

CS 677: Parallel Programming for Many-core Processors

Lecture 9

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Logistics

- Homeworks 2 and 3
- Homework 4 - not yet
- Exam - no
- Projects
- Grades:
 - Homeworks 40%
 - Quizzes 7%
 - Project from 35% to 43% including proposal and midpoint report

Outline

- Pinned Memory
- Streams
- Thrust

Pinned Memory

- *Page-locked* or *pinned* memory transfers attain the highest bandwidth between host and device
 - Ensures that host buffer does not get moved to virtual memory
- Allocated using the `cudaMallocHost()`
- Pinned memory should not be overused
 - Excessive use can reduce overall system performance
 - How much is too much is difficult to tell in advance

Asynchronous Transfers and Overlapping Transfers with Computation

- Data transfers between host and device using `cudaMemcpy()` are blocking transfers
 - Control is returned to the host thread only after the data transfer is complete.
- The `cudaMemcpyAsync()` function is a nonblocking variant of `cudaMemcpy()`
 - Unlike `cudaMemcpy()` the asynchronous transfer version requires pinned host memory

Asynchronous Transfers and Overlapping Transfers with Computation

```
cudaMemcpyAsync(a_d, a_h, size,  
    cudaMemcpyHostToDevice, stream);  
kernel<<<grid, block>>>(a_d);  
cpuFunction();
```

- Memory transfer and device execution are performed in parallel with host execution
- Last argument of `cudaMemcpyAsync()` specifies stream
 - 0 is the default - only nonzero streams are asynchronous (more details soon)
 - Kernel does not begin execution until memory transfer is complete

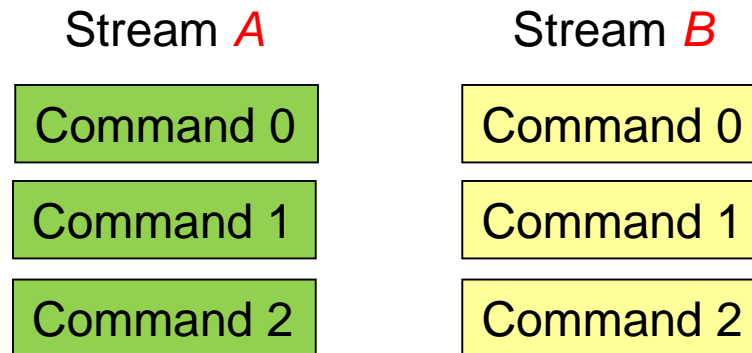
CUDA Streams

Patrick Cozzi
University of Pennsylvania
CIS 565 - Spring 2011

Steve Rennich
NVIDIA

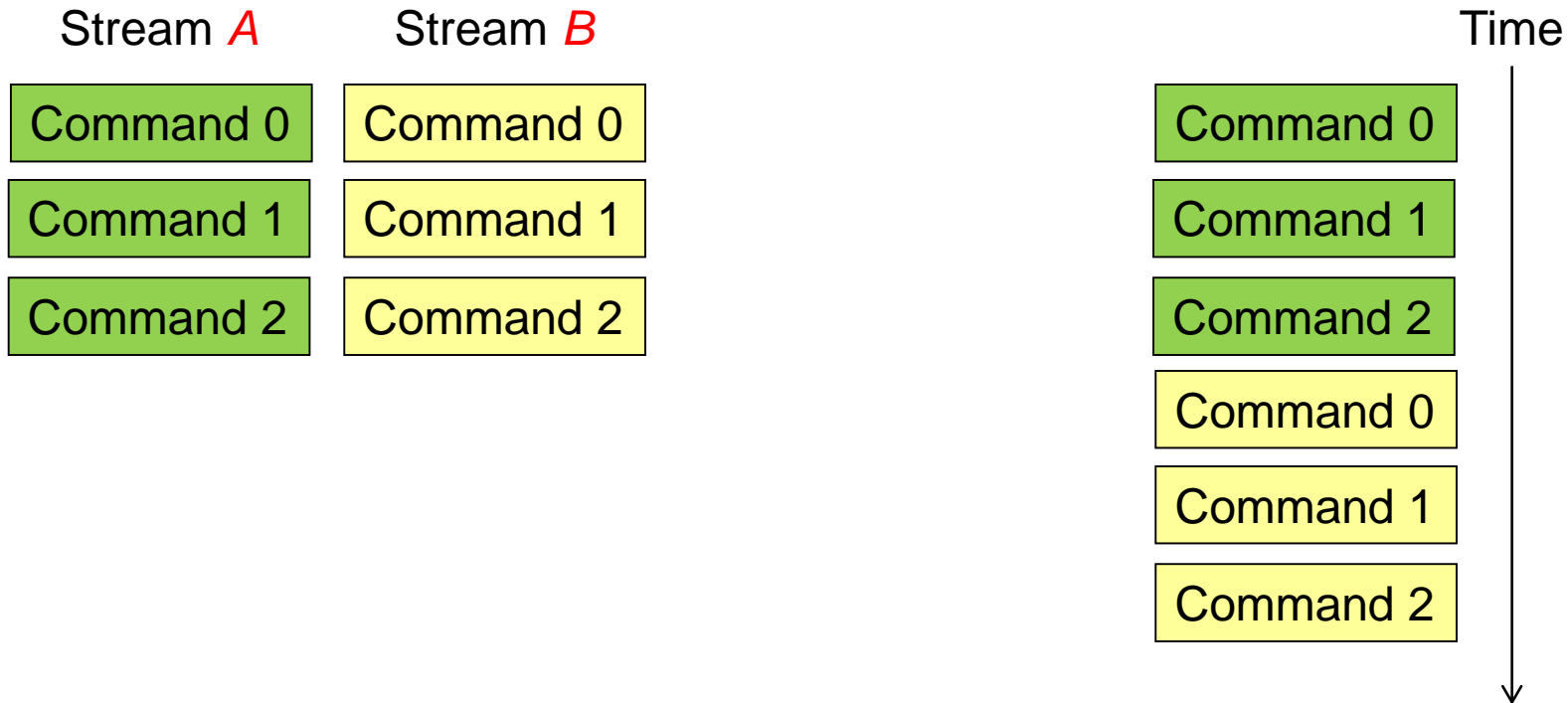
Streams

- **Stream**: Sequence of commands that execute in order
- Streams may execute their commands out-of-order or concurrently with respect to other streams



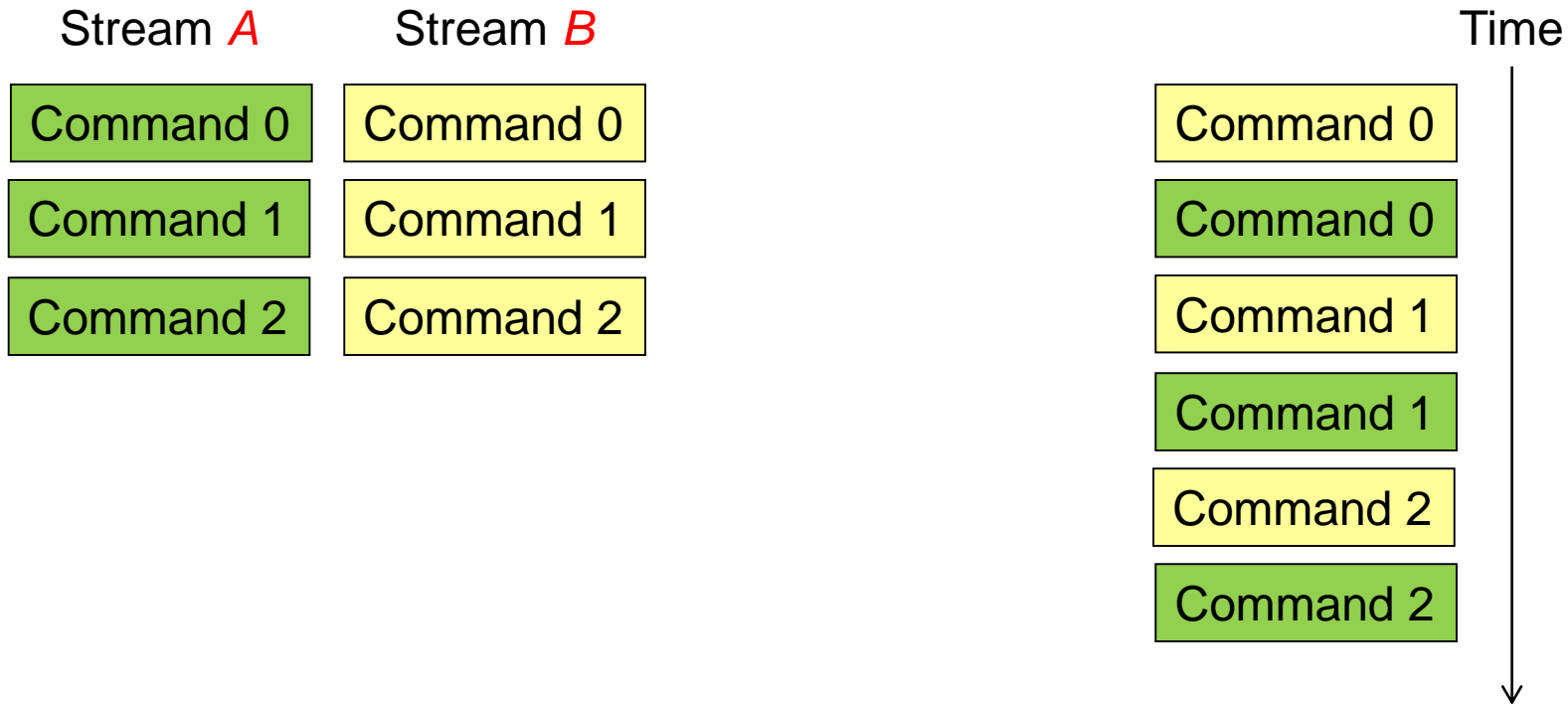
Streams

- Is this a possible order?



