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
Accelerating Arkouda with GPUs

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

<table>
<thead>
<tr>
<th></th>
<th>CPU-DRAM</th>
<th>GPU-HBM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Summit (2018)</td>
<td>340 GB/s</td>
<td>2,700 GB/s</td>
</tr>
<tr>
<td>Frontier (2022)</td>
<td>205 GB/s</td>
<td>13,080 GB/s</td>
</tr>
</tbody>
</table>

- Challenges:
  - algorithmic portability
  - memory management
  - programmability
How our GPU code fits into Arkouda

**Python3 Client**

- ZMQ Socket

**Chapel Server**

- Dispatcher
  - Indexing
  - Arithmetic
  - Sorting
  - Generation
  - I/O

**Code Modules**

- Distributed Object Store

**Platform**

- MPP, SMP, Cluster, Laptop, etc.
- Accelerator devices (GPUs)

Develop semantic mapping between Chapel abstractions and accelerators.

**GPU-specific code (generated or GPUAPI)**
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, ...)`

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

https://github.com/milthorpe/arkouda
https://github.com/milthorpe/chapel-gpu
Example: Sum on GPU (unified memory), GPU API

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

```
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 Significant 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


ak_df.sort_values()
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

ak_df.sort_values()
Sort (Frontier, multi-node)

- **Arkouda (CPU)**
  - `radixSortLSD_keys`

- **Kernel:**
  - CUB library
    - `DeviceRadixSort::SortKeys`
  - merge on CPU:
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  - GPU merge:
    - peer-to-peer swap and merge


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

- `ak_df.sort_values()`
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
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
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

```chapel
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;
            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

```chapel
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)

```chapel
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

<table>
<thead>
<tr>
<th>GPU 0</th>
<th>GPU 1</th>
<th>GPU 2</th>
<th>GPU 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>B</td>
<td>A</td>
<td>B</td>
</tr>
</tbody>
</table>

2 \( \log_2(N) - 1 \) rounds

Need to access individual elements across all GPU chunks and copy chunks between arrays

1. 

2. 

3. 

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;
}
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,
            cudaMemcpyDeviceToHost, *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, cudaMemcpyDeviceToHost, *device_buffers->GetPrimaryStream(right_device)));
    }
    ...
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
  
  ```chapel
  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
  
  ```chapel
  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
  
  ```chapel
  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
  o Granularity met with limitations and tedious, difficult to debug implementation

• Frontier and AMD specific issues
  o ROCM bugs

• Frontier and Chapel incompatibility
  o HBM through GPUs, not host
  o Chapel Arrays are not NUMA aware

• Chapel GPU Code Gen
  o Realize is work in progress
  o Feedback on potential solutions to solve issues caused by high granularity of Georgia Tech GPU API