Asynchronous 3-D FFTs using OpenMP offload for extreme problem sizes

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What is the (3D) Fourier Transform, and why is it important?

Representing complex signals as sums of sines and cosines

- In wavenumber: $f(x) = \sum_k \hat{f}(k) \exp(ikx)$ or in frequency: $g(t) = \sum_\omega \hat{g}(\omega) \exp(i\omega t)$
- Forward transform: obtain set of coefficients from function values
- Inverse transform: obtain function values from the coefficients
- Can be extended to 3D in space: $f(\mathbf{x}) = \sum_{\mathbf{x}} \hat{f}(\mathbf{k}) \exp(i\mathbf{k} \cdot \mathbf{x})$
- Transforming one direction at a time:

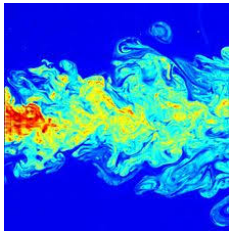
$$f(x,y,z) = \mathcal{F}_x^{-1}\left\{\mathcal{F}_y^{-1}\left\{\mathcal{F}_z^{-1}\left\{\hat{f}(k_x,k_y,k_z)\right\}\right\}\right\}$$

As effective methods of numerical solution of PDEs

- In some cases, equations governing $\hat{f}$ may be more readily solved numerically (which is our prime motivation in this talk)

Science Motivation: The Challenge of Fluid Turbulence

- Disorderly fluctuations over a wide range of scales in 3D space and time
- A physical problem of great complexity, and a critical factor in many disciplines



- Governing equations are known, but mathematically intractable
- Experiments, theory, modeling, computation all useful yet imperfect.
- Better physical understanding is required (e.g. think Covid-19)

Computing Turbulence: Direct Numerical Simulations

- Separate instantaneous velocity field into the sum of an averged state, and departures (fluctuations) from that state
- Form and solve (numerically) equations for the fluctuations
- Simplified geometries: periodic boundary conditions compatible with Fourier decompositions are numerically advantageous and physically useful.
- State-of-the-art around 2000 was 1024^3
- 4096^3 (Kaneda *et al*) on Earth Simulator in Japan, 2003
- In 2019 we reached world-leading $18,432^3$ using CUDA Fortran on Summit

Looking towards even larger problem sizes using OpenMP offload for portability

Navier-Stokes equations and Fourier pseudo-spectral methods

- Numerical solution of PDE governing velocity field $\mathbf{u}(\mathbf{x}, t)$

$$\partial \mathbf{u}/\partial t + (\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla(p/\rho) + \nu\nabla^2\mathbf{u} + \mathbf{f}$$

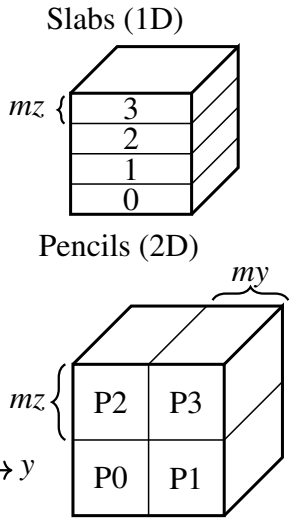
- Fourier decomposition: $\mathbf{u}(x,t) = \sum_{\mathbf{k}} \hat{\mathbf{u}}(\mathbf{k}) \exp(i\mathbf{k}\cdot\mathbf{x})$. In equation for Fourier coefficients nonlinear terms lead to convolution integrals, requiring $\sim N^6$ operations
- "Pseudo-spectral": form products first by multiplication in physical space, before transforming to wavenumber space. Fast Fourier Transform (FFT) $\propto N^3 \ln_2 N$ — but communication is required to make complete lines of data available.
- Aliasing errors in nonlinear terms: use truncation and phase-shifts (Rogallo 1981)
- Cost of simulation per step tied to a number of forward and backward transforms.

Efficient distributed 3D FFT on GPUs forms a key component

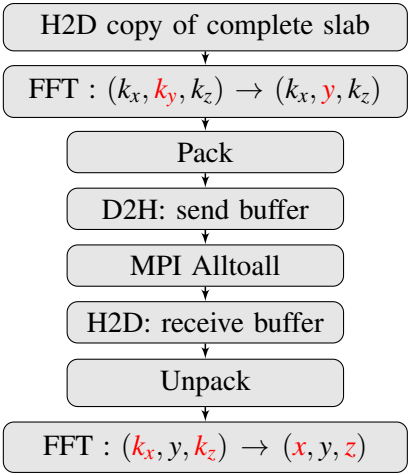
Domain Decomposition: 1D or 2D?

