Braiding a Million Threads: Scalable GPU Sort on Frontier

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Path of Research

- Transition from Summit to Frontier
- Georgia Tech GPU API – Akihiro Hiyashi
- Performance on Frontier
- Chapel GPU Code Generation

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Accelerating Arkouda with GPUs

https://github.com/Bears-R-Us/arkouda

- Arkouda promises 'HPC-enabled exploratory data analytics'
- Compute on large data → memory bandwidth

	CPU-DRAM	GPU-HBM
Summit (2018)	340 GB/s	2,700 GB/s
Frontier (2022)	205 GB/s	13,080 GB/s

- Challenges:
  - algorithmic portability
  - memory management
  - programmability

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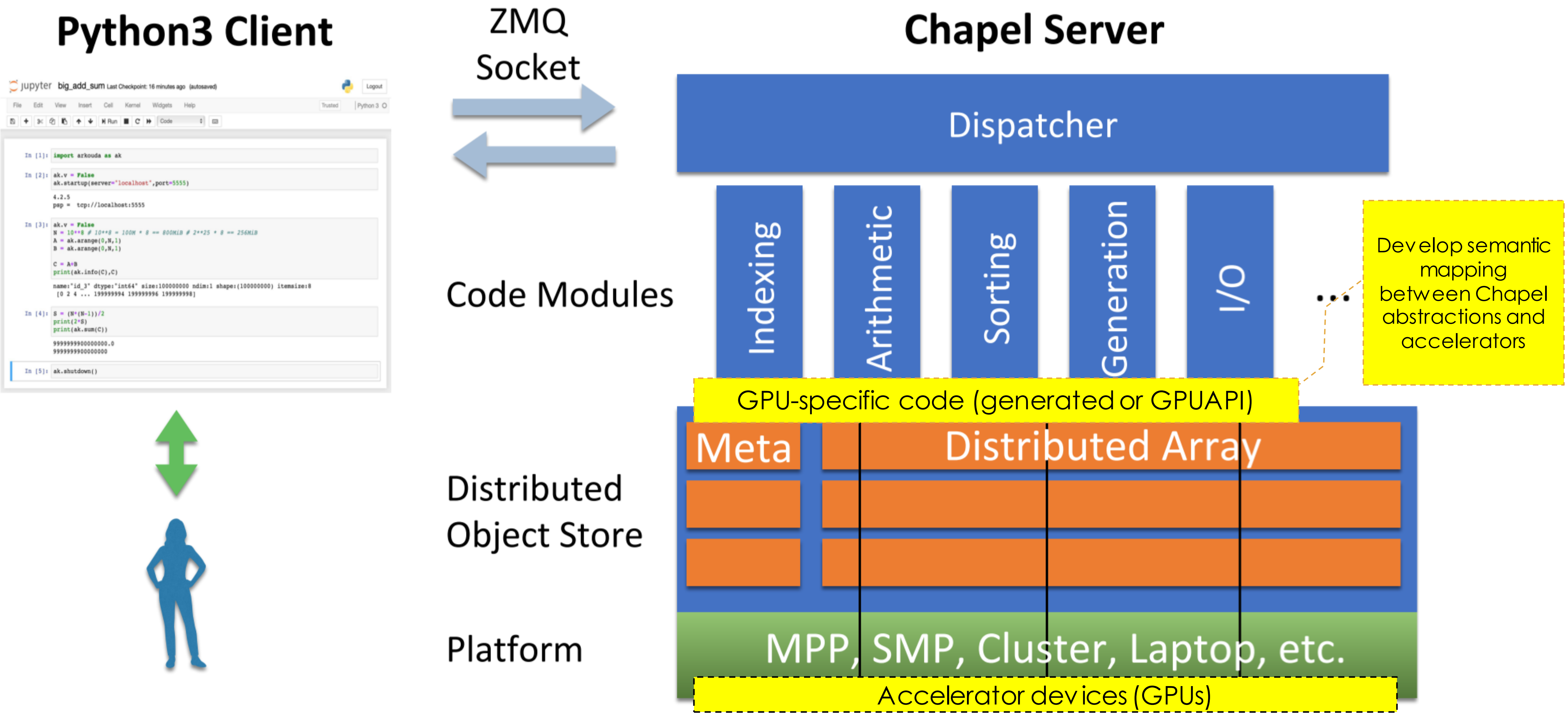
How our GPU code fits into Arkouda



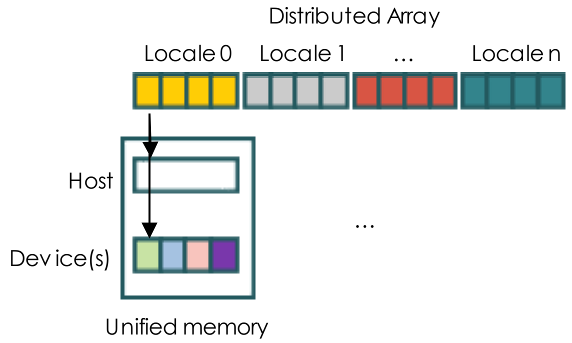
Georgia Tech Chapel GPU API

- Georgia Tech-developed framework abstracting over GPU programming models (CUDA, HIP, DPC++, SYCL)
- `GPUIterator`: exposing parallelism for kernel launch
  - low-level
- `GPUAPI`: device and memory management
  - low-mid-level: C-interoperability wrappers around device functions
  - mid-level: `GPUArray` to manage memory allocation, transfer
  - there is no high-level

GPUUnifiedDist: Arkouda Arrays in Shared Virtual Memory

- Host and device(s) share pointers to a single unified memory space
- Any access to memory that is currently in a different physical memory will result in a page fault, handled transparently with hardware support
- User-defined Chapel distribution `GPUUnifiedDist`
  - based on `BlockDist`
  - allocates memory for `LocGPUUnifiedArr` using `makeArrayFromPtr(umemPtr, …)`

```
module SymArrayDmapCompat …
proc makeDistDom(size:int, param GPU:bool = false) where GPU == true {
  select MyDmap {
    when Dmap.blockDist {
      return {0..#size} dmapped gpuUnifiedDist(…);
    }
    …
  }
}
```

