OpenMP

SC'20 Booth Talk Series

Targeting Accelerator using OpenMP with GenASiS: A Simple and Effective Fortran Experience

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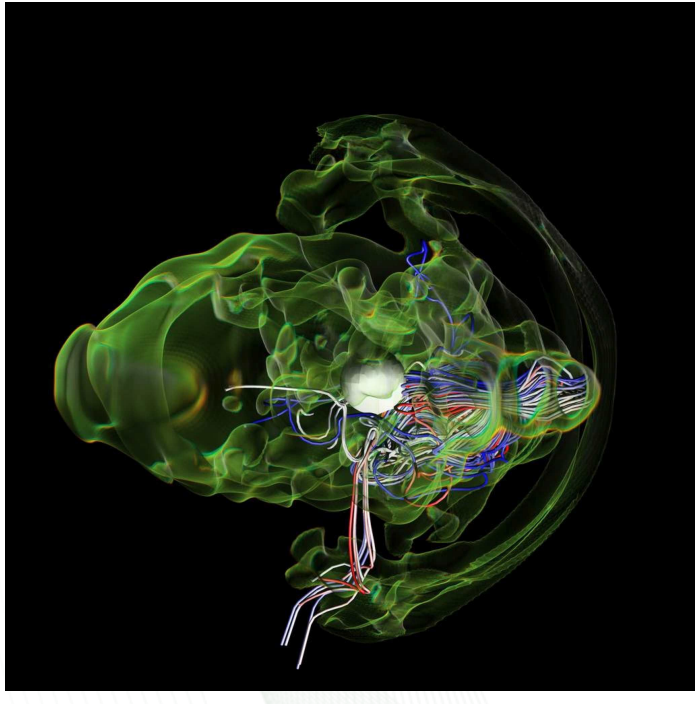
The Application

General ***A***strophysics ***Si***mulation ***S***ystem (GenASiS)

- Designed for parallel, large scale simulations
  - weak-scale to ~100 thousands MPI processes
- Written entirely in modern Fortran (2003, 2008)
- Modular, object-oriented design, and extensible
- Multi-physics solvers:
  - (Magneto)-hydrodynamics (HLL, HLLC solvers)
  - Explicit 2nd order time-integration
  - Self-gravity, polytropic & nuclear EoS
  - Grey and spectral neutrino transport
- CPU only code with OpenMP for threading (prior to this work)

The Application

- Studied the role fluid instabilities --- convection and Standing Accretion Shock Instability (SASI) --- in supernova dynamics
- Discovered exponential magnetic field amplification by SASI in progenitor star → origin of neutron star magnetic fields
- Refactored to three major subdivisions: *Basics*, *Mathematics*, *Physics* → allowing unit testing, ad-hoc/standalone tests, mini-apps



Paths to Targeting Accelerators

- "Native" accelerator programming model (e.g. CUDA, HIP, …)
  - requires rewrite of all computational kernels
  - loss of Fortran semantics (multi-d arrays, pointer/array remapping)
  - requires interfacing with the rest of the (Fortran) code
- Extensions to Fortran (e.g. CUDA Fortran)
  - non standard extension to Fortran only supported by few compilers non-uniformly
  - cannot easily fall back to standard Fortran for host-only code
- OpenMP offload
  - standardized directives
  - retain Fortran semantics
  - increasing support by more compilers (with existing implementation on our current target platform, OLCF Summit)

Higher-level GenASiS Functionality

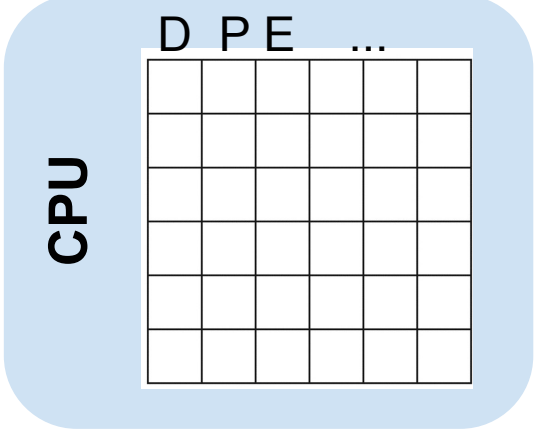
- StorageForm :
  - a class for data and metadata; the 'heart' of data storage facility in GenASiS
  - metadata includes units, variable names (for I/O, visualization)
  - used to group together a set of related physical variables (e.g. Fluid)
  - render more generic and simplified code for I/O, ghost exchange, prolongation & restriction (AMR mesh)