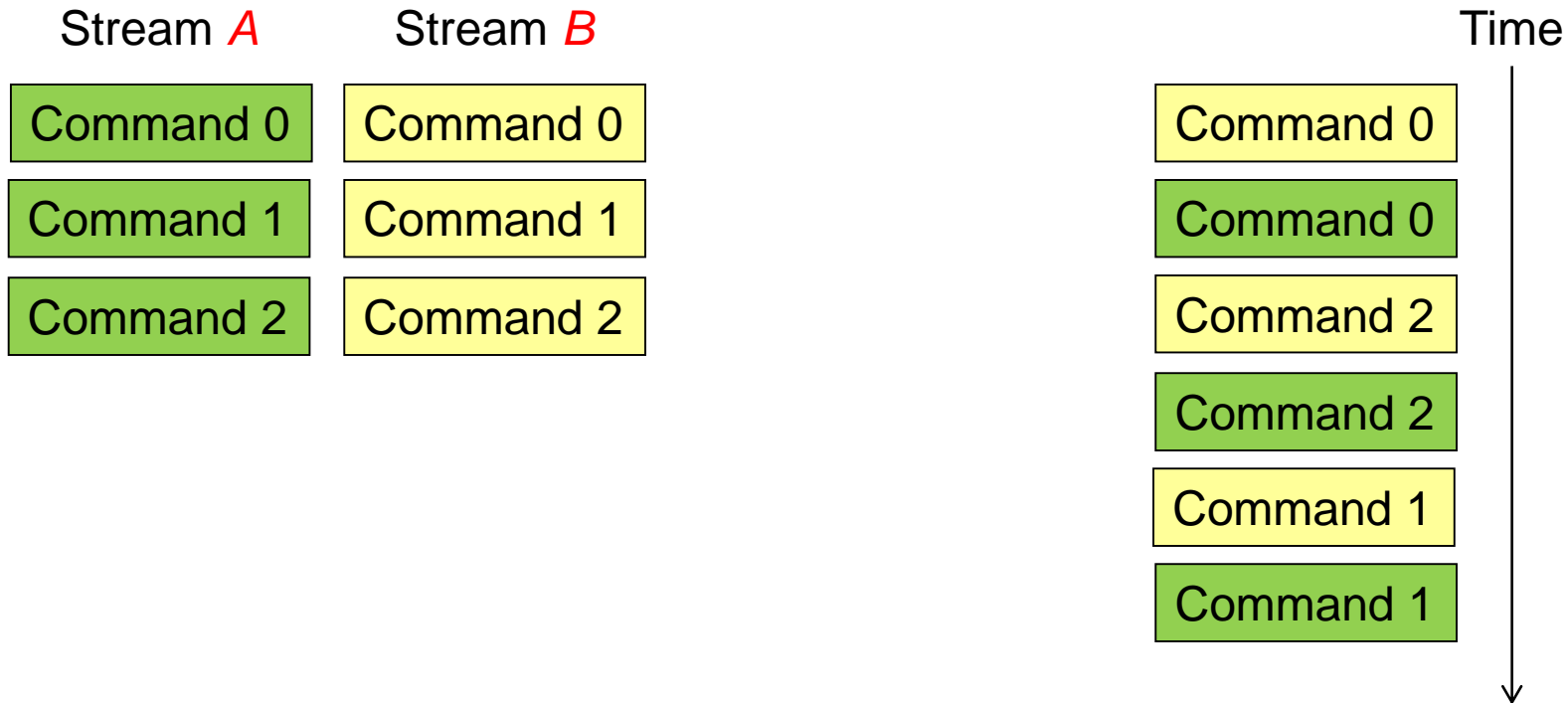
Streams

- Is this a possible order?



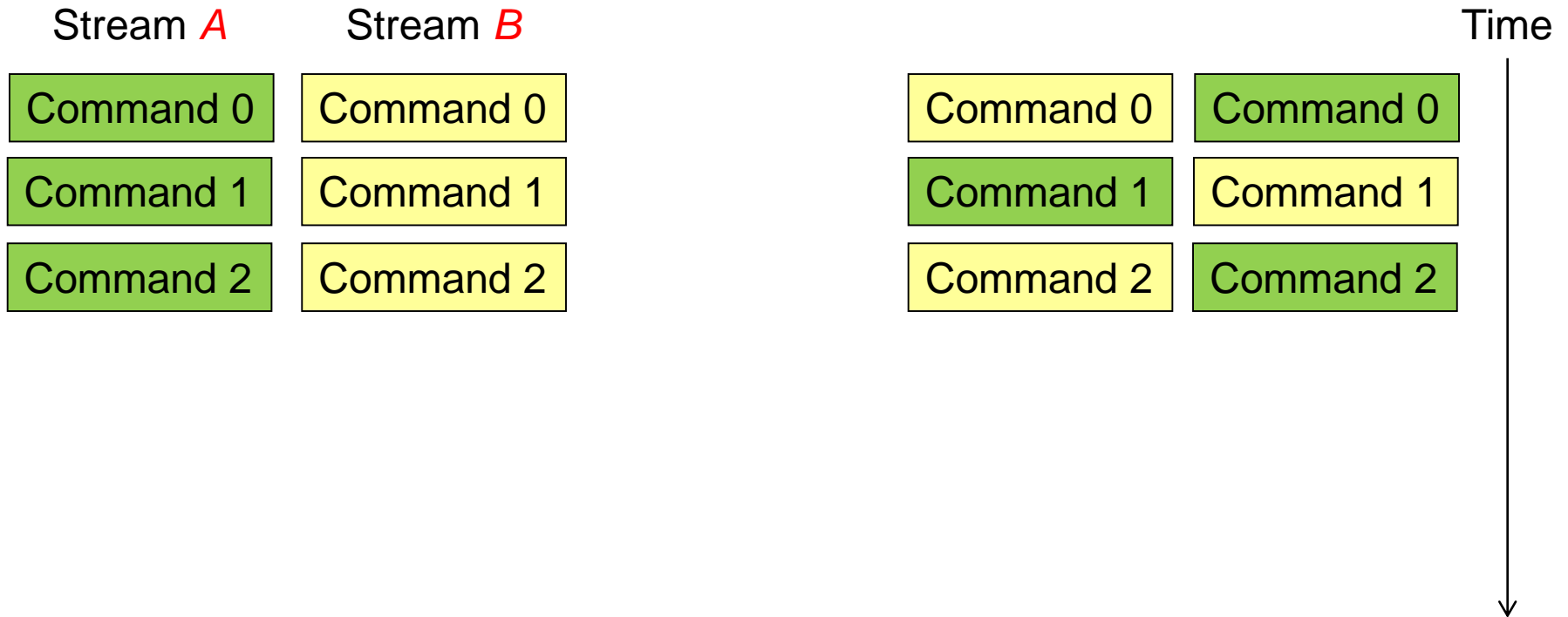
Streams

- Is this a possible order?




Streams

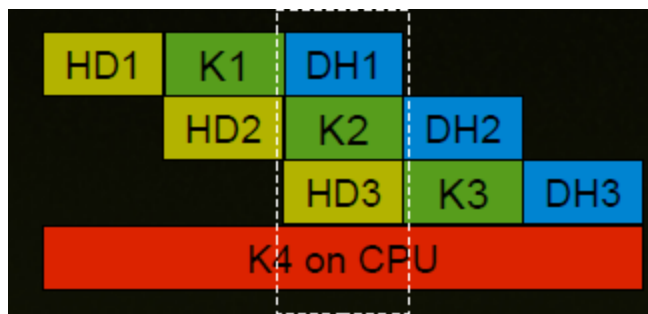
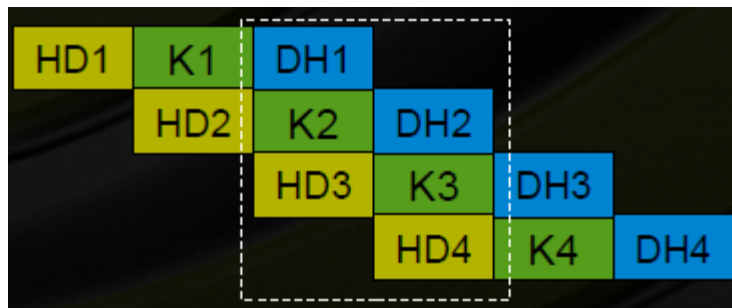
- Is this a possible order?



Streams

- In CUDA, what commands go in a stream?
 - Kernel launches
 - Host  device memory transfers

Amount of Concurrency



Default Stream (Stream '0')

- Stream used when no stream is specified
- Completely synchronous w.r.t. host and device
 - As if `cudaDeviceSynchronize()` inserted before and after every CUDA operation
- Exceptions - asynchronous w.r.t. host
 - Kernel launches in the default stream
 - `cudaMemcpy*Async`
 - `cudaMemset*Async`
 - `cudaMemcpy` within the same device
 - H2D `cudaMemcpy` of 64kB or less

Requirements for Concurrency

- CUDA operations must be in different, non-0, streams
- cudaMemcpyAsync with host from 'pinned' memory
 - Page-locked memory
 - Allocated using cudaMallocHost() or cudaHostAlloc(*) (*)
- Sufficient resources must be available
 - cudaMemcpyAsyncs in different directions
 - Device resources (SMEM, registers, blocks, etc.)

* Both commands are roughly equivalent, but not in all versions of CUDA

Streams

- Code Example
 1. Create two streams
 2. Each stream:
 1. Copy page-locked memory to device
 2. Launch kernel
 3. Copy memory back to host
 3. Destroy streams

Stream Example (Step 1 of 3)

```
cudaStream_t stream[2];  
for (int i = 0; i < 2; ++i)  
{  
    cudaStreamCreate(&stream[i]);  
}
```

Create two streams

```
float *hostPtr;  
cudaMallocHost(&hostPtr, 2 * size);
```

Stream Example (Step 1 of 3)

```
cudaStream_t stream[2];  
for (int i = 0; i < 2; ++i)  
{  
    cudaStreamCreate(&stream[i]);  
}
```

```
float *hostPtr;
```

```
cudaMallocHost(&hostPtr, 2 * size);
```

Allocate two buffers in page-locked memory

Stream Example (Step 2 of 3)

```
for (int i = 0; i < 2; ++i)
{
    cudaMemcpyAsync(/* ... */,
        cudaMemcpyHostToDevice, stream[i]);
    kernel<<<100, 512, 0, stream[i]>>>
        (/* ... */);
    cudaMemcpyAsync(/* ... */,
        cudaMemcpyDeviceToHost, stream[i]);
}
```

Commands are assigned to, and executed by streams

Stream Example (Step 3 of 3)