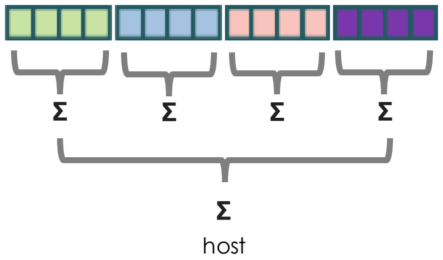


https://github.com/milthorpe/chapel-gpu
https://github.com/milthorpe/arkouda

Example: Sum on GPU (unified memory), GPU API

$$\sum_{i=0}^{n-1} A_i$$

`ak_arr.sum()`



Device memory allocation

Data transfer

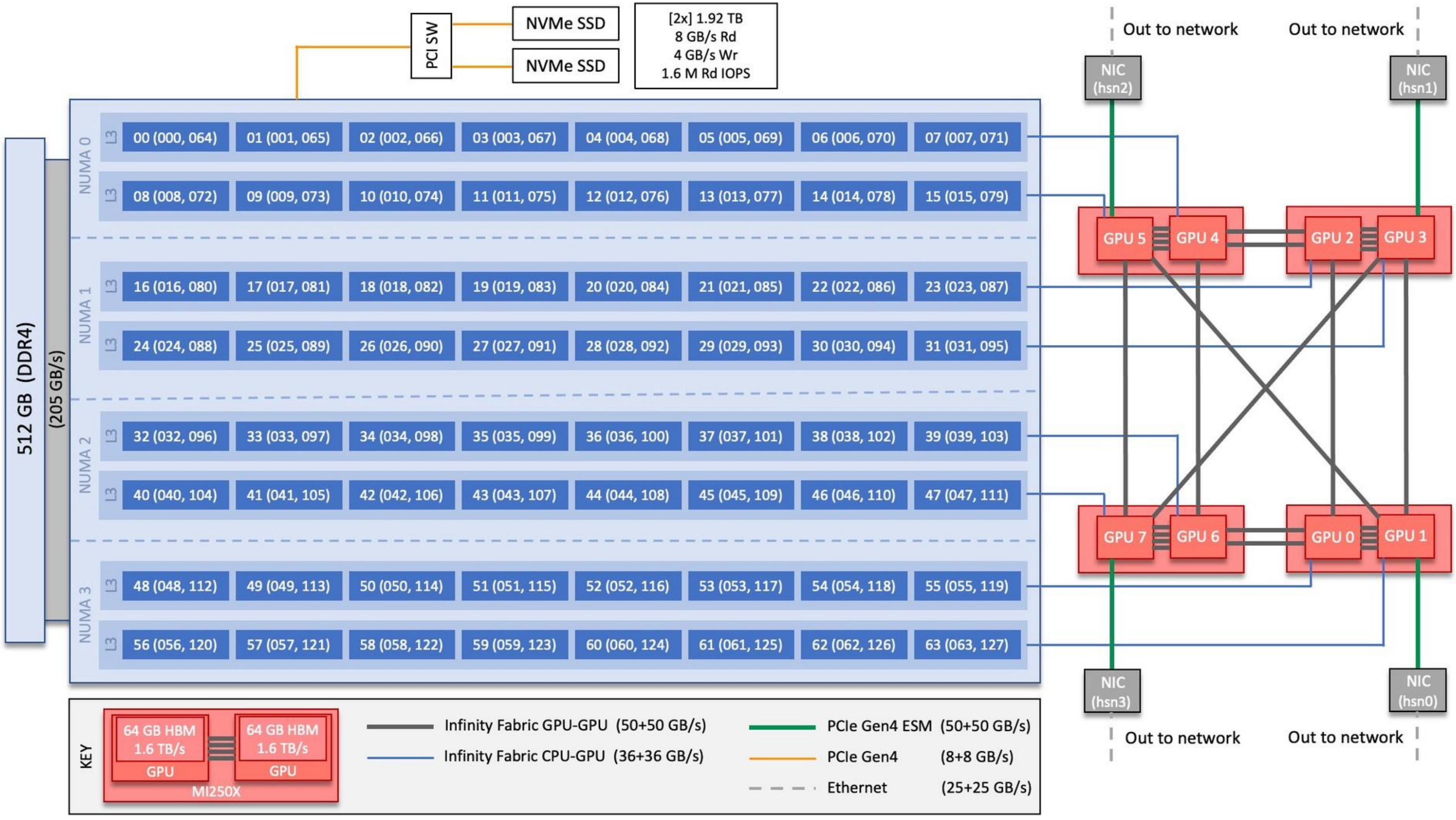
Synchronization

```
use GPUIterator;
use GPUAPI;

extern proc launchSum(devInPtr: c_void_ptr, devOutPtr: c_void_ptr, n: int): etype;

proc cubSum(ref e: SymEntry) where e.GPU == true {
  var deviceSum: [0..#nGPUs] e.etype;
  var sumCallback = lambda(lo: int, hi: int, n: int) {
    var devOut = new GPUArray(deviceSum[deviceId]);
    var deviceId: int(32);
    GetDevice(deviceId);
    e.prefetchLocalDataToDevice(lo, hi, deviceId);
    launchSum(e.c_ptrToLocalData(lo), devOut.dPtr(), n);
    DeviceSynchronize();
    devOut.fromDevice();
  };
  forall i in GPU(e.a.localSubdomain(), sumCallback) { }
  return (+ reduce deviceSum);
}
```

Frontier - Experimental Evaluation

- Evaluation platform: OLCF Frontier (+Crusher)
  - 1 × 64-core AMD EPYC 7A53 CPU @ 2.75GHz
  - 512 GiB DDR4 DRAM
  - 4 × AMD MI250X GPUs with 128 GiB HBM2E
  - Logically divided into 8 GPUs / 64 GiB HBM
  - ROCM 5.4.0
  - AMD driver version 6.1.5
- Arkouda Radix Sort LSD (Least Signficant Digit)
- Timing server-side Arkouda Chapel code directly (not from Python client)
  - Doesn't allow batching of communications

