# CME 213

## SPRING 2019

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# Thrust

- Writing CUDA code is not that easy!
- Difficulty of writing code with good performance
- Portability problem: what if my computer does not have an NVIDIA GPU?

- Thrust offers a clever solution to some of these problems!

# What is Thrust?

- It's the STL (standard template library) of CUDA!
- It's a C++ template library that does many things:
- Implement several standard algorithms like sort, reduction, scan
- Allows the user to easily specify "custom" operations if they are not in the library.
- Provides a high-performance implementation. All the hard work has been done for you already!

- That's magic.
- Works beautifully but requires good knowledge of templates.
- "Think STL"

# Multiple backends

- Provides multiple back-ends: CUDA, OpenMP, TBB (Threading Building Blocks by Intel), and regular C++.

- Compilation option examples:

OpenMP

```
-Xcompiler -fopenmp \
-DTHRUST_DEVICE_SYSTEM=THRUST_DEVICE_SYSTEM_OMP -lgomp
```

TBB

```
-DTHRUST_DEVICE_SYSTEM=THRUST_DEVICE_SYSTEM_TBB -ltbb
```

- You can compile with nvcc or just g++.

# Backend preprocessing macro options

- Default:

```
THRUST_DEVICE_SYSTEM_CUDA

THRUST_DEVICE_SYSTEM_OMP
THRUST_DEVICE_SYSTEM_TBB
THRUST_DEVICE_SYSTEM_CPP
```

# Vectors

- Data is stored as vectors.
- Two types of vectors: host and device.
- Device vector lives on the GPU but we can be used like a regular STL vector!

# Host vector

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

#include <iostream>

int main(void) {
    // H has storage for 4 integers
    thrust::host_vector<int> H(4);

    // initialize individual elements
    H[0] = 14;
    H[1] = 20;
    H[2] = 38;
    H[3] = 46;

    // H.size() returns the size of vector H
    std::cout << "H has size " << H.size() << std::endl;

    // print contents of H
    for(size_t i = 0; i < H.size(); i++) {
        std::cout << "H[" << i << "] = " << H[i] << std::endl;
    }
```

# Device vector

Same syntax.

Lives on the GPU but no difference for the programmer.

```
// Copy host_vector H to device_vector D
thrust::device_vector<int> D = H;

// elements of D can be modified
D[0] = 99;
D[1] = 88;

// print contents of D
for(size_t i = 0; i < D.size(); i++) {
    std::cout << "D[" << i << "] = " << D[i] << std::endl;
}
```

# Containers

- STL has many containers!
  - vector, list, deque, set, multiset, map, multimap, hash_set, hash_multiset, hash_map, hash_multimap
- Thrust only allows vector.
- This is because this is the only container that fits well the GPU computing model.
- Thrust is still compatible with the STL.

# Static dispatching

Thrust is a clever system. It figures out based on the type of the arguments whether an algorithm should be run on the host or device.

```
// initialize all ten integers of a device_vector to 1
thrust::device_vector<int> D(10, 1);

// set the first seven elements of a vector to 9
thrust::fill(D.begin(), D.begin() + 7, 9);

// initialize a host_vector with the first five elements of D
thrust::host_vector<int> H(D.begin(), D.begin() + 5);

// set the elements of H to 0, 1, 2, 3, ...
thrust::sequence(H.begin(), H.end());
```

Runs on the GPU

Runs on the CPU

Decision is based on type: host or device

# Pointer types

- Casting between pointer types is often needed.
- Thrust assumes that a regular pointer lives on the host. But this is not always true!