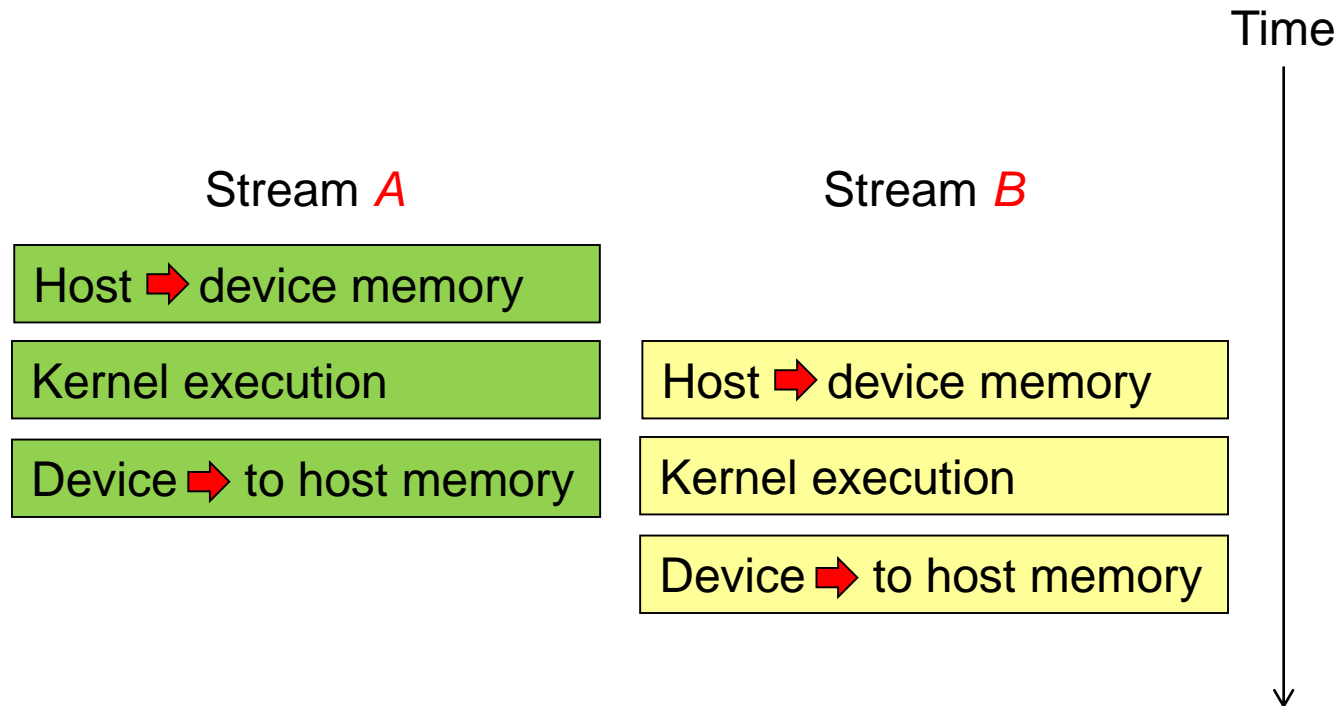
```
for (int i = 0; i < 2; ++i)
{
    // Blocks until commands complete
    cudaStreamDestroy(stream[i]);
}
```

Streams

- Assume compute capability 1.1 and above:
 - Overlap of data transfer and kernel execution
 - Concurrent kernel execution
 - Concurrent data transfer
- How can the streams overlap?

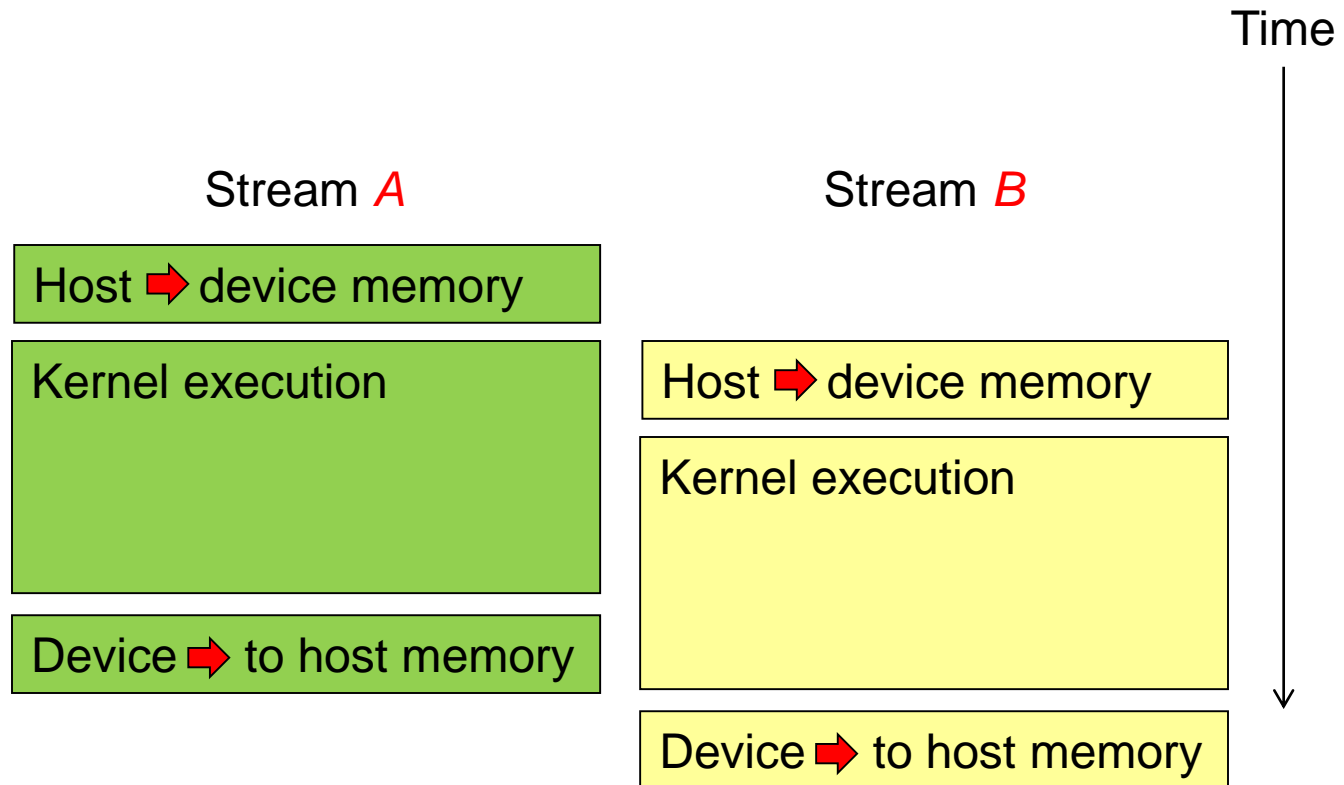
Streams

- Can we have more overlap than this?



Streams

- Can we have this?



Streams

- *Implicit Synchronization*
 - An operation that requires a dependency check to see if a kernel finished executing:
 - *Blocks* all kernel launches *from any stream* until the checked kernel is finished
- `cudaStreamQuery()` can be used to test if a stream has completed all operations

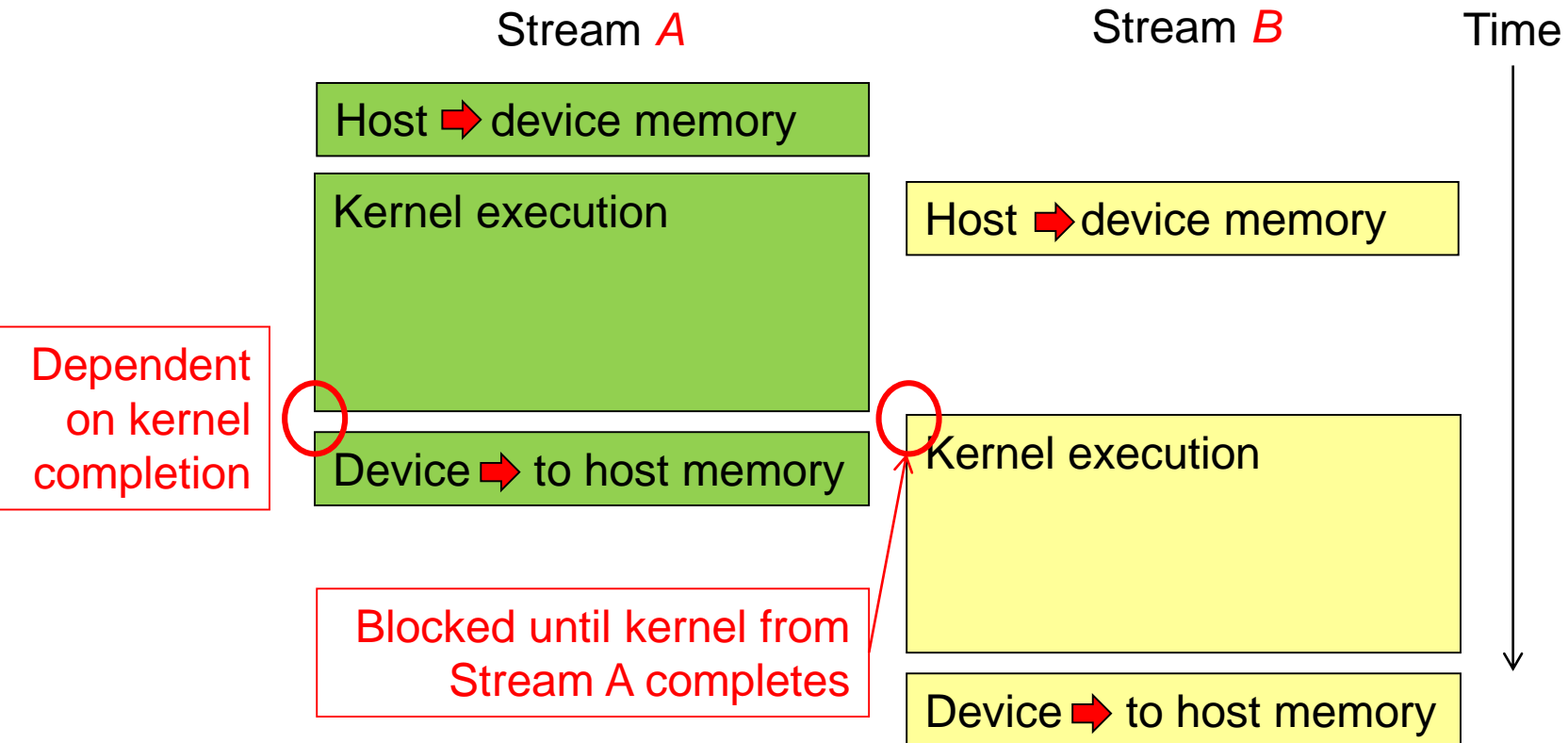
See 3.2.6.5.3 in the NVIDIA CUDA C Programming Guide for all limitations (version 3.2)

Implicit Synchronization

- These operations implicitly synchronize all other CUDA operations
 - Page-locked memory allocation
 - `cudaMallocHost`
 - `cudaHostAlloc`
 - Device memory allocation
 - `cudaMalloc`
 - Non-Async version of memory operations
 - `cudaMemcpy*` (no Async suffix)
 - `cudaMemset*` (no Async suffix)
 - Change to L1/shared memory configuration
 - `cudaDeviceSetCacheConfig`

Streams

- Can we have this?