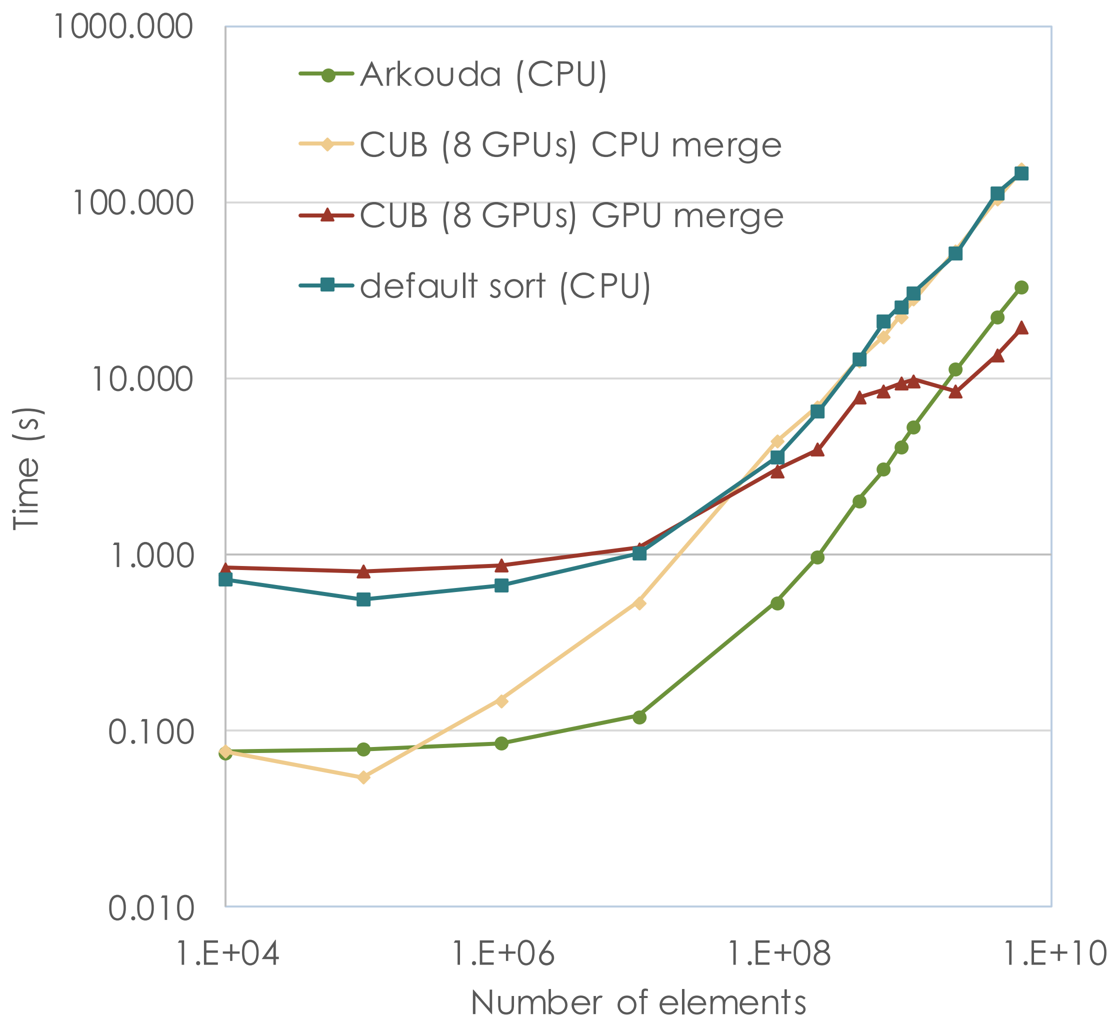
Frontier - Compute Node Schema



Sort (Frontier, single-node)

- Arkouda (CPU)
  `radixSortLSD_keys`
- Kernel:
  - CUB library
    `DeviceRadixSort::SortKeys`
  - merge on CPU:
    K-way merge
  - GPU merge:
    peer-to-peer swap and merge

Tobias Maltenberger, Ivan Ilic, Ilin Tolovski, and Tilmann Rabl. (2022) *Evaluating multi-GPU sorting with modern interconnects.* Intl. Conf. Management of Data. https://doi.org/10.1145/3514221.3517842




```
ak_df.sort_values()
```

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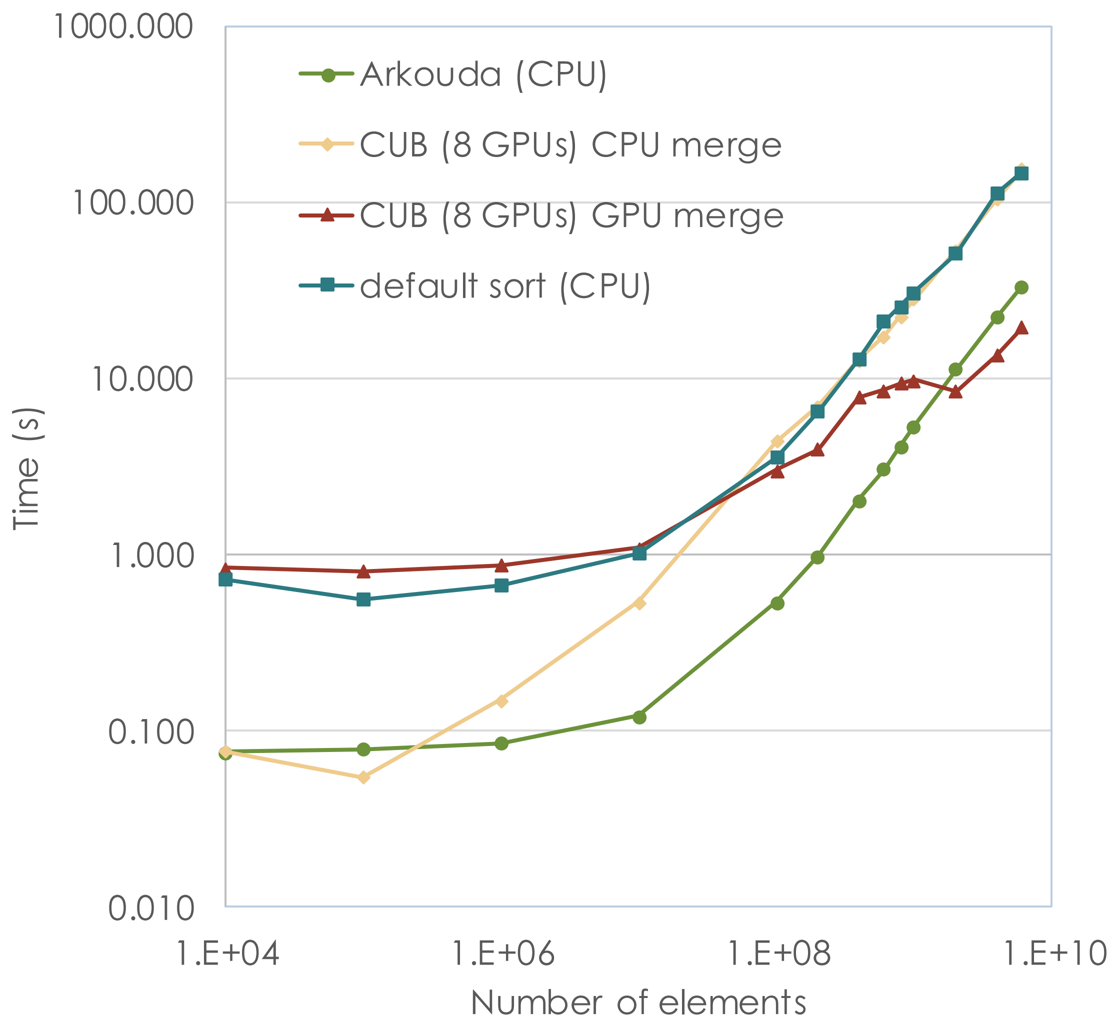
Sort (Frontier, single-node cont.)