```
// raw pointer to device memory
int* raw_ptr;
cudaMalloc((void**) &raw_ptr, N * sizeof(int));

// wrap raw pointer with a device_ptr
thrust::device_ptr<int> dev_ptr(raw_ptr);

// use device_ptr in thrust algorithms
thrust::fill(dev_ptr, dev_ptr + N, (int) 0);
```

Without the cast, the function would run on the host

- This allows using Thrust in the middle of other CUDA code.

# Raw pointers

Similarly, there are cases where Thrust produces some output result that we want to use

```
// create a device_ptr
thrust::device_ptr<int> dev_ptr = thrust::device_malloc<int>(N);

// extract raw pointer from device_ptr
int* raw_ptr = thrust::raw_pointer_cast(dev_ptr);
```

Convert a device pointer back to a regular pointer

This means you can freely go back and forth between CUDA and Thrust.

# Let's get to work!

- Let's calculate a saxpy: $Y \leftarrow aX + Y$

- We take as input (a, x[i], y[i]) and return a*x[i]+y[i]
- For this, STL-like transform functions are required.
- What is a transform?

```
OutputIterator thrust::transform ( InputIterator    first,
                                   InputIterator    last,
                                   OutputIterator   result,
                                   UnaryFunction    op
                                 )
```

```
Input → Output
```

```
OutputIterator thrust::transform ( InputIterator1   first1,
                                   InputIterator1   last1,
                                   InputIterator2   first2,
                                   OutputIterator   result,
                                   BinaryFunction   op
                                 )
```

```
(Input1,Input2) → Output
```

# Operators

- How do we define an operator?
- Generally speaking, this is simply an object `f` for which we can define `f(x,y)`.
- See `saxpy.cu` example.

What's a functor?
Answer: a class that defines an operator ()

A binary function takes two inputs, and returns one output

```
struct saxpy_functor : public thrust::binary_function<float,float,float> {
    const float a;

    saxpy_functor(float _a) : a(_a) {}

    __host__ __device__
    float operator()(const float& x, const float& y) const {
        return a * x + y;
    }
};
```

That's the () operator! The type of the variables must match **`binary_function`**

# Applying the transform

```
void saxpy(float A, thrust::device_vector<float>& X,
           thrust::device_vector<float>& Y) {
    // Y <- A * X + Y
    thrust::transform(X.begin(), X.end(), Y.begin(), Y.begin(), saxpy_functor(A));
}
```

**Input 1** **Input 2** **Output** **Functor**

# Exercise

- Open **`adj_diff.cu`**
- Complete the **`TODO`** missing code
- All the asserts should pass when your implementation is correct.

# Algorithms

That’s good but I already know how to do that.

Remember that the backend can be GPU or CPU. That should count!

More importantly, Thrust provides many STL algorithms:

- Reduce
- Scan
- Sort
- Reorder/copy
- Search

# Example: sort

May sorts possible using the same framework.

`sort.cu`

# Basic sort

```
std::cout << "sorting integers\n";
{
    thrust::device_vector<int> keys(N);
    initialize(keys);
    print(keys);
    thrust::sort(keys.begin(), keys.end());
    print(keys);
}
```

```
sorting integers
 79 78 62 78 94 40 86 57 40 16 28 54 77 87 93 98
 16 28 40 40 54 57 62 77 78 78 79 86 87 93 94 98
```

# User-defined

```
std::cout << "\nsorting integers (user-defined comparison)\n";
{
    thrust::device_vector<int> keys(N);
    initialize(keys);
    print(keys);
    thrust::sort(keys.begin(), keys.end(), evens_before_odds());
    print(keys);
}
```

```
struct evens_before_odds {
    __host__ __device__
    bool operator()(int x, int y) {
        if(x % 2 == y % 2) {
            return x < y;
        } else if(x % 2) {
            return false;
        } else {
            return true;
        }
    }
};
```

```
sorting integers (user-defined comparison)
 79 78 62 78 94 40 86 57 40 16 28 54 77 87 93 98
 16 28 40 40 54 62 78 78 86 94 98 57 77 79 87 93
```

# Key-value sorting

```
std::cout << "\nkey-value sorting\n";
{
    thrust::device_vector<int> keys(N);
    thrust::device_vector<int> values(N);
    initialize(keys, values);
    print(keys, values);
    thrust::sort_by_key(keys.begin(), keys.end(), values.begin());
    print(keys, values);
}
```