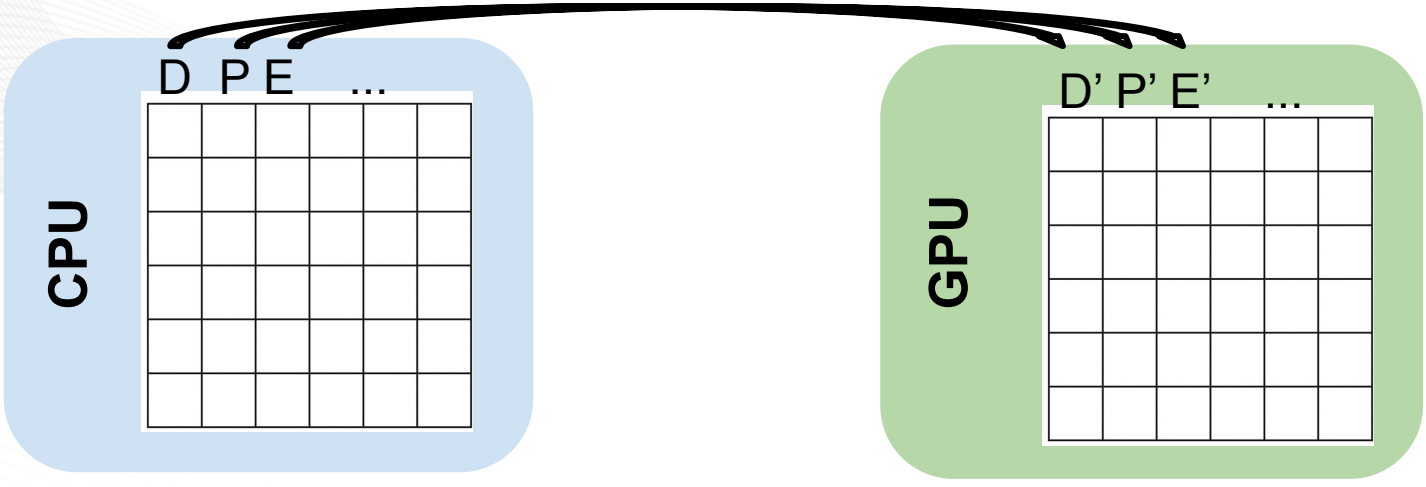
- Data :
  - `StorageForm % Value ( nCells, nVariables )`
  - use as, e.g.
```
Pressure => StorageForm % Value ( :, 1 ),
Density  => StorageForm % Value ( :, 2 )
```

- Methods:
  - `call S % Initialize ( )` ← **allocate** data on **host**
  - `call S % AllocateDevice ( )` ← **allocate** and **associate** data **on GPU**
  - `call S % Update{Device,Host} ( )` ← **transfer** data

Higher-level GenASiS Functionality (2)

- call StorageForm % Initialize &
  (Shape = [6, 6], &
  VariableOption = [“Pressure”, “Density”, &
  “Energy”, …])






```
real ( KDR ), dimension ( :, : ), pointer :: Scratch
type ( c_ptr ) :: D_Value

call AllocateDevice ( S % nValues * S % nVariables, D_Value )

call c_f_pointer ( D_Value, Scratch, [ S % nValues, S % nVariables ] )

do iV = 1, S % nVariables

  D_Value = c_loc ( Scratch ( :, iV ) )
  Variable => S % Value ( :, iV )
  call AssociateHost ( D_Value, Variable )

end do
```

Tells OpenMP data location on GPU
→avoid (implicit) allocation & transfer

Lower-Level GenASiS Functionality

- Fortran wrappers to OpenMP APIs
  - call AllocateDevice(Value, D_Value)
    → omp_target_alloc()

    call AssociateHost(D_Value, Value)
    → omp_target_associate_ptr()

    call UpdateDevice(Value, D_Value),
    call UpdateHost(Value, D_Value)
    → omp_target_memcpy()