- GPU peer-to-peer merge beats Arkouda CPU for large data
- Approx. 60% of time is data transfer to/from GPU – can be eliminated if Arkouda arrays reside in GPU HBM

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Sort (Frontier, multi-node)

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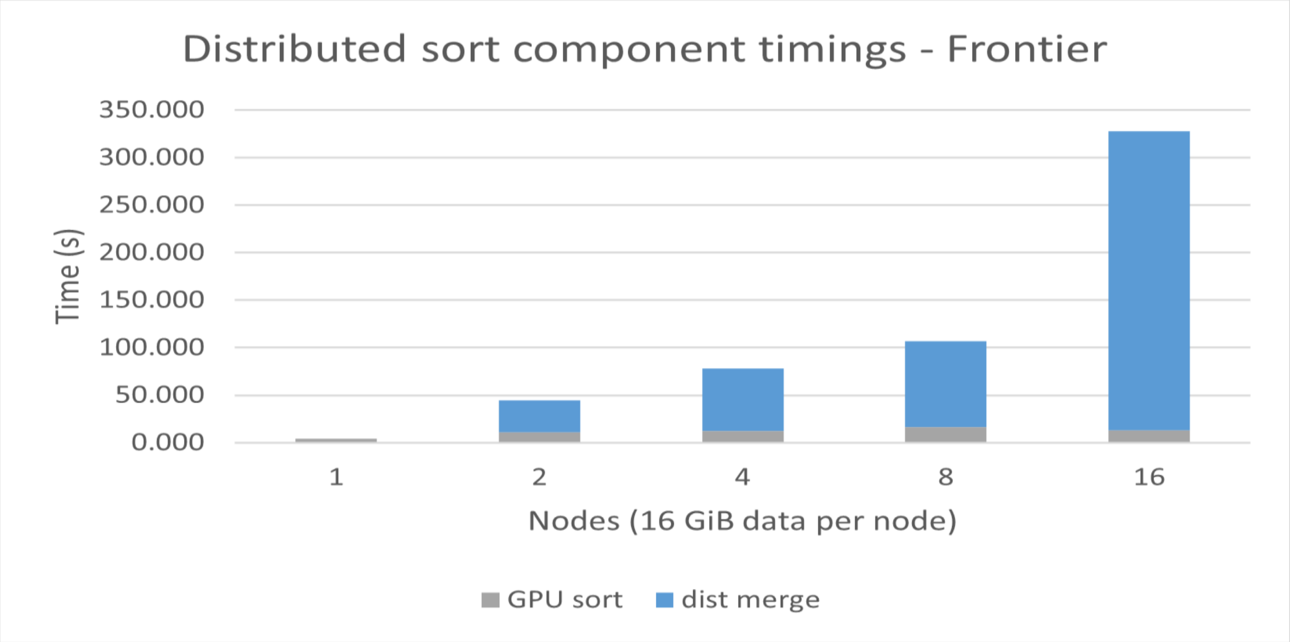
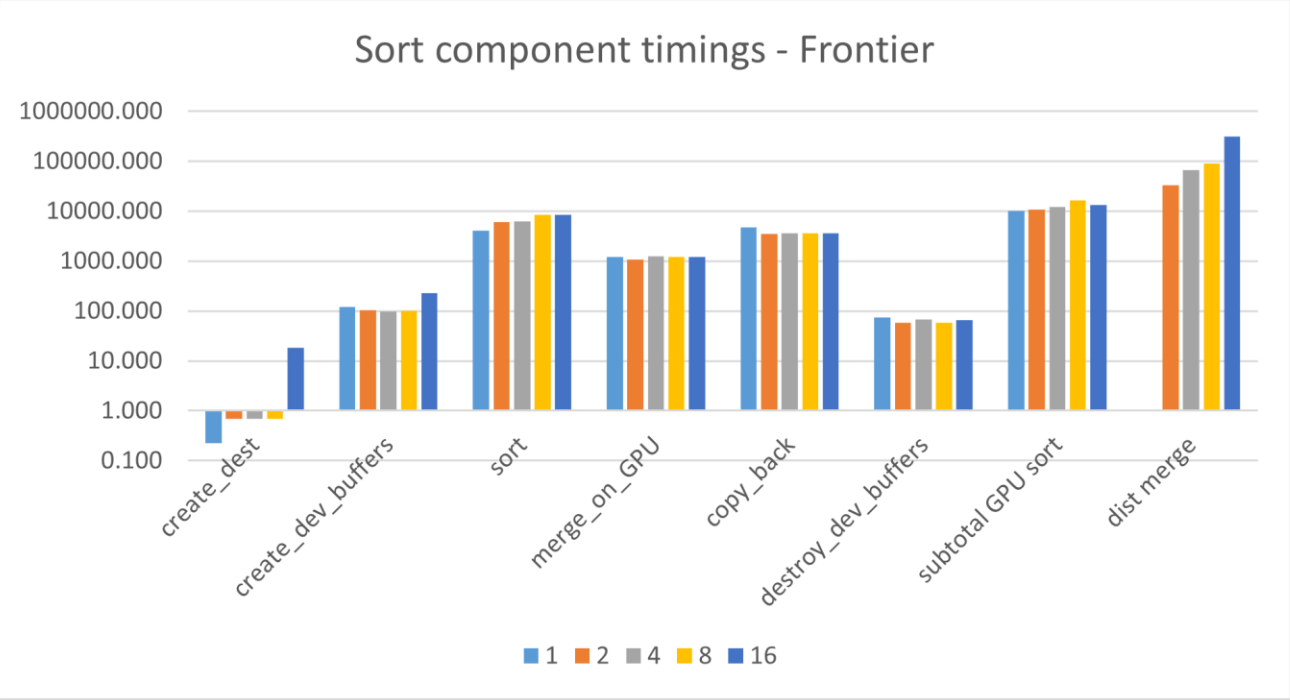
  - Inter-node merge:
    peer-to-peer swap and merge
    in host memory - O(n log n)

