NVIDIA DEEP LEARNING INSTITUTE

MULTI-GPU PROGRAMMING FOR CUDA C++

Dr. Momme Allalen | LRZ | 30.11.2021

COPY/COMPUTE OVERLAP CONSIDERATIONS

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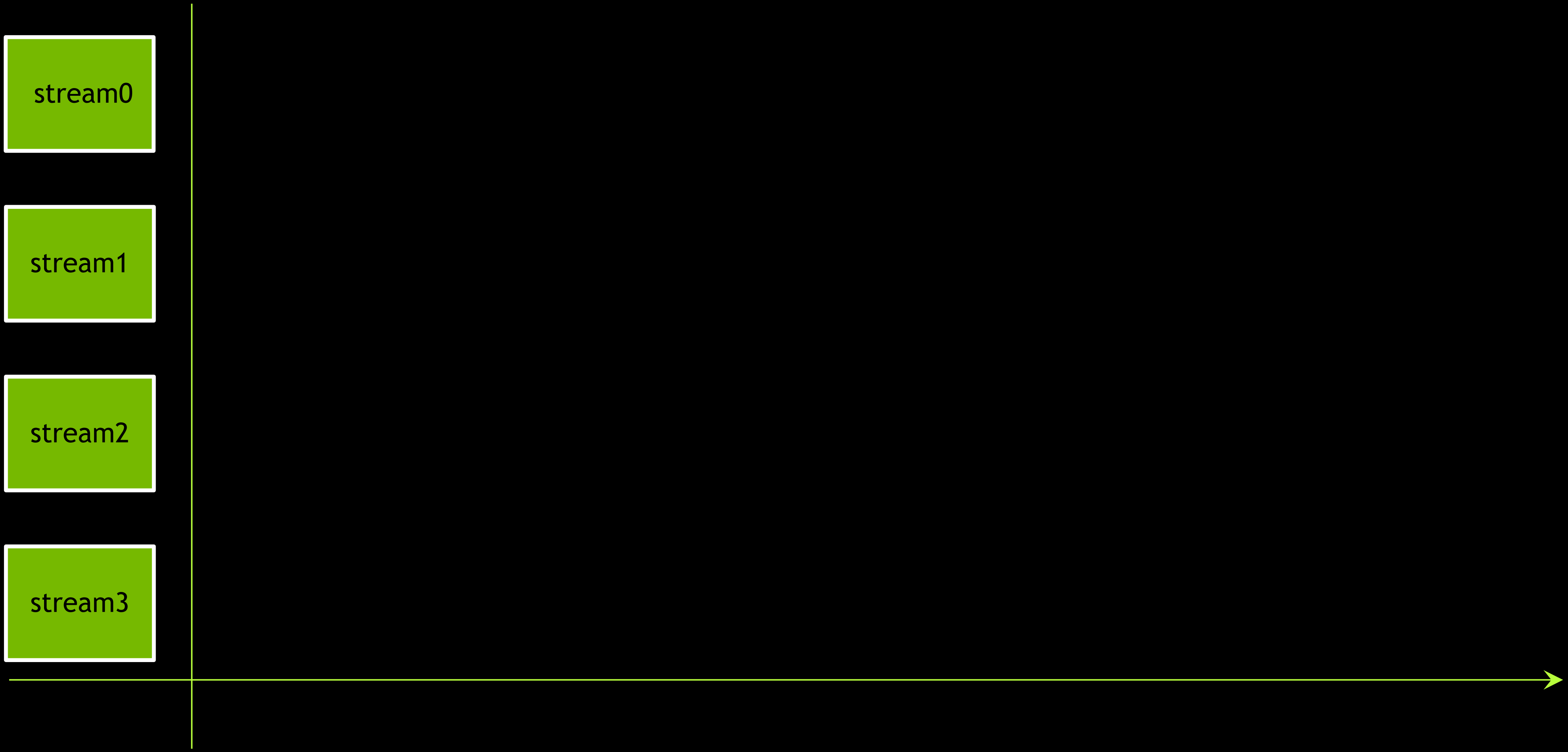
Copy/Compute Overlap with Streams

Copy/Compute Overlap Indexing

COPY/COMPUTE OVERLAP WITH STREAMS

Using the default stream, a typical 3-step CUDA program will perform HtoD copy, compute, and DtoH copy serially