```
key-value sorting
 (79, 0) (78, 1) (62, 2) (78, 3) (94, 4) (40, 5) (86, 6) (57, 7) (40, 8) (16, 9) (28,10) (54,11) (77,12) (87,13) (93,14) (98,15)
 (16, 9) (28,10) (40, 5) (40, 8) (54,11) (57, 7) (62, 2) (77,12) (78, 1) (78, 3) (79, 0) (86, 6) (87,13) (93,14) (94, 4) (98,15)
```

More examples in **`sort.cu`**

# Kernel fusion or composability

More general calculations are allowed by chaining kernels together.

Imagine for example that we want to compute the norm of a vector.

This involves two steps:

- Computing the square of each entry
- Summing up all the values (reduce)

Each step is supported by Thrust, but there is no function in Thrust that does both.

Is it still possible to make it work?

# Transform iterators

A clever trick. How does it work?

Take a vector:

```
thrust::device_vector<int> input(N);
```

Here is a simple reduce:

```
sum = thrust::reduce(input.begin(), input.end());
```

We need to take the square of the entries.

`input.begin()` is an iterator. It can be dereferenced to get a value

```
5 ⇦ (*it)
```

We want an iterator which when dereferenced returns the square

```
5*5 ⇦ (*…)
```

This works by writing this as

```
5*5 ⇦ square(5) ⇦ 5 ⇦ (*it)
```

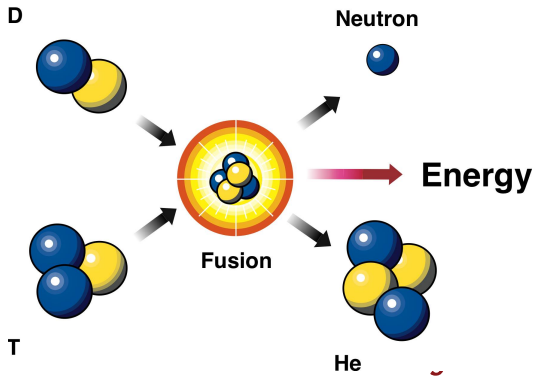
You have to chain or fuse operations.

Input iterator

Function applied to iterator (*it)

```
int sum = thrust::reduce(
            thrust::make_transform_iterator(
                input.begin(), square()),
            thrust::make_transform_iterator(
                input.end(), square()));
```

Create a new iterator = fusion!



```
struct square : public thrust::unary_function<int,int> {
    __host__ __device__
    int operator()(const int x) const {
        return x * x;
    }
};
```

- A unary functor is required
- **`transform_iterator`** allows composing kernels together.
- This greatly expands the number of things you can do using Thrust.

# Histogram

Thrust can be used in creative ways to do a lot of things.
Say for example that you want to calculate a histogram.

Input data:

3 4 3 5 8 5 6 6 4 4 5 3 2 5 6 3 1 3 2 3 6 5 3 3 3 2 4 2 3 3 2 5 5 5 8 2 5 6 6 3

Bins

0 1 2 3 4 5 6 7 8

Count

0 1 6 12 4 9 6 0 2

# Implementation

Let's break it down step by step.

First, sort!

```
// sort data to bring equal elements together
thrust::sort(data.begin(), data.end());
```

```
initial data  3 4 3 5 8 5 6 6 4 4 5 3 2 5 6 3 1 3 2 3 6 5 3 3 3 2 4 2 3 3 2 5 5 5 8 2 5 6 6 3
 sorted data  1 2 2 2 2 2 2 3 3 3 3 3 3 3 3 3 3 3 4 4 4 4 5 5 5 5 5 5 5 5 5 6 6 6 6 6 6 8 8
```

```
initial data  3 4 3 5 8 5 6 6 4 4 5 3 2 5 6 3 1 3 2 3 6 5 3 3 3 2 4 2 3 3 2 5 5 5 8 2 5 6 6 3
 sorted data  1 2 2 2 2 2 2 3 3 3 3 3 3 3 3 3 3 3 3 4 4 4 4 5 5 5 5 5 5 5 5 5 6 6 6 6 6 6 8 8
```

That's how many bins we need

We need to count how many repeats we have in this sequence.

# Use upper_bound


- We are getting deeper into Thrust voodoo territory.
- **upper_bound** searches the position where a value can be inserted without violating the ordering.

| | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Input | 1 | 2 | 2 | 2 | 2 | 2 | 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | … |
| Position | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | … |
| Values | | | | | | | | 2 | | | | | | | | | | | | 3 | |

```
Upper bound of 2 is:  7
Upper bound of 3 is:  19
```

# Cumulative sum

**`upper_bound`** basically gives a cumulative sum of the histogram we are looking for.