Streams

- Performance Advice
 - Issue all independent commands before dependent ones
 - Delay synchronization (implicit or explicit) as long as possible

Streams

- Rewrite this to allow concurrent kernel execution

```
for (int i = 0; i < 2; ++i)
{
    cudaMemcpyAsync(/* ... */, stream[i]);
    kernel<<< /*... */ stream[i]>>>();
    cudaMemcpyAsync(/* ... */, stream[i]);
}
```

Streams

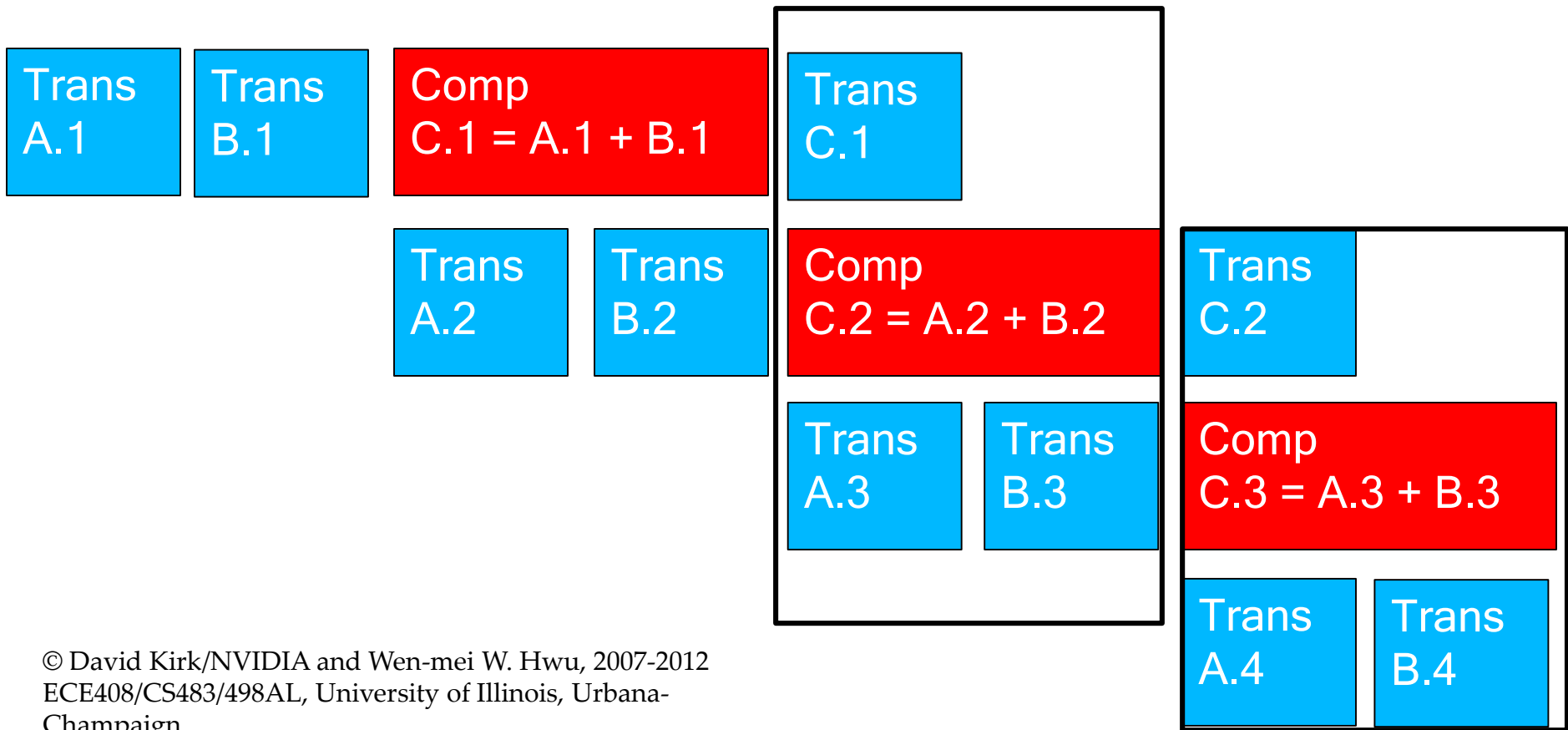
```
for (int i = 0; i < 2; ++i) // to device
    cudaMemcpyAsync(/* ... */, stream[i]);
```

```
for (int i = 0; i < 2; ++i)
    kernel<<< /*... */ stream[i]>>>();
```

```
for (int i = 0; i < 2; ++i) // to host
    cudaMemcpyAsync(/* ... */, stream[i]);
```

Overlapped (Pipelined) Timing

- Divide large vectors into segments
- Overlap transfer and compute of adjacent segments



Explicit Synchronization

- `cudaDeviceSynchronize()`
 - Blocks until commands in all streams finish
 - `cudaThreadSynchronize()` has been deprecated
- `cudaStreamSynchronize(streamid)`
 - Blocks until commands in a specific stream finish

Synchronization using Events

- Create specific 'Events', within streams, to use for synchronization
- `cudaEventRecord (event, streamid)`
- `cudaEventSynchronize (event)`
- `cudaStreamWaitEvent (stream, event)`
- `cudaEventQuery (event)`

Explicit Synchronization Example

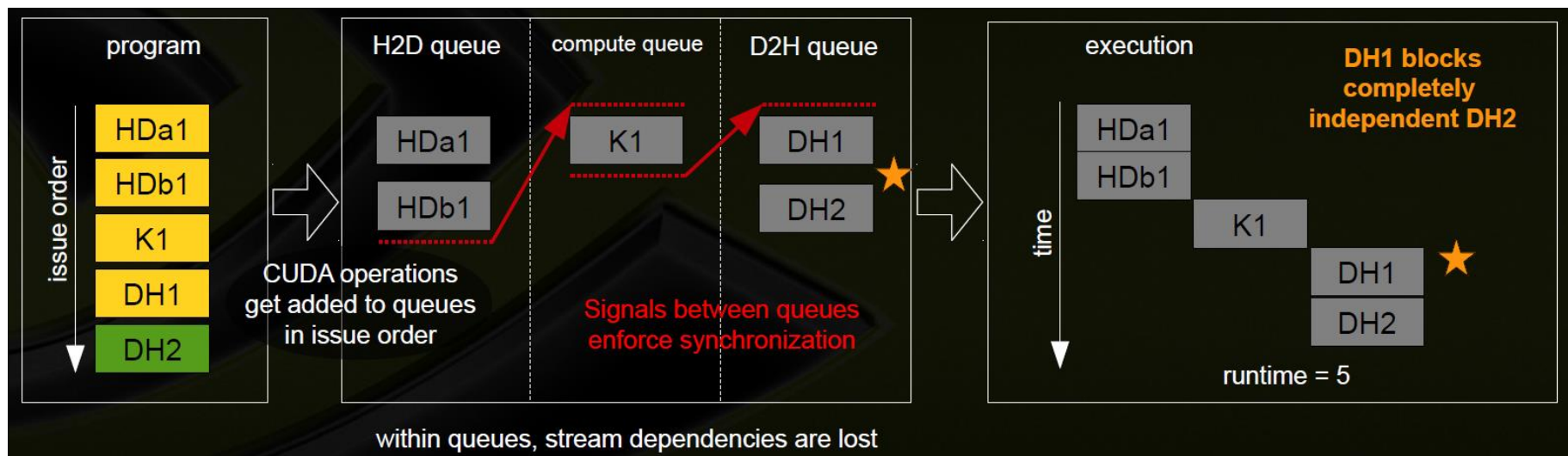
```
{  
    cudaEvent_t event;  
    cudaEventCreate (&event); // create event  
  
    // 1) H2D copy of new input  
    cudaMemcpyAsync ( d_in, in, size, H2D, stream1 );  
    cudaEventRecord (event, stream1);                // record event  
  
    // 2) D2H copy of previous result  
    cudaMemcpyAsync ( out, d_out, size, D2H, stream2 );  
    cudaStreamWaitEvent ( stream2, event );           // wait for event in stream1  
  
    kernel <<< , , , stream2 >>> ( d_in, d_out );    // 3) must wait for 1 and 2  
    asynchronousCPUMethod ( ... );  
}
```

Stream Scheduling

- Fermi hardware has 3 queues
 - 1 Compute Engine queue
 - 2 Copy Engine queues - one for H2D and one for D2H
- CUDA operations are dispatched to HW in the sequence they were issued
 - Placed in the relevant queue
 - Stream dependencies between engine queues are maintained, but lost within an engine queue
- A CUDA operation is dispatched from the engine queue if:
 - Preceding calls in the same stream have completed,
 - Preceding calls in the same queue have been dispatched, and
 - Resources are available
- CUDA kernels may be executed concurrently if they are in different streams
 - Threadblocks for a given kernel are scheduled if all threadblocks for preceding kernels have been scheduled and there still are SM resources available
- Note that a blocked operation blocks all other operations in the queue, even in other streams

