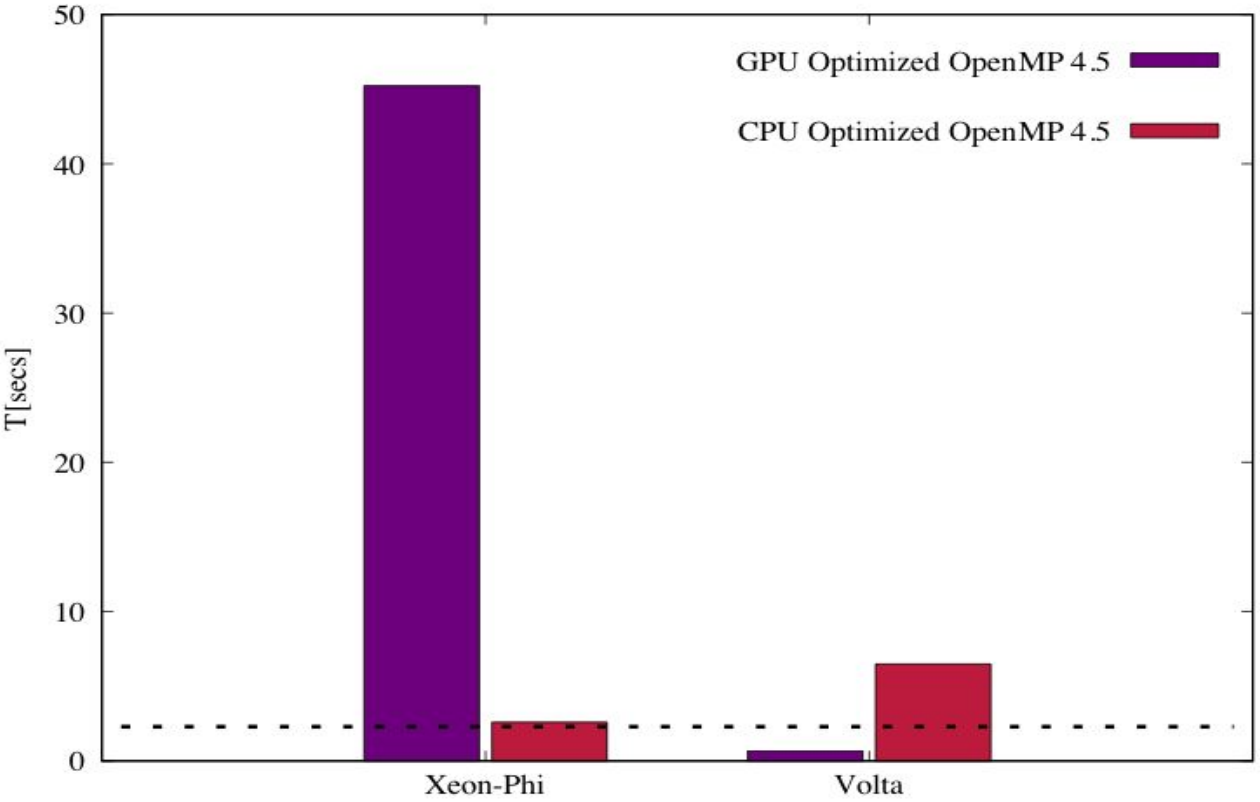
- OpenACC version improved by 30%
- OpenMP implementation (xl and clang) gave a 2X performance improvement
- xlc-OpenMP and CUDA-V2 give similar runtime performance
    - 4X faster than Xeon Phi

OpenMP 4.5 on CPUs

```
#pragma omp target enter data map(alloc:input[0:X])
#pragma omp target update to(input[0:X], …)
#pragma omp target teams distribute collapse(2)\
map(to:...) \
reduction(+:output_re{0,1,2}, output_im{0,1,2})
for(N){
 for(X){
#pragma omp parallel for \
      reduction(+:output_re{0,1,2}, output_im{0,1,2})
   for(M){
    for(iw){
      //Compute and store in local variables
      }
     output_re{0,1,2} += …;
     output_re{0,1,2} += …;
   }
 }
}
#pragma omp target exit data map(delete:input[0:X])
```

- Compiler on Cori - intel/2018
- Creates a single team and associates all threads to the team
- `X` and `N` loops are collapsed and run sequentially
- `M-loop` is distributed among the threads

GPU optimized vs CPU optimized



- GPU optimized OpenMP 4.5 is 18X slower on Xeon Phi
- CPU optimized OpenMP 4.5 is 12X slower on Volta

Summary

- Effort needed to port a kernel onto CPU and GPU using OpenMP
- Current state of OpenMP 4.5
    - Comparison with OpenACC and CUDA
    - Effect on the performance due to loop ordering
- OpenMP 4.5 on CPUs
    - Interpretation of OpenMP 4.5 directives on CPUs by intel compilers
    - Comparison of CPU optimized versus GPU optimized performance on GPU and CPUs respectively

Thank you &&

Questions ?

OpenMP 4.5 vs OpenACC on V100

Kernel Generated

	Grid	Thread	Registers
OpenMP (xl)	(1280,1,1)	(512, 1,1)	114
OpenACC (pgi)	(65535, 1,1)	(128,1,1)	136

Hardware metrics (nvprof)

	Dram utilization	Global hit-rate	Occupancy
OpenMP (xl)	7	84.6%	0.27
OpenACC (pgi)	8	54.05%	0.19

- OpenACC generates ~50X more threadblocks, whereas OpenMP has 4X more threads per threadblock
- Volta has only 80 SM
- Latency of misses is hidden by the additional threadblocks that are created