`ak_df.sort_values()`





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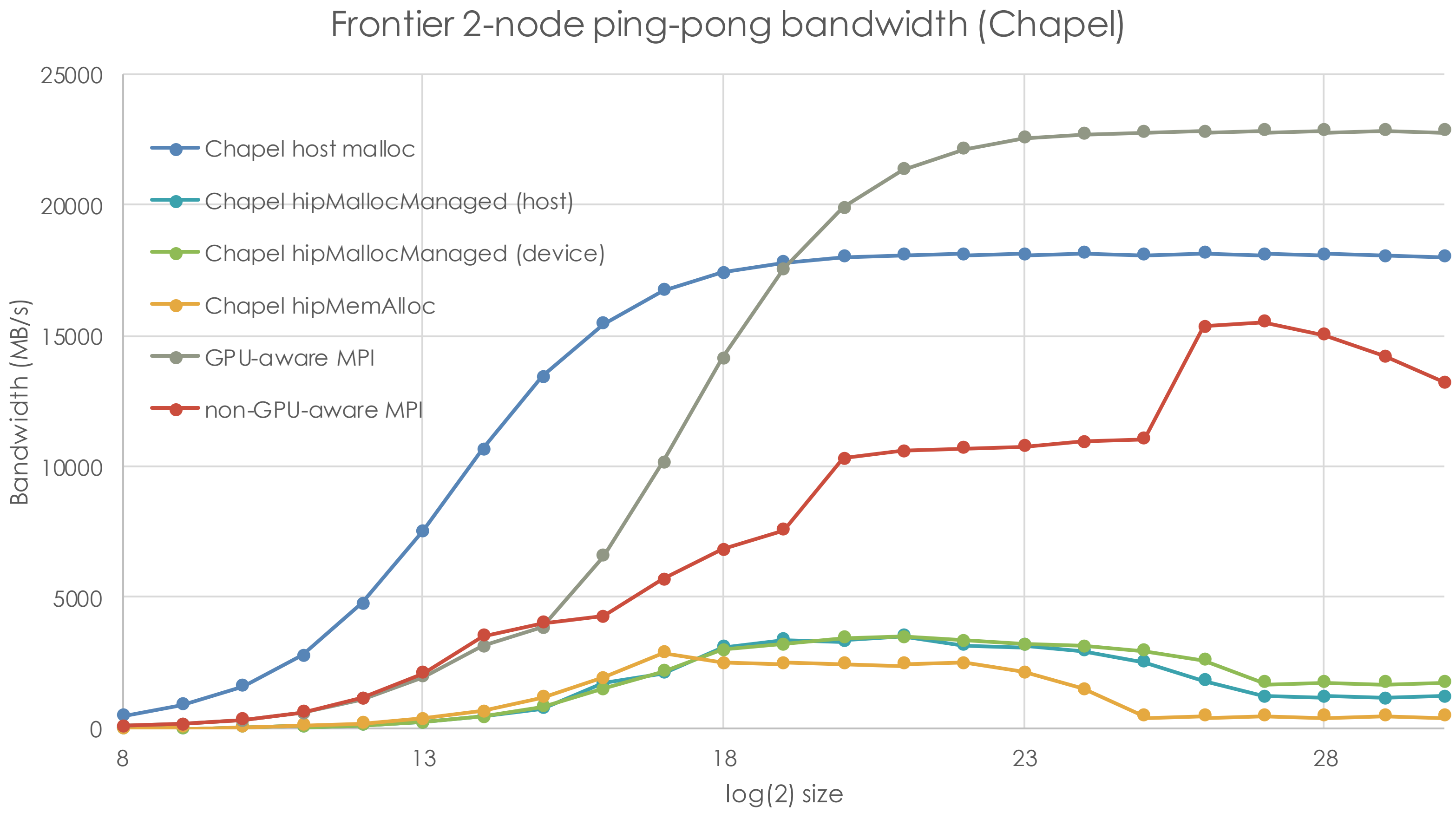
Limitations

- Inter-node communications paging through host, non-GPU memory
    - Lower available bandwidth than GPU-direct comms
- Repeated communications in same session become slower! (Memory leak?)
- NUMA-awareness of GPU arrays
- Prefetch does not improve kernel time (unlike Summit/NVIDIA – is it even implemented?)

Internode Communications on GPU-connected EX

- Chapel comms bandwidth is significantly below GPU-aware MPI
  - Regardless of how memory is allocated