How best to distribute memory among P MPI tasks?

- 1D: Each MPI rank holds a slab
  — one global transpose among all processes ($x-y$ to $x-z$)
- 2D: Each rank holds a pencil
  — two transposes, within row and column communicators
- Pencils used for most large simulations (e.g. we ran 8192^3 using 262,144 MPI tasks on Blue Waters at NCSA)
- Fatter nodes and more GPUs per node: return to slabs?
  — GPU parallelism instead of distributed memory (MPI)
  — fewer nodes (and MPI tasks) in communication
  — associated pack and unpack operations are simplified



A basic (Synchronous) GPU algorithm

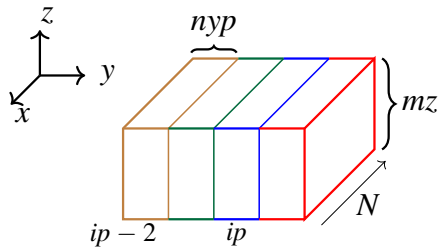


- Copy entire slab from CPU (host (H)) to GPU (device (D)) and back to CPU at end
- 1D FFTs in y, z, x directions using cufft library
- Pack and unpack data on GPU: faster than CPU
- MPI Alltoall among all tasks to transpose $x-y$ to $x-z$ slabs
- D2H and H2D copies of send and receive buffers before and after Alltoall
- Similar operations to transform back to wavenumber space from physical space

Large problem that may not fit on GPU? Any asynchronism possible?

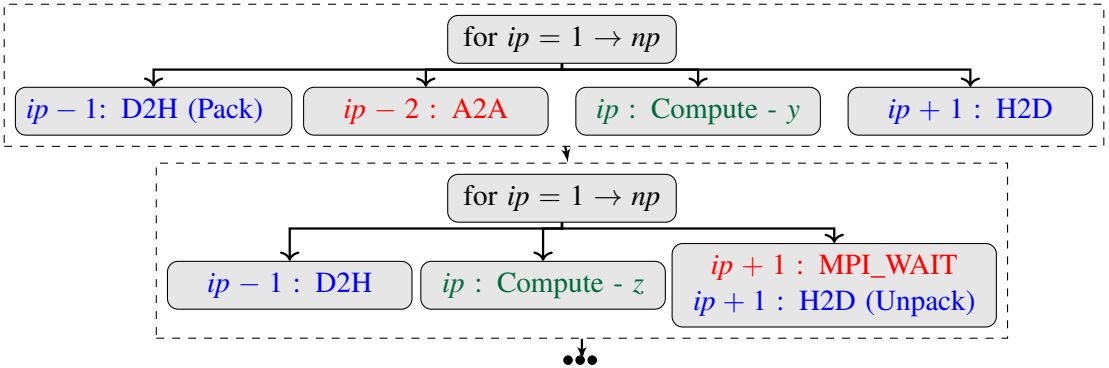
New batched asynchronous algorithm

- Divide slab into *np* pencils and process each pencil separately ($nyp = nxp = N/np$)
- Overlap operations on different pencils to hide some data transfer and compute costs



- Overlap using one stream each (in CUDA Fortran) for data transfer and compute
- Overlap: Compute on *ip*, HtoD on $ip + 1$, DtoH on $ip - 1$ and all-to-all on $ip - 2$
- Non-blocking all-to-all allows overlap, `MPI_WAIT` ensures completion
- GPU-Direct can be used to avoid copies before and after all-to-all
- Repeat until all pencils (*np*) processed on GPU and transposed

Batched asynchronism: Illustrated via operations in y and z



- Operations on same row executed asynchronously but launched from left to right
- Pack and unpack: strided data copy to avoid reordering data before transpose
- Non-blocking all-to-all allows overlap. Call MPI_WAIT before compute

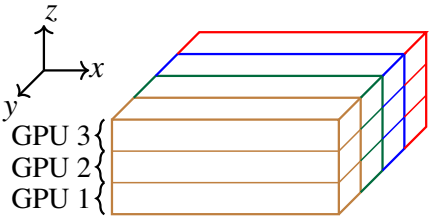
How many tasks per node?