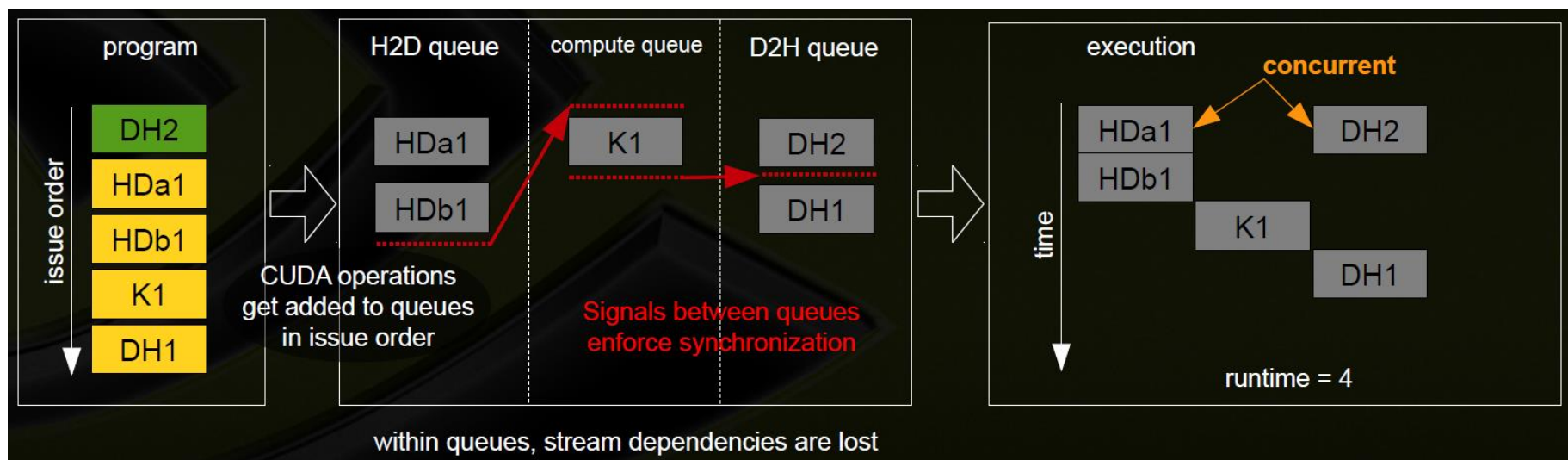
Example - Blocked Queue

- Two streams, stream 1 is issued first
 - Stream 1 : HDa1, HDb1, K1, DH1 (issued first)
 - Stream 2 : DH2 (completely independent of stream 1)



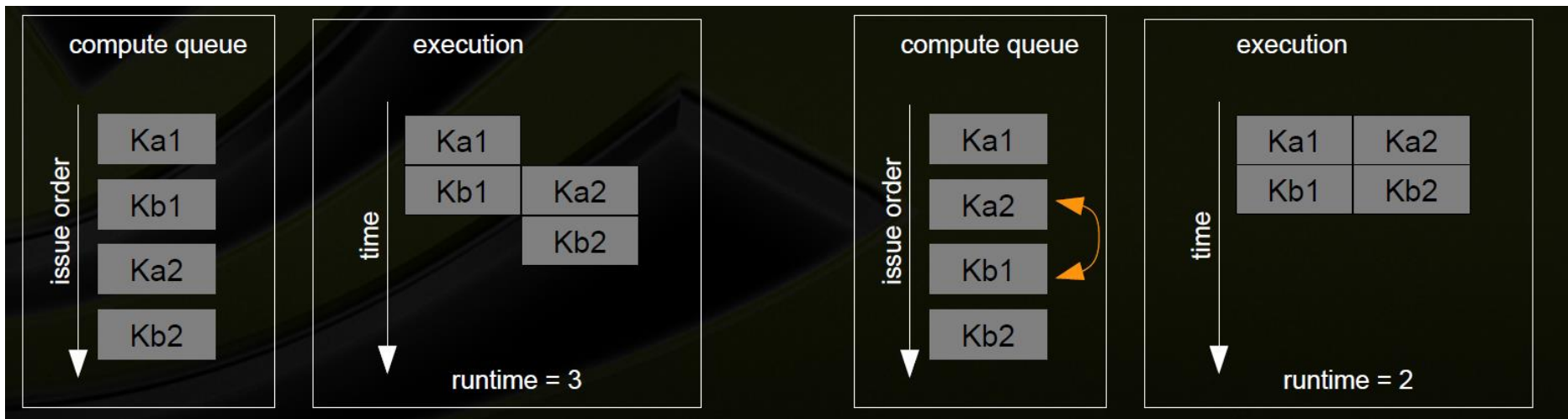
Example - Blocked Queue

- Two streams, stream 1 is issued first
 - Stream 1 : HDa1, HDb1, K1, DH1
 - Stream 2 : DH2 (issued first)



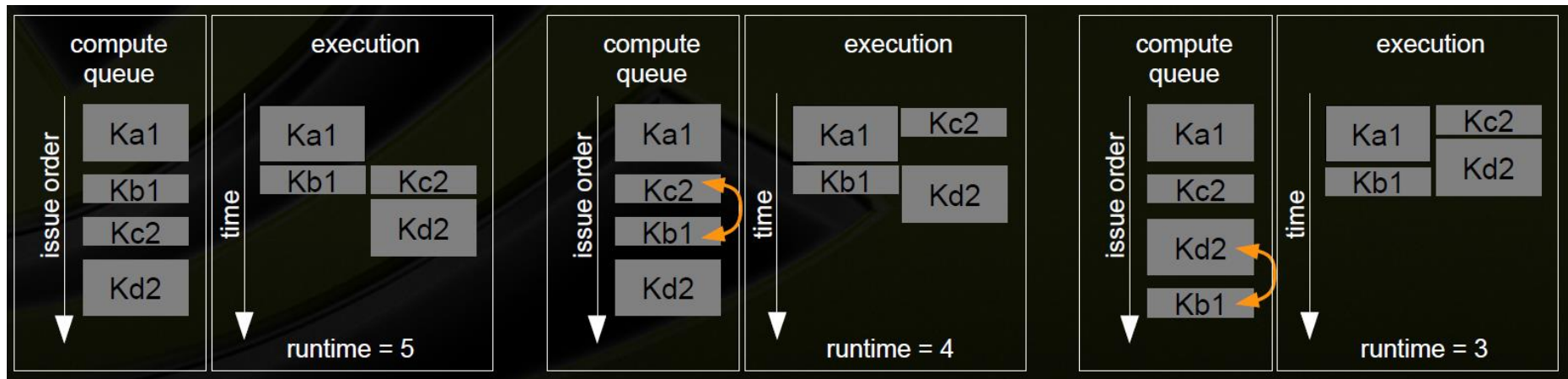
Example - Blocked Kernel

- Two streams - just issuing CUDA kernels
 - Stream 1 : Ka1, Kb1
 - Stream 2 : Ka2, Kb2
 - Kernels are similar size, fill $\frac{1}{2}$ of the SM resources



Example - Optimal Concurrency can Depend on Kernel Execution Time

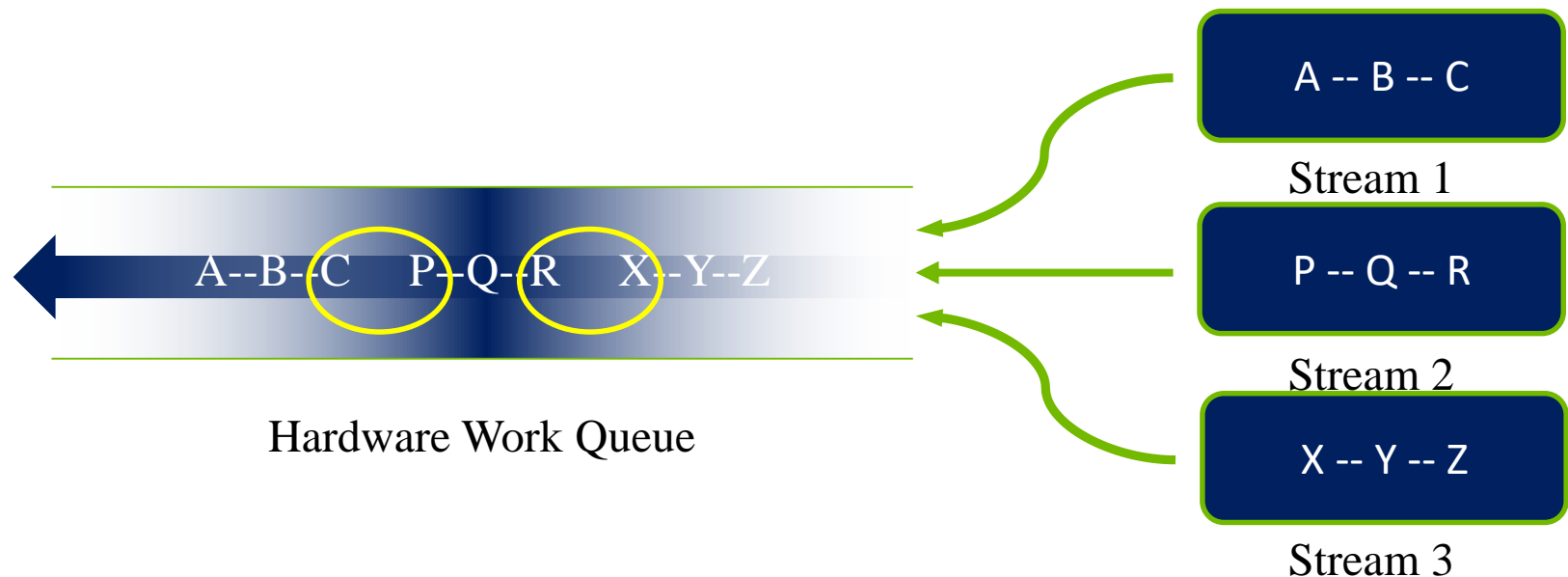
- Two streams - just issuing CUDA kernels - but kernels are different 'sizes'
 - Stream 1 : Ka1 {2}, Kb1 {1}
 - Stream 2 : Kc2 {1}, Kd2 {2}
 - Kernels fill $\frac{1}{2}$ of the SM resources



Hyper Queue

- Provide multiple real queues for each engine
- Allow much more concurrency by allowing some streams to make progress for an engine while others are blocked

