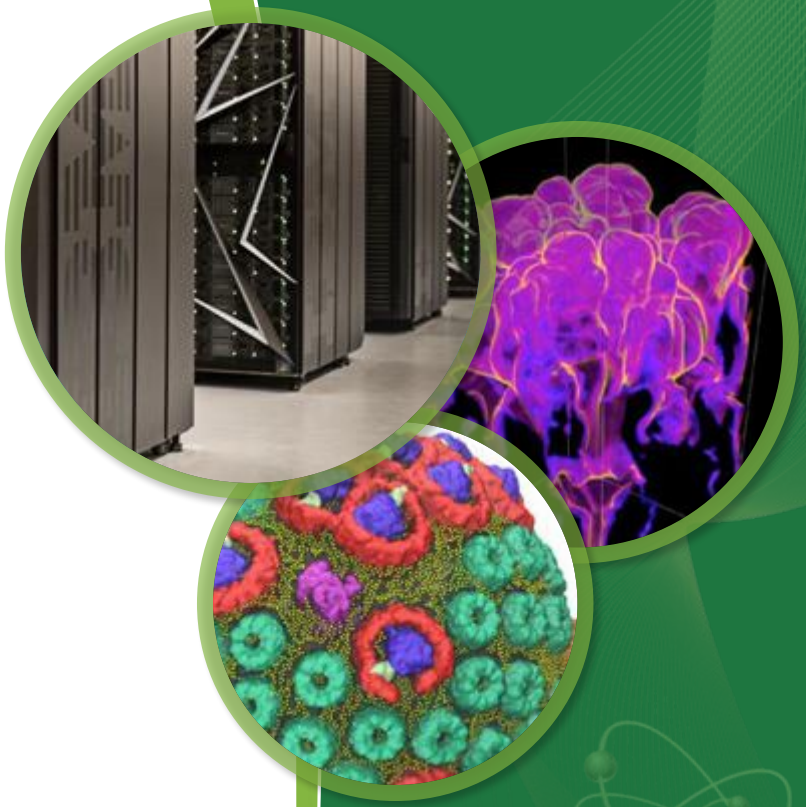
Targeting GPUs using OpenMP Directives on Summit with GenASiS: A Simple and Effective Fortran Experience



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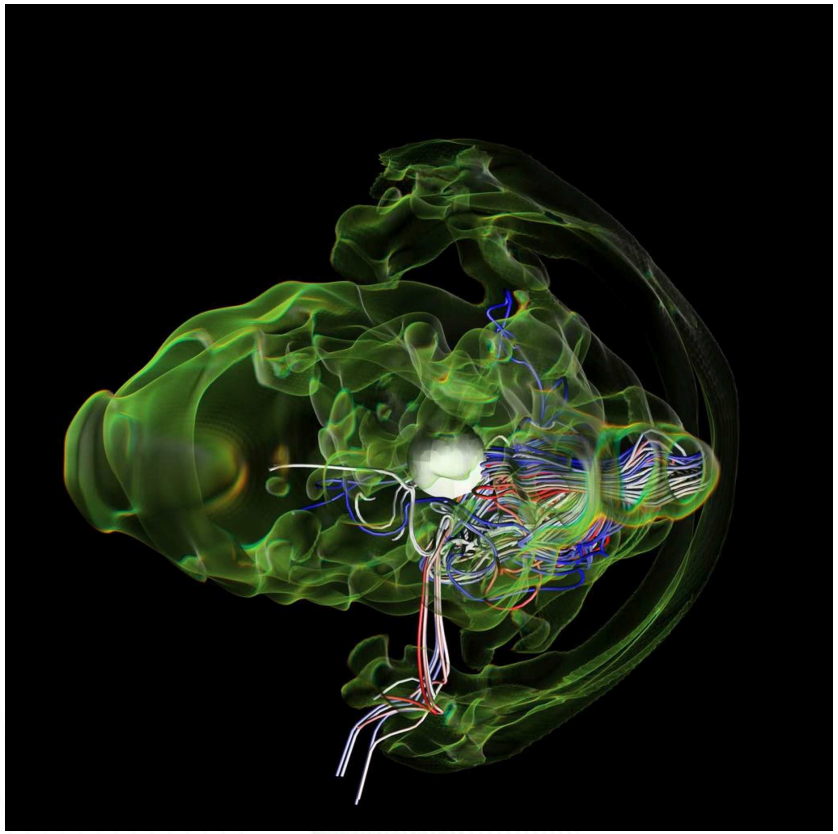
The Application