Based on Summit node architecture

- 6 tasks per node: 1 task per GPU
- 2 tasks per node: 3 GPUs per task
  - — OpenMP threads to launch operations to GPUs
  - — 3 times fewer MPI tasks, 3 times larger message size

Number of pencils per all-to-all

- Does it affect the performance?
- 1 pencil at a time
  - — overlap MPI with data movement and compute
- Entire slab (*np* pencils) at a time
  - — no MPI overlap with data movement and compute
  - — *np* times larger message size and fewer MPI calls



Each pencil further divided vertically among multiple GPUs

MPI performance and strided copies

MPI performance occupies a significant fraction of runtime

- Message size between processes in *all-to-all* increases as number of processes decrease: reduce communication overhead and latency
- Transpose multiple pencils together: further increases message size

Many strided copies are needed: compute on part of slab, pack, unpack

- *zero-copy* (Appelhans 2018): GPU initiates many small transfers to/from host pinned memory; uses GPU compute resources for data transfer
- `cudaMemCpy2DAsync`: CUDA library call can handle simple strides without using GPU compute resources

More details on optimization can be found in Ravikumar *et al.* 2019

Fewer MPI tasks; zero-copy & MemCpy2D: optimal strided copies

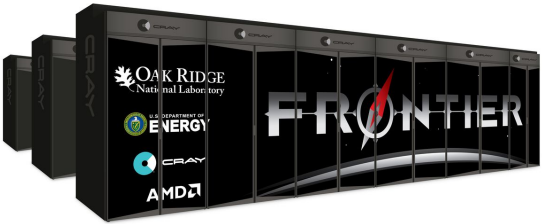
Batched asynchronous code performance (CUDA Fortran)

- Performance data collected on Summit
  — 2nd order Runge Kutta, 3 inverse and 5 forward transforms, 2 substages per timestep

Nodes	Problem Size	Time(s)			
		Sync CPU (Pencils)	Async GPU		
			6 tasks/node	2 tasks/node	
				1 pencil/A2A	1 slab/A2A
16	3072^3	34.38	8.09	6.70	7.50
128	6144^3	40.18	12.17	8.66	8.07
1024	12288^3	47.57	13.63	12.62	10.14
3072	18432^3	41.96	25.44	22.30	14.24

- 2 tasks/node performs better than 6 task/node for all problem sizes tested
- 128 nodes and above: 1 slab/A2A better than 1 pencil/A2A
  — suggests better overall performance without MPI overlapping GPU operations
- $18{,}432^3$: $\sim$ 3X speedup to pencils CPU version; communication bound code

Porting to future exascale architectures



- AMD CPU w/ 4 AMD GPUs per node
- Program GPUs: HIP, OpenMP

- 2 Intel CPUs w/ 6 Intel GPUs per node
- Program GPUs: oneAPI, OpenMP

Support for CUDA Fortran is not likely. Need efficient portable implementation.

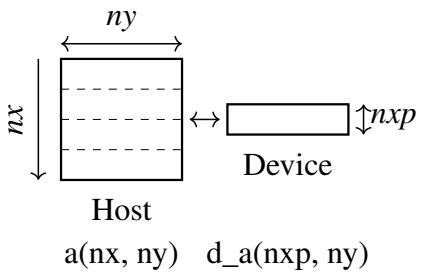
OpenMP is widely accepted standard and a clear favorite for Fortran

Non-contiguous maps and strided copies

- FFTs in *y*: need only *a(1:nxp, 1:ny)* on device
- In CUDA Fortran use: `cudaMemCpy2DAsync`

How to do it in OpenMP?

- `MAP(to:a(1:nxp, 1:ny))`: not 5.0 compliant
- Using `omp_target_memcpy_rect`
  — copy rectangular subvolume from a nD array
  — similar to 2D strided copies in CUDA
  — `TASK` for asynchronism (5.1: async version)
  — need C-FORTRAN interface (5.0 and lower)
- Using *zero-copy* kernels: GPU initiates many small transfers to/from host pinned memory [Appelhans GTC 2018]




```
1 omp_target_memcpy_rect (dst, src, elem_size, &
2     ndims, vol, dst_offset, src_offset, dst_dims, &
3     src_dims, dst_dev, src_dev)
```

OpenMP 4.5+: `omp_target_memcpy_rect`?