```
thrust::counting_iterator<IndexType> search_begin(0);
thrust::upper_bound(data.begin(), data.end(),
                    search_begin, search_begin + num_bins,
                    histogram.begin());
```

Counts from 0 to num_bins
0 1 2 3 4 5 6 7 8

Output goes there

```
Dense Histogram
          initial data  3 4 3 5 8 5 6 6 4 4 5 3 2 5 6 3 1 3 2 3 6 5 3 3 3 2 4 2 3 3 2 5 5 5 8 2 5 6 6 3
           sorted data  1 2 2 2 2 2 2 3 3 3 3 3 3 3 3 3 3 3 4 4 4 4 5 5 5 5 5 5 5 5 5 6 6 6 6 6 6 8 8
  cumulative histogram  0 1 7 19 23 32 38 38 40
```

# Dense histogram

Take differences to get the histogram

```
thrust::adjacent_difference(histogram.begin(), histogram.end(),
                            histogram.begin());
```

```
Dense Histogram
          initial data  3 4 3 5 8 5 6 6 4 4 5 3 2 5 6 3 1 3 2 3 6 5 3 3 3 2 4 2 3 3 2 5 5 5 8 2 5 6 6 3
           sorted data  1 2 2 2 2 2 2 3 3 3 3 3 3 3 3 3 3 3 3 4 4 4 4 5 5 5 5 5 5 5 5 5 6 6 6 6 6 6 8 8
  cumulative histogram  0 1 7 19 23 32 38 38 40
      histogram values  0 1 2 3 4 5 6 7 8
      histogram counts  0 1 6 12 4 9 6 0 2
```

# Sparse histogram

- Actually simpler.

- We want to print only the bins that contain at least 1 value (e.g., skip bin 7).

Two steps:

1. Count how many unique bins are required (histogram bins for which we have at least one value)
2. Calculate the number of values in each bin

# Count the number of bins needed

Clever use of **`inner_product`**

Voodoo[2]

```
  initial data  3 4 3 5 8 5 6 6 4 4 5 3 2 5 6 3 1 3 2 3 6 5 3 3 3 2 4 2 3 3 2 5 5 5 8 2 5 6 6 3
   sorted data  1 2 2 2 2 2 2 3 3 3 3 3 3 3 3 3 3 3 3 4 4 4 4 5 5 5 5 5 5 5 5 5 6 6 6 6 6 6 8 8
  shifted data  2 2 2 2 2 2 3 3 3 3 3 3 3 3 3 3 3 3 4 4 4 4 5 5 5 5 5 5 5 5 6 6 6 6 6 6 8 8
not equal data  1 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 1 0 0 0 1 0 0 0 0 0 0 0 0 1 0 0 0 0 0 1 0
```

This is what we are after!

Shifted data

```
int num_bins = thrust::inner_product(data.begin(), data.end() - 1,
                                     data.begin() + 1,
                                     1,
                                     thrust::plus<int>(),
                                     thrust::not_equal_to<int>());
```

Starting value

The addition

The multiplication!

# One call to Thrust is enough!

1 1 1 1 1 …

```
thrust::reduce_by_key(data.begin(), data.end(),
                      thrust::constant_iterator<int>(1),
                      histogram_values.begin(),
                      histogram_counts.begin());
```