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 GPU

- CUDA
  - 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
- CUDA Fortran
  - non standard extension to Fortran (XL, PGI)
  - cannot easily fall back to standard Fortran
- Directives (OpenMP)
  - retain Fortran semantics
  - OpenMP 4.5 has excellent support from IBM XL (Summit), CCE (Titan)
    - with excellent support for modern Fortran

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

- Affirmative control of data movement
- Persistent memory allocation on the device

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 )`

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

Sidebar: OpenMP Memory for Offload

- OpenMP maps host (CPU) variables to device (GPU) (explicitly or implicitly)
  - default copy to-from
- *Presence check*: if fail, new variable is created on device
  - sometime requires explicit association to avoid unintentional data movement

Offloading Computational Kernel

```
 1 subroutine AddKernel ( A, B, D_A, D_B, D_C, C )
 2
 3   real ( KDR ), dimension ( : ), intent ( in ) :: A, B
 4   type ( c_ptr ), intent ( in ) :: D_A, D_B, D_C
 5   real ( KDR ), dimension ( : ), intent ( out ) :: C
 6
 7   integer ( KDI ) :: i
 8
 9   call AssociateHost ( D_A, A )
10   call AssociateHost ( D_B, B )
11   call AssociateHost ( D_C, C )
12
13   !$OMP target teams distribute parallel do schedule ( static, 1 )
14   do i = 1, size ( C )
15     C ( i ) = A ( i ) + B ( i )
16   end do
17   !$OMP end target teams distribute parallel do
18
19   call DisassociateHost ( C )
20   call DisassociateHost ( B )
21   call DisassociateHost ( A )
22
23 end subroutine AddKernel
```

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

```
call F % Initialize &
                    iables])
                    eDevice ( )
call F % UpdateDevice ( )
call AddKernel &
  ( F % Value ( :, 1 ),
    F % Value ( :, 2 ), &
    F % D_Value ( 1 ),
    F % D_Value ( 2 ), &
    F % D_Value ( 3 ),
    F % Value ( :, 3 ) )
```

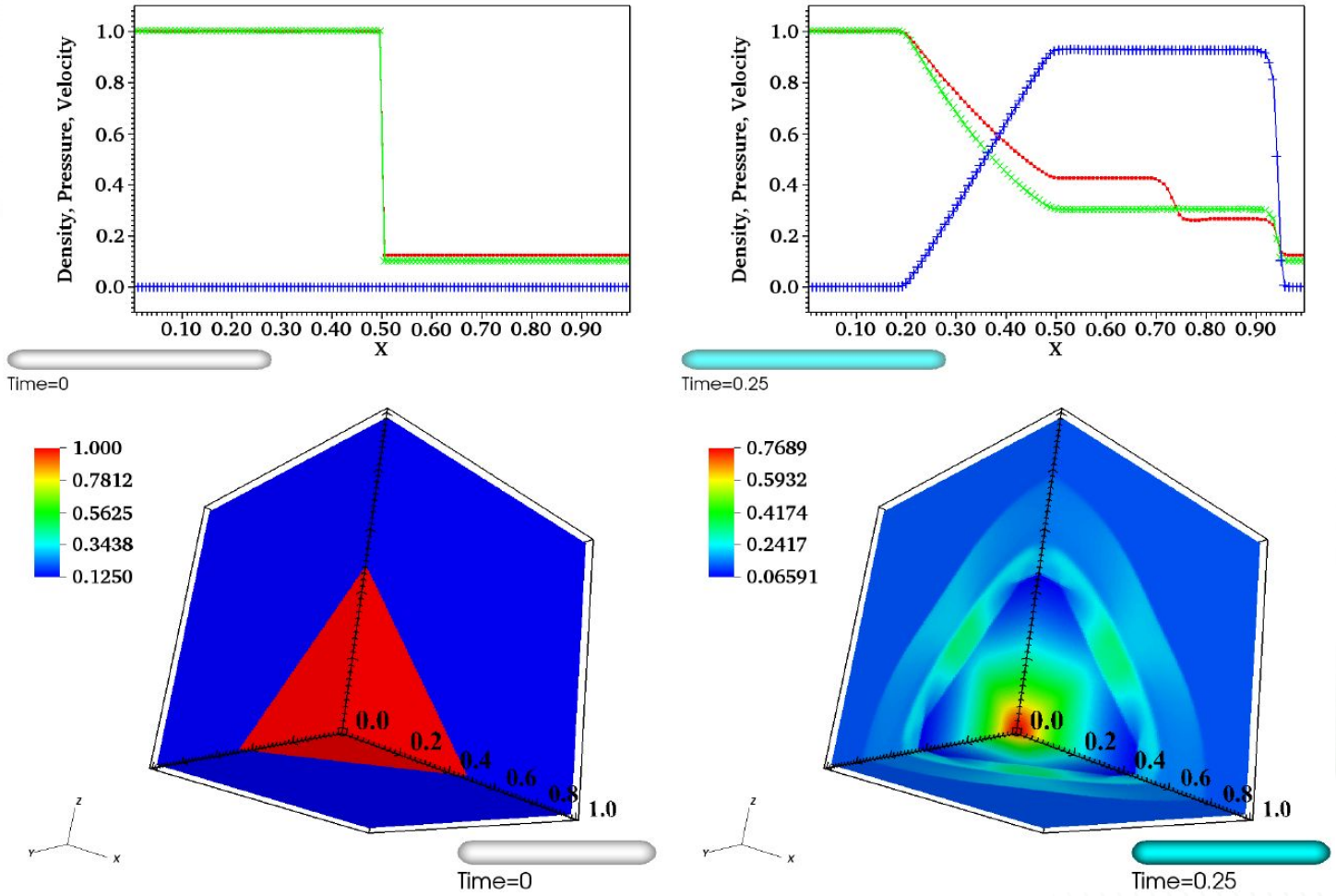
Example of Kernel with Pointer Remapping

```
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, F % D_Value ( iV), ... )
```