- Copy rectangular subvolume from a multi-dimensional array
- Callable from C/C++, use C-Fortran interface
- *ndims*: no. of dimensions in array
- *vol*: no. of elements to copy in each dimension
- *offset*: no. of elements from *base of each dimension*, after which to copy data from/to
  – In 5.0: from *origin of dst (src)*, need clarity
- *dims*: no. of elements in each dimension
- Need to account for C vs. Fortran ordering
  – first dimension along row (*ny*) even though in Fortran it is along column

```
1  ! src on host of shape (nx, ny)
2  ! dst on device of shape (nxp, ny)
3
4  ! copy src(1:nxp, 1:ny) to dst(1:nxp, 1:ny)
5
6  num_dims = 2
7  vol(1) = ny ; vol(2) = nxp
8   dst_offset (1) = 0 ;  dst_offset (2) = 0
9   src_offset (1) = 0 ;  src_offset (2) = 0
10 dst_dims(1) = ny ; dst_dims(2) = nxp
11 src_dims(1) = ny ; src_dims(2) = nx
12
13 omp_target_memcpy_rect(dst, src, elem_size,
    ndims, vol, dst_offset , src_offset ,
    dst_dims, src_dims, dst_dev, src_dev)
```

Zero-copy kernels for complex strided copies

```
1  TARGET ENTER DATA MAP(to:d_buf) &
2  DEPEND(IN:indep) DEPEND(OUT:tdep) NOWAIT
3
4  TARGET TEAMS DISTRIBUTE PARALLEL DO &
5  COLLAPSE(4) IS_DEVICE_PTR(h_buf) &
6  DEPEND(INOUT:tdep) NOWAIT
7  do yg=1,numtasks
8     do z=1,mz
9        do y1=1,my
10          do x=1,nx
11             y = my*(yg-1)+y1
12             d_buf(x,y,z) = h_buf(x,z,y1,yg)
13          end do
14       end do
15    end do
16 end do
17 END TARGET TEAMS DISTRIBUTE PARALLEL DO
18
19 TARGET EXIT DATA MAP(from:d_buf) &
20 DEPEND(IN:tdep) DEPEND(OUT:outdep) NOWAIT
```

- GPU threads copy data to device buffer (`d_buf`) by directly accessing host resident **pinned** memory (`h_buf`)
- `IS_DEVICE_PTR` to make the host buffer accessible to GPU threads
- `h_buf` is dummy argument, separate subroutine with `h_buf` passed into it
- Strided read and write, transpose y and z
- Uses GPU compute resources for copy, slows down other computes
- Best for more complex stride patterns, like unpacking

Interoperability between OpenMP and non-blocking libraries

```
1  TARGET DATA MAP(tofrom: a)
2
3  TASK DEPEND(out:var)                                    Ⓐ
4
5  TARGET DATA USE_DEVICE_PTR(a)
6  FFTExecute (a, forward, stream)
7  FFTExecute (a, inverse , stream)
8  END TARGET DATA
9
10 END TASK
11
12 ! Copy or compute on other data                         Ⓒ
13
14 TARGET TEAMS DISTRIBUTE DEPEND(IN:var) NOWAIT
15 a(:, :, :) = a(:, :, :)/nx                              Ⓑ
16 END TARGET TEAMS DISTRIBUTE
17
18 END TARGET DATA
```

- Ⓐ: launch FFT kernel to GPUs
- Ⓑ waits as dependent on Ⓐ
- Ⓒ executes asynchronously
- Ⓐ finishes prematurely once FFTs launched, does not wait for kernels to finish executing on GPU
- Ⓑ starts to run before FFTs complete on GPU, incorrect results

Timeline: OpenMP and non-blocking library

Asynchronous execution of cudaFFT library and OpenMP TARGET loop

- `TASK DEPEND` used to establish synchronization between FFT & TARGET loop
- Host thread launches FFT & then GPU compute before FFT completes
- `Detach` in OpenMP 5.0: signals event completion for depending tasks to continue

OpenMP 5.0 features critical for asynchronism

DETACH to enforce synchronization

```
1  TARGET DATA MAP(tofrom: a)
2
3  TASK DEPEND(out:var) DETACH(event)
4
5  TARGET DATA USE_DEVICE_PTR(a)  Ⓐ
6  FFTExecute (a, forward, stream)
7  FFTExecute (a, inverse , stream)
8  END TARGET DATA
9
10 cudaStreamAddCallback (stream, ptr_callback, C_LOC(event), 0)
11 END TASK
12
13 ! Copy or compute on other data  Ⓒ
14
15 TARGET TEAMS DISTRIBUTE DEPEND(IN:var) NOWAIT
16 a (:, :, :) = a (:, :, :) /nx                    Ⓑ
17 END TARGET TEAMS DISTRIBUTE
18
19 END TARGET DATA
```

```
1 subroutine callback (stream, status, event)
2   type( c_ptr ) :: event
3   integer(kind=omp_event_handle_kind) :: f_event
4   call C_F_POINTER (event, f_event)
5   call omp_fulfill_event( f_event )
6 end subroutine callback
```

