Accelerating Data Analytics with Arkouda on GPUs

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Accelerating Arkouda with GPUs

αρκούδα
massive scale
data science

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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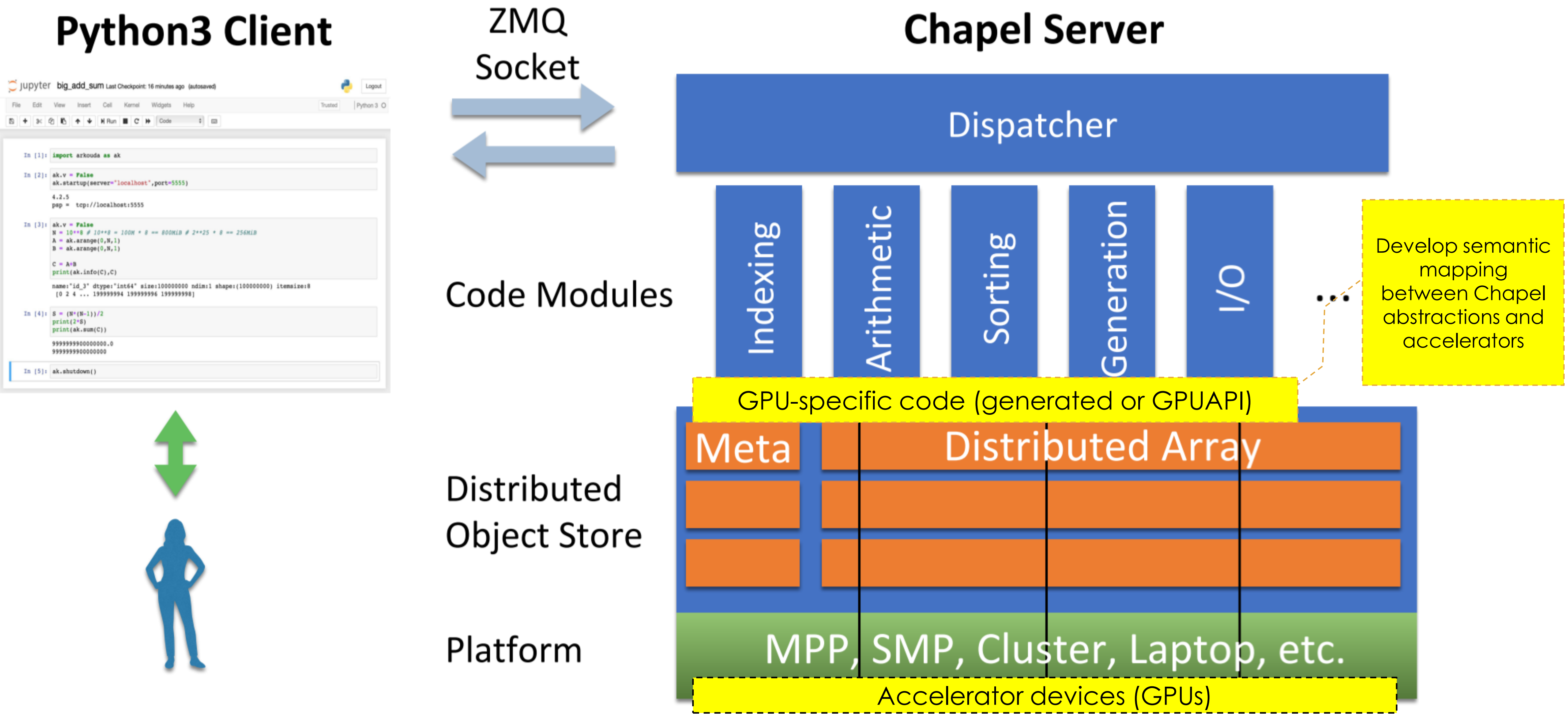
Arkouda Architecture



Chapel GPUAPI

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

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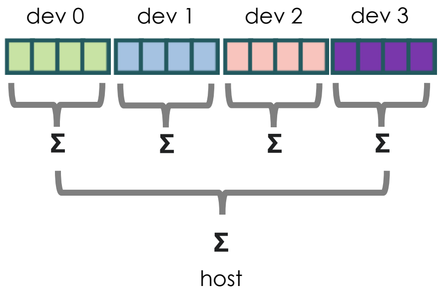
Example: Sum on GPU (mid-level GPUAPI)

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

`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 sum(A: [?aDom] ?etype) {
  var deviceSum: [0..#nGPUs] etype;
  var sumCallback = lambda(lo: int, hi: int, n: int) {
    var devA = new GPUArray(A.localSlice(lo .. hi));
    var devOut = new GPUArray(deviceSum[deviceId]);
    var deviceId: int(32);
    GetDevice(deviceId);
    devA.toDevice();
    launchSum(devA.dPtr(), devOut.dPtr(), n);
    DeviceSynchronize();
    devOut.fromDevice();
  };
  forall i in GPU(A.localSubdomain(), sumCallback) { }
  return (+ reduce deviceSum);
}
```

CUDA / OpenCL

Arkouda GPU Device Cache

- Common pattern
  - new GPUArray for local chunk
  - copy host-to-device
  - kernel launch[es]
  - [copy device-to-host]
- Where possible, leave arrays on GPU between operations

MultiTypeSymEntry.chpl

```
class SymEntry : GenSymEntry {
  proc createDeviceCache() {
  class DeviceCache {
    var isCurrent = false;
    /* Range of data for each GPU device */
    var deviceChunks: [gpuDevices] range;
    /* GPU arrays for each device */
    var deviceArrays: [gpuDevices] shared GPUArray?;
    proc toDevice(deviceId) {
      if (!isCurrent) {
        deviceArrays[deviceId]!.toDevice();
        isCurrent = true;
      }
    }
    proc fromDevice(deviceId) { … }
  }
}
```

Example: Histogram on GPU (Device Cache)

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

`ak_arr.sum()`

Device memory allocation

Data transfer

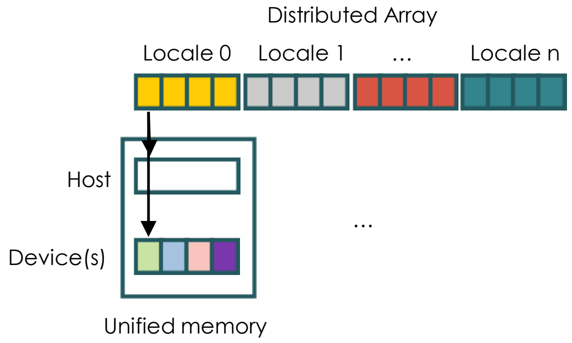
Synchronization

```
use GPUIterator;
use GPUAPI;

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

proc sum(e: SymEntry) {
  e.createDeviceCache(); // idempotent
  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.toDevice(deviceId); // idempotent
    launchSum(e.getDeviceArray(deviceId).dPtr(),
devOut.dPtr(), n);
    DeviceSynchronize();
    devOut.fromDevice();
  };
  forall i in GPU(e.a.localSubdomain(), sumCallback) { }
  return (+ reduce deviceSum);
}
```

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



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

Example: Histogram on GPU (unified memory)

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

`ak_arr.sum()`

```
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);
}
```

Device memory allocation

Data transfer

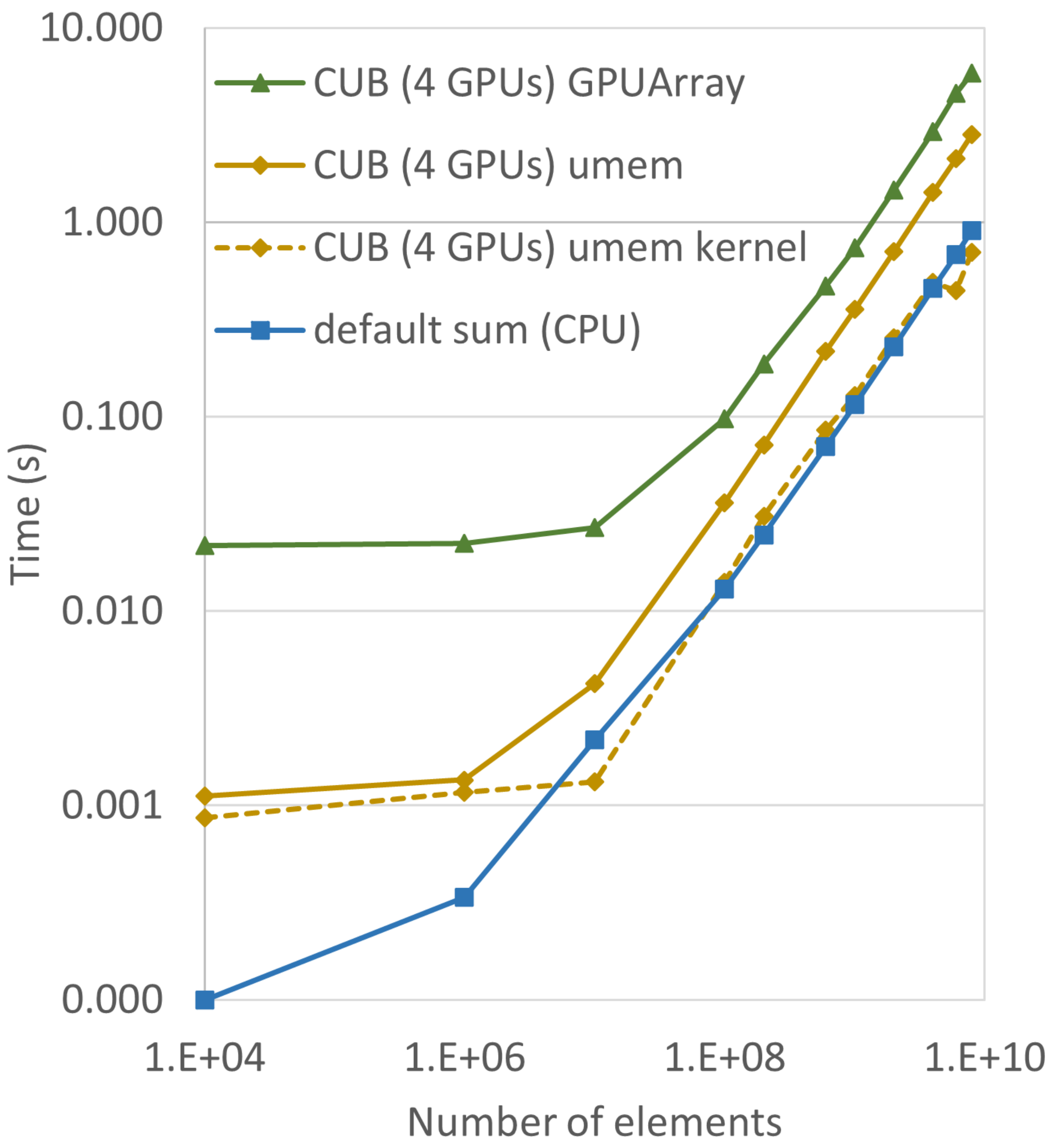
Synchronization

Experimental Evaluation

- Evaluation platform: NVIDIA DGX workstation
  - 2 × 20-core Intel Xeon E5-2698s @ 2.2GHz
  - 256GiB of DRAM
  - 4 × Tesla V100 GPUs with 32 GiB HBM
  - Chapel 1.30
  - NVHPC toolkit v22.11 (CUDA v11.8)
  - CUDA driver version 530.30.02
- Timing server-side Arkouda Chapel code directly (not from Python client)
  - Doesn't allow batching of communications

Reduction

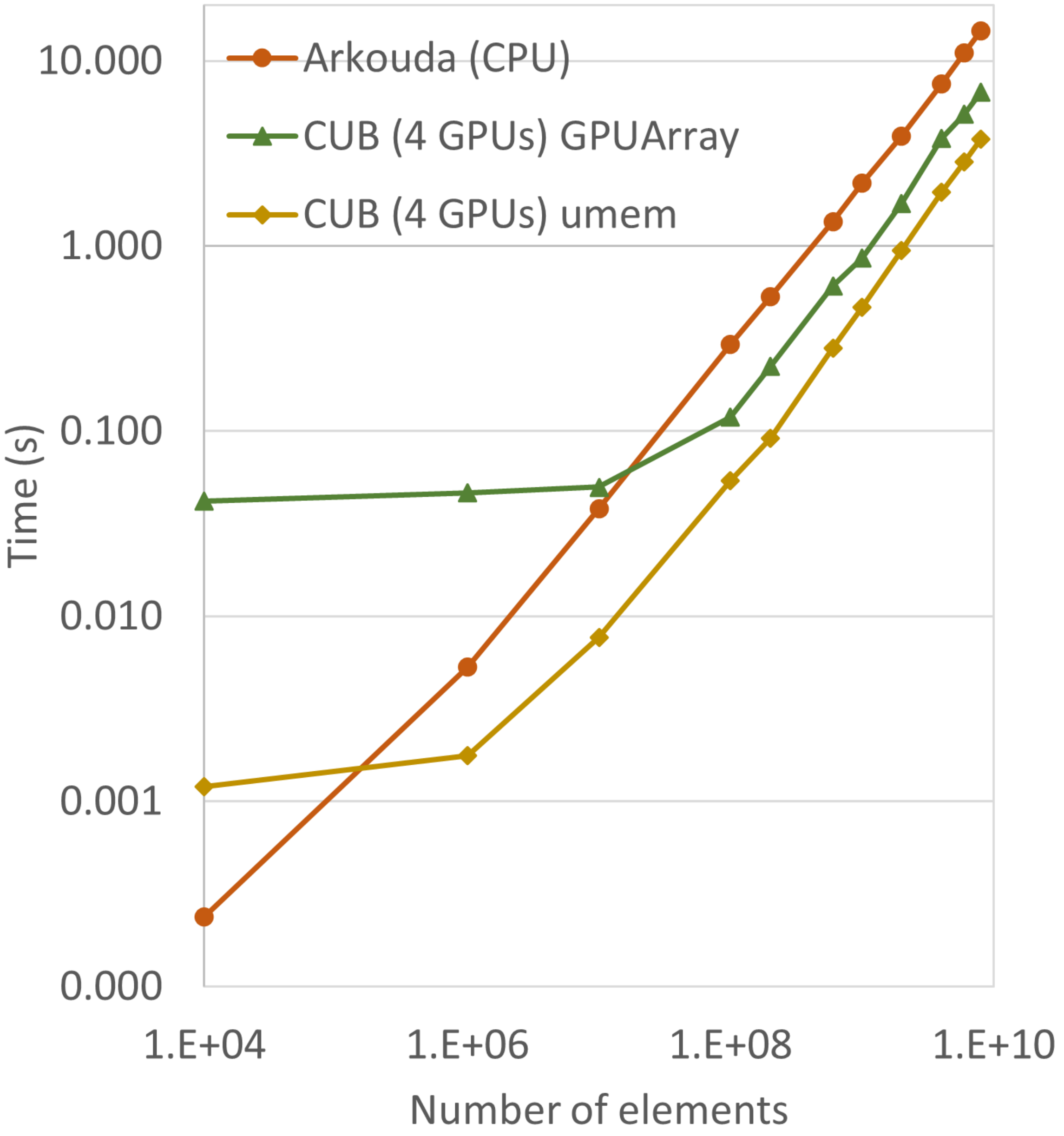
- GPUArray
  `DeviceCache`
- umem
  `GPUUnifiedDist`
- Kernel:
  - CUB library
    `DeviceReduce::Sum`
  - NCCL
    `ncclReduce`




```
ak_arr.sum()
```

Histogram

- Arkouda (CPU)
  `histogramGlobalAtomic`
- Kernel:
  - CUB library
    `DeviceHistogram::HistogramEven`
  - NCCL
    `ncclAllReduce`

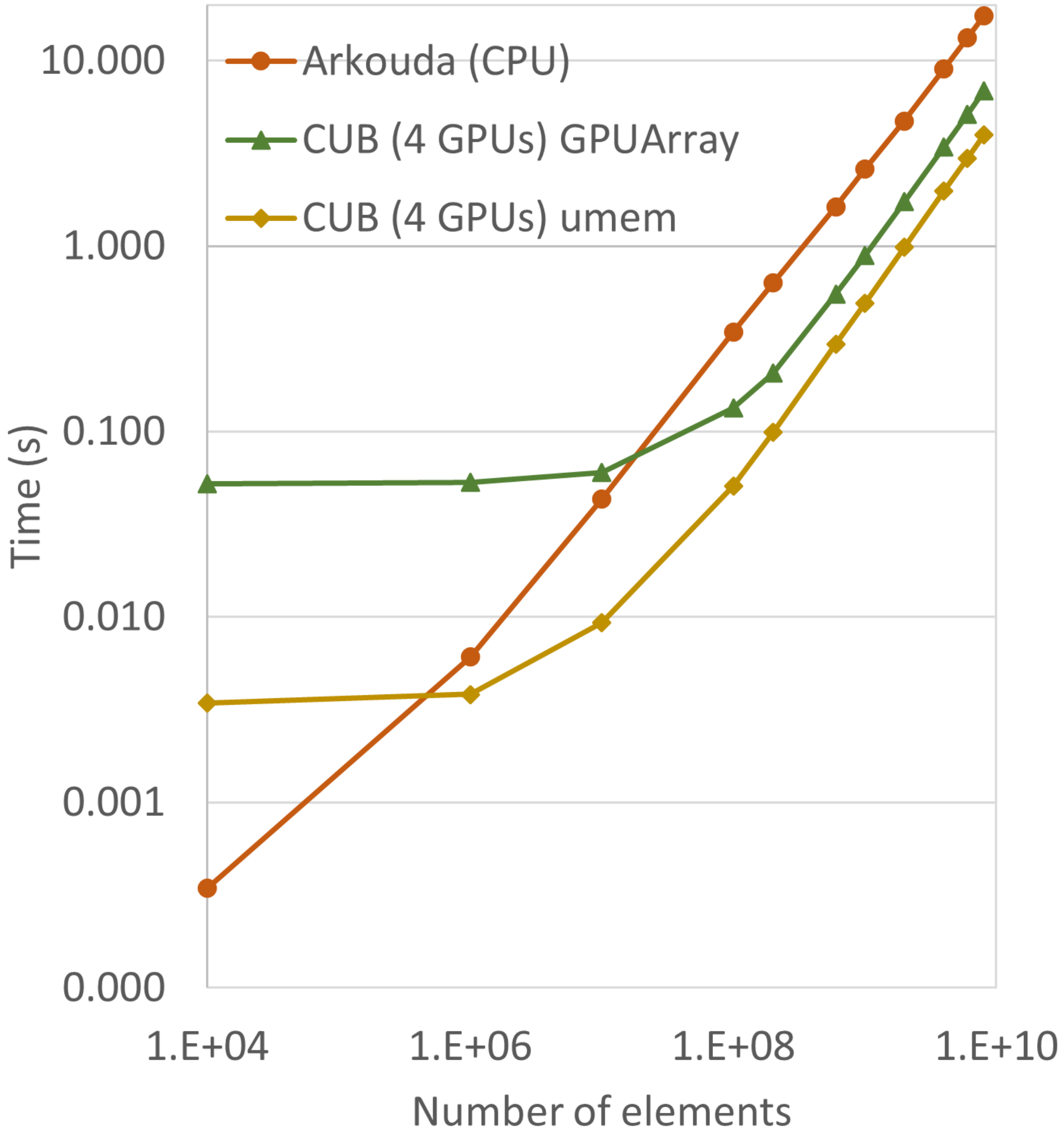



```
ak.histogram(A, sqrt(A.size))
```

Chained Operations

- DeviceCache / Unified Memory avoids multiple host-device transfers

```
A.sum()
A.min()
A.max()
ak.histogram(A, sqrt(A.size))
```



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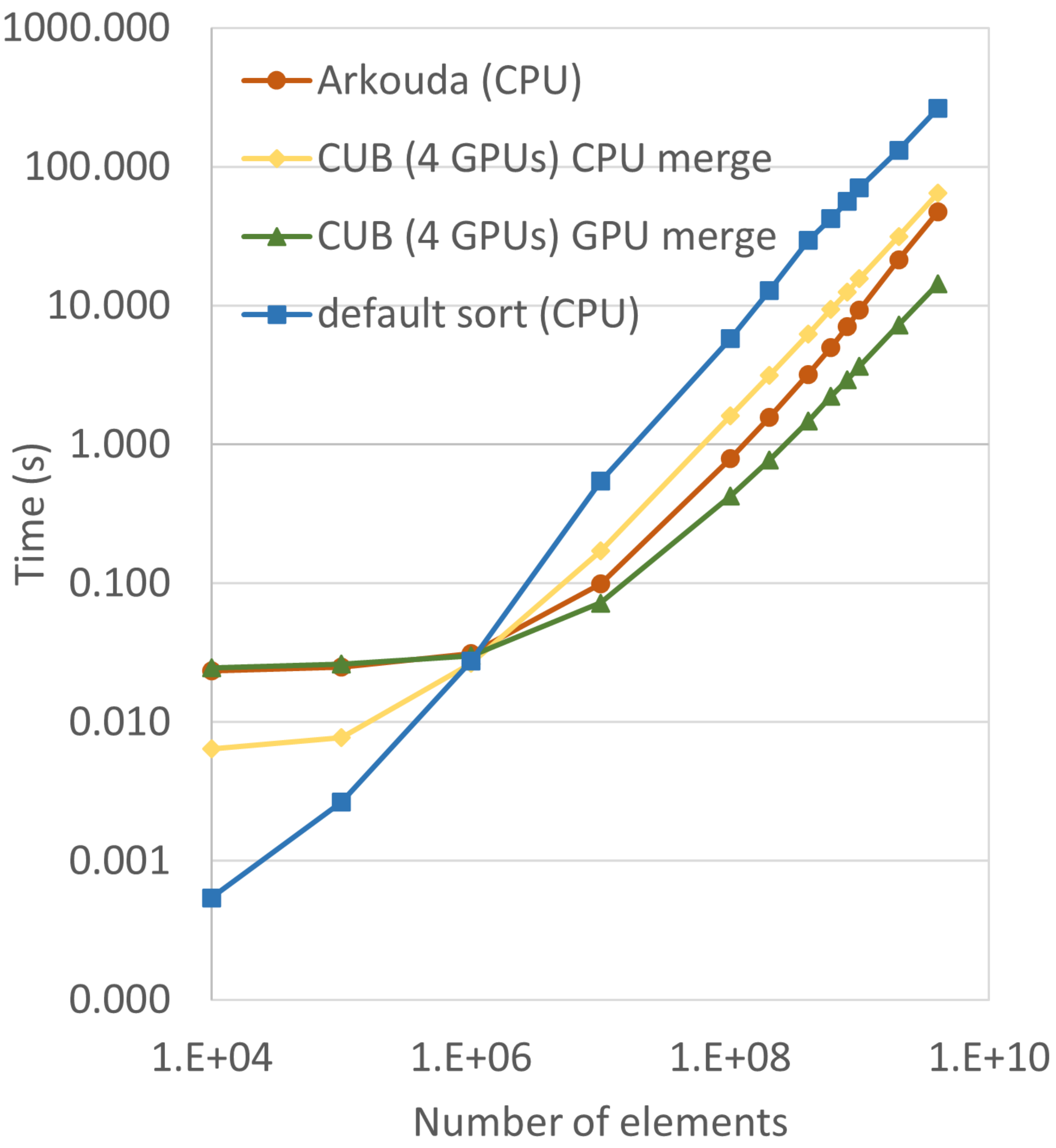
Milthorpe: Accelerating Data Analytics with Arkouda on GPUs (CHIUW 2023)

Sort

- 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()`

Summary and Future Work

- Chapel GPUAPI combined with unified memory can support productive, high-performance development of GPU-accelerated data analytics
  - algorithmic portability still a challenge
- Future:
  - Application Workflows: real data analytics pipelines
    - e.g. astronomical image/spectroscopic post-processing and analysis
  - Port to AMD GPUs (HIP/ROCm)
  - Chapel GPU code generation

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