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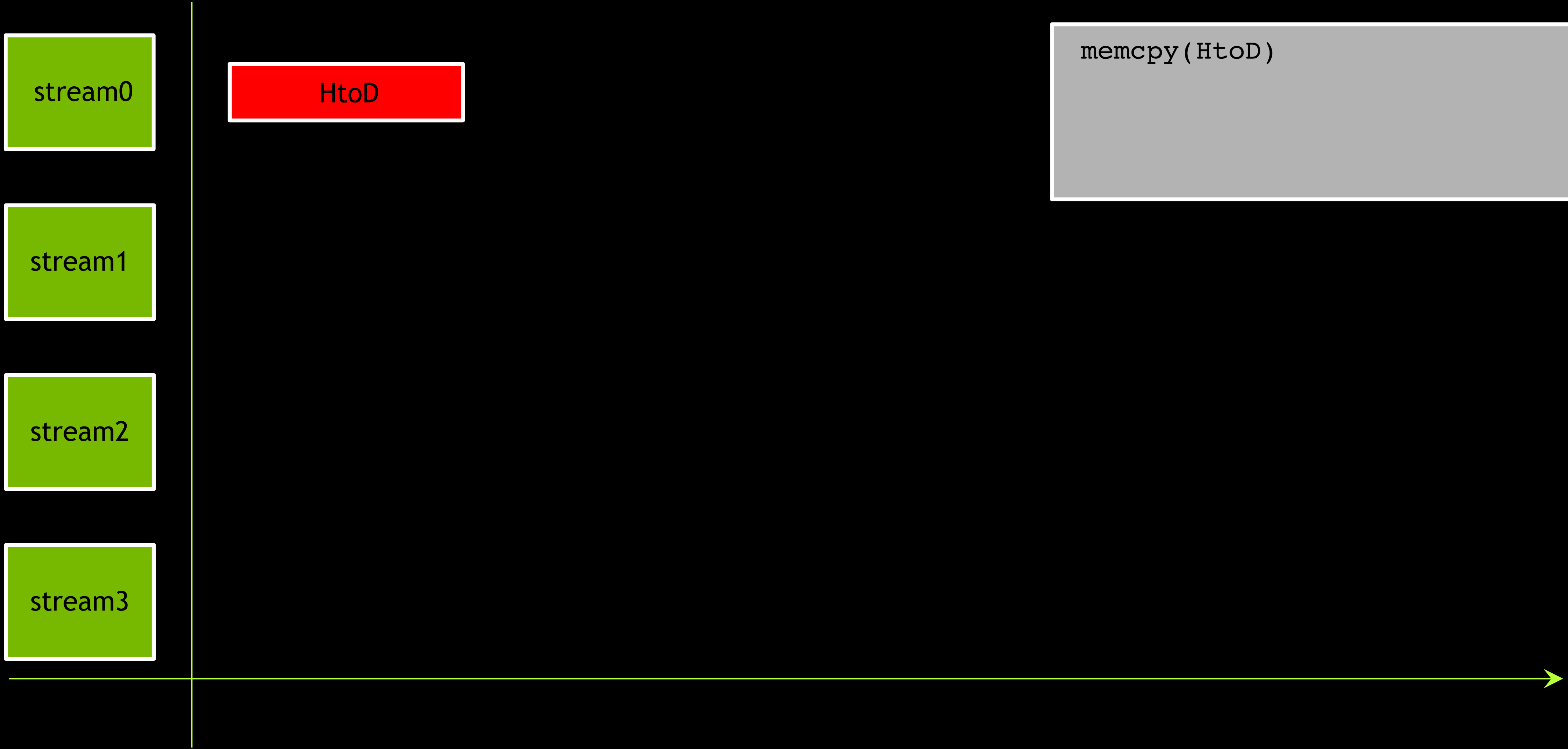


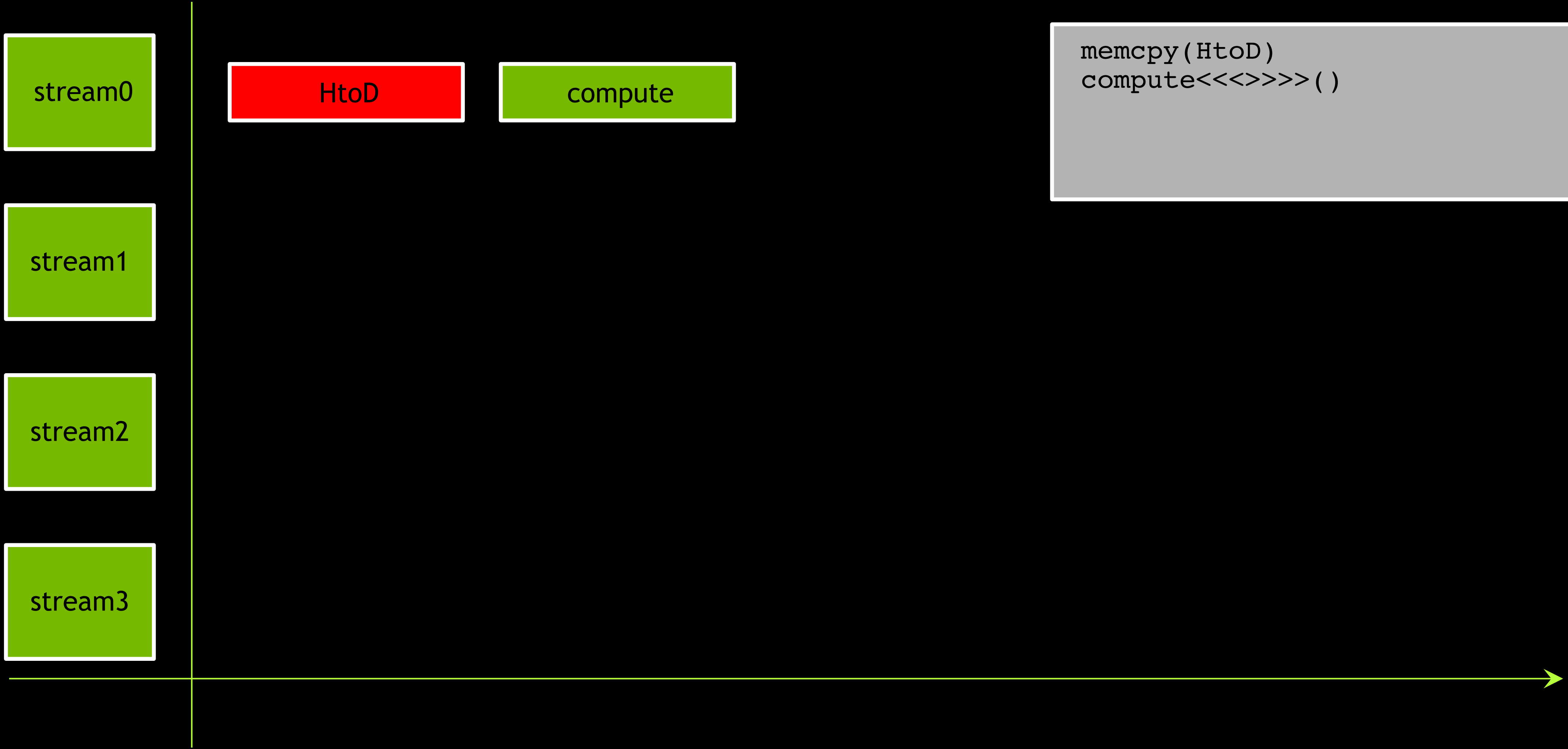

```
memcpy(HtoD)
```

Note: we will be using shorthand code in these slides for ease of presentation

```
memcpy(HtoD)
```