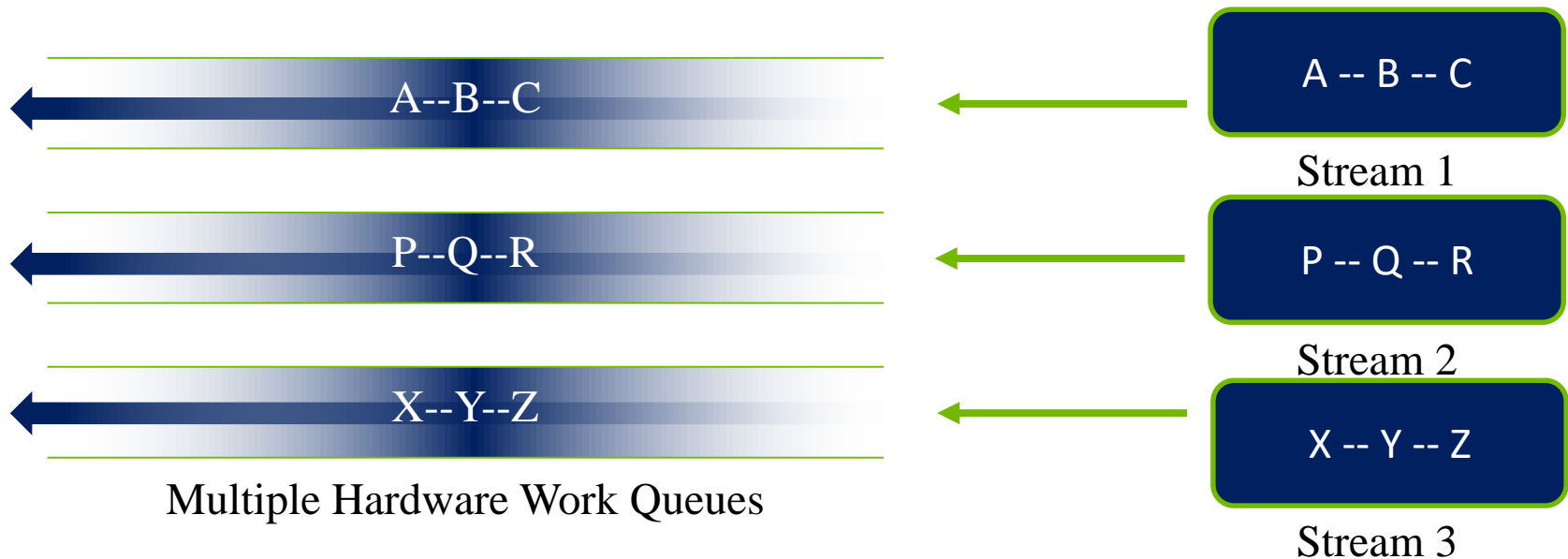
Fermi (and older) Concurrency



Fermi allows 16-way concurrency

- Up to 16 grids can run at once
- But CUDA streams multiplex into a single queue
- Overlap only at stream edges

Improved Concurrency



Kepler allows 32-way concurrency

- One work queue per stream
- Concurrency at full-stream level
- No inter-stream dependencies

Pascal also supports 32-way concurrency

- One work queue per stream
- Dynamic scheduling

Thrust

Jared Hoberock and Nathan Bell
Modified by P. Mordohai (March 2013)

A Simple Example

```
#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(int i = 0; i < H.size(); i++)
    std::cout << "H[" << i << "] = " << H[i] << std::endl;

// resize H
H.resize(2);

std::cout << "H now has size " << H.size() << std::endl;

// 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(int i = 0; i < D.size(); i++)
    std::cout << "D[" << i << "] = " << D[i] << std::endl;

// H and D are automatically deleted when the function
returns
return 0;
}
```

Diving In

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

int main(void)
{
    // generate 16M random numbers on the host
    thrust::host_vector<int> h_vec(1 << 24);
    thrust::generate(h_vec.begin(), h_vec.end(), rand);

    // transfer data to the device
    thrust::device_vector<int> d_vec = h_vec;

    // sort data on the device
    thrust::sort(d_vec.begin(), d_vec.end());

    // transfer data back to host
    thrust::copy(d_vec.begin(), d_vec.end(), h_vec.begin());
}
```

Objectives

- Programmer productivity
 - Rapidly develop complex applications
 - Leverage parallel primitives
- Encourage generic programming
 - Don't reinvent the wheel
 - E.g. one reduction to rule them all
- High performance
 - With minimal programmer effort
- Interoperability
 - Integrates with CUDA C/C++ code

What is Thrust?

- C++ template library for CUDA
 - Mimics Standard Template Library (STL)
- Containers
 - `thrust::host_vector<T>`
 - `thrust::device_vector<T>`
- Algorithms
 - `thrust::sort()`
 - `thrust::reduce()`
 - `thrust::inclusive_scan()`
 - Etc.

Namespaces

- C++ supports namespaces
 - Thrust uses `thrust` namespace
 - `thrust::device_vector`
 - `thrust::copy`
 - STL uses `std` namespace
 - `std::vector`
 - `std::list`
- Avoids collisions
 - `thrust::sort()`
 - `std::sort()`
- For brevity
 - `using namespace thrust;`

Containers

- Make common operations concise and readable
 - Hides `cudaMalloc`, `cudaMemcpy` and `cudaFree`

```
// allocate host vector with two elements
thrust::host_vector<int> h_vec(2);
```

```
// copy host vector to device
thrust::device_vector<int> d_vec = h_vec;
```

```
// manipulate device values from the host
d_vec[0] = 13;
d_vec[1] = 27;
```

```
std::cout << "sum: " << d_vec[0] + d_vec[1] << std::endl;
```

```
// vector memory automatically released w/ free() or cudaFree()
```

Containers

- Compatible with STL containers
 - Eases integration
 - vector, list, map, ...

```
// list container on host
std::list<int> h_list;
h_list.push_back(13);
h_list.push_back(27);
```

```
// copy list to device vector
thrust::device_vector<int> d_vec(h_list.size());
thrust::copy(h_list.begin(), h_list.end(), d_vec.begin());
```

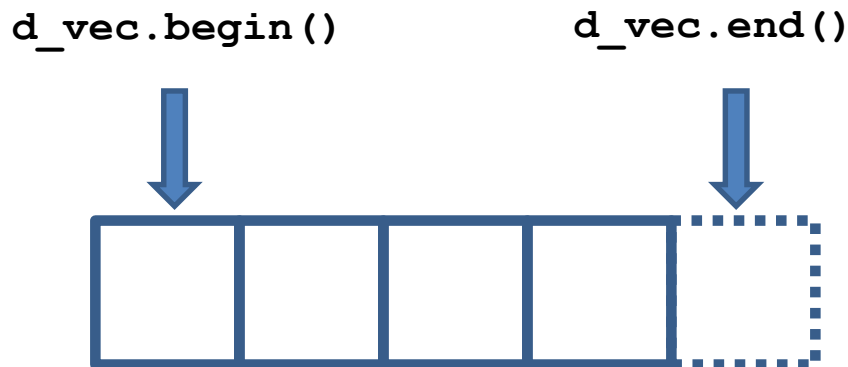
```
// alternative method
thrust::device_vector<int> d_vec(h_list.begin(), h_list.end());
```

Note: initializing an STL container with a device_vector works, but results in one cudaMemcpy() for each element instead of a single cudaMemcpy for the entire vector.

Iterators

- Sequences defined by pair of iterators

```
// allocate device vector  
thrust::device_vector<int> d_vec(4);  
  
d_vec.begin(); // returns iterator at first element of d_vec  
d_vec.end()   // returns iterator one past the last element of d_vec  
  
// [begin, end) pair defines a sequence of 4 elements
```



Iterators

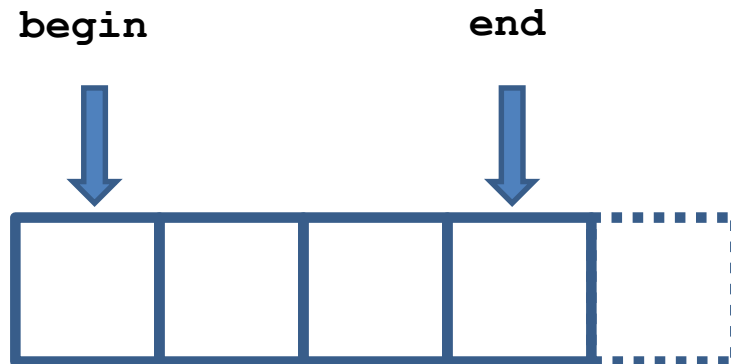
- Iterators act like pointers

```
// allocate device vector
thrust::device_vector<int> d_vec(4);

thrust::device_vector<int>::iterator begin = d_vec.begin();
thrust::device_vector<int>::iterator end   = d_vec.end();

int length = end - begin; // compute size of sequence [begin, end)

end = d_vec.begin() + 3;  // define a sequence of 3 elements
```



Iterators

- Use iterators like pointers

```
// allocate device vector
thrust::device_vector<int> d_vec(4);

thrust::device_vector<int>::iterator begin = d_vec.begin();

*begin = 13;           // same as d_vec[0] = 13;
int temp = *begin;     // same as temp = d_vec[0];

begin++;               // advance iterator one position

*begin = 25;           // same as d_vec[1] = 25;
```

Iterators

- Track memory space (host/device)
 - Guides algorithm dispatch

```
// initialize random values on host
thrust::host_vector<int> h_vec(1000);
thrust::generate(h_vec.begin(), h_vec.end(), rand);

// copy values to device
thrust::device_vector<int> d_vec = h_vec;

// compute sum on host
int h_sum = thrust::reduce(h_vec.begin(), h_vec.end());

// compute sum on device
int d_sum = thrust::reduce(d_vec.begin(), d_vec.end());
```


Iterators

- Convertible to raw pointers

```
// allocate device vector  
thrust::device_vector<int> d_vec(4);
```

```
// obtain raw pointer to device vector's memory  
int * ptr = thrust::raw_pointer_cast(&d_vec[0]);
```

```
// use ptr in a CUDA C kernel  
my_kernel<<<N/256, 256>>>(N, ptr);
```

```
// Note: ptr cannot be dereferenced on the host!  
// raw pointers do not know where they live  
// Thrust iterators do
```

Iterators

- Wrap raw pointers with `device_ptr`

```
int N = 10;

// 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);

// access device memory through device_ptr
dev_ptr[0] = 1;

// extract raw pointer from device_ptr
int * raw_ptr2 = thrust::raw_pointer_cast(dev_ptr);

// free memory
cudaFree(raw_ptr);
```

Recap

- Containers
 - Manage host & device memory
 - Automatic allocation and deallocation
 - Simplify data transfers
- Iterators
 - Behave like pointers
 - Keep track of memory spaces
 - Convertible to raw pointers
- Namespaces
 - Avoid collisions

C++ Background

- Function templates

```
// function template to add numbers (type of T is variable)
template< typename T >
T add(T a, T b)
{
    return a + b;
}

// add integers
int x = 10; int y = 20; int z;
z = add<int>(x,y);      // type of T explicitly specified
z = add(x,y);          // type of T determined automatically

// add floats
float x = 10.0f; float y = 20.0f; float z;
z = add<float>(x,y);   // type of T explicitly specified
z = add(x,y);         // type of T determined automatically
```

C++ Background

- Function objects (Functors)