```
thrust::pair<OutputIterator1,OutputIterator2> thrust::reduce_by_key ( InputIterator1  keys_first,
                                                                       InputIterator1  keys_last,
                                                                       InputIterator2  values_first,
                                                                       OutputIterator1 keys_output,
                                                                       OutputIterator2 values_output
                                                                     )
```

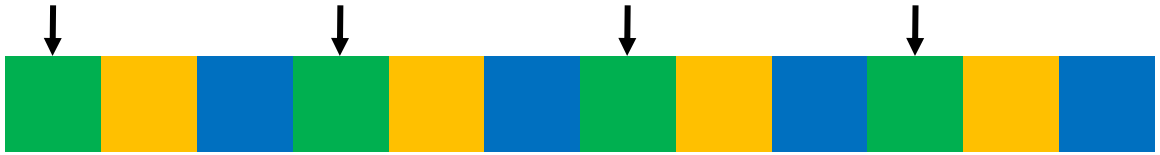
- For each of group of consecutive keys that are equal, perform a reduction.
- Write the key (“data”) to **`keys_output`**, and the result of the reduction (histogram) to **`values_output`**.

No 7 because it is a sparse histogram

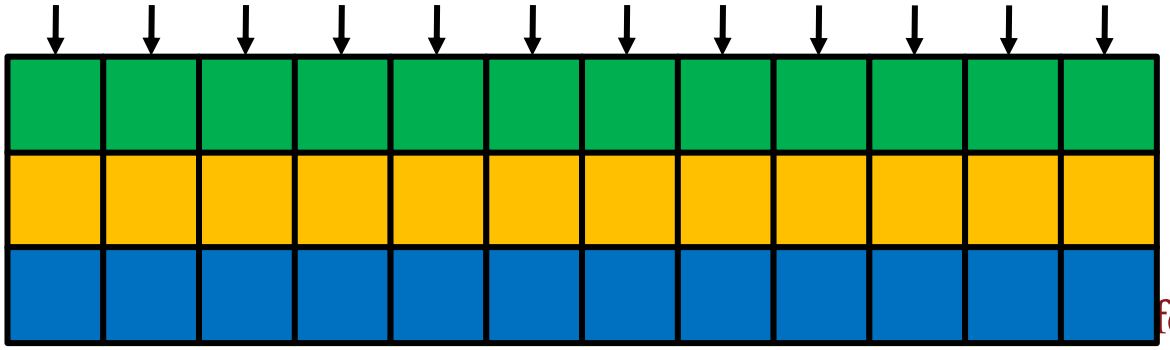
```
    initial data  3 4 3 5 8 5 6 6 4 4 5 3 2 5 6 3 1 3 2 3 6 5 3 3 3 2 4 2 3 3 2 5 5 5 8 2 5 6 6 3
     sorted data  1 2 2 2 2 2 2 3 3 3 3 3 3 3 3 3 3 3 3 4 4 4 4 5 5 5 5 5 5 5 5 6 6 6 6 6 6 8 8
    shifted data  2 2 2 2 2 2 3 3 3 3 3 3 3 3 3 3 3 4 4 4 4 5 5 5 5 5 5 5 5 6 6 6 6 6 6 8 8
   not equal data 1 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 1 0 0 0 0 0 0 0 0 1 0 0 0 0 0 1 0
histogram values  1 2 3 4 5 6 8
histogram counts  1 6 12 4 9 6 2
```

# Zippers

- There are many cases where a function expects one argument but we need many.
- What should we do then?
- This can be quite common in fact.
- Usually, for convenience, we define structs and put all our variables in them.
- This is the Array of Structs approach.
- However, on a GPU, this leads to uncoalesced memory access.
- It is better to use a **Struct of Arrays.**



Stride 3



Stride 1

# Zippers are the way to go

- Say we have two arrays of 3D vectors.
- We want to calculate the dot product of all these vectors.
- **`(A0, A1, A2)`** is array A of 3D vectors.
- **`(B0, B1, B2)`** is array B.