Example of Kernel with Pointer Remapping

```
 1 subroutine ComputeDifference_X ( V, D_V, D_dV, dV )
 2
 3   real ( KDR ), dimension ( -1:, -1:, -1: ), intent ( in ) :: V
 4   type ( c_ptr ), intent ( in ) :: D_V, D_dV
 5   real ( KDR ), dimension ( -1:, -1:, -1: ), intent ( out ) :: dV
 6
 7   integer ( KDI ) :: i, j, k
 8
 9   call AssociateHost ( D_V, V )
10   call AssociateHost ( D_dV, dV )
11
12   !$OMP target teams distribute parallel do collapse ( 3 ) schedule ( static, 1 )
13   do k = 1, nZ
14     do j = 1, nY
15       do i = 0, nX + 2
16         dV ( i, j, k ) = V ( i, j, k ) - V ( i - 1, j, k )
17       end do
18     end do
19   end do
20   !$OMP end target teams distribute parallel do
21
22   call DisassociateHost ( dV )
23   call DisassociateHost ( V )
24
25 end subroutine ComputeDifferences_X
```

Porting a Fluid Dynamics Application: RiemannProblem



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

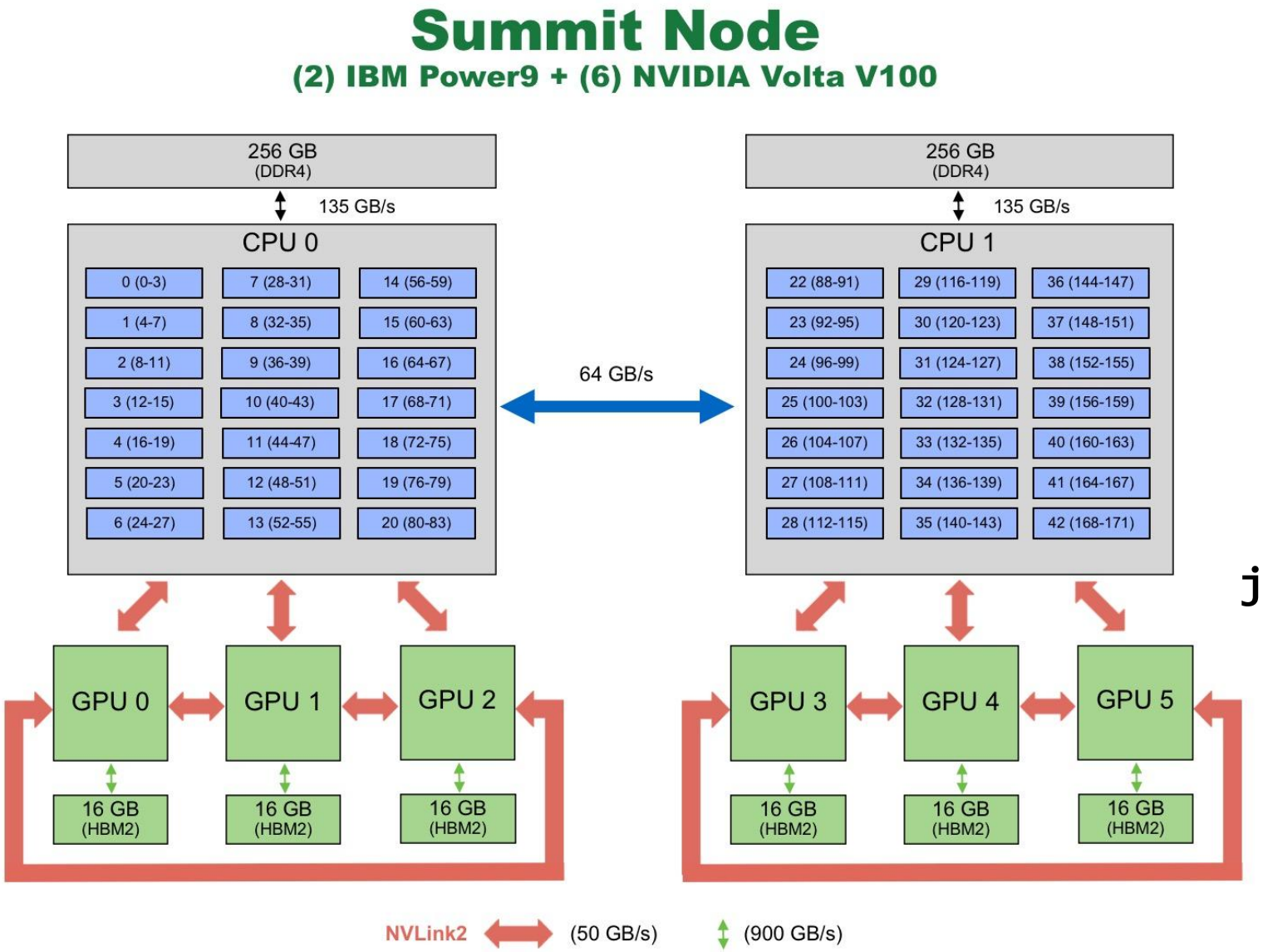
Fluid Evolution on CPU

```
 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

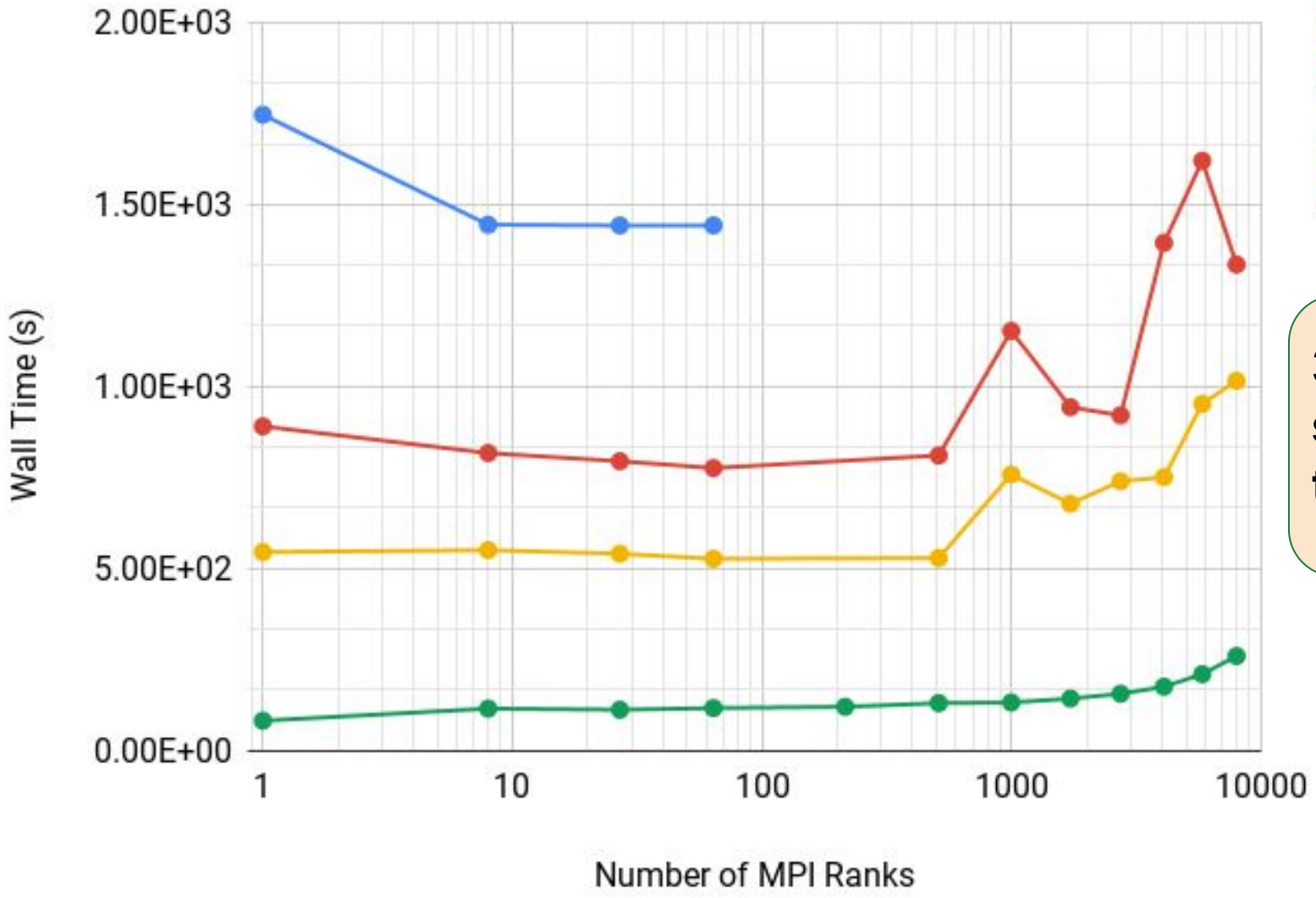


"Proportional resource tests":
7 CPU cores vs. 1 GPU

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