```
// templated functor to add numbers
```

```
template< typename T >  
class add  
{  
    public:  
    T operator() (T a, T b)  
    {  
        return a + b;  
    }  
};
```

```
int x = 10; int y = 20; int z;  
add<int> func;    // create an add functor for T=int  
z = func(x,y);   // invoke functor on x and y
```

```
float x = 10; float y = 20; float z;  
add<float> func; // create an add functor for T=float  
z = func(x,y);   // invoke functor on x and y
```

```

// this is a functor
// unlike functions, it can contain state
struct add_x {
    add_x(int x) : x(x) {}
    int operator()(int y) { return x + y; }

private:
    int x;
};

// Now you can use it like this:
add_x add42(42); // create an instance of the functor class
int i = add42(8); // and "call" it
assert(i == 50); // and it added 42 to its argument

std::vector<int> in; // assume this contains a bunch of values)
std::vector<int> out;
// Pass a functor to std::transform, which calls the functor on every
// element in the input sequence, and stores the result to the output
// sequence
// unlike a function pointer this can be resolved and inlined at
// compile time
std::transform(in.begin(), in.end(), out.begin(), add_x(1));
assert(out[i] == in[i] + 1); // for all i

```

C++ Background

- Generic Algorithms

```
// apply function f to sequences x, y and store result in z
template <typename T, typename Function>
void transform(int N, T * x, T * y, T * z, Function f)
{
    for (int i = 0; i < N; i++)
        z[i] = f(x[i], y[i]);
}

int N = 100;
int x[N]; int y[N]; int z[N];

add<int> func; // add functor for T=int

transform(N, x, y, z, func); // compute z[i] = x[i] + y[i]

transform(N, x, y, z, add<int>()); // equivalent
```

Algorithms

- Thrust provides many standard algorithms
 - Transformations
 - Reductions
 - Prefix Sums
 - Sorting
- Generic definitions
 - General Types
 - Built-in types (`int`, `float`, ...)
 - User-defined structures
 - General Operators
 - reduce with `plus` operator
 - scan with `maximum` operator

Algorithms

- General types and operators

```
#include <thrust/reduce.h>
```

```
// declare storage
```

```
device_vector<int>    i_vec = ...
```

```
device_vector<float> f_vec = ...
```

```
// sum of integers (equivalent calls)
```

```
reduce(i_vec.begin(), i_vec.end());
```

```
reduce(i_vec.begin(), i_vec.end(), 0, plus<int>());
```

Initial value of sum



```
// sum of floats (equivalent calls)
```

```
reduce(f_vec.begin(), f_vec.end());
```

```
reduce(f_vec.begin(), f_vec.end(), 0.0f, plus<float>());
```

```
// maximum of integers
```

```
reduce(i_vec.begin(), i_vec.end(), 0, maximum<int>());
```

Algorithms

- General types and operators

```
struct negate_float2
{
    __host__ __device__
    float2 operator()(float2 a)
    {
        return make_float2(-a.x, -a.y);
    }
};

// declare storage
device_vector<float2> input  = ...
device_vector<float2> output = ...

// create functor
negate_float2 func;

// negate vectors
transform(input.begin(), input.end(), output.begin(), func);
```

Algorithms

- General types and operators

```
// compare x component of two float2 structures
```

```
struct compare_float2  
{  
    __host__ __device__  
    bool operator()(float2 a, float2 b)  
    {  
        return a.x < b.x;  
    }  
};
```

```
// declare storage  
device_vector<float2> vec = ...
```

```
// create comparison functor  
compare_float2 comp;
```

```
// sort elements by x component  
sort(vec.begin(), vec.end(), comp);
```

Algorithms

- Operators with State

```
// compare x component of two float2 structures
struct is_greater_than
{
    int threshold;

    is_greater_than(int t) { threshold = t; }

    __host__ __device__
    bool operator()(int x) { return x > threshold; }
};

device_vector<int> vec = ...

// create predicate functor (returns true for x > 10)
is_greater_than pred(10);

// count number of values > 10
int result = count_if(vec.begin(), vec.end(), pred);
```

Recap

- Algorithms
 - Generic
 - Support general types and operators
 - Statically dispatched based on iterator type
 - Memory space is known at compile time
 - Have default arguments
 - `reduce(begin, end)`
 - `reduce(begin, end, init, binary_op)`

Fancy Iterators

- Behave like “normal” iterators
 - Algorithms don't know the difference
- Examples
 - `constant_iterator`
 - `counting_iterator`
 - `transform_iterator`
 - `permutation_iterator`
 - `zip_iterator`

Fancy Iterators

- `constant_iterator`
 - Mimics an infinite array filled with a constant value

```
// create iterators
constant_iterator<int> begin(10);
constant_iterator<int> end = begin + 3;

begin[0]    // returns 10
begin[1]    // returns 10
begin[100] // returns 10

// sum of [begin, end)
reduce(begin, end);    // returns 30 (i.e. 3 * 10)
```



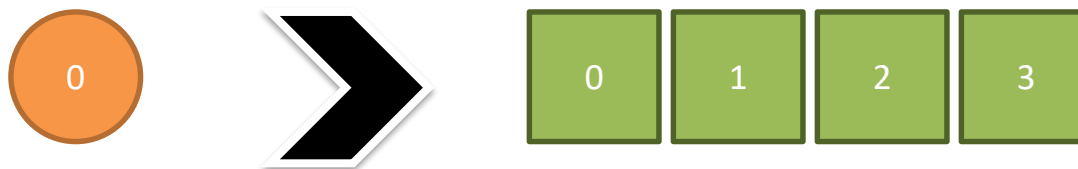
Fancy Iterators

- `counting_iterator`
 - Mimics an infinite array with sequential values

```
// create iterators  
counting_iterator<int> begin(10);  
counting_iterator<int> end = begin + 3;
```

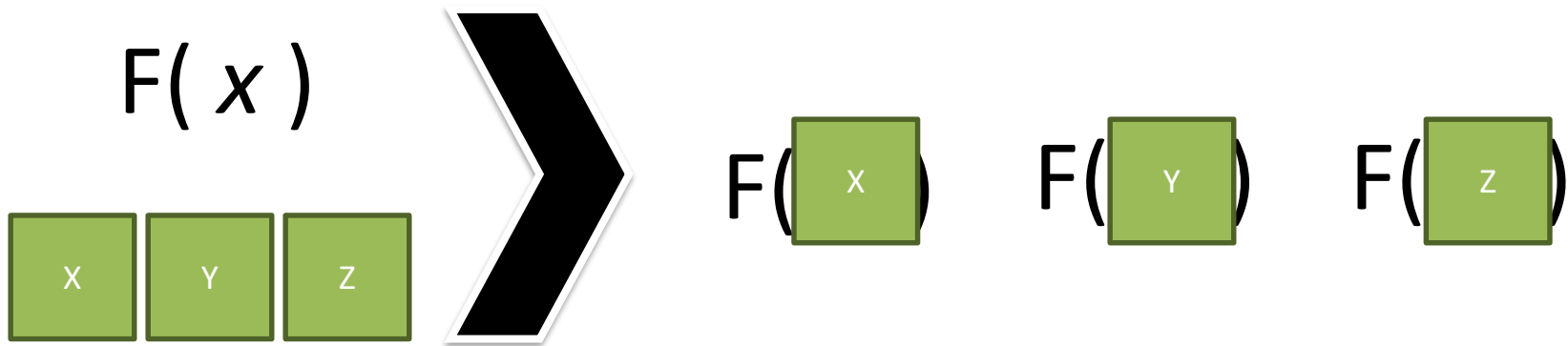
```
begin[0]    // returns 10  
begin[1]    // returns 11  
begin[100]  // returns 110
```

```
// sum of [begin, end)  
reduce(begin, end);    // returns 33 (i.e. 10 + 11 + 12)
```



Fancy Iterators

- `transform_iterator`
 - Yields a transformed sequence
 - Facilitates kernel fusion (e.g. sum of squares)



Fancy Iterators

- `transform_iterator`
 - Conserves memory capacity and bandwidth

```
// initialize vector
device_vector<int> vec(3);
vec[0] = 10; vec[1] = 20; vec[2] = 30;

// create iterator (type omitted)
first = make_transform_iterator(vec.begin(), negate<int>());
last  = make_transform_iterator(vec.end(),   negate<int>());

first[0]    // returns -10
first[1]    // returns -20
first[2]    // returns -30

// sum of [begin, end)
reduce(first, last);    // returns -60 (i.e. -10 + -20 + -30)
```

Fancy Iterators

- `zip_iterator`
 - Looks like an array of structs (AoS)
 - Stored in structure of arrays (SoA)



Fancy Iterators

- `zip_iterator`

```
// initialize vectors
device_vector<int>  A(3);
device_vector<char> B(3);
A[0] = 10;  A[1] = 20;  A[2] = 30;
B[0] = 'x'; B[1] = 'y'; B[2] = 'z';

// create iterator (type omitted)
first = make_zip_iterator(make_tuple(A.begin(), B.begin()));
last  = make_zip_iterator(make_tuple(A.end(),   B.end()));

first[0]    // returns tuple(10, 'x')
first[1]    // returns tuple(20, 'y')
first[2]    // returns tuple(30, 'z')

// maximum of [begin, end)
maximum< tuple<int,char> > binary_op;
reduce(first,last, first[0], binary_op); // returns tuple(30,'z')
// tuple() defines a comparison operator
```

Best Practices

- Fusion
 - Combine related operations together
- Structure of Arrays
 - Ensure memory coalescing
- Implicit Sequences
 - Eliminate memory accesses

Fusion

- Combine related operations together
 - Conserves memory bandwidth
- Example: SNRM2
 - Square each element
 - Compute sum of squares and take `sqrt()`
 - The fused implementation reads the array once while the un-fused implementation performs 2 reads and 1 write per element

Fusion

- Unoptimized implementation

```
// define transformation f(x) -> x^2
struct square
{
    __host__ __device__
    float operator()(float x)
    {
        return x * x;
    }
};

float snrm2_slow(device_vector<float>& x)
{
    // without fusion
    device_vector<float> temp(x.size());
    transform(x.begin(), x.end(), temp.begin(), square());

    return sqrt( reduce(temp.begin(), temp.end()) );
}
```

Fusion

- Optimized implementation (3.8x faster)

```
// define transformation f(x) -> x^2
```

```
struct square
```

```
{
    __host__ __device__
    float operator()(float x)
    {
        return x * x;
    }
};
```