Value : Fortran array
D_Value : type(c_ptr), GPU address

Offloading Computational Kernel

Persistent **allocation** and **association**

```
call F % Initialize &
  ([nCells, nVariables])
call F % AllocateDevice ( )
call F % UpdateDevice ( )
call AddKernel &
  ( F % Value ( :, 1 ),
    F % Value ( :, 2 ), &
    F % Value ( :, 3 ) )
```

```
1  subroutine AddKernel ( A, B, C )
2
3    real ( KDR ), dimension ( : ), intent ( in ) :: A, B
4    real ( KDR ), dimension ( : ), intent ( out ) :: C
5
6    integer ( KDI ) :: i
7
8    !$OMP target teams distribute parallel do schedule ( static, 1 )
9    do i = 1, size ( C )
10     C ( i ) = A ( i ) + B ( i )
11   end do
12   !$OMP end target teams distribute parallel do
13
14 end subroutine AddKernel
```

No implicit data transfer,
no explicit **map()**

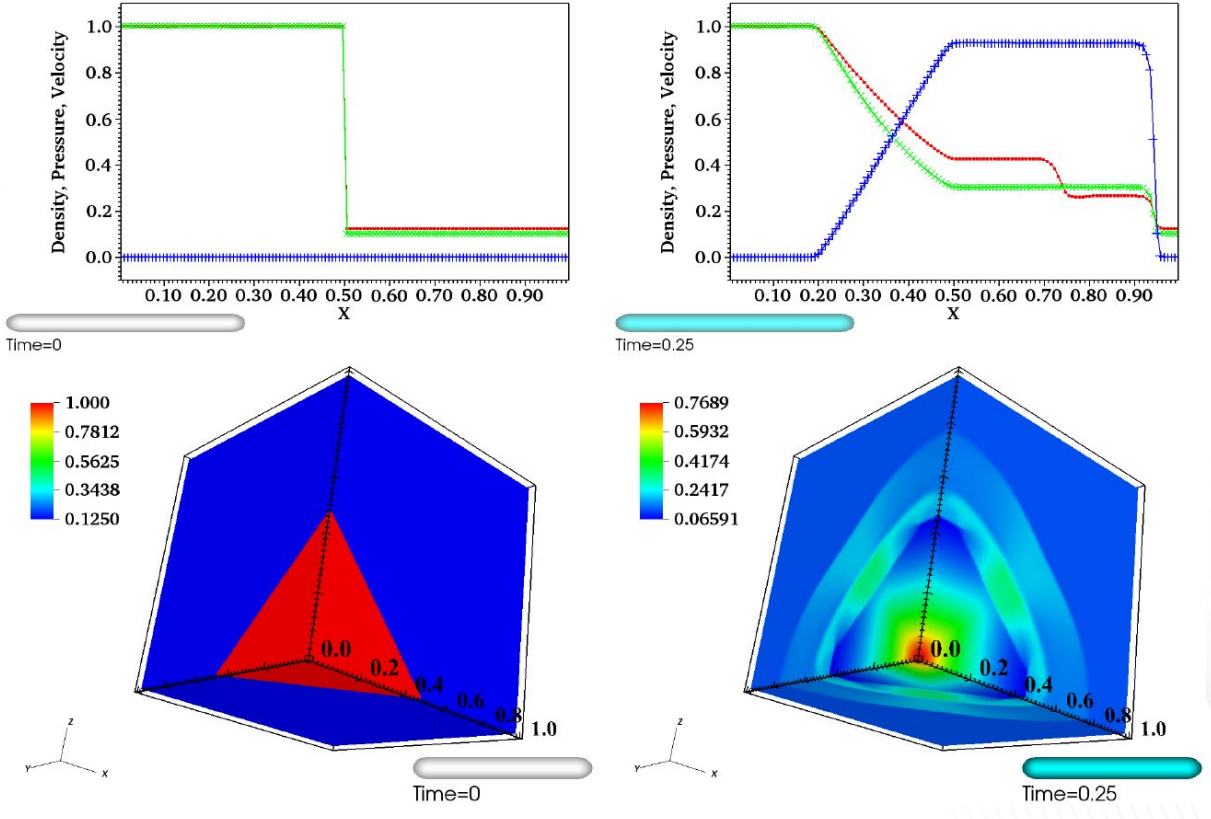
Example of Kernel with Pointer Remapping

```
real ( KDR ), dimension ( :, :, : ), pointer
  :: V, dV

V ( -1:nX+2, -1:nY+2, -1:nZ+2 ) => F % Value ( : , iV )
dV ( -1:nX+2 , -1:nY+2 , -1:nZ+2 ) => dF % Value ( : , iV )

call ComputeDifferences_X ( V, dV )
```