Using the default stream, a typical 3-step CUDA program will perform HtoD copy, compute, and DtoH copy serially

```
memcpy(HtoD)
compute<<<>>>()
```



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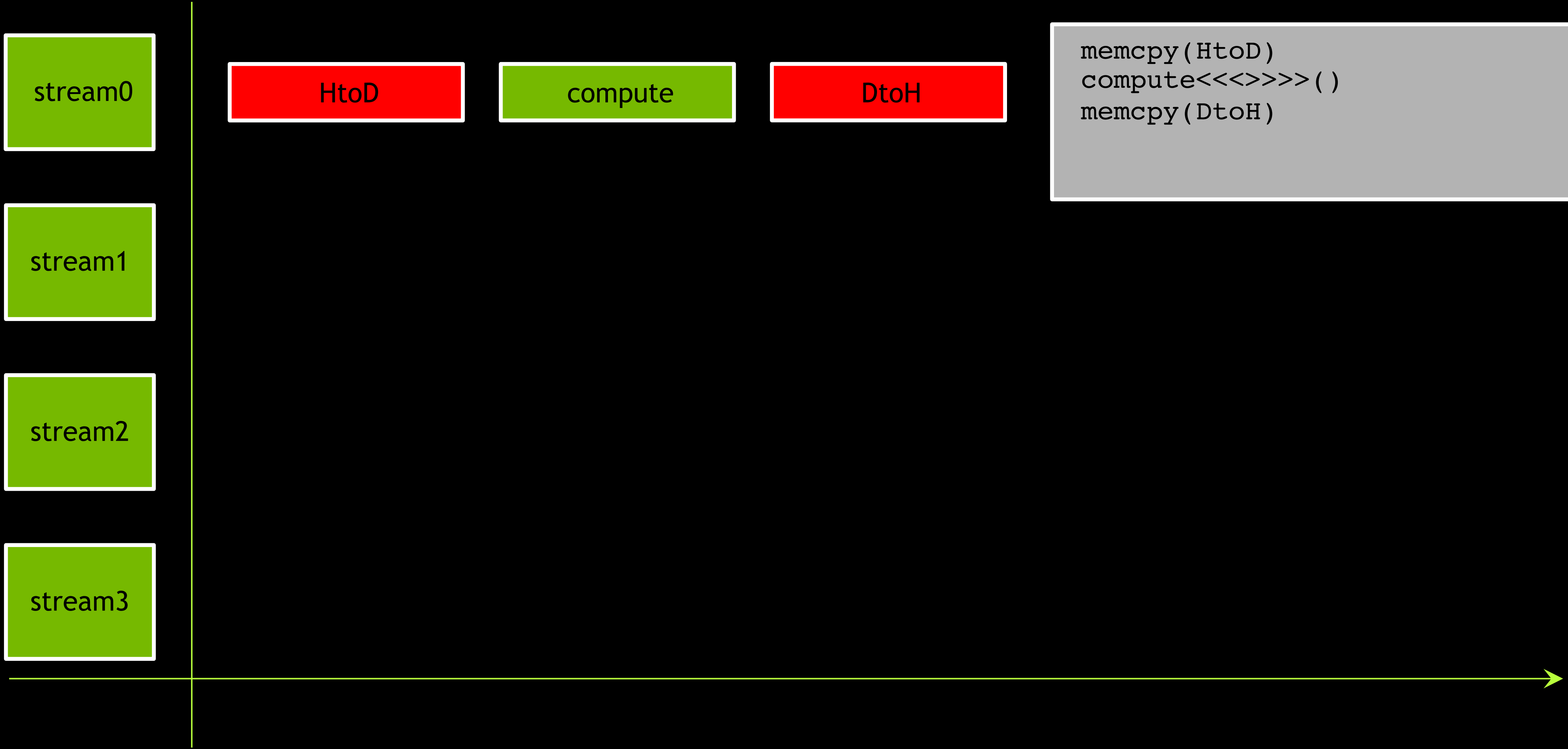
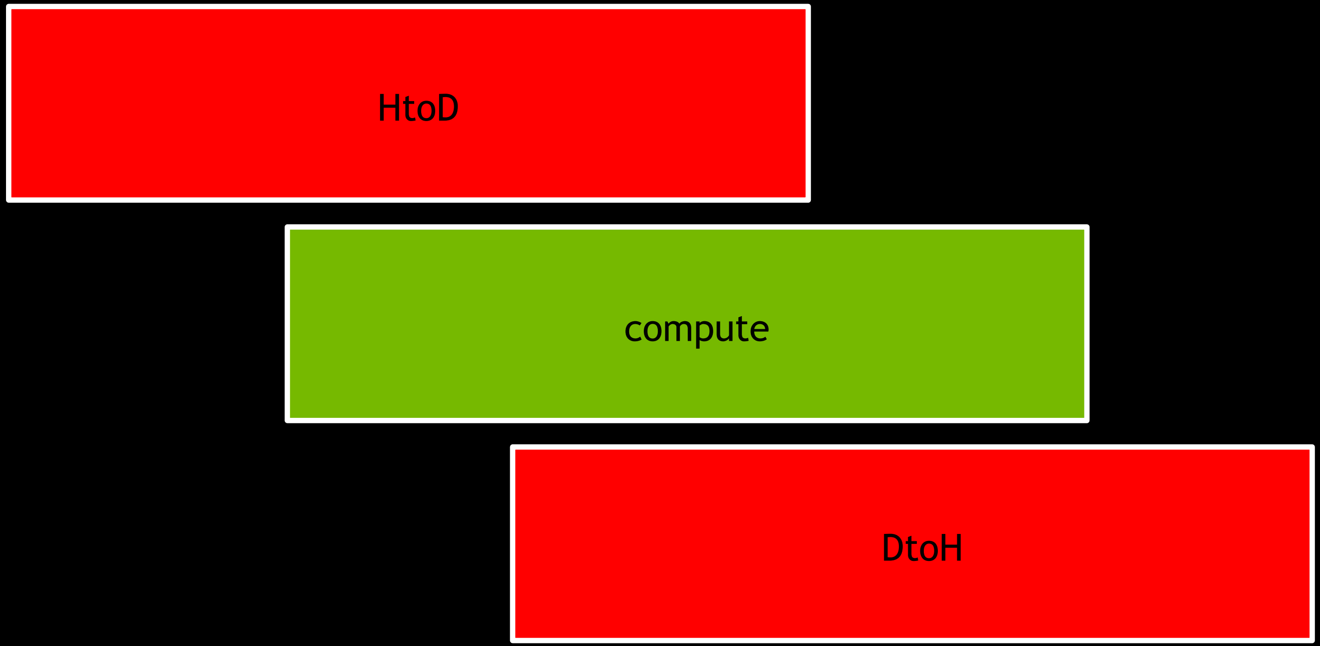
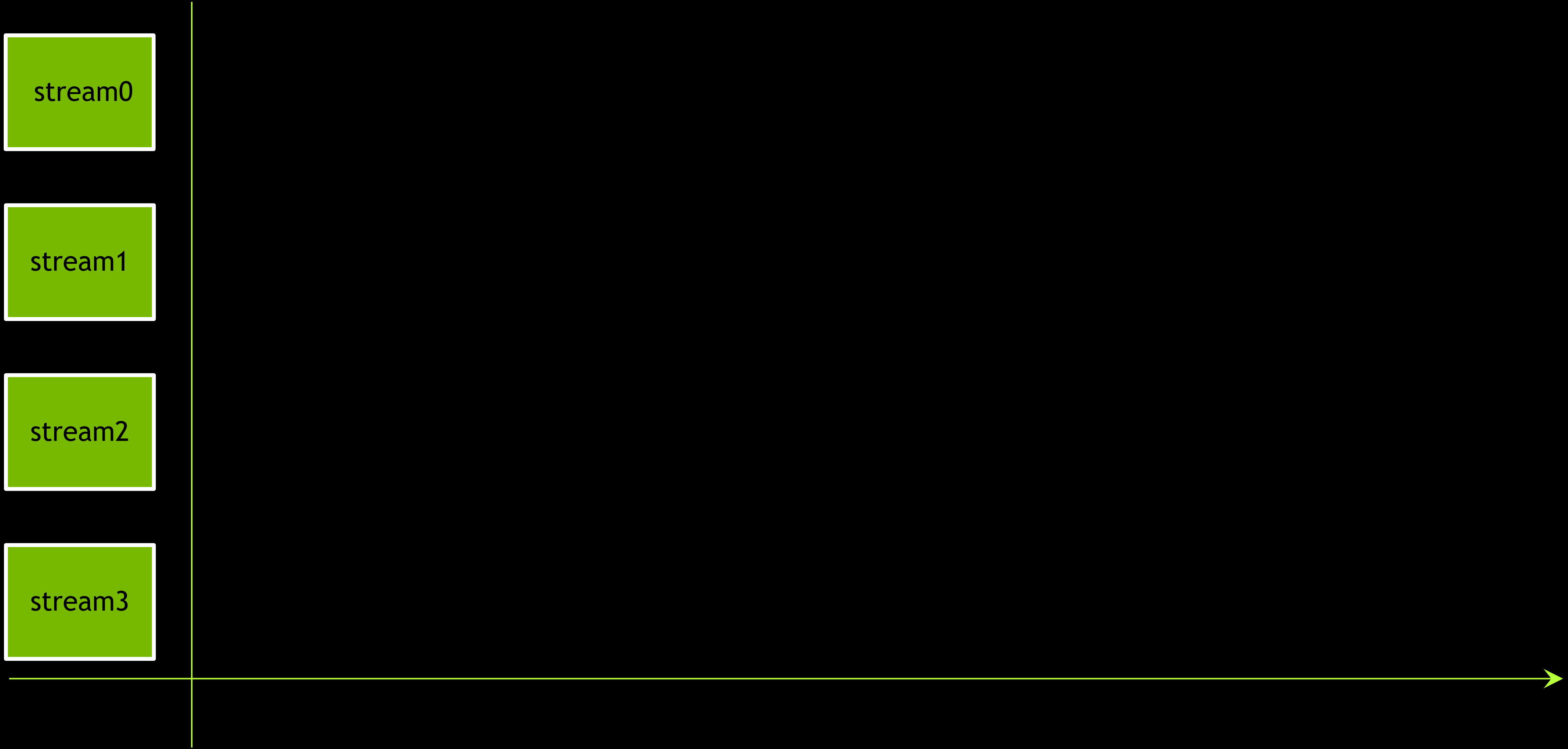



```
memcpy(HtoD)
compute<<<>>>()
memcpy(DtoH)
```