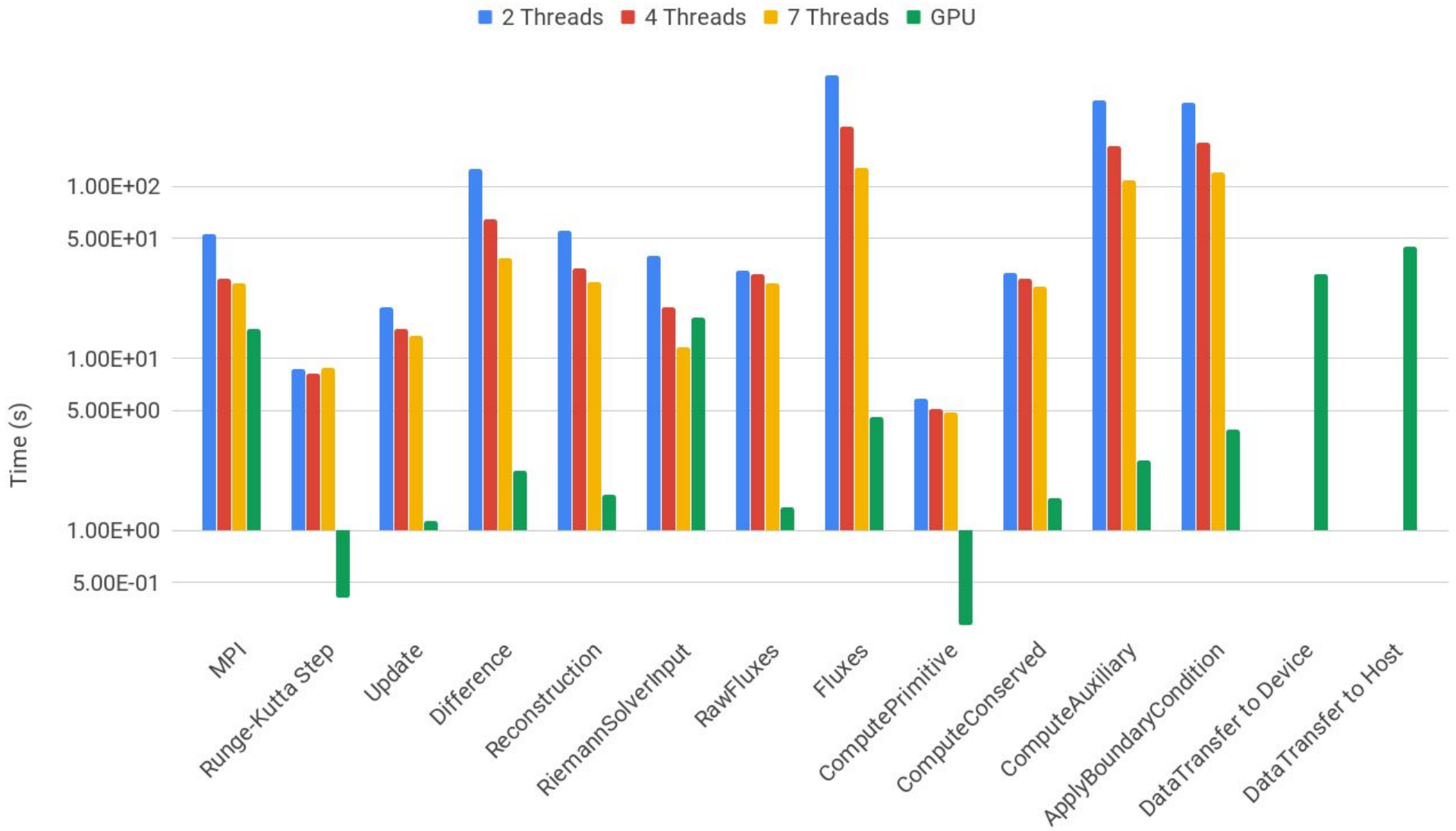
```
jsrun -r6 -c7 -g1 -a1 -bpacked:7
```

Performance Results: Weak-Scaling 3D RiemannProblem

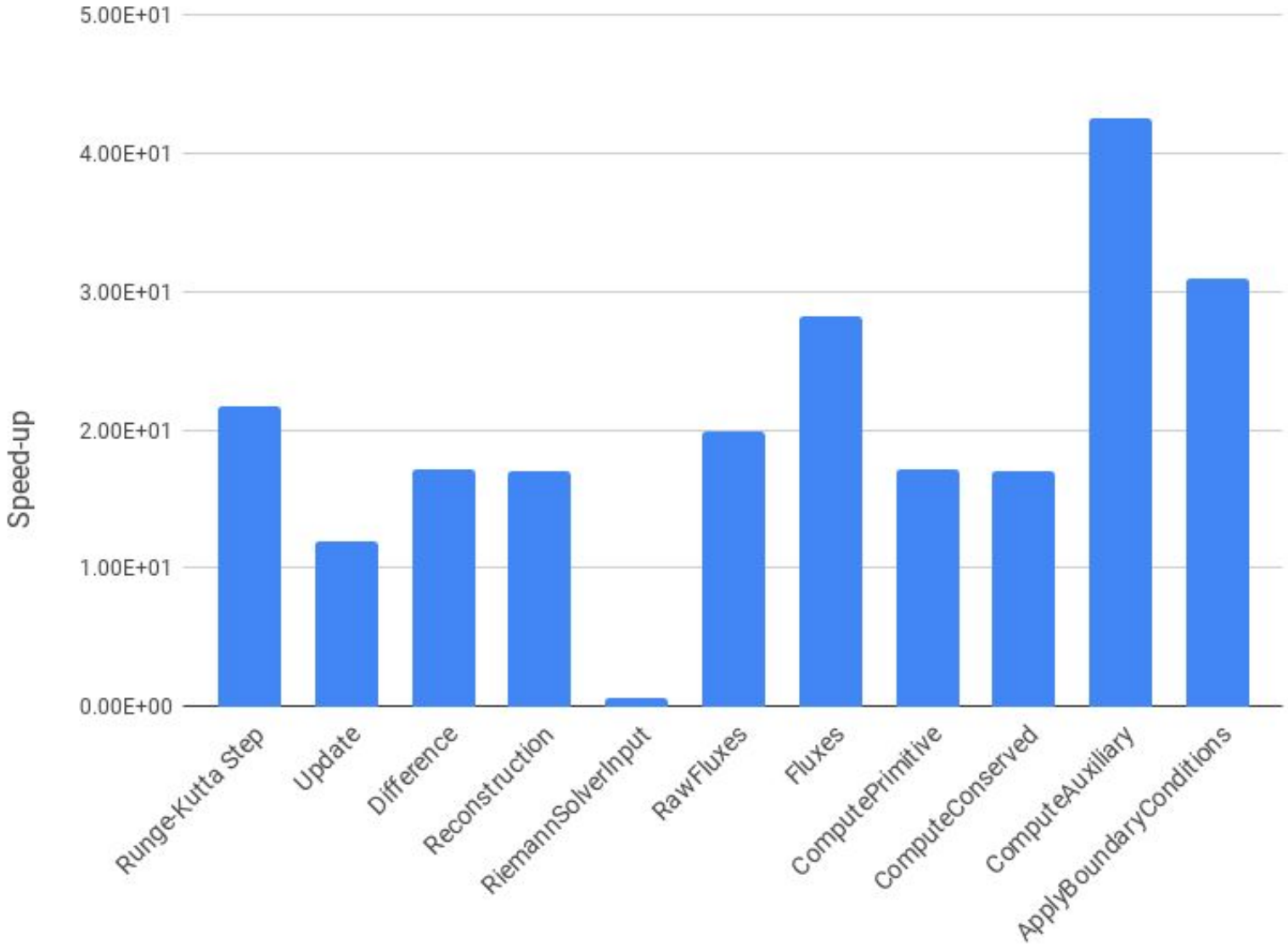


3.92X - 6.71X speedup from 7 CPU threads to GPU

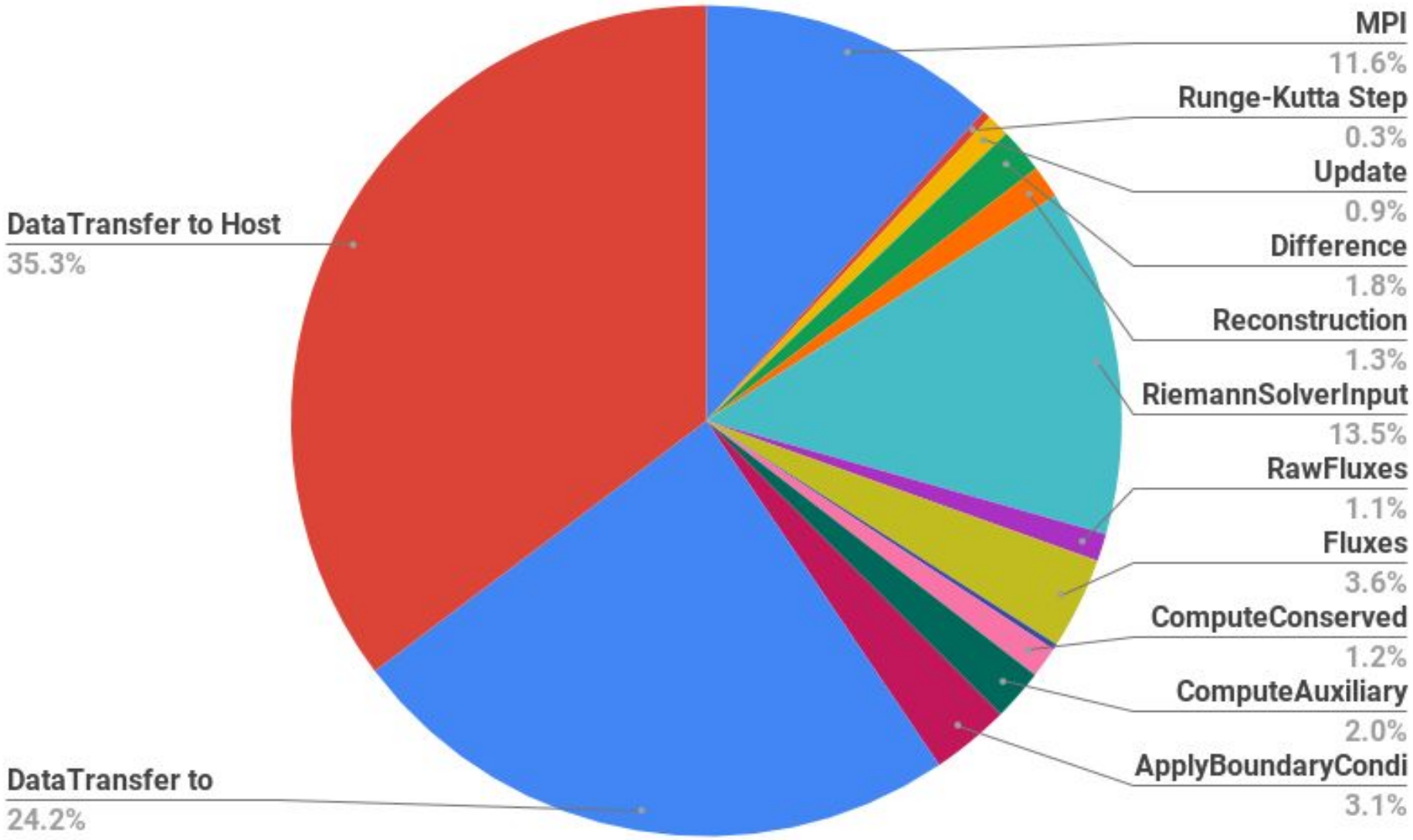
Performance Results: Kernel Timings



Performance Results: Kernel Speedups



Performance Results: Timing Distribution

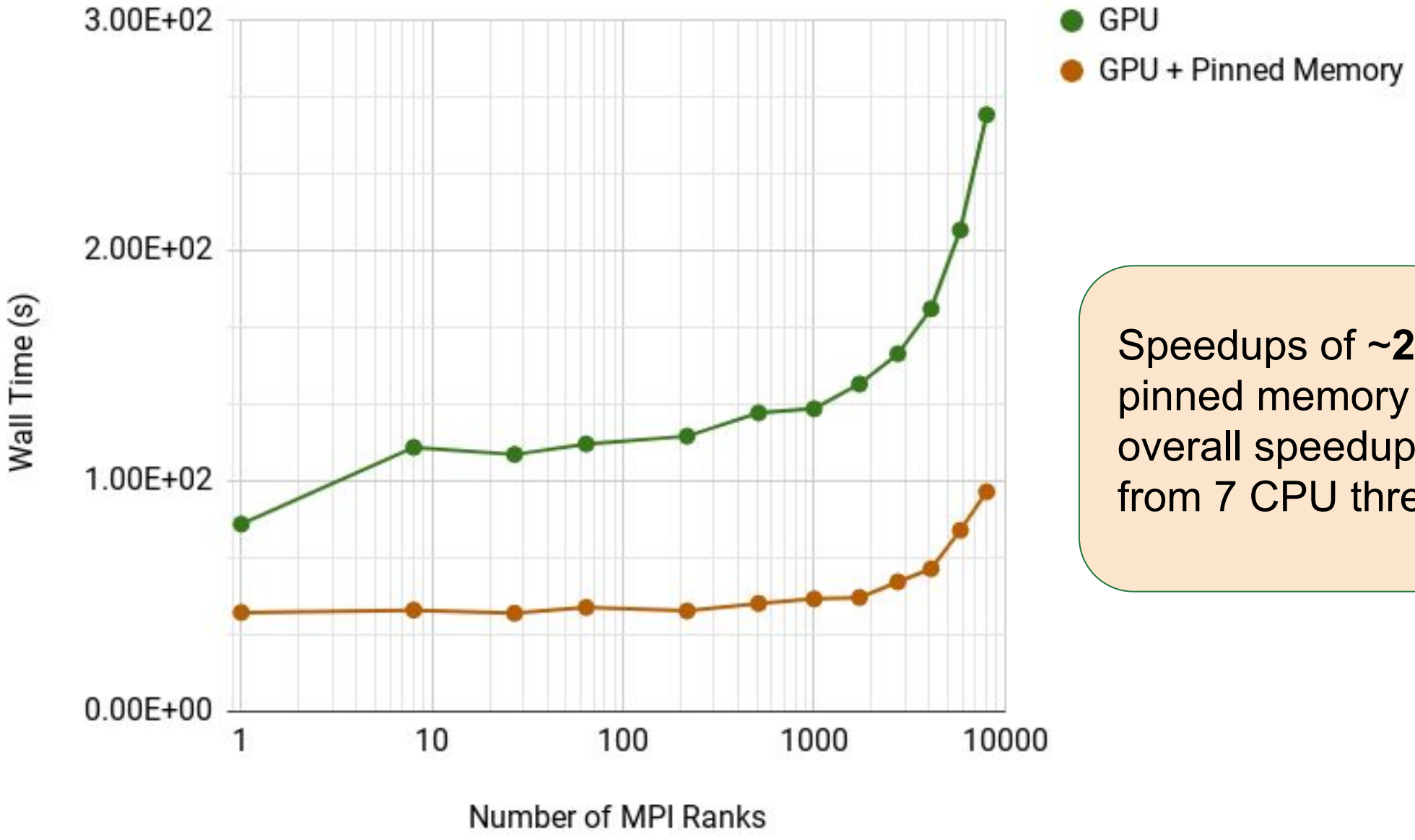


Beyond OpenMP: Using Pinned Memory

To optimize data transfers:

- pinned memory: page-locked host memory allocated using `cudaMallocHost()` or `cudaHostAlloc()`
