Parallel Computing with GPUs: Sorting and Libraries

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Last Week

- We learnt about Performance optimisation
- APOD cycle
- Use of guided analysis to find important kernels
- Use of guided analysis to find optimisation routes for code

- ❑Sorting Networks
- ❑Merge and Bitonic sort
- ❑Thrust Parallel Primitives Library
- ❑Applications of sorting (binning)

Serial Sorting Examples

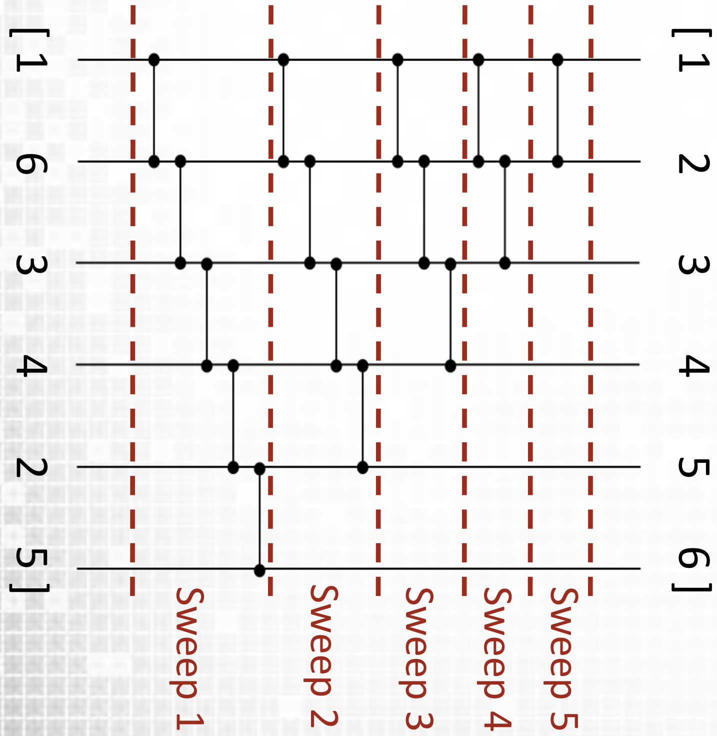
- Insertion Sort
  - Insert a new element into a sorted list.
    - E.g. [1 6 3 4 2 5]
      - [1] -> [1 6] -> [1 3 6] -> [1 3 4 6] -> [1 2 3 4 6] -> [1 2 3 4 5 6]
- Bubble Sort
  - Exchange and Sweep to compare each pair of adjacent elements
  - $O(n^2)$ worst-case and average case, $O(n)$ best case.
    - E.g. [1 6 3 4 2 5]
      - [1 6 3 4 2 5] -> [1 **3 6** 4 2 5] -> [1 3 **4 6** 2 5] -> [1 3 4 **2 6** 5] -> [1 3 4 2 **5 6**]
      - [1 3 **2 4** 5 6]
      - [1 **2 3** 4 5 6]

Classifying Sort Techniques/Implementations

- ❑Data driven
  - ❑Each step of the algorithm depends on the previous step version
  - ❑Highly serial
- ❑Data independent
  - ❑The algorithms performs fixed steps and does not change its processing based on data
  - ❑Well suited to parallel implementations
  - ❑Can be expressed as a sorting network…

Sorting Networks

- A sorting network is a comparator network that sorts all input sequences
  - Following the same execution of stages
- Consider the previous Bubble Sort [1 6 3 4 2 5]



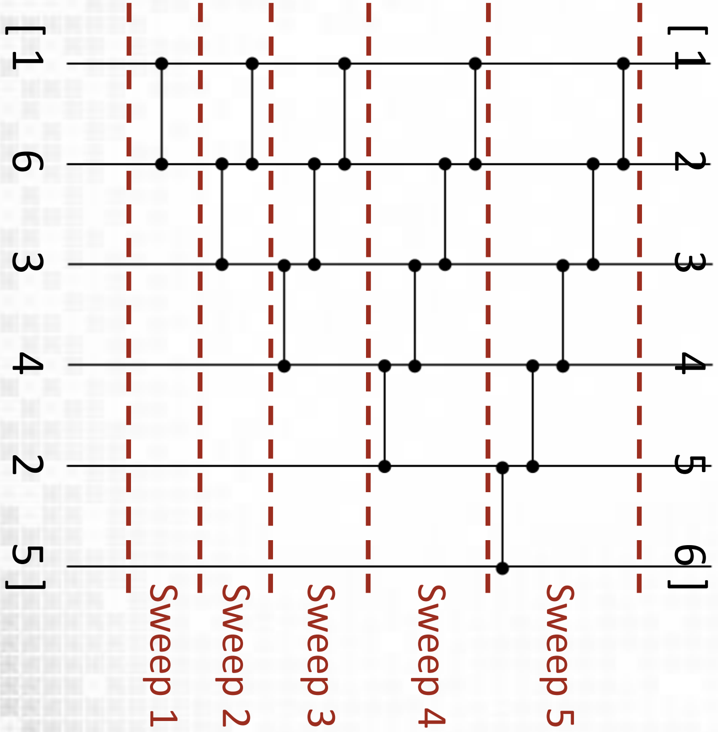
[1 6 3 4 2 5] -> [1 **3 6** 4 2 5] -> [1 3 **4 6** 2 5] -> [1 3 4 **2 6** 5] -> [1 3 4 2 **5 6**]
[1 3 4 2 5 6] -> [1 3 4 2 5 6] -> [1 3 **2 4** 5 6] -> [1 3 2 4 5 6]
[1 3 2 4 5 6] -> [1 2 3 4 5 6] -> [1 2 3 4 5 6]
[1 3 2 4 5 6] -> [1 **2 3** 4 5 6]
[1 2 3 4 5 6]

Sweeps

Not considered
Compared not swapped
Compared and swapped

Sorting Networks

- And Insertion Sort…

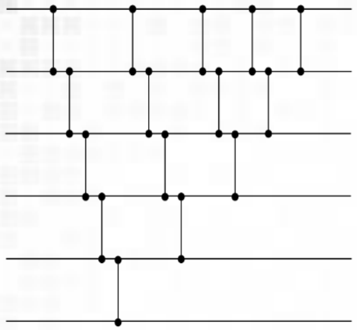


[1 6 3 4 2 5]
[1 3 6 4 2 5] -> [1 3 6 4 2 5]
[1 3 4 6 2 5] -> [1 3 4 6 2 5] -> [1 3 4 6 2 5]
[1 3 4 2 6 5] -> [1 3 2 4 6 5] -> [1 2 3 4 6 5] -> [1 2 3 4 6 5]
[1 2 3 4 5 6] -> [1 2 3 4 5 6] -> [1 2 3 4 5 6] -> [1 2 3 4 5 6] -> [1 2 3 4 5 6]

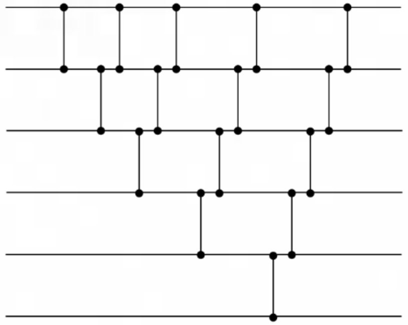
Sweeps

Not considered
Compared not swapped
Compared and swapped

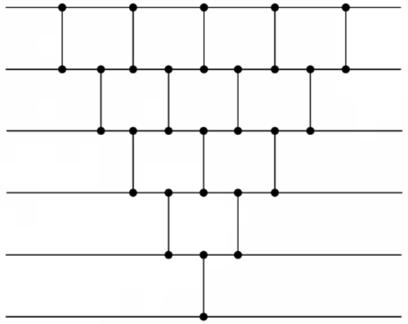
Parallel Sorting Networks



Bubble



Insertion



[**1 6** 3 4 2 5]
[1 **3 6** 4 2 5]
[1 3 **4 6** 2 5]
[1 3 4 **2 6** 5]
[1 3 **2 4 5 6**]
[1 **2 3** 4 5 6]
[1 2 3 4 5 6]
[1 2 3 4 5 6]
[1 2 3 4 5 6]

Sweeps = 9

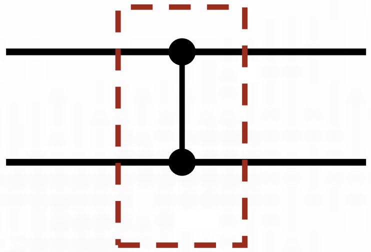
- Parallel Bubble and Insertion sorting network is still not very efficient
  - $2n - 3$ sweeps
  - $n(n-1)/2$ comparisons - $O(n^2)$ complexity

- Sorting Networks
- Merge and Bitonic sort
- Thrust Parallel Primitives Library
- Applications of sorting (binning)

Merge Sort

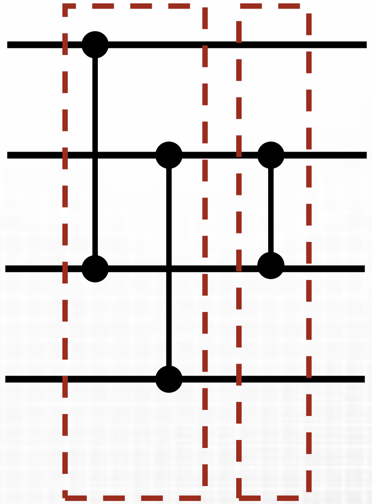
- To reduce the $O(n^2)$ overhead we need a better sorting network
- The odd-even merge sort network (for power of 2 n)
  - Sort all odd and even keys separately and then merge m values of a stage
  - Merge a sorted sequence of elements on lines $< a_1, \ldots, an >$ with those on lines $< a_{n+1}, \ldots, a_{2n} >$
  - Each merge requires $\log(n)$ passes
  - Total complexity of $O(n \log(n^2) \ + \ \log(n))$

$n = 1$



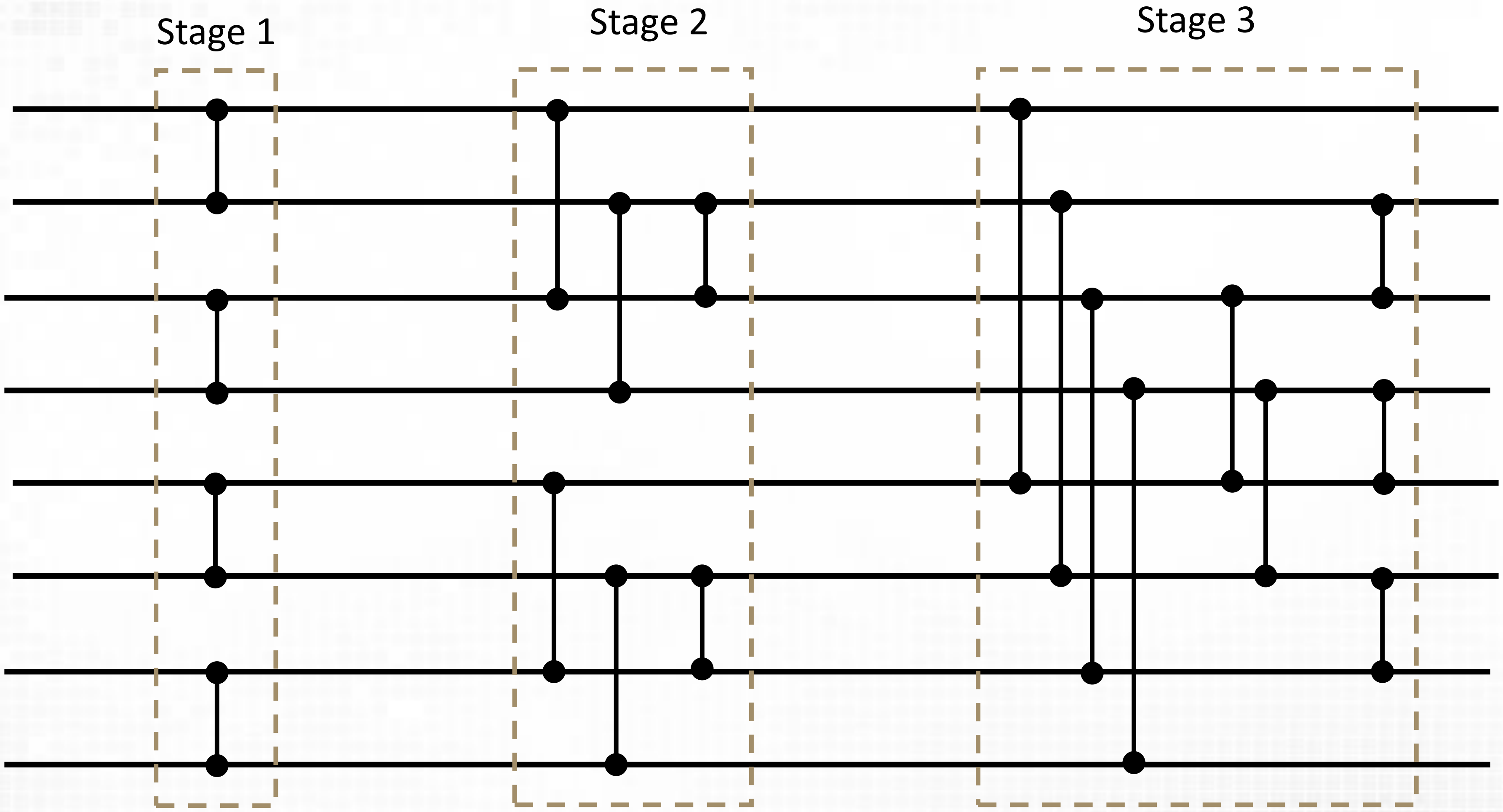
pass 1

$n = 2$

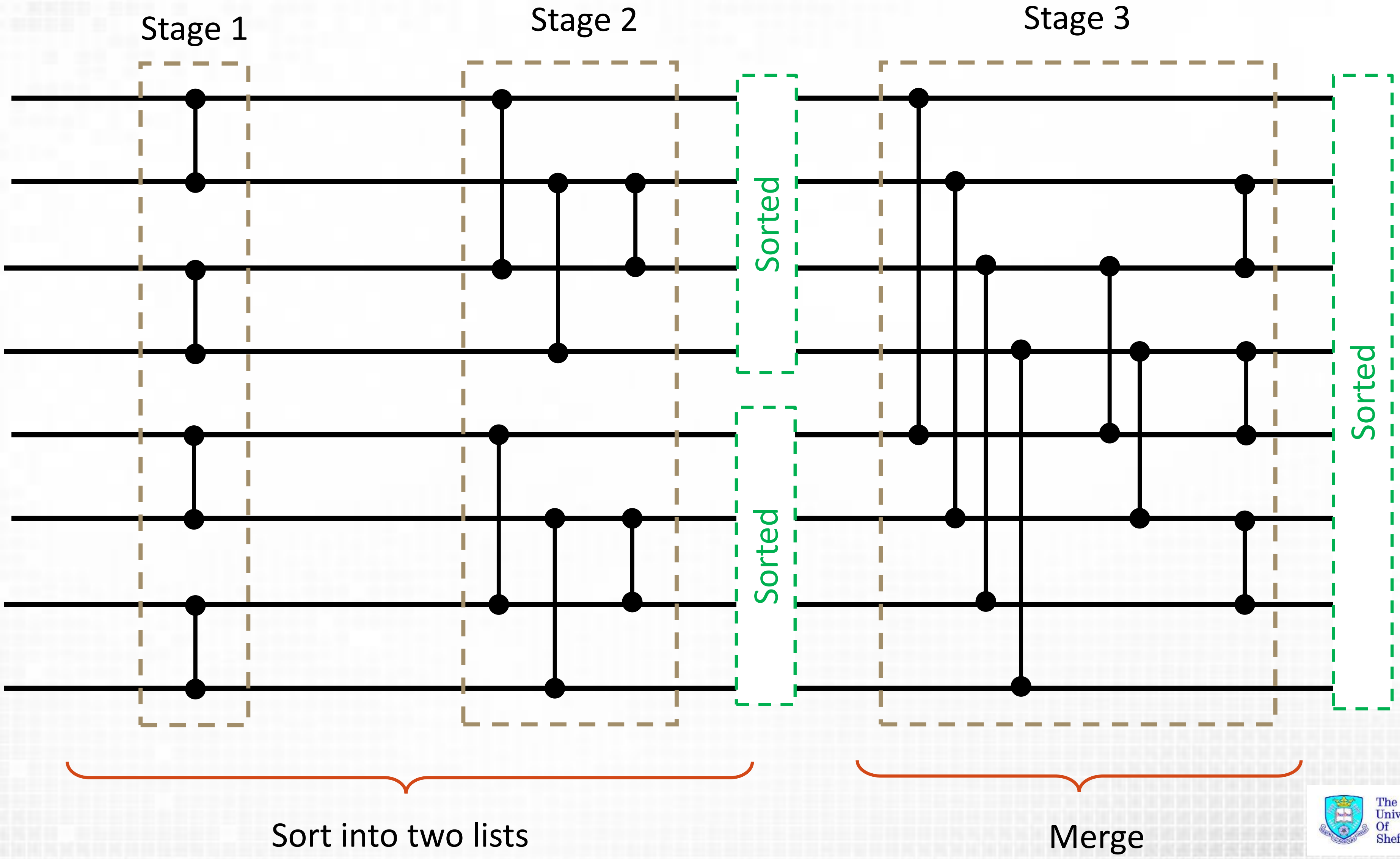


pass 1 pass 2

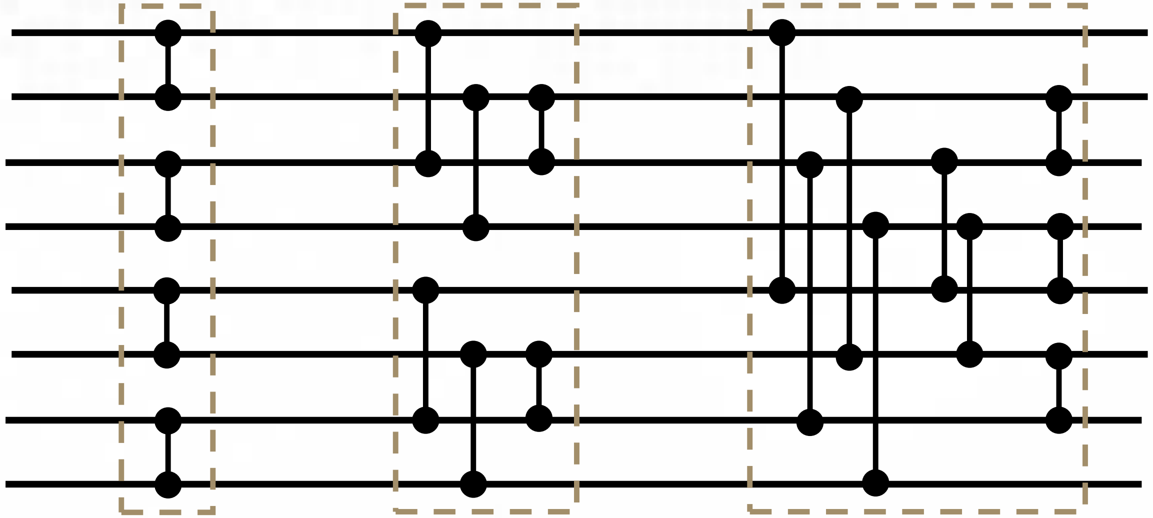
Merge Sorting (n=8)



Merge Sorting (n=8)



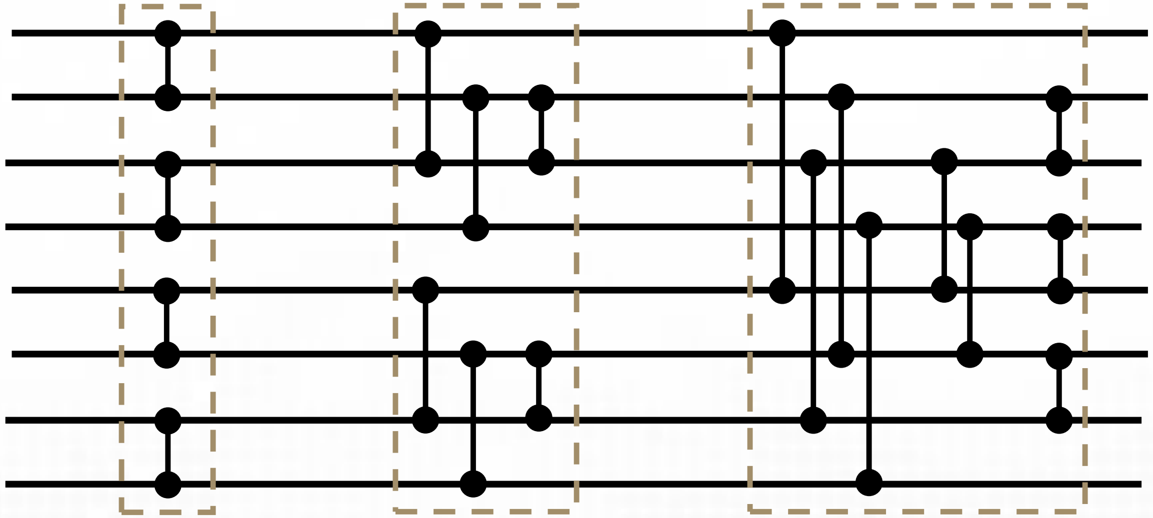
Merge Sorting (n=8) example



Input	Stage 1	Stage 2			Stage 3							Output
8	1	1			1							1
1	8		5	3			3				2	2
5	3	3		5		5			2		3	3
3	5		8					8		4	4	4
6	2	2			2				5		5	5
2	6		6	4			4			8	6	6
4	4	4		6		6					8	8
9	9		9					9				9

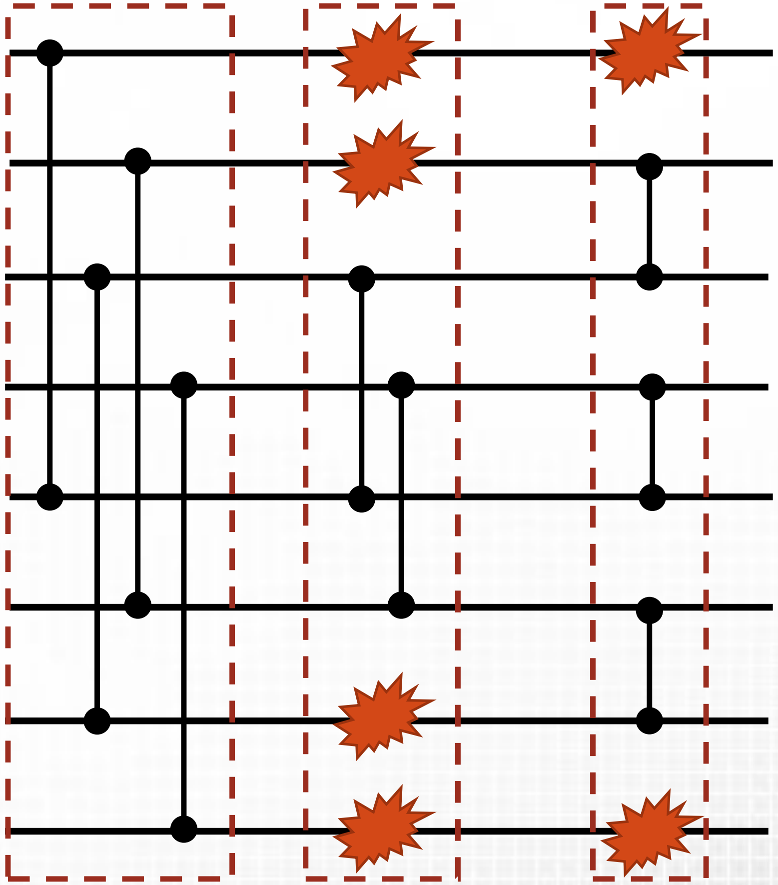
Limitations of Merge Sort?

- What is potentially wrong with a merge sort GPU implementation?
  - Hint: Think about workload per thread



Limitations of Merge Sort

- What is potentially wrong with a merge sort GPU implementation?
  - Irregular memory accesses
  - Not all values are compared in each pass (uneven workload per thread)



The University Of Sheffield.

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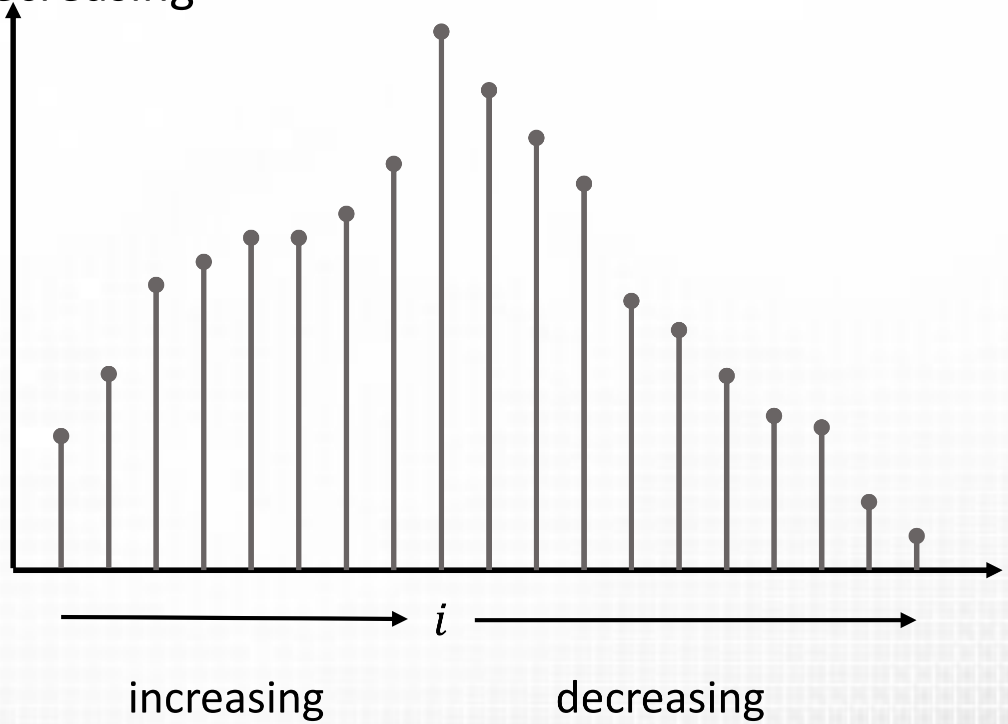
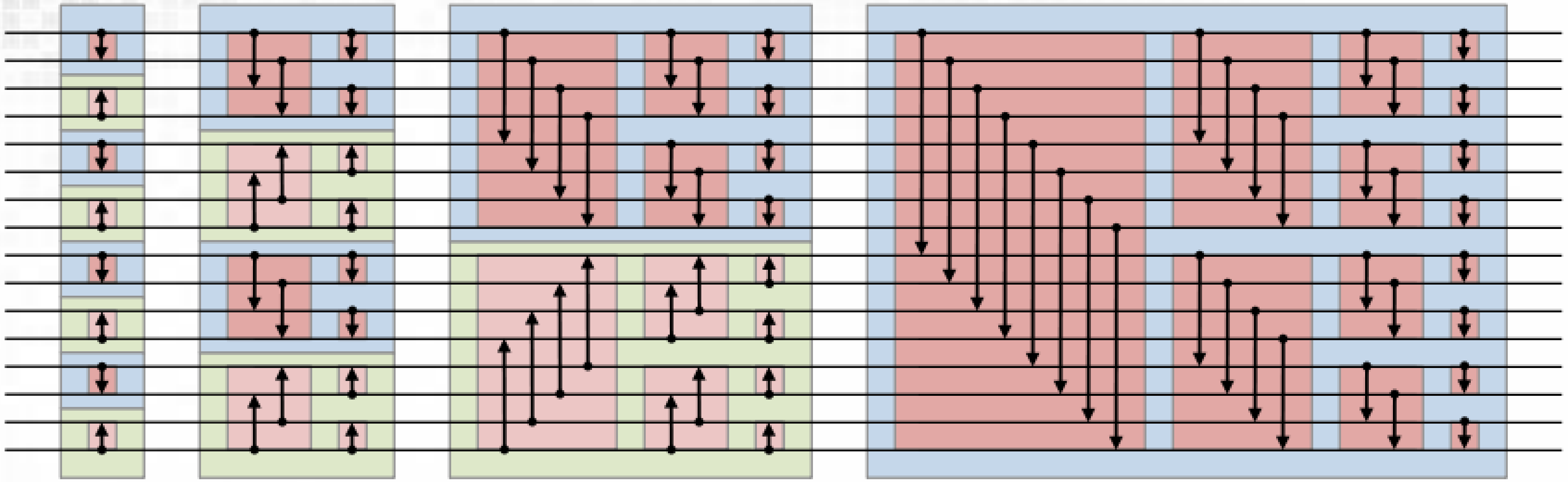
Solution: Bitonic Sort

- Bitonic sorting network
  - Iterative splitting and merging of inputs into increasing large bionic sequences
  - A sequence is bitonic if
    - There is an i, such that , a_0 …, a_i is monotonically increasing and a_i …, a_n is monotonically decreasing



Bitonic Sorting Network

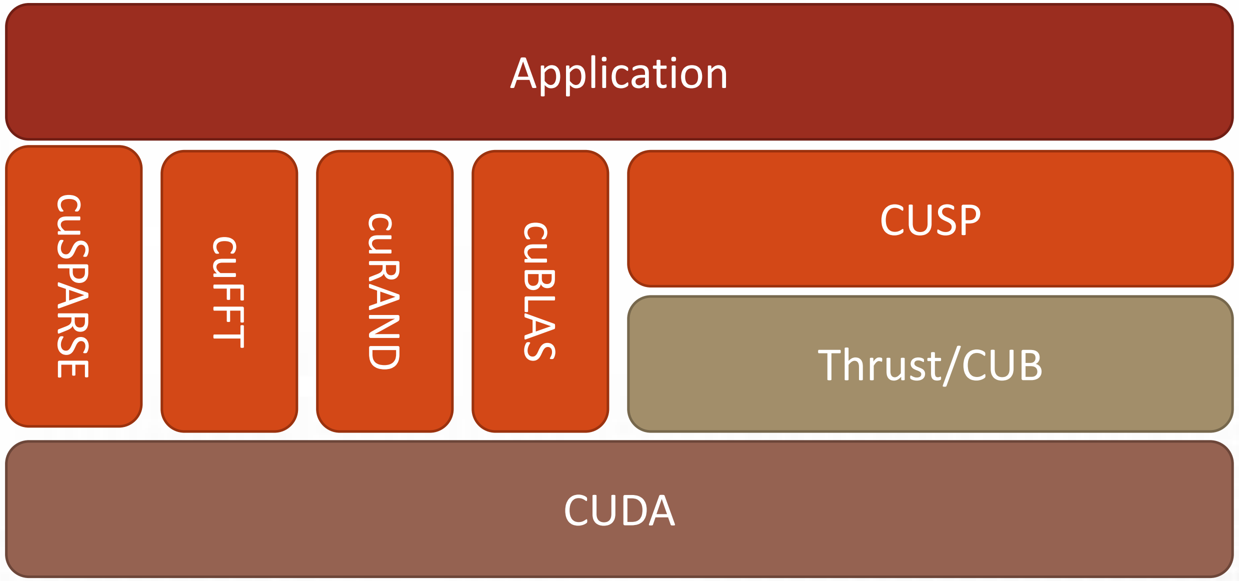


- ❑Sorting and Merging increasing large bionic sequences
  - ❑When $n = 2^k$ there are k levels with $\frac{n}{2}$ comparisons each
- ❑GPU Implementation
  - ❑Regular access strides :-)
  - ❑Efficiently balanced workload :-)
  - ❑Requires multiple kernel launches to merge over n > block size

- ❑Sorting Networks
- ❑Merge and Bitonic sort
- ❑Thrust Parallel Primitives Library
- ❑Applications of sorting (binning)

CUDA libraries

- Abstract CUDA model away from programmer
- Highly optimised implementations of common tools
  - Mainly focused on linear algebra



Thrust

- Template Library for CUDA
  - Implements many parallel primitives (scan, sort, reduction etc.)
  - Part of standard CUDA release
  - Level of Abstraction which hides kernels, mallocs and memcpy’s
- Designed for C++ programmers
  - Similar in design and operation as the C++ Standard Template Library (STL)
  - Only a small amount of C++ required..

Thrust containers

- Thrust uses <u>only</u> high level *vector* containers
  - `host_vector`: on host
  - `device_vector`: on GPU
- Other STL containers include
  - queue
  - list
  - tack
  - queue
  - priority_queue
  - set
  - multiset
  - map
  - multimap
  - bitset
- STL containers can be used to initialise a Thrust vector

```
#include <thrust/host_vector.h>
#include <thrust/device_vector.h>

int main()
{
  //create a vector on the host
  thrust::host_vector<int> h_vec(10);

  //create a vector on the device
  thrust::device_vector<int> d_vec = h_vec;

  //device data manipulated directly from host
  for (int i = 0; i < 10; i++)
    d_vec[i] = i;

  //vector memory automatically released
  return 0;
}
```

Thrust Iterators

- They point to regions of a vector
- Can be used like pointers
  - Explicit cast when dereferencing very important

```
thrust::device_vector<int>::iterator begin = d_vec.begin();
thrust::device_vector<int>::iterator end = d_vec.end();
printf("d_vec at begin=%d", (int)*begin);
begin++;//move on a single position
printf("d_vec at begin++=%d", (int)*begin);
*end = 88;
printf("d_vec at end=%d", (int)*end);
```

```
d_vec at begin=0
d_vec at begin++=1
d_vec at end=88
```

Thrust Iterators

- Can be converted to a raw pointer

```
int * d_ptr = thrust::raw_pointer_cast(begin);
int * d_ptr = thrust::raw_pointer_cast(begin[0]);

kernel<BLOCKS, TPB>(d_ptr);
```

- Raw pointers can be used in Thrust
  - BUT not exactly the same as a vector

```
int* d_ptr;
cudaMalloc((void**)&d_ptr, N);
thrust::device_ptr<int> d_vec =  thrust::device_pointer_cast(d_ptr);
//or
thrust::device_ptr<int> d_vec = thrust::device_ptr<int>(d_ptr)
cudaFree(d_ptr);
```

Thrust Algorithms

- Transformations
  - Application of a function to each element within the range of a vector
- Reduction
  - Reduction of a set of values to a single value using binary associative operator
  - Can also be used to count occurrences of a value
- Prefix Sum
  - Both inclusive and exclusive scans
- Sort
  - Can sort keys or key value pairs
- Binary Search
  - Position of a target value

Thrust Transformations

- Some examples of the many transformations

```
thrust::copy(d_vec.begin(), d_vec.begin() + 10, d_vec_cpy.begin());

thrust::fill(d_vec.begin(), d_vec.begin() + 10, 0);

//rand is a predefined Thrust generator
thrust::generate(d_vec.begin(), d_vec.begin() + 10, rand);

// fill d_vec with {0, 1, 2, 3, 4, 5, 6, 7, 8, 9}
thrust::sequence(d_vec.begin(), d_vec.begin() + 10);

//all occurrences of the value 1 are replaced with the value 10
thrust::replace(d_vec.begin(), d_vec.end(), 1, 10);
```

Thrust Algorithms

- Either in-place or to output vector

```
thrust::device_vector<int> d_vec(10);
thrust::device_vector<int> d_vec_out(10);

//fill d_vec with {0, 1, 2, 3, 4, 5, 6, 7, 8, 9}
thrust::sequence(d_vec.begin(), d_vec.begin() + 10);

//inclusive scan to output vector
thrust::inclusive_scan(d_vec.begin(), d_vec.end(),
d_vec_out.begin());

//inclusive scan in place
thrust::inclusive_scan(d_vec.begin(), d_vec.end(),
d_vec.begin());

//generate random data (actually a transformation)
thrust::generate(d_vec.begin(), d_vec.end(), rand);

//sort in place
thrust::sort(d_vec.begin(), d_vec.end());
```

Custom Transformations

```
thrust::device_vector<int> d_vec(10);
thrust::device_vector<int> d_vec_out(10);

//fill d_vec with {0, 1, 2, 3, 4, 5, 6, 7, 8, 9}
d_vec = thrust::sequence(d_vec.begin(), d_vec.begin() + 10);


//declare a custom operator
struct add_5{
  __host__ __device__ int operator()(int a){
     return a + 5;
  }
};

add_5 func;

//apply custom transformation
thrust::transform(d_vec.begin(), d_vec.end(), d_vec_out.begin(), func);

//d_vec is now {5, 6, 7, 8, 9, 10, 11, 12, 13, 14}
```

Thrust Fusion

- For best performance it is necessary to fuse operations

```
struct absolute{
  __host__ __device__ int operator()(int a){
    return a < 0 ? -a : a ;
  }
};
absolute func;

//custom transformation to calculate absolute value
thrust::transform(d_vec.begin(), d_vec.end(), d_vec.begin(), func);
//apply reduction, maximum binary associate operator
int result = thrust::reduce(d_vec.begin(), d_vec.end(), 0, thrust::maximum<int>());
```

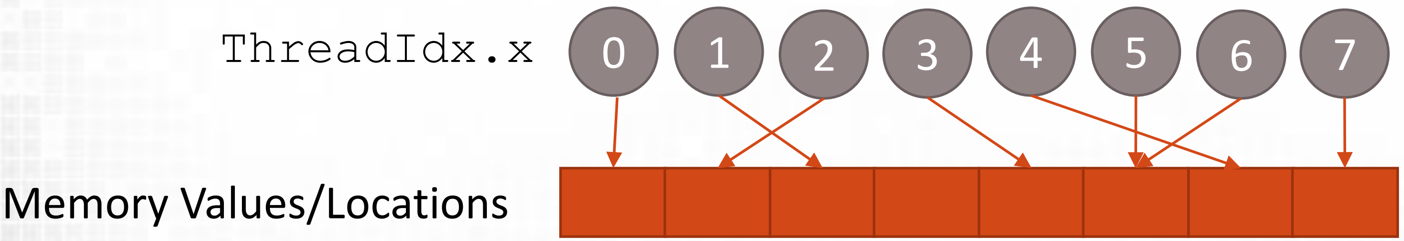
```
struct absolute{
  __host__ __device__ int operator()(int a){
    return a < 0 ? -a : a ;
  }
};
absolute func;

//apply transform reduction maximum binary associate operator
int result = thrust::transform_reduce(d_vec.begin(), d_vec.end(), func, 0, thrust::maximum<int>());
```

- ❑ Sorting Networks
- ❑ Merge and Bitonic sort
- ❑ Thrust Parallel Primitives Library
- ❑ Applications of sorting (binning)

Sorting and parallel primitives

- ❑Can be very useful for building data structures
  - ❑We can use prefix sum for writing multiple values per element
- ❑Remember Gather vs Scatter
  - ❑What if our outputs are scattered to output
  - ❑Very common in particle simulations etc.
    - ❑Outputs might represent spatial bins



Scatter operation

- ❑ Write to a number of locations
- ❑ Random access write?

- ❑ How to read multiple values afterwards?

Binning and Sorting

`ThreadIdx.x`	0	1	2	3	4	5	6	7
Desired Write_Index for the thread	0	2	1	4	6	5	5	7
thrust::sort(Write_Index)	0	1	2	4	5	5	6	7

Build a data structure

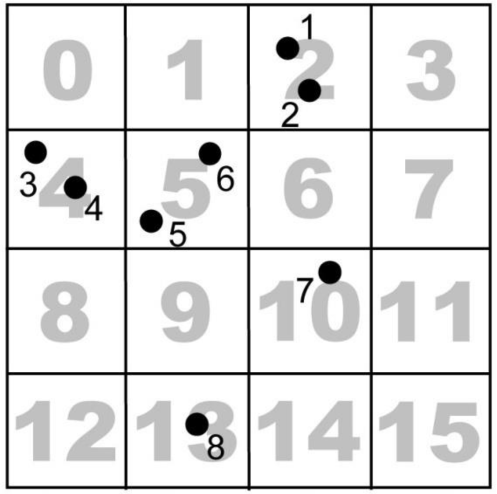
Unique write indices	0	1	2	3	4	5	6	7
Count(Write_Index)	1	1	1	0	1	2	1	1
thrust::inclusive_scan(count)	0	1	2	3	3	4	6	7

i.e. how many threads want to write to this index

- We can now read varying values from each bin
  - E.g. for location 5
    - inclusive_scan gives starting index of 4
    - Iterate from index 4 for a count of 2 to find all values of write_index 5

Particle interaction example

- As with previous slide use sorting
  - Divide the environment according to some interaction radius
  - Output particle key value pairs (keys are location determined through some hash function)
  - Sort Keys
  - Reorder particles based on key pairs
  - Generate a partition boundary table
    - Histogram count and prefix sum
  - Each particle needs to read all particles in its own location and any neighbouring location
    - Guarantees particle interactions within the interaction radius



Partition	First agent	Last agent
0		
1		
2	1	2
3		
4	3	4
5	5	6
6		
7		
8		
9		
10	7	7
11		
12		
13	8	8
14		
15		

Summary

- Sorting networks allow data independent sort algorithms to map easily parallel architectures
- Choice of a sorting network will dictate the memory access pattern and hence the performance on a GPU
- Merge sort and Bitonic sort are popular choices for GPUs
- Thrust implements many parallel primitives
- Thrust is based on the idea of containers, iterators, transformations and algorithms
- Sorting can be used to improve complex problems such as particle systems over a fixed range

Acknoledgements and Further Reading

- Comparison on sorting approaches on GPU
  - http://arxiv.org/ftp/arxiv/papers/1511/1511.03404.pdf

- https://devblogs.nvidia.com/parallelforall/expressive-algorithmic-programming-thrust/