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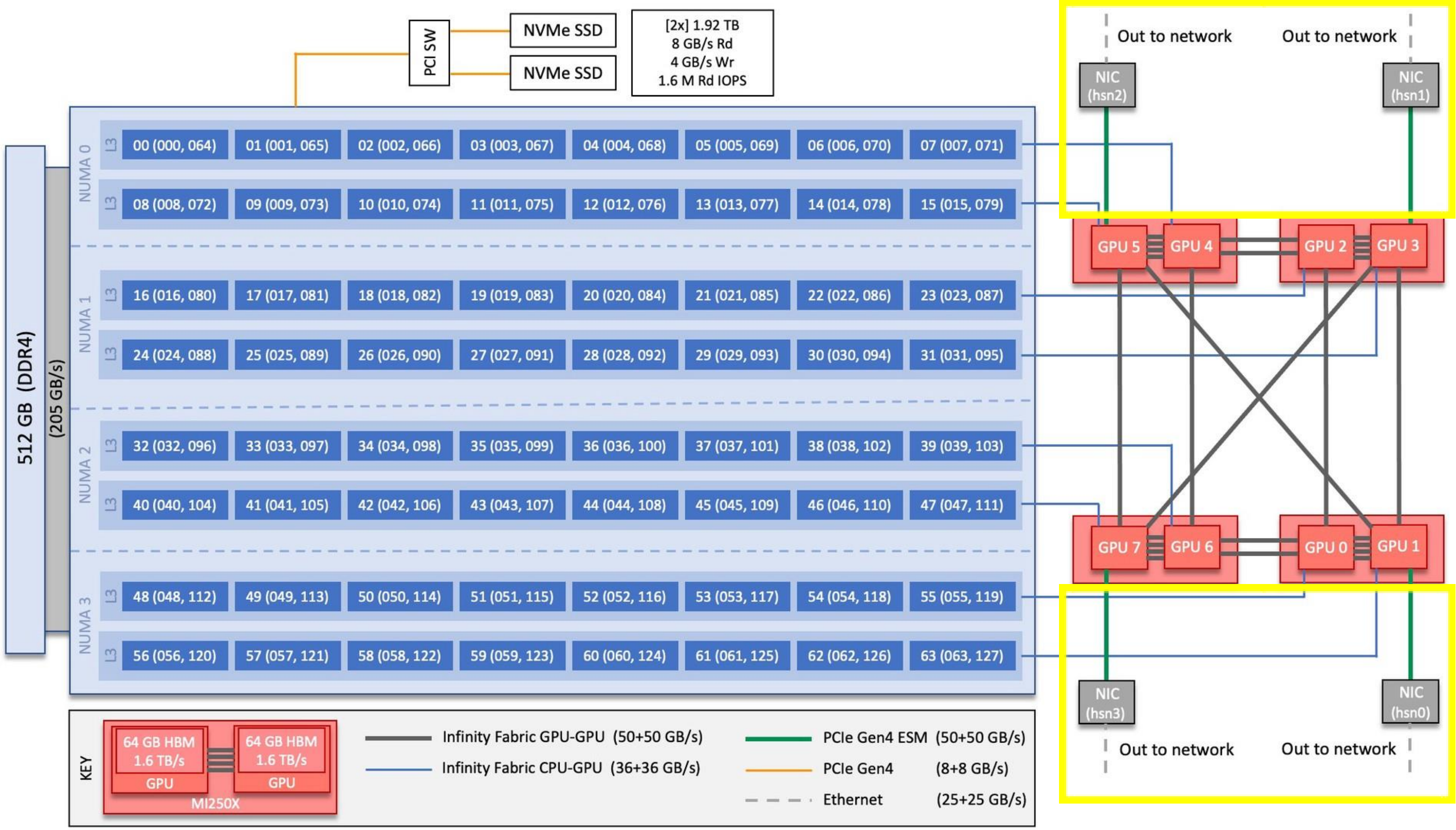
Chapel OFI Comms Layer Changes

- Frontier network interface cards (NICs) are directly connected to GPUs
- Chapel OFI comms layer doesn't utilise libfabric FI_HMEM intranode device support
- Need to register device memory regions - new memory allocator



https://docs.olcf.ornl.gov/systems/frontier_user_guide.html

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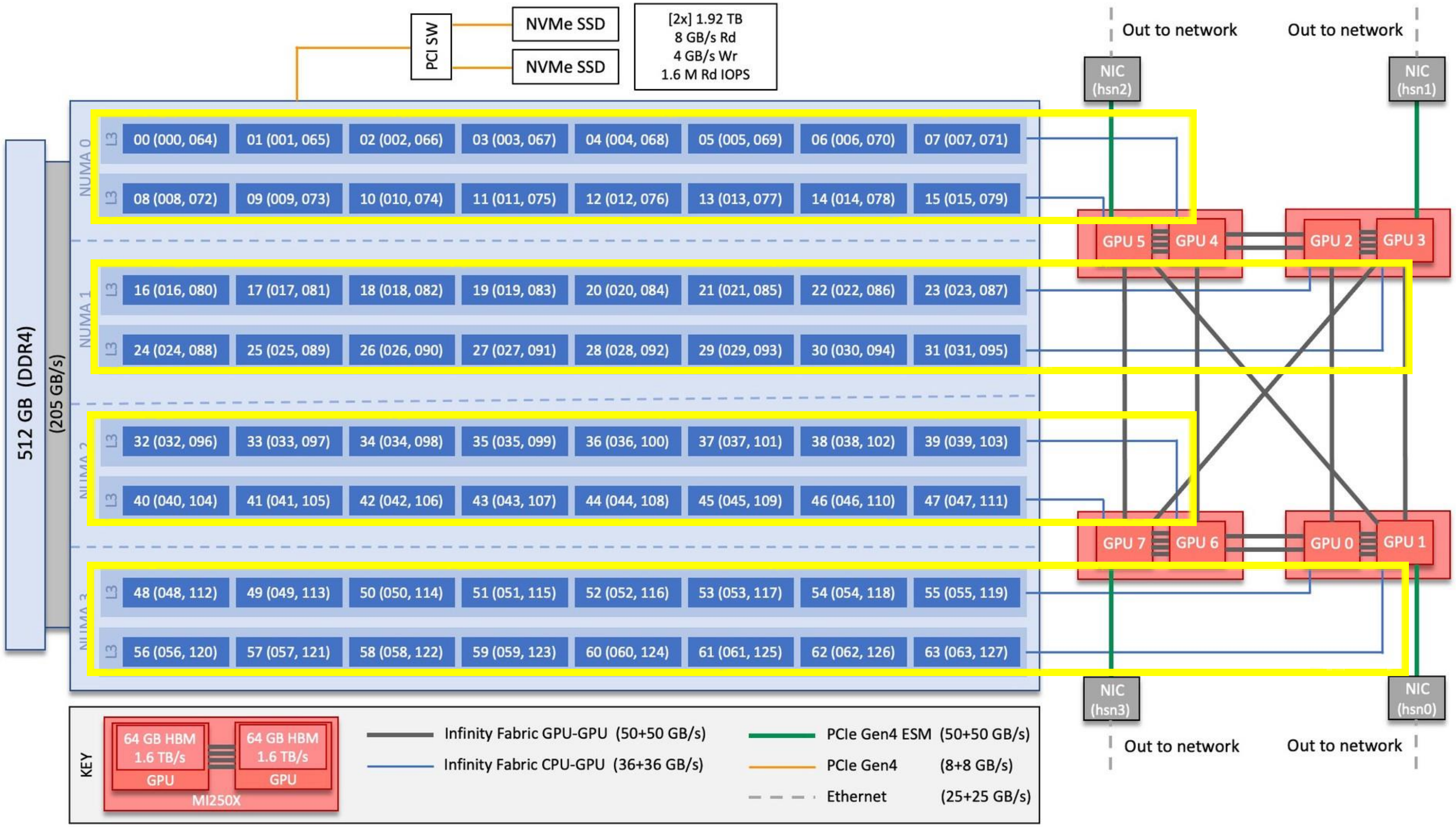
NUMA on Frontier