Let's consider how we might perform copy/compute overlap

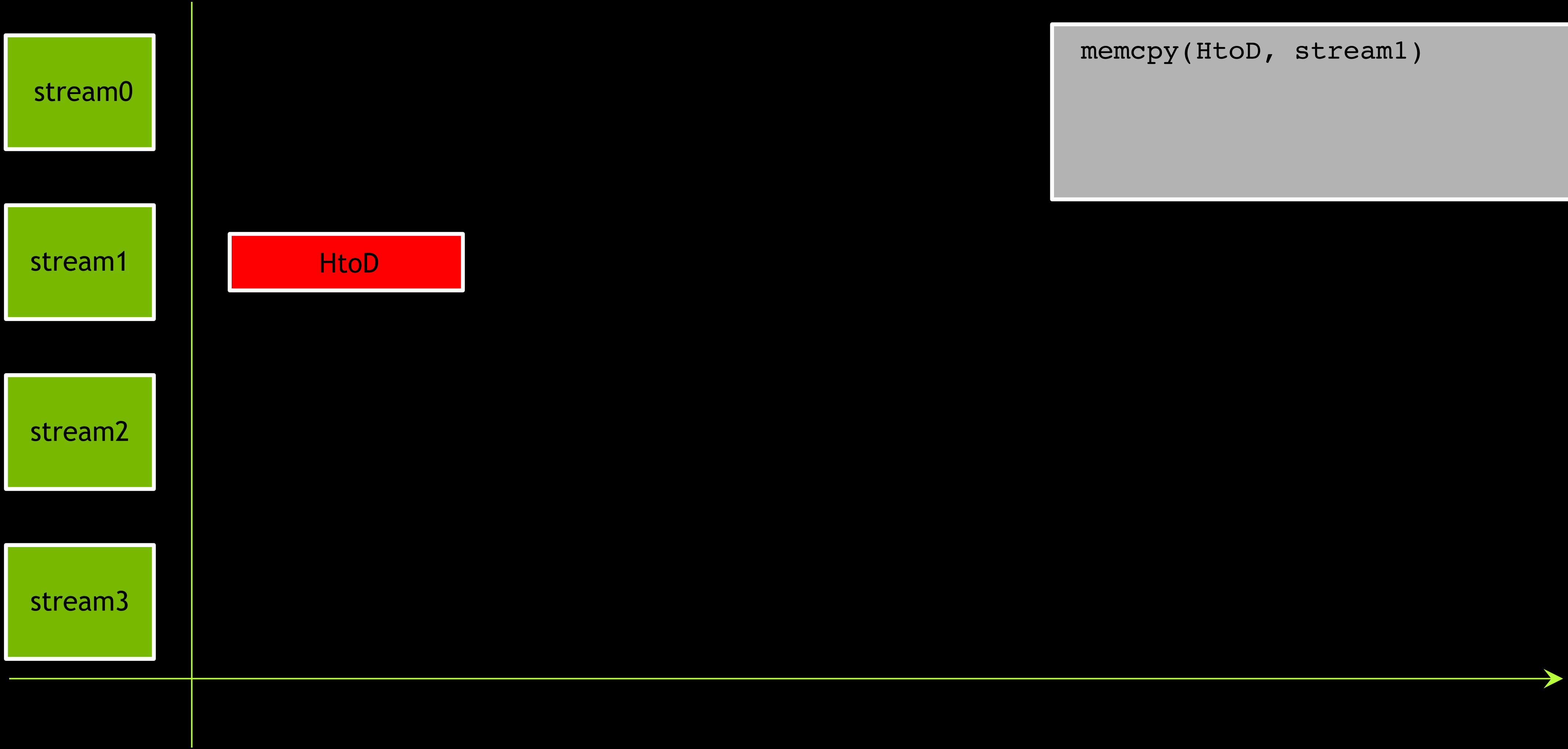


One naïve approach might be to simply issue each of these 3 operations in different non-default streams



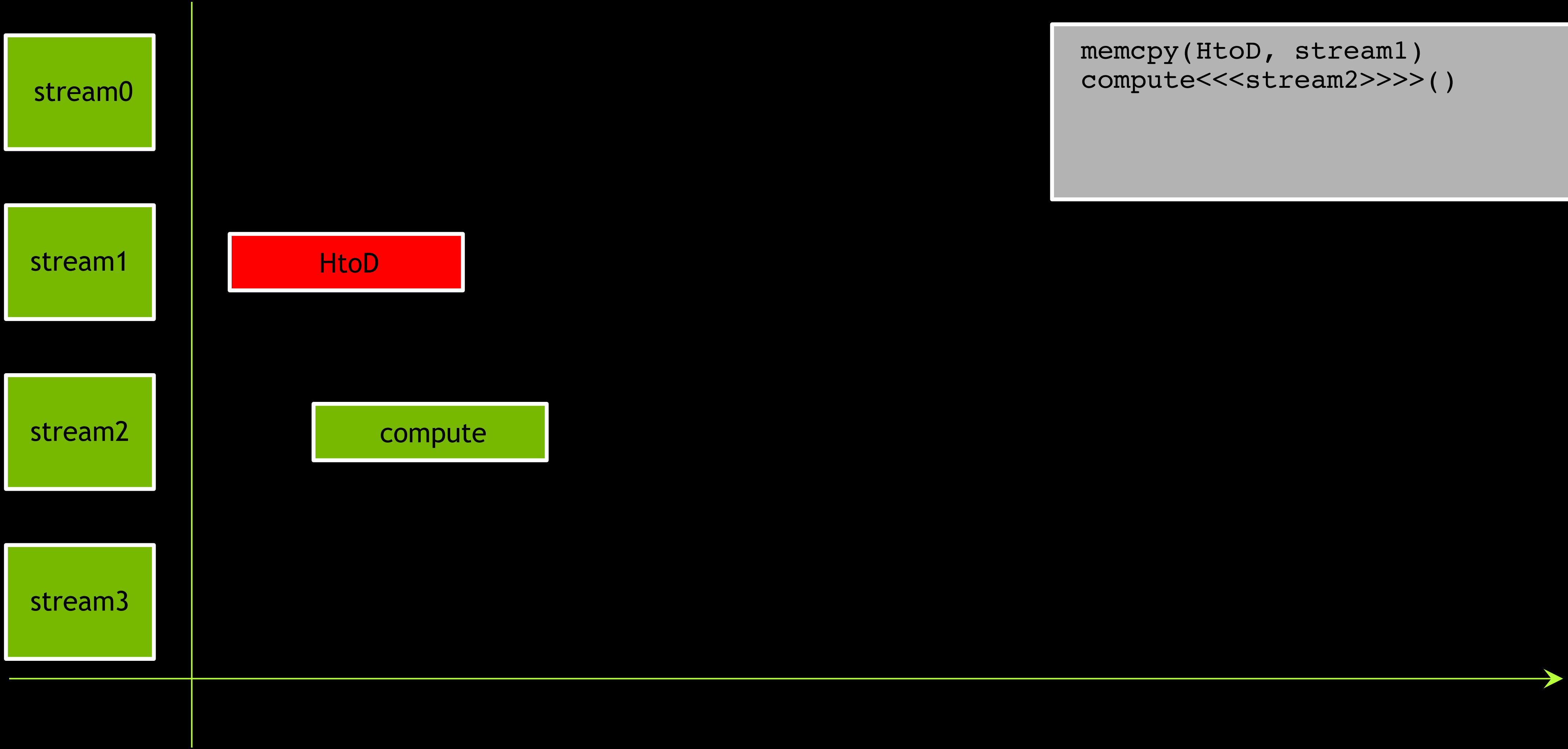
One naïve approach might be to simply issue each of these 3 operations in different non-default streams

```
memcpy(HtoD, stream1)
```



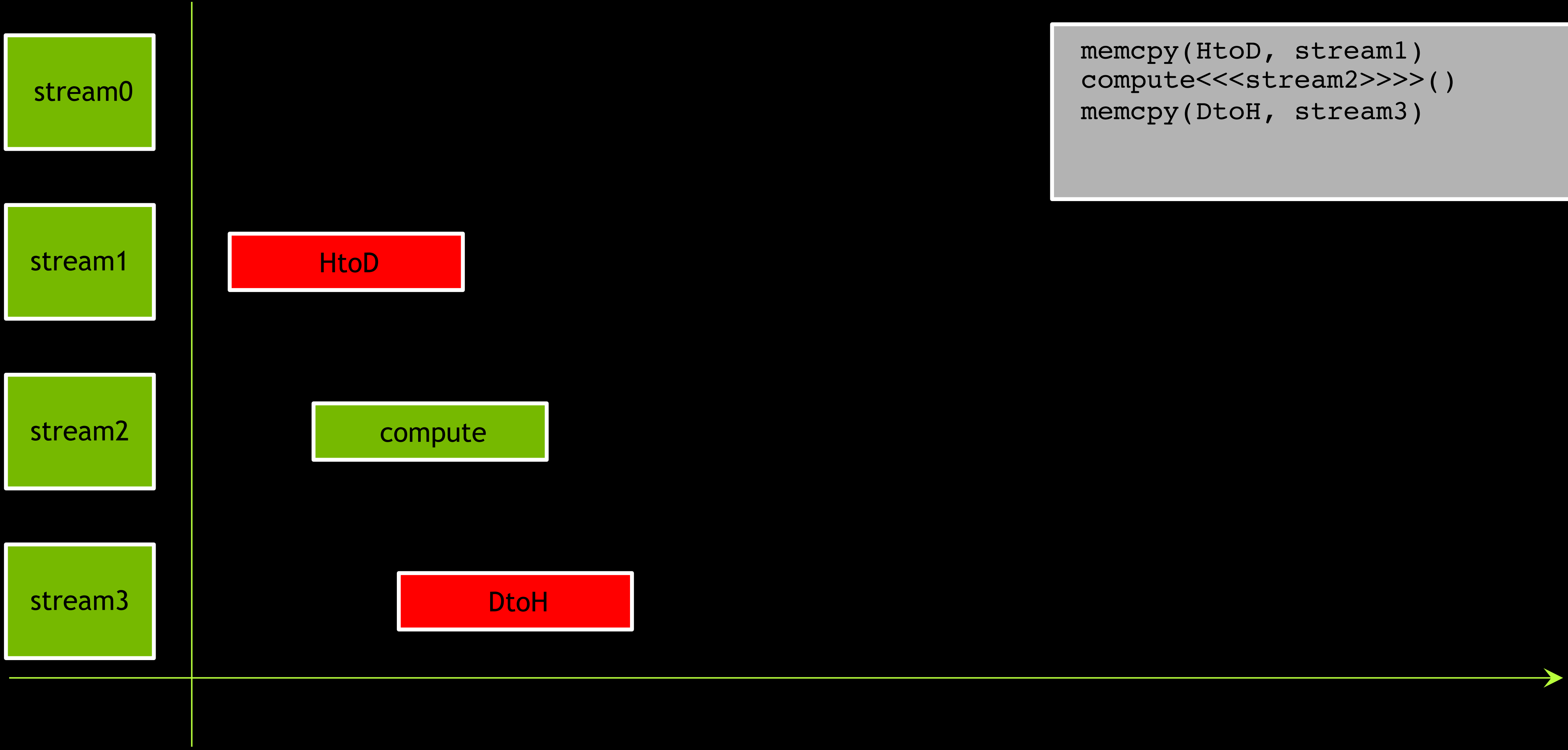
One naïve approach might be to simply issue each of these 3 operations in different non-default streams

```
memcpy(HtoD, stream1)
compute<<<stream2>>>>()
```



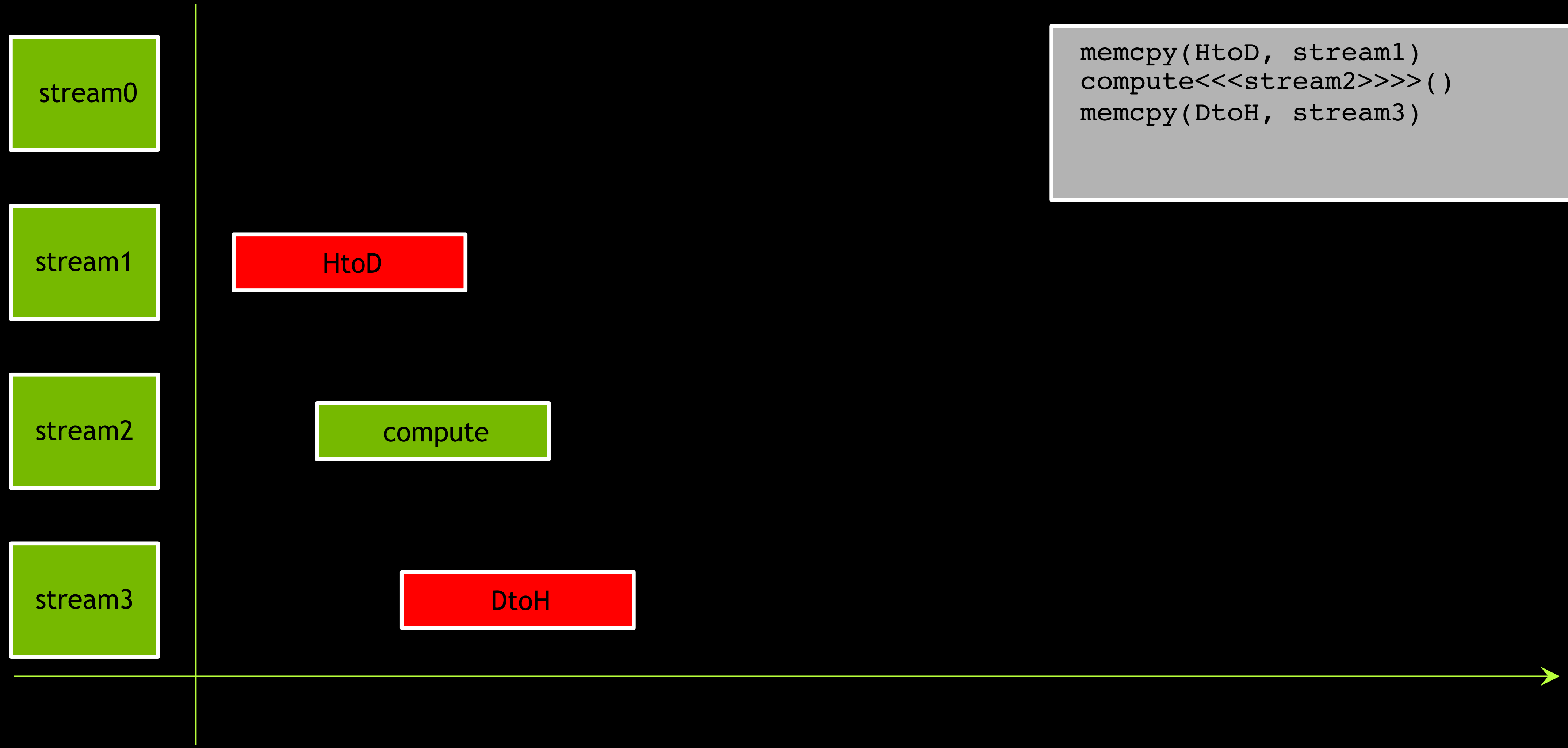
One naïve approach might be to simply issue each of these 3 operations in different non-default streams

```
memcpy(HtoD, stream1)
compute<<<stream2>>>>()
memcpy(DtoH, stream3)
```



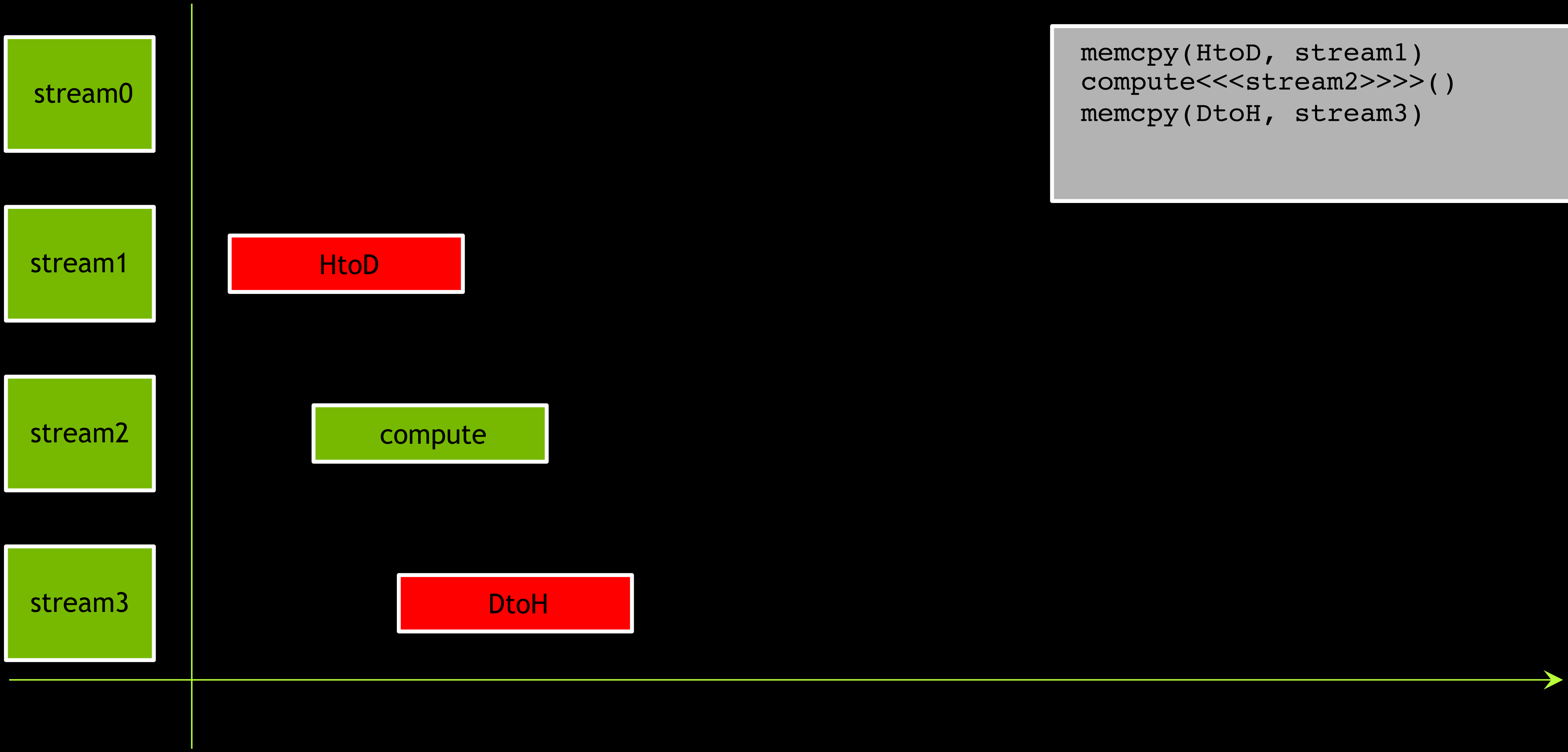
Would this work?

```
memcpy(HtoD, stream1)
compute<<<stream2>>>>()
memcpy(DtoH, stream3)
```



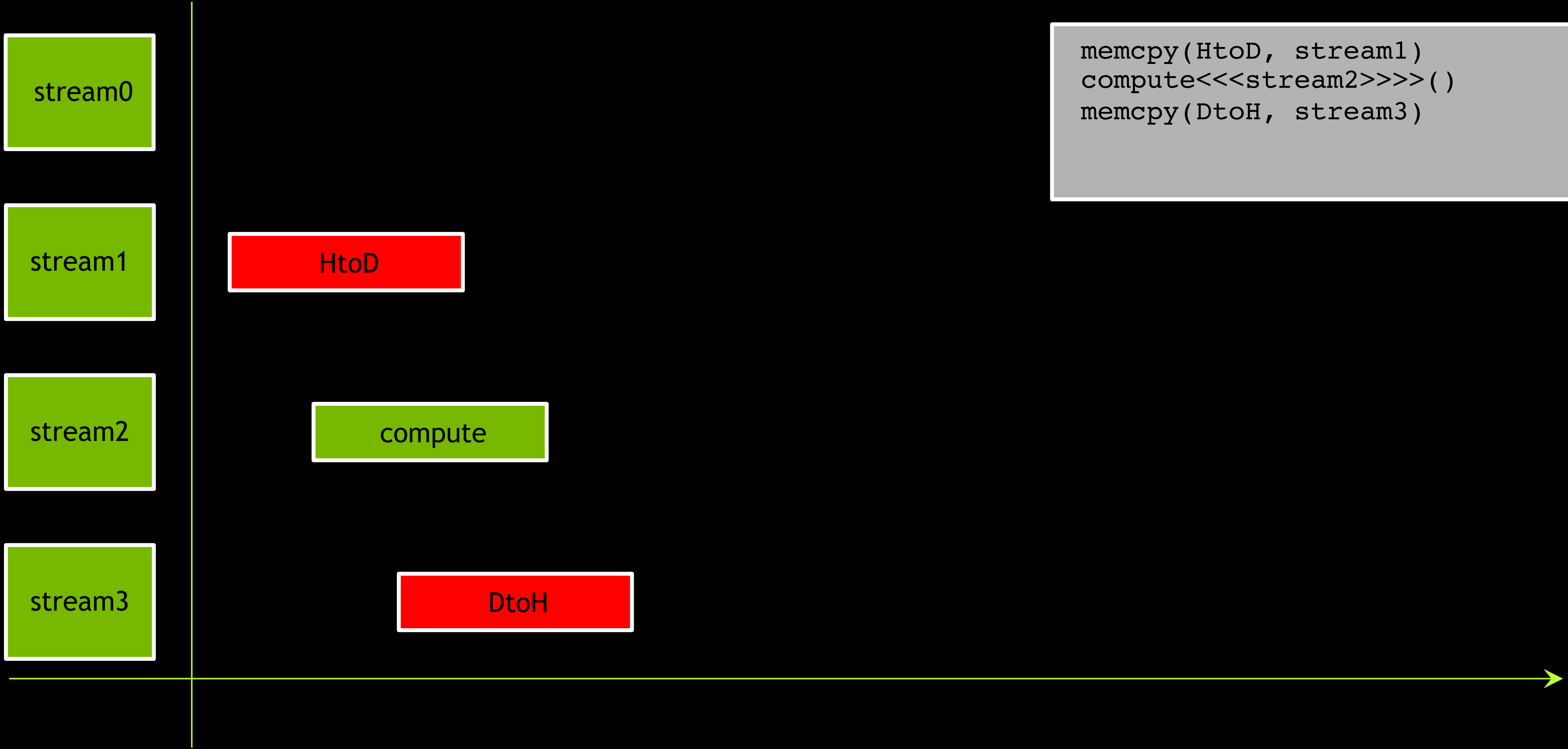
Would this work?
No

```
memcpy(HtoD, stream1)
compute<<<stream2>>>>()
memcpy(DtoH, stream3)
```