- Ⓐ: launch FFT, add *callback* in stream where FFT will run
- Ⓑ waits as dependent on Ⓐ, Ⓒ executes asynchronously
- Ⓐ finishes after event fulfilled by *callback*

Porting asynchronous CUDA Fortran to OpenMP

```
1  do ip=1,np
2      NEXT = mod(ip+1,3); CURR = mod(ip,3);
3      PREV = mod(ip−1,3); COMM = mod(ip−2,3);
4      cudaStreamWaitEvent (trans_stream, DtoH(NEXT), 0)
5      cudaMemCpy2DAsync (abuf(NEXT),a(ip+1),trans_stream)
6      cudaEventRecord (HtoD(NEXT),trans_stream)
7      cudaStreamWaitEvent (comp_stream, HtoD(CURR), 0)
8      FFTExecute  (abuf(CURR), comp_stream)
9      cudaEventRecord (comp(CURR), comp_stream)
10     cudaStreamWaitEvent (trans_stream, comp(PREV), 0)
11     cudaMemCpy2DAsync (snd(ip-1), abuf(PREV), &
12         trans_stream)
13     cudaEventRecord (DtoH(PREV), trans_stream)
14     cudaEventSynchronize (DtoH(COMM))
15     MPI_IALLTOALL (snd(ip-2))
16 end do
```

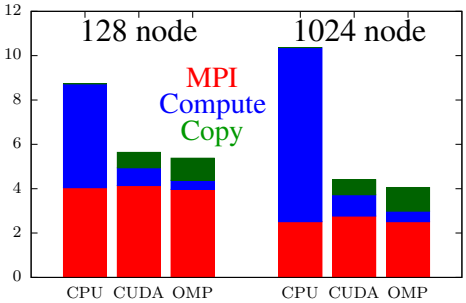
```
1  do ip=1,np
2      NEXT = mod(ip+1,3); CURR = mod(ip,3);
3      PREV = mod(ip−1,3); COMM = mod(ip−2,3);
4      TASK DEPEND (IN:DtoH(NEXT), OUT:HtoD(NEXT))
5      omp_target_memcpy_rect (abuf(NEXT), a(ip+1))
6
7      TASK DEPEND (IN:HtoD(CURR), OUT:comp(CURR))
8          DETACH(event)
9      FFTExecute  (abuf(CURR), comp_stream)
10     TASK DEPEND (IN:comp(PREV), OUT:DtoH(PREV))
11     omp_target_memcpy_rect (snd(ip−1),  abuf(PREV))
12
13
14     TASK DEPEND(IN:DtoH(COMM))
15     MPI_IALLTOALL (snd(ip-2))
16 end do
```

- `DEPEND` clause replaces `cudaEventRecord` & `cudaStreamWaitEvent`
- `omp_target_memcpy_rect` replaces `cudaMemCpy2DAsync`

Performance: Non-Batched synchronous version

Summit (XL compiler) up to 1024 nodes ($\sim 22\%$ of full machine) using 1 task/GPU
Timings for 3 pairs of forward and inverse transforms

# Nodes	Prob. Size	Time (s)		
		CPU	CUDA	OMP
2	1536^3	5.21	2.39	2.41
16	3072^3	6.79	3.30	3.16
128	6144^3	9.10	5.26	5.01
1024	12288^3	10.59	4.30	4.12