```
float snrm2_fast(device_vector<float>& x)
```

```
{
    // with fusion
    return sqrt( transform_reduce(x.begin(), x.end(),
                                   square(), 0.0f, plus<float>()) );
}
```


Structure of Arrays (SoA)

- Array of Structures (AoS)
 - Often does not obey coalescing rules
 - `device_vector<float3>`
- Structure of Arrays (SoA)
 - Obeys coalescing rules
 - Components stored in separate arrays
 - `device_vector<float> x, y, z;`
- Example: Rotate 3d vectors
 - SoA is 2.8x faster

Array of Structures (AoS)

```
struct rotate_float3
{
    __host__ __device__
    float3 operator()(float3 v)
    {
        float x = v.x;
        float y = v.y;
        float z = v.z;

        float rx = 0.36f*x + 0.48f*y + -0.80f*z;
        float ry = -0.80f*x + 0.60f*y + 0.00f*z;
        float rz = 0.48f*x + 0.64f*y + 0.60f*z;

        return make_float3(rx, ry, rz);
    }
};

...

device_vector<float3> vec(N);

transform(vec.begin(), vec.end(), vec.begin(), rotate_float3());
```

Structure of Arrays (SoA)

```
struct rotate_tuple
{
    __host__ __device__
    tuple<float,float,float> operator() (tuple<float,float,float> v)
    {
        float x = get<0>(v);
        float y = get<1>(v);
        float z = get<2>(v);

        float rx = 0.36f*x + 0.48f*y + -0.80f*z;
        float ry = -0.80f*x + 0.60f*y + 0.00f*z;
        float rz = 0.48f*x + 0.64f*y + 0.60f*z;

        return make_tuple(rx, ry, rz);
    }
};

...

device_vector<float> x(N), y(N), z(N);

transform(make_zip_iterator(make_tuple(x.begin(), y.begin(), z.begin())),
          make_zip_iterator(make_tuple(x.end(), y.end(), z.end())),
          make_zip_iterator(make_tuple(x.begin(), y.begin(), z.begin())),
          rotate_tuple());
```

Implicit Sequences

- Avoid storing sequences explicitly
 - Constant sequences
 - `[1, 1, 1, 1, ...]`
 - Incrementing sequences
 - `[0, 1, 2, 3, ...]`
- Implicit sequences require no storage
 - `constant_iterator`
 - `counting_iterator`
- Example
 - Index of the smallest element

Implicit Sequences

```
// return the smaller of two tuples
struct smaller_tuple
{
    tuple<float,int> operator()(tuple<float,int> a, tuple<float,int> b)
    {
        if (a < b)
            return a;
        else
            return b;
    }
};

int min_index(device_vector<float>& vec)
{
    // create explicit index sequence [0, 1, 2, ... )
    device_vector<int> indices(vec.size());
    sequence(indices.begin(), indices.end());

    tuple<float,int> init(vec[0],0);
    tuple<float,int> smallest;

    smallest = reduce(make_zip_iterator(make_tuple(vec.begin(), indices.begin())),
                     make_zip_iterator(make_tuple(vec.end(), indices.end())),
                     init,
                     smaller_tuple());

    return get<1>(smallest);
}
```

Implicit Sequences

```
// return the smaller of two tuples
struct smaller_tuple
{
    tuple<float,int> operator()(tuple<float,int> a, tuple<float,int> b)
    {
        if (a < b)
            return a;
        else
            return b;
    }
};

int min_index(device_vector<float>& vec)
{
    // create implicit index sequence [0, 1, 2, ... )
    counting_iterator<int> begin(0);
    counting_iterator<int> end(vec.size());

    tuple<float,int> init(vec[0],0);
    tuple<float,int> smallest;

    smallest = reduce(make_zip_iterator(make_tuple(vec.begin(), begin)),
                     make_zip_iterator(make_tuple(vec.end(), end)),
                     init,
                     smaller_tuple());

    return get<1>(smallest);
}
```

Recap

- Best Practices
 - Fusion
 - 3.8x faster
 - Structure of Arrays
 - 2.8x faster
 - Implicit Sequences
 - 3.4x faster

Additional Resources

- Thrust
 - Homepage <http://thrust.github.io/>
 - More
<http://docs.nvidia.com/cuda/thrust/index.html>
<https://developer.nvidia.com/thrust>

Processing Rainfall Data

day	[0 0 1 2 5 5 6 6 7 8 ...]
site	[2 3 0 1 1 2 0 1 2 1 ...]
measurement	[9 5 6 3 3 8 2 6 5 10 ...]

Notes

- 1) Time series sorted by day
- 2) Measurements of zero are excluded from the time series

Storage Options

- Array of structures

```
struct Sample {  
    int day;  
    int site;  
    int measurement;  
};  
thrust::device_vector<Sample> data;
```

- Structure of arrays (Best Practice)

```
struct Data  
{  
    thrust::device_vector<int> day;  
    thrust::device_vector<int> site;  
    thrust::device_vector<int> measurement;  
};  
Data data;
```

Number of Days with Rainfall

```
int compute_number_of_days_with_rainfall( const Data &data)
{
    return thrust::inner_product(data.day.begin(), data.day.end() - 1,
        data.day.begin() + 1, 1,
        thrust::plus<int>(), // + functor
        thrust::not_equal_to<int>()); // * functor }
```



Total Rainfall at each Site

```
template <typename Vector>
void compute_total_rainfall_per_site(const Data &data, Vector &site, Vector &measurement)
{
    // Copy data to keep the original data as it is.
    Vector tmp_site(data.site), tmp_measurement(data.measurement);

    // Sort the "pairs" (site, measurement) by increasing value of site.
    thrust::sort_by_key(tmp_site.begin(), tmp_site.end(), tmp_measurement.begin());

    // Reduce measurements by site (Assumption: site/measurement are big enough).
    thrust::reduce_by_key(tmp_site.begin(), tmp_site.end(), tmp_measurement.begin(),
                        site.begin(),
                        measurement.begin());
}
```

tmp_site	[0 = 0	1 = 1 = 1 = 1	2 = 2 = 2	3	...]
tmp_measurement	[6 + 2	3 + 3 + 6 + 10	9 + 8 + 5	5	...]



site	[0	1	2	3	...]
measurement	[8	22	22	5	...]

Number of Days where Rainfall Exceeds 5

```
using namespace thrust::placeholders;

int count_days_where_rainfall_exceeded_5(const Data &data)
{
    size_t N = compute_number_of_days_with_rainfall(data);

    thrust::device_vector<int> day(N);
    thrust::device_vector<int> measurement(N);

    thrust::reduce_by_key(
        data.day.begin(), data.day.end(),
        data.measurement.begin(),
        day.begin(),
        measurement.begin());

    return thrust::count_if(measurement.begin(), measurement.end(), _1 > 5);
}
```

Number of Days where Rainfall Exceeds 5

```
struct greater_than
{
    int threshold;
    greater_than( int threshold ) : threshold( threshold ) {}
    __device__ __host__ bool operator()( int i ) { return i > threshold; }
};
```

Sort Unsorted Input

day	[0	5	1	6	5	7	2	0	8	6	...]
site	[2	2	0	0	1	2	1	3	1	1	...]
measurement	[9	8	6	2	3	5	3	5	10	6	...]

Sort by day and site



day	[0	0	1	2	5	5	6	6	7	8	...]
site	[2	3	0	1	1	2	0	1	2	1	...]
measurement	[9	5	6	3	3	8	2	6	5	10	...]

Sort Unsorted Input

```
struct day_site_cmp
{
    template <typename Tuple0, typename Tuple1>
    __device__ __host__ bool operator()(const Tuple0 &t0, const Tuple1 &t1)
    {
        int day0  = thrust::get<0>(t0);
        int day1  = thrust::get<0>(t1);
        int site0 = thrust::get<1>(t0);
        int site1 = thrust::get<1>(t1);

        return day0 < day1 || (day0 == day1 && site0 < site1);
    }
};

void sort_data(Data &data)
{
    thrust::sort_by_key(
        thrust::make_zip_iterator(thrust::make_tuple(data.day.begin(), data.site.begin())),
        thrust::make_zip_iterator(thrust::make_tuple(data.day.end(), data.site.end())),
        data.measurements.begin(),
        day_site_cmp());
}
```


Sort Unsorted Input (faster)

▪ 40M elements sorted on a Tesla M2090:

– 1st version: 990.76ms

– 2nd version: 131.05ms

```
void sort_data(Data &data)
{
    thrust::device_vector<int64> tmp(data.day.size());

    // Pack (day, site) pairs into 64-bit integers.
    thrust::transform(
        thrust::make_zip_iterator(thrust::make_tuple(data.day.begin(), data.site.begin())),
        thrust::make_zip_iterator(thrust::make_tuple(data.day.end(), data.site.end())),
        tmp.begin(),
        pack());

    // Sort using the 64-bit integers as keys.
    thrust::sort_by_key(tmp.begin(), tmp.end(), data.measurement.begin());

    // Unpack (day, site) pairs from 64-bit integers.
    thrust::transform(
        tmp.begin(),
        tmp.end(),
        thrust::make_zip_iterator(thrust::make_tuple(data.day.begin(), data.site.begin())),
        unpack());
}
```

Sort Unsorted Input (faster)

```
struct pack
{
    template <typename Tuple>
    __device__ __host__ int64 operator()(const Tuple &t)
    {
        return ( static_cast<int64>( thrust::get<0>(t) ) << 32 ) | thrust::get<1>(t);
    }
};

struct unpack
{
    __device__ __host__ thrust::tuple<int,int> operator()(int64 p)
    {
        int d = static_cast<int>(p >> 32);
        int s = static_cast<int>(p & 0xffffffff);
        return thrust::make_tuple(d, s);
    }
};
```

Total Rainfall at Given Site

```
struct one_site_measurement
{
    int site;
    one_site_measurement(int site) : site(site) {}

    __host__ __device__ int operator()(thrust::tuple<int,int> t)
    {
        if( thrust::get<0>(t) == site )
            return thrust::get<1>(t);
        else
            return 0;
    }
};

int compute_total_rainfall_at_one_site(int i, const Data &data)
{
    // Fused transform-reduce (best practice).
    return thrust::transform_reduce(
        thrust::make_zip_iterator(thrust::make_tuple(data.site.begin(), data.measurement.begin())),
        thrust::make_zip_iterator(thrust::make_tuple(data.site.end(), data.measurement.end())),
        one_site_measurement(i),
        0,
        thrust::plus<int>());
}
```