- Chapel distributed arrays aren't NUMA-aware
- Full host-device flood bandwidth (200GB/s) requires NUMA-aware placement of host array segments



https://docs.olcf.ornl.gov/systems/frontier_user_guide.html

Opportunities for Chapel GPU Code Generation

- With GPU code generation, some algorithms may be appropriate for both multi-GPU and distributed computation

```
proc selectPivot(A: [], targetLocs: [] locale) {
  var endLH = A.localSubdomain(targetLocs[targetLocs.size/2 - 1]).last;
  var startRH = A.localSubdomain(targetLocs[targetLocs.size/2]).first;
  var partitionSize = A.localSubdomain(targetLocs.first).size;
  var lo = 0;
  var hi = partitionSize * targetLocs.size/2;
  while lo < hi {
    var mid = hi - (hi - lo) / 2;
    if A[endLH-mid+1] <= A[startRH + mid-1] then
      hi = mid - 1;
    else
      lo = mid;
    }
  return lo;
}
```

This code is from DistMerge.chpl; currently, each node is a single locale; but it would work equally well if targetLocs referred to GPU devices

```
proc mergePartitions(ref src, ref tmp, const targetLocs: [] locale) {
  if targetLocales.size > 2 then
    coforall i in 0..1 {
      var localesSubset: [0..# targetLocs.size / 2] locale;
      localesSubset = targetLocs((i * (targetLocs.size / 2))
         .. #(targetLocales.size / 2));
      mergePartitions(src, tmp, localesSubset);
  }
  var pivot = selectPivot(src, targetLocales);
  if pivot > 0 {
    var locsToMerge = swapPartitions(src, tmp, targetLocs, pivot);
    coforall (loc, cut) in locsToMerge do on loc {
      mergeSortedKeysAtCut(src, tmp, cut);
    }
  }
  // recursive merge again
}
```

Opportunities for Chapel GPU Code Generation (2)

- This code works for inter-locale swap (doesn't work for GPUs)

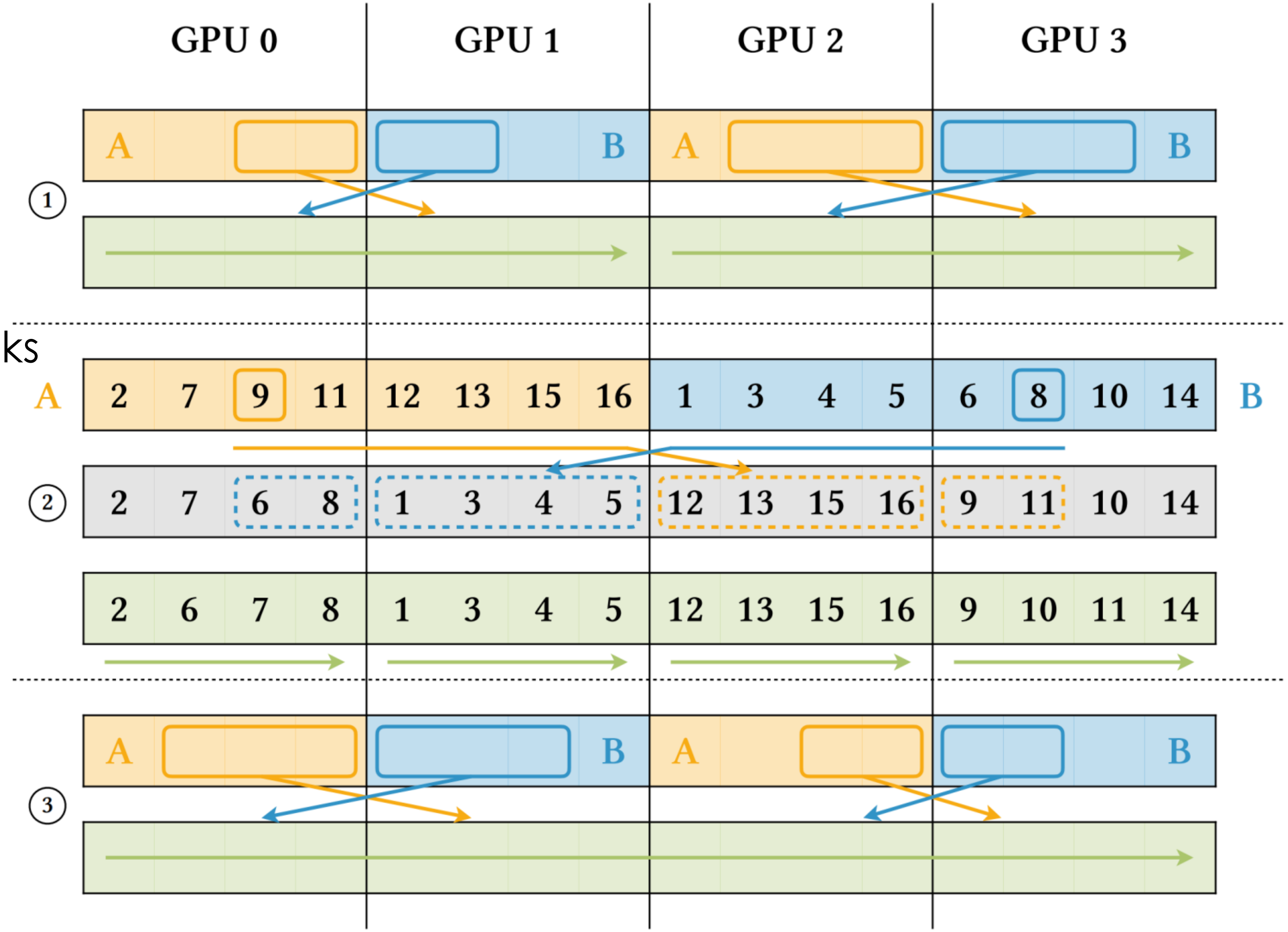
```
proc swapPartitions(ref src, ref tmp, const targetLocales: [] locale, in pivot: int) {
    var partitionSize = src.size / src.domain.targetLocales().size;
    var localesToSwap = pivot / partitionSize;
    …
    coforall i in 0..localesToSwap with (const targetLocales, ref localesToMerge) {
        const leftLocale = …;
        const rightLocale = …;
        const numElements = if (i == localesToSwap) then pivot else partitionSize;

        const leftStart = src.localSubdomain(leftLocale).first + partitionSize - numElements;
        const rightStart = src.localSubdomain(rightLocale).first;

        cobegin {
            on leftLocale do tmp.localSlice[leftStart..#numElements] = src[rightStart..#numElements];
            on rightLocale do tmp.localSlice[rightStart..#numElements] = src[leftStart..#numElements];
        }
        ...
    }
}
```