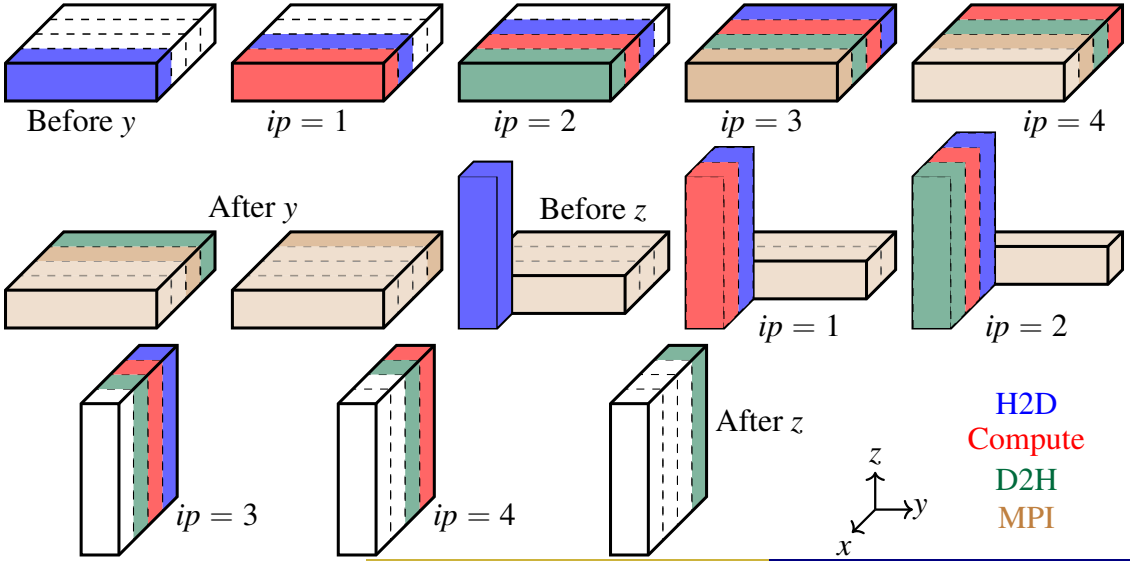


- OpenMP & CUDA show similar performance ($\sim$ 2.6X speedup for $12k^3$)
- GPU: compute negligible but additional cost due to copies, 62% in MPI
- OpenMP data copies slower than in CUDA, but compute faster !
- OpenMP code also works with CCE compiler and AMD GPUs

Summary and Future Work

- Developed algorithm for Summit using CUDA Fortran to run 18432^3 problem size
- Preliminary steps taken towards portability using OpenMP for offload
- Some challenges of portability overcome, some pending full OMP 5.0 availability
- Strided copy b/w small device & larger host arrays: `omp_target_memcpy_rect`
- Synchronizing non-blocking GPU library calls & OpenMP tasks: `DETACH`
- Future work towards 3D FFTs at massive scale, at resolution beyond $18{,}432^3$
  - Batched asynchronism algorithm (using `DETACH`) needed for optimal performance
  - A framework for portable GPU parallelism for communication-intensive applications

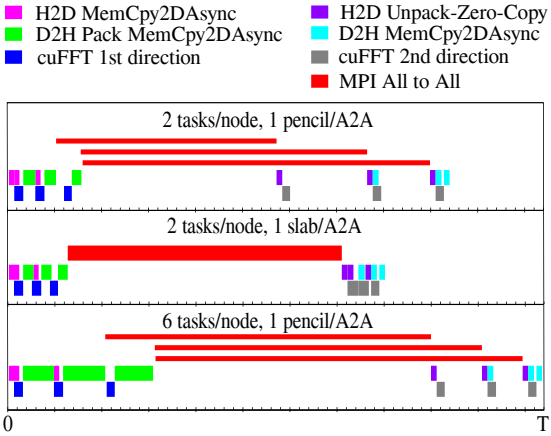
Batched async. algorithm: additional details



Timeline and asynchronous MPI analysis

- Slab/A2A better to pencil/A2A?
  - Faster MPI of data as one large msg
- Why is 2 tasks/node better than 6?
  - Each MPI longer: small P2P, more tasks
  - Slow pack: 3X Cpy2D, high overhead
  - Use ZC: steals GPU resources slowing 2 tasks/node

Normalized timeline of $12,288^3$ on 1024 nodes



MPI dominates runtime; No MPI overlap shows best performance

Performance: Batched version

- OpenMP version: copy on host from large buffer to small buffer before `UPDATE` (workaround)
  – `omp_target_memcpy_rect` slow compared to workaround and `cudaMemCpy2D`
- $6k^3$ OMP is 16.1s slower than CUDA async
  – 12.4s to copy one buffer to another on host
  – 3.7s (or 20%) saving due to asynchronism?
- Work in progress: optimize OpenMP version
  – Fast rectangular copy to avoid host operations
  – DETACH will help enable asynchronism
- Both OMP codes work with CCE & AMD GPUs

6 pencils per slab
Performance on Summit using XL
OpenMP version uses workaround

# Nodes	Prob. Size	Time (s)	
		CUDA async	OMP sync
4	3072^3	10.14	26.20
32	6144^3	13.53	29.64

Production code using CUDA: $18k^3$ on $3k$ nodes, $\sim$ 3X speedup