Example of Kernel with Pointer Remapping

```
1  subroutine ComputeDifference_X ( V, dV )
2
3    real ( KDR ), dimension ( -1:, -1:, -1: ), &
4      intent ( in ) :: &
5        V
6    real ( KDR ), dimension ( -1:, -1:, -1: ), &
7      intent ( out ) :: &
8        dV
9
10   integer ( KDI ) :: i, j, k
11
12   !$OMP target teams distribute parallel do collapse ( 3 ) schedule ( static, 1 )
13   do k = 1, nZ
14     do j = 1, nY
15       do i = 0, nX + 2
16         dV ( i, j, k ) &
17           = V ( i, j, k ) - V ( i - 1, j, k )
18       end do
19     end do
20   end do
21   !$OMP end target teams distribute parallel do
22
23 end subroutine ComputeDifferences_X
```

Porting a Fluid Dynamics Application: RiemannProblem



Initial (left) and final (right) density of 1D and 3D RiemannProblem

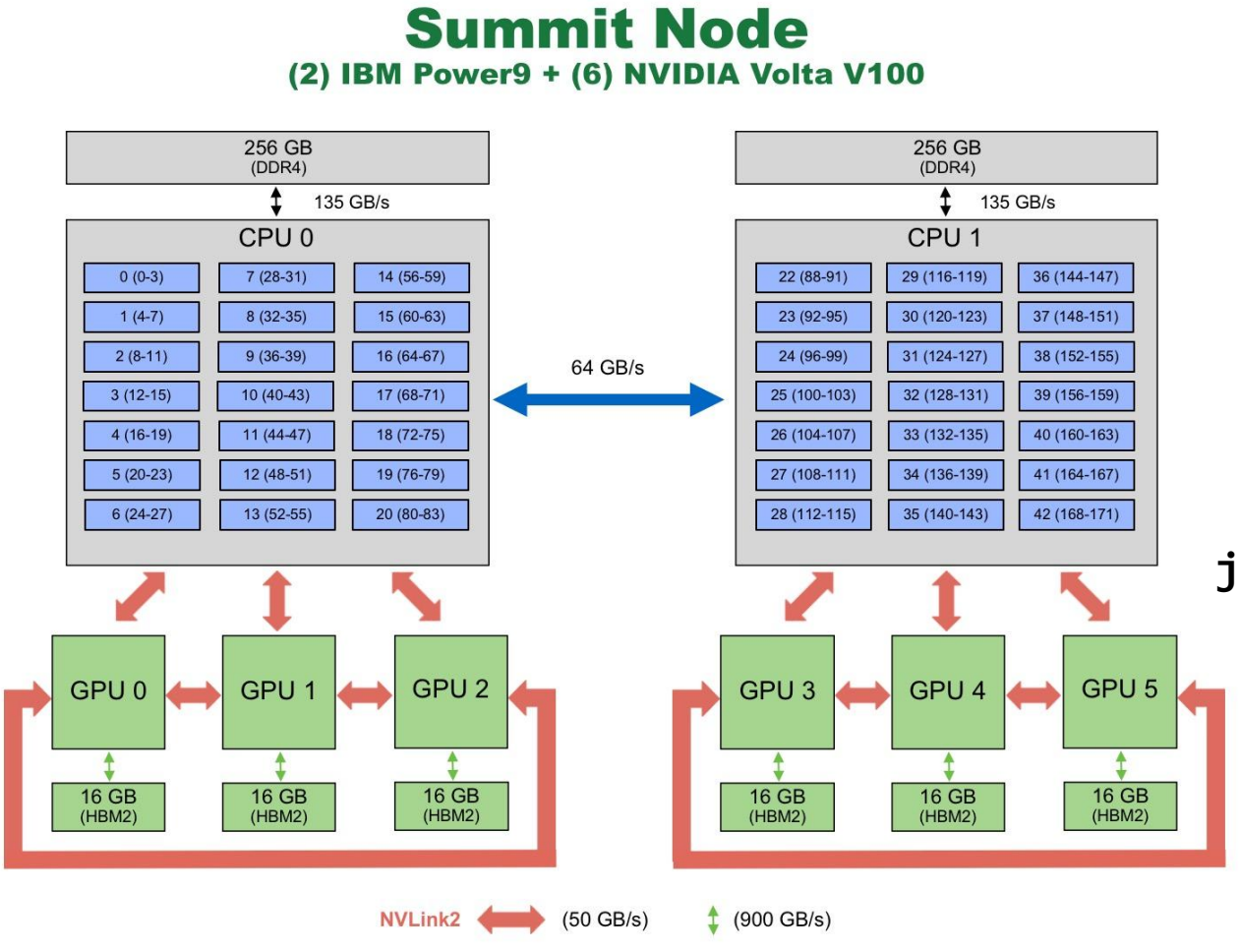
Fluid Evolution on CPU

```
 1: Call: Initialize ( )
 2: Call: GhostExchange ( )
 3: Set: Time = StartTime
 4: while Time < FinishTime do
 5:    Call: ComputeTimeStep ( ) → TimeStep
 6:    Set: FluidOld = FluidCurrent
 7:
 8:    Call: ComputeDifferences ( )
 9:    Call: ComputeReconstruction ( )
10:    Call: ComputeFluxes ( )
11:    Call: ComputeUpdate ( TimeStep ) → FluidUpdate
12:    Set: FluidCurrent = FluidOld + FluidUpdate
13:
14:    Call: GhostExchange ( )
15:
16:    Call: ComputeDifferences ( )
17:    Call: ComputeReconstruction ( )
18:    Call: ComputeFluxes ( )
19:    Call: ComputeUpdate ( TimeStep )
20:    Set: FluidCurrent = 0.5 * (FluidOld + FluidCurrent + FluidUpdate)
21:
22:    Call: GhostExchange ( )
23: end while
```

Fluid Evolution on GPU

```
 1: HOST: Call: Initialize ( )
 2: Call: GhostExchange ( )
 3: HOST: Set: Time = StartTime
 4: while Time < FinishTime do
 5:    HOST: Call: ComputeTimeStep ( ) → TimeStep
 6:    TRANSFER: Call: FluidCurrent % UpdateDevice ( )
 7:    DEVICE: Set: FluidOld = FluidCurrent
 8:
 9:    DEVICE: Call: ComputeDifferences ( )
10:    DEVICE: Call: ComputeReconstruction ( )
11:    DEVICE: Call: ComputeFluxes ( )
12:    DEVICE: Call: ComputeUpdate ( TimeStep ) → FluidUpdate
13:    DEVICE: Set: FluidCurrent = FluidOld + FluidUpdate
14:
15:    TRANSFER: Call: FluidCurrent % UpdateHost ( )
16:    HOST: Call: GhostExchange ( )
17:    TRANSFER: Call: FluidCurrent % UpdateDevice ( )
18:
19:    DEVICE: Call: ComputeDifferences ( )
20:    DEVICE: Call: ComputeReconstruction ( )
21:    DEVICE: Call: ComputeFluxes ( )
22:    DEVICE: Call: ComputeUpdate ( TimeStep )
23:    DEVICE: Set: FluidCurrent = 0.5 * (FluidOld + FluidCurrent + FluidUpdate)
24:
25:    TRANSFER: Call: FluidCurrent % UpdateHost ( )
26:    Call: GhostExchange ( )
27: end while
```

Performance Results

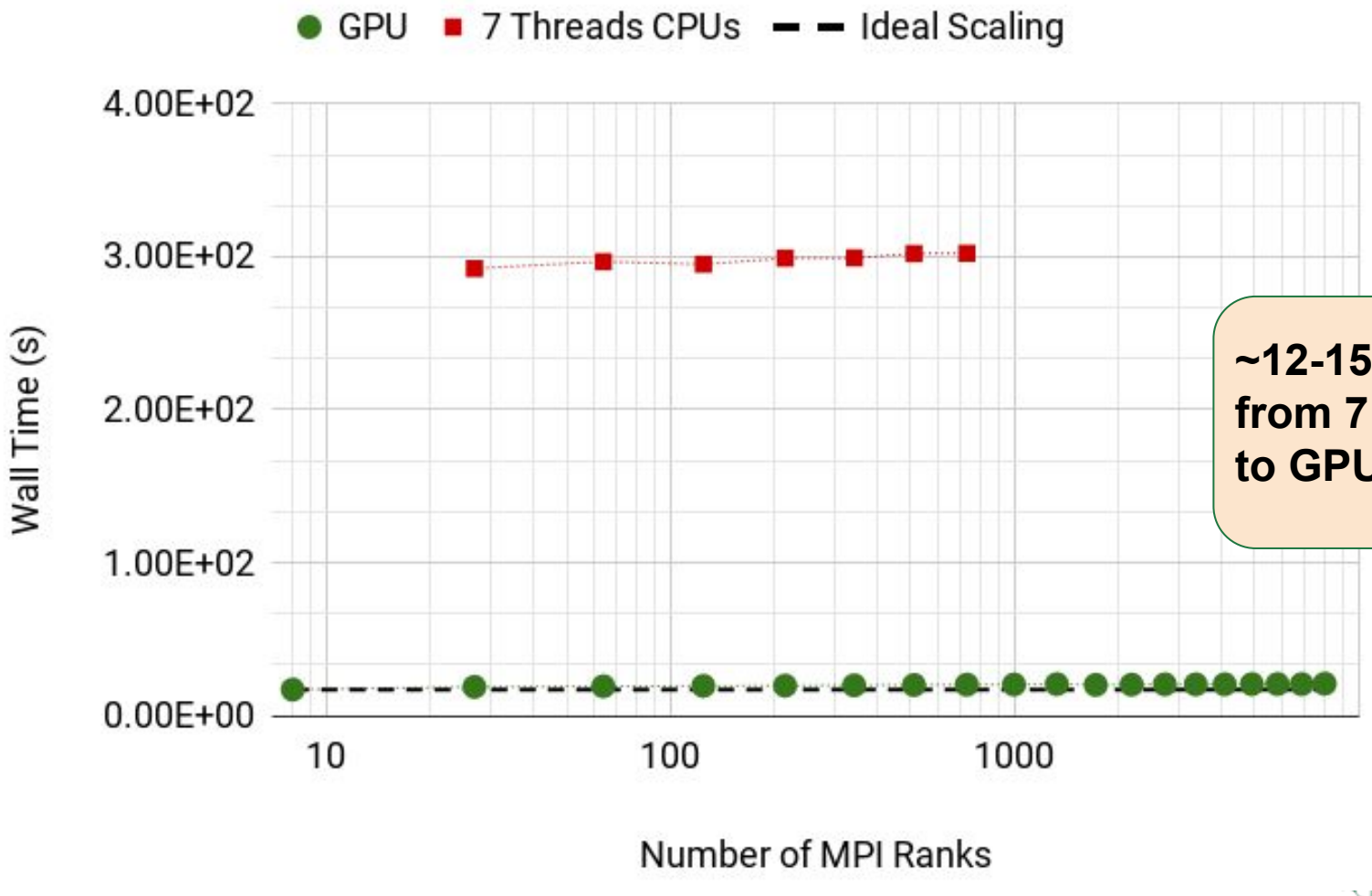


"Proportional resource tests":
7 CPU cores vs. 1 GPU

6 RS per host,
1 MPI (+OpenMP) per RS

```
jsrun -r6 -c7 -g1 -a1 -bpacked:7
```

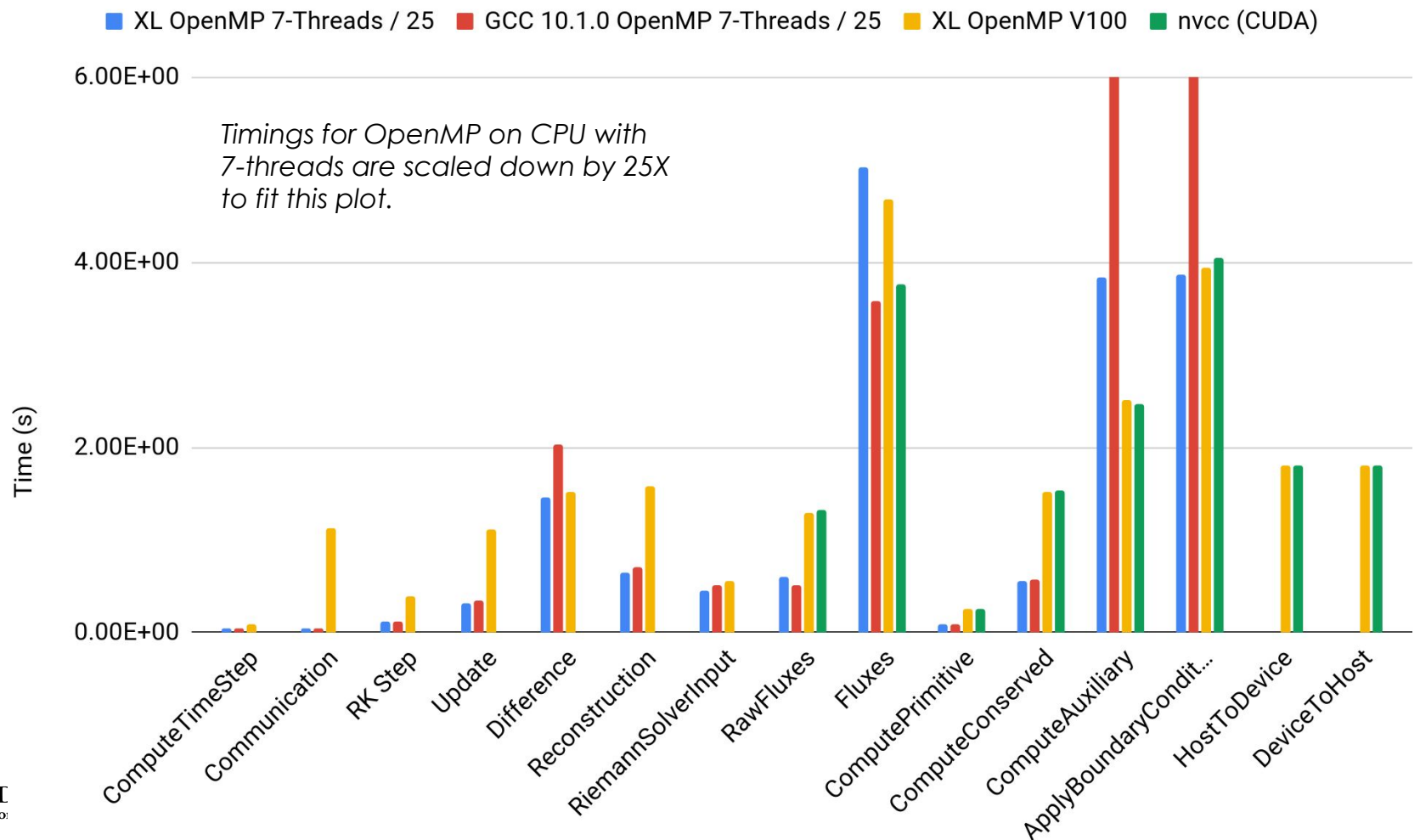
Results: Weak-Scaling 3D RiemannProblem



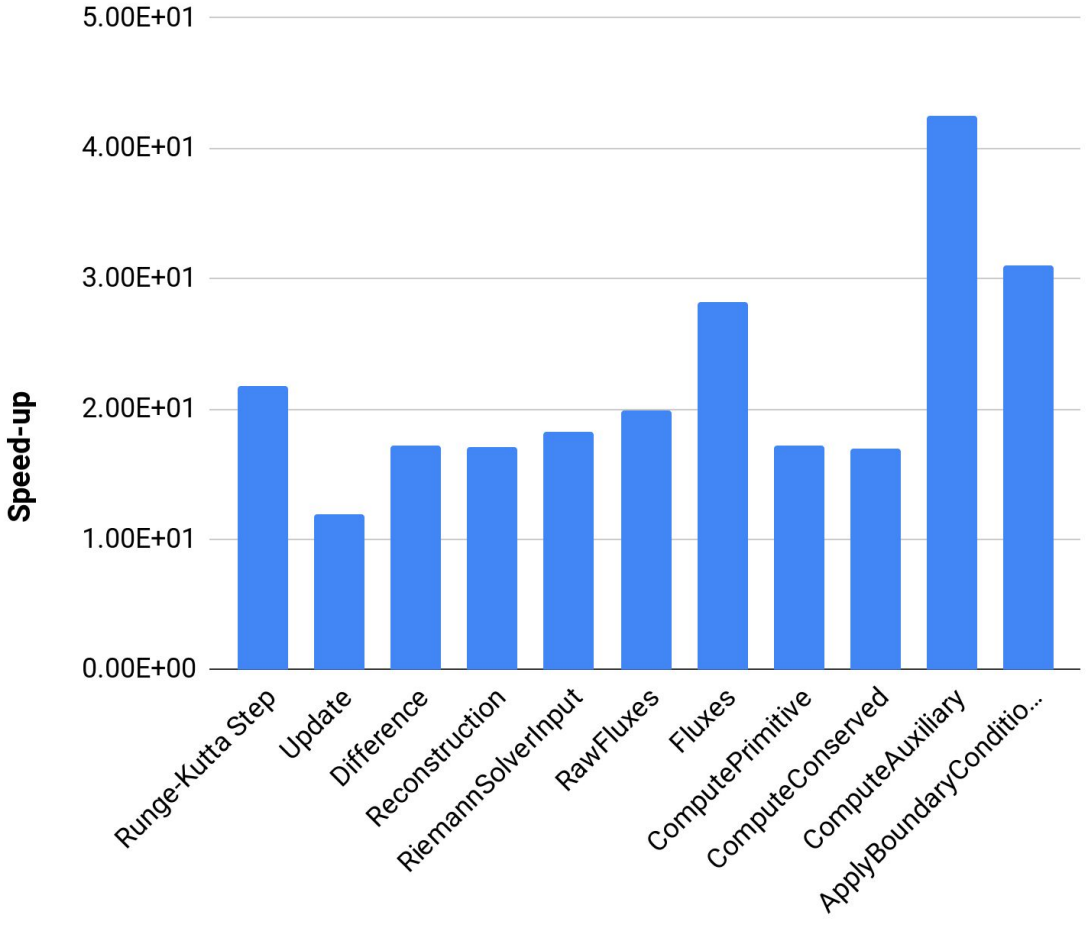
~12-15X speedup from 7 CPU threads to GPU

Results: GenASiS Basics RiemannProblem

Kernel timings for 50 cycles, 3D - 256^3 cells per GPU (**lower is better/faster**)



Performance Results: Kernel Speedups



Conclusion

- OpenMP provides a simple and effective path to port Fortran code to run on accelerators
  - more compilers are supporting OpenMP offload (XL, GCC, CCE, Intel, PGI, LLVM-based)

- **Performance parity** between OpenMP offload and vendor-specific accelerator programming model (e.g. CUDA) is achievable
  - OpenMP is more portable and can be more “natural” to the application
  - compilers need to do a good job of optimization
  - no need to rewrite kernels, simpler to port from multi-threading to GPU offload
  - can continue to exploit base language feature (Fortran)

- Code and paper: github.com/GenASiS arxiv.org/abs/1812.07977

OpenMP

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openmp.org OpenMP API specs, forum, reference guides, and more

link.openmp.org/sc20 Videos and PDFs of OpenMP SC'20 presentations