Multi-GPU Swap and Merge Algorithm

2 log2(N) -1 rounds

Need to access individual elements across all GPU chunks

and copy chunks between arrays



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GPU API

```
template <typename T>
inline __device__ void GetValueFromVirtualPartition(size_t partition_size, T** virtual_partition, size_t index,
                                                     T* value) {
  *value = virtual_partition[index / partition_size][index % partition_size];
}

template <typename T>
__global__ void SelectPivot(size_t partition_size, size_t num_partitions, T** local_virtual_partition,
                            T** remote_virtual_partition, size_t* result_pivot) {
  size_t low = 0;
  size_t high = partition_size * num_partitions;

  while (low < high) {
    const size_t mid = high - (high - low) / 2;
    T a;
    GetValueFromVirtualPartition<T>(partition_size, local_virtual_partition, partition_size * num_partitions - mid, &a);
    T b;
    GetValueFromVirtualPartition<T>(partition_size, remote_virtual_partition, mid - 1, &b);
    if (a <= b) {
      high = mid - 1;
    } else {
      low = mid;
    }
  }
  *result_pivot = low;
}
```

Swap partitions – CUDA/HIP - called from GPU API

```
template <typename T>
std::array<int, 2> SwapPartitions(DeviceBuffers<T>* device_buffers, size_t pivot, const std::vector<int>& devices) {
  const size_t partition_size = device_buffers->GetPartitionSize();
  size_t devices_to_swap = pivot / partition_size;
  ...
#pragma omp parallel for
  for (size_t i = 0; i <= devices_to_swap; ++i) {
    const int left_device = ...;
    const int right_device = ...;
    const size_t num_elements = (i == devices_to_swap) ? pivot : partition_size;

    CheckCudaError(cudaSetDevice(left_device));

    CheckCudaError(cudaMemcpyAsync(
        thrust::raw_pointer_cast(device_buffers->AtSecondary(left_device)->data() + partition_size - num_elements),
        thrust::raw_pointer_cast(device_buffers->AtPrimary(right_device)->data()), sizeof(T) * num_elements,
        cudaMemcpyDeviceToDevice, *device_buffers->GetPrimaryStream(left_device)));

    CheckCudaError(cudaSetDevice(right_device));

    CheckCudaError(cudaMemcpyAsync(
        thrust::raw_pointer_cast(device_buffers->AtSecondary(right_device)->data()),
        thrust::raw_pointer_cast(device_buffers->AtPrimary(left_device)->data() + partition_size - num_elements),
        sizeof(T) * num_elements, cudaMemcpyDeviceToDevice, *device_buffers->GetPrimaryStream(right_device)));
    ...
  }
```

Merge Partitions – CUDA/HIP

```
template <typename T>
void MergePartitions(DeviceBuffers<T>* device_buffers, HostVector<T>* elements, const std::vector<int>& devices,
                     size_t num_fillers) {
  if (devices.size() > 2) {
#pragma omp parallel for
    for (size_t i = 0; i < 2; ++i) {
      MergePartitions(
          device_buffers, elements,
          {devices.begin() + (i * (devices.size() / 2)), devices.begin() + ((i + 1) * (devices.size() / 2))},
          num_fillers);
    }
  }
  const size_t pivot = FindPivot<T>(device_buffers, devices);
  if (pivot > 0) {
    const std::array<int, 2> devices_to_merge = SwapPartitions<T>(device_buffers, pivot, devices);
    MergeLocalPartitions<T>(device_buffers, elements, pivot, devices_to_merge, devices, num_fillers);
  }
  // recursive merge again
```

Chapel GPU Code Generation can make our lives easier

- Note – below is fictional code that we envision as nice to haves as developers when implementing algorithms, such as ones that require system specific optimizations (Frontier)

- Allocating a distributed GPU array across all GPUs on a node

```
var Dom: domain(1) dmapped blockDist({0..n}, targetLocales=here.gpus) = {0..n};
```

- Direct copy between portions of an array allocated to different devices on a single node

```
const gpu0Dom = A.dom.localSubdomain(here.gpus[0]);
const gpu7Dom = A.dom.localSubdomain(here.gpus[7]);
A[gpu0Dom] = A[gpu7Dom];
```

- Direct copy between portions of an array allocated to devices on different nodes

```
const localGpu0Dom = A.dom.localSubdomain(here.gpus[0]);
const remoteGpu0Dom = A.dom.localSubdomain(Locales[1].gpus[0]);
A[localGpu0Dom] = A[remoteGpu0Dom];
```

Summary and Future Work

- Georgia Tech GPU API
  - Granularity met with limitations and tedious, difficult to debugs implementation
- Frontier and AMD specific issues
  - ROCM bugs
- Frontier and Chapel incompatability
  - HBM through GPUs, not host
  - Chapel Arrays are not NUMA aware
- Chapel GPU Code Gen
  - Realize is work in progress
  - Feedback on potential solutions to solve issues caused by high granularity of Georgia Tech GPU API

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