- created another Fortran wrapper in GenASiS, used in `StorageForm` initialization method as an option
  `StorageForm % Initialize ( ..., PinnedOption = .true.)`
- No mechanism to do this with OpenMP 4.5 (but perhaps in 5.x)

Performance Results: Using Pinned Memory



Speedups of **~2.6X** when pinned memory is used → overall speedups of **over 12X** from 7 CPU threads

Implications (Then and Now)

- c. 2010: 1024^3 cells with 64000 processors (Jaguar), ~3s per timestep
  Now: 64 GPUs (11 nodes) on Summit, ~1.2s per timestep

- Enable us to do higher-fidelity simulations, ensemble studies for trends in observables
  - plan to perform ~200 2D grey transport supernova simulations, tens of 3D grey transport, and a handful of 3D spectral transport simulations

- First step towards full Boltzmann radiation transport (6-D problem + time) with exascale computing

Remaining Issues and Future Work

- A single code-base with OpenMP for multi-threading and offload
  - Fall back to multi-threading with `target if`-clause is problematic
  - `team distribute` directive introduce deleterious effects for multi-threading
- Kernel-launch parallelism and CUDA streams
  - no mechanism within OpenMP to affect and select stream
- Better compilers support for OpenMP 4.5 - 5.x
- Using CUDA-aware MPI for GPU Direct
  - benefit (vs. manual staging on host) depends on message sizes

Conclusion

- Using OpenMP allows for a simple and effective porting of Fortran code to target GPU
  - 2 - 3 months “walltime” efforts for this project
  - ~1 day / week “person time” efforts
- OpenMP 4.5 (and later) is a path to port code to GPU
  - more compilers are supporting OpenMP offload (XL, GCC, CCE, Intel, PGI, LLVM-based)
- Code available on http://github.com/GenASiS
  - paper describing this work in preparation