

Performance Portable Magnetohydrodynamics for the Exascale Era

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The Renaissance Simulations (O'Shea et al. 2015)

Movie c/o Donna Cox, Bob Patterson, NCSA Advanced Visualization Laboratory

CPU



Xeon Phi



Stampede 2



Cori (12)
LBNL



NVIDIA

BLUE WATERS
SUSTAINED PETASCALE COMPUTING



Summit (1)



Perlmutter

GPU



Aurora
ANL



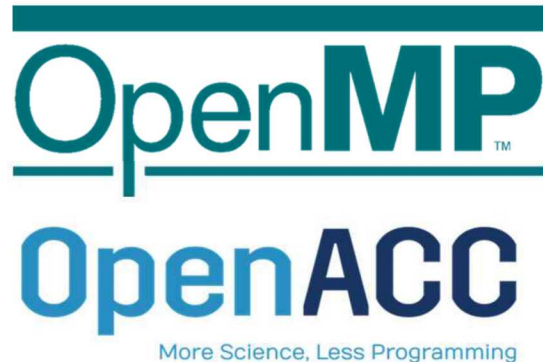
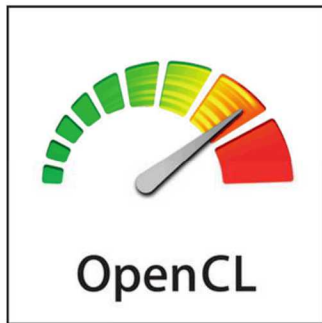
AMD



Performance Portability APIs

Typical Solutions

- OpenCL
- OpenACC
- OpenMP 4.5, 5.0



Abstraction Layers

- OCCA
- RAJA
- Kokkos

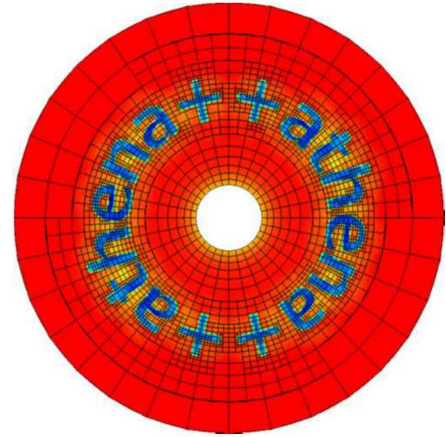


K-Athena: Performance Portable MHD

- Conversion of Athena++ with Kokkos
- Minimal code changes
- Performance Portable
 - Ready for CPUs, GPUs
- Freely available on GitLab

<https://gitlab.com/pgrete/kathena>

<https://arxiv.org/abs/1905.04341>



Kokkos Conversion

Athena++

```
for( int k = ks; k < ke; k++){  
  for( int j = js; j < je; j++){  
    #pragma omp simd  
    for( int i = is; i < ie; i++){  
      /* Loop Body */  
      u(k, j, i) = ...  
    }  
  }  
}
```

K-Athena

```
using namespace Kokkos;  
parallel_for( MDRangePolicy<Rank<3>>  
  ({ks, js, is}, {ke, je, ie}),  
  KOKKOS_LAMBDA(int k, int j, int i){  
    /* Loop Body */  
    u(k, j, i) = ...  
  });
```

Loop Heading Changes



Data Changes to Kokkos::View



Loop Body Unchanged



Parallelism Flexibility

Flat Parallelism

```
using namespace Kokkos;  
parallel_for( MDRangePolicy<Rank<3>>  
    ({ks, js, is}, {ke, je, ie}),  
    KOKKOS_LAMBDA(int k, int j, int i){  
        /* Loop Body */  
        u(k, j, i) = ...  
    });
```

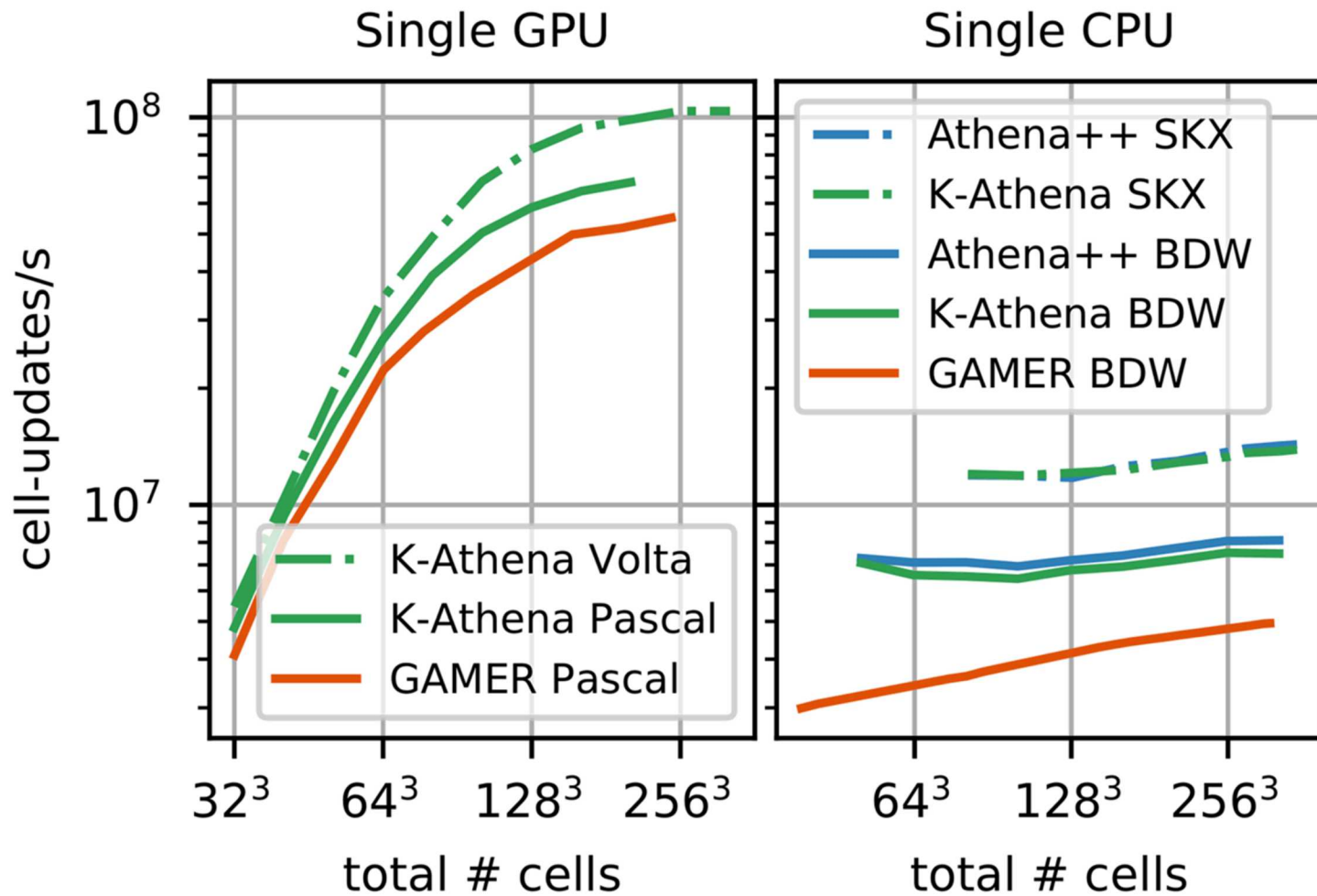
Teams: CPU Cores on a Socket, SMs on GPU

Threads: HT on CPU, Warps on GPU

Vectors: SIMD on CPU, Threads on GPU

Hierarchical Parallelism

```
using namespace Kokkos;  
parallel_for(team_policy(nk*nj, AUTO),  
    KOKKOS_LAMBDA(member_type team_mem){  
        int lr = team_mem.league_rank();  
        int k = lr / nj + ks;  
        int j = lr % nj + js;  
        parallel_for(  
            TeamThreadRange<>(team_mem, is, ie),  
            [&](int i) {  
                /* Loop Body */  
                u(k, j, i) = ...  
            });  
    });
```

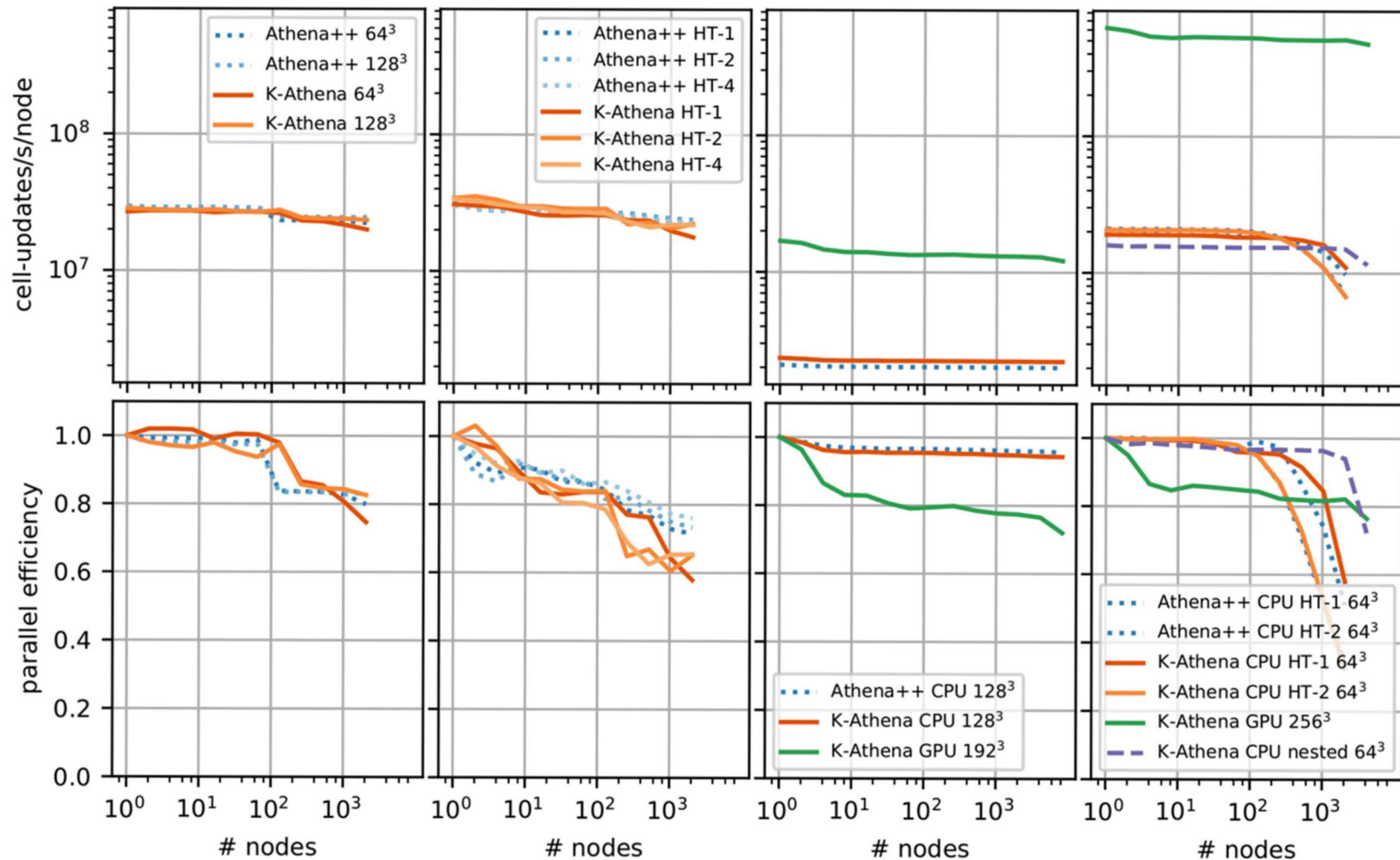


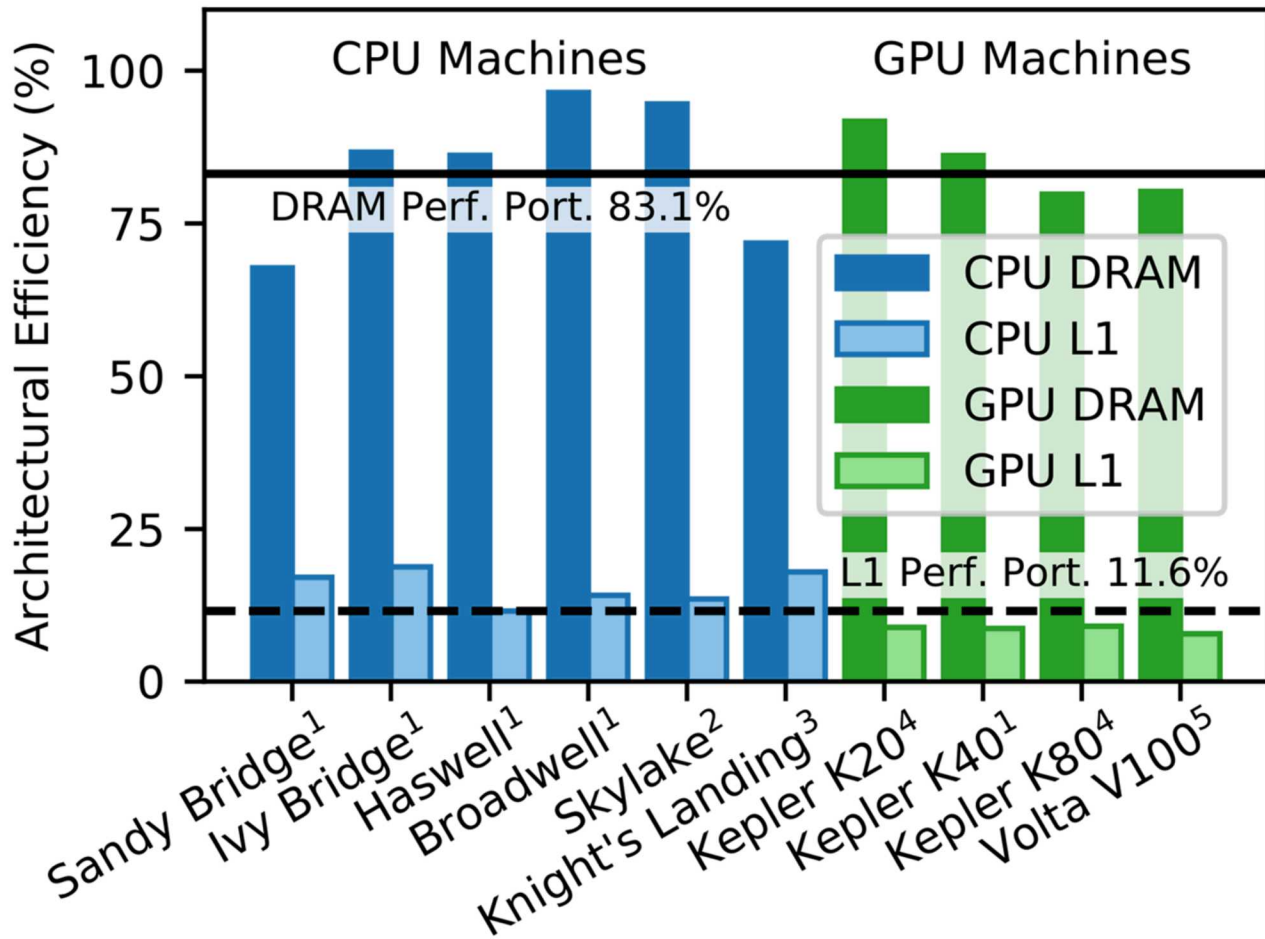
Electra Skylake CPU

Theta Knights Landing

Titan Opteron/Kepler GPU

Summit Power9/Volta GPU





¹Pleiades, ²Electra, ³Stampede 2, ⁴MSU HPCC, ⁵Summit

K-Athena

- Performance Portable Ideal MHD
 - Available for CPU, GPU, future architectures (Aurora, Frontier, ARM)
 - Adaptive Mesh Refinement soon
 - Special Relativistic and General Relativistic MHD can be made available
- MHD Turbulence Simulations on Blue Waters, XSEDE systems
- Magnetized Galaxy Cluster simulations
- Kokkos for future projects (Enzo-E)

<https://gitlab.com/pgrete/kathena>

<https://arxiv.org/abs/1905.04341>

References

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We acknowledge funding by NASA Astrophysics Theory Program grant #NNX15AP39G. Code development, testing, and benchmarking was made possible through various computing grants including allocations on NASA Pleiades (SMD-16-7720), OLCF Titan (AST133), OLCF Summit (AST146), ALCF Theta (Athena performance), XSEDE Comet (TG-AST090040), and Michigan State University's High Performance Computing Center.

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