```
thrust::device_vector<float> A0 =
    random_vector(N, rng);  // x components of the 'A' vectors
thrust::device_vector<float> A1 =
    random_vector(N, rng);  // y components of the 'A' vectors
thrust::device_vector<float> A2 =
    random_vector(N, rng);  // z components of the 'A' vectors

thrust::device_vector<float> B0 =
    random_vector(N, rng);  // x components of the 'B' vectors
thrust::device_vector<float> B1 =
    random_vector(N, rng);  // y components of the 'B' vectors
thrust::device_vector<float> B2 =
    random_vector(N, rng);  // z components of the 'B' vectors
```

# Zip it!

Zip it to create a single iterator for A, and another one for B.

```
Float3Iterator A_first = thrust::make_zip_iterator(
                            make_tuple(A0.begin(), A1.begin(), A2.begin()));
Float3Iterator A_last  = thrust::make_zip_iterator(
                            make_tuple(A0.end(), A1.end(), A2.end()));
Float3Iterator B_first = thrust::make_zip_iterator(
                            make_tuple(B0.begin(), B1.begin(), B2.begin()));
```

# Then run the kernel

The kernel is run as usual using the zip iterators.

```
thrust::transform(A_first, A_last, B_first, result.begin(), DotProduct());


// We use a 3-tuple to store the 3 components of our vector
typedef thrust::tuple<float,float,float> Float3;

// This functor implements the dot product between 3d vectors
struct DotProduct : public thrust::binary_function<Float3,Float3,float> {
    __host__ __device__
    float operator()(const Float3& a, const Float3& b) const {
        return thrust::get<0>(a) * thrust::get<0>(b) +    // x components
               thrust::get<1>(a) * thrust::get<1>(b) +    // y components
               thrust::get<2>(a) * thrust::get<2>(b);     // z components
    }
};
```

Standard C++ tuple syntax

# Shortcuts!

```
thrust::transform(X.begin(), X.end(),   // input range #1
                  Y.begin(),            // input range #2
                  Y.begin(),            // output range
                  a * _1 + _2);         // placeholder expression
```

The placeholder expression

```
a * _1 + _2
```

means to add `a` times the first argument, `_1`, to the second argument, `_2`.

# C++11 lambda expressions

- Functor no longer required
- Replaced by a lambda expression
- Allows to write more compact, elegant code.
- Compile with:

**`-std=c++11 --expt-extended-lambda`**

```
thrust::transform(X.begin(),
                  X.end(),
                  Y.begin(),
                  Y.begin(),
                  [=] __host__ __device__ (float x, float y) {
                    return a * x + y;
                  }
                 );
```

# Relevant CUDA libraries

CUBLAS - Basic Linear Algebra Subroutines

CUSPARSE - Sparse Matrix library

CURAND - Random Number Generation library

CUFFT - Fast Fourier Transform library

NPP - Performance Primitives library; collection of GPU-accelerated image, video, and signal processing functions

Closely related to Thrust:

CUB - library of parallel primitives and other utilities; provides an abstraction layer over block-level, warp-level, and thread-level operations.

- ***Parallel primitives***
  - ***Warp-wide "collective" primitives***
    - Cooperative warp-wide prefix scan, reduction, etc.
    - Safely specialized for each underlying CUDA architecture
  - ***Block-wide "collective" primitives***
    - Cooperative I/O, sort, scan, reduction, histogram, etc.
    - Compatible with arbitrary thread block sizes and types
  - ***Device-wide primitives***
    - Parallel sort, prefix scan, reduction, histogram, etc.
    - Compatible with CUDA dynamic parallelism
- ***Utilities***
  - ***Fancy iterators***
  - ***Thread and thread block I/O***
  - ***PTX intrinsics***
  - ***Device, kernel, and storage management***

# We have only scratched the surface…

https://thrust.github.io/ Thrust homepage

https://github.com/thrust/thrust/wiki/Quick-Start-Guide

The complete documentation

https://github.com/thrust/thrust/wiki/Documentation

Use Google to search

Check the code examples to get ideas

Nothing on TV tonight? Check out some videos on Thrust:

- GTC 2011 video on Thrust by Nathan Bell
- Introduction to Thrust slides by Hoberock and Bell
- GTC 2011 video on Thrust by Hoberock and Bell
- Thrust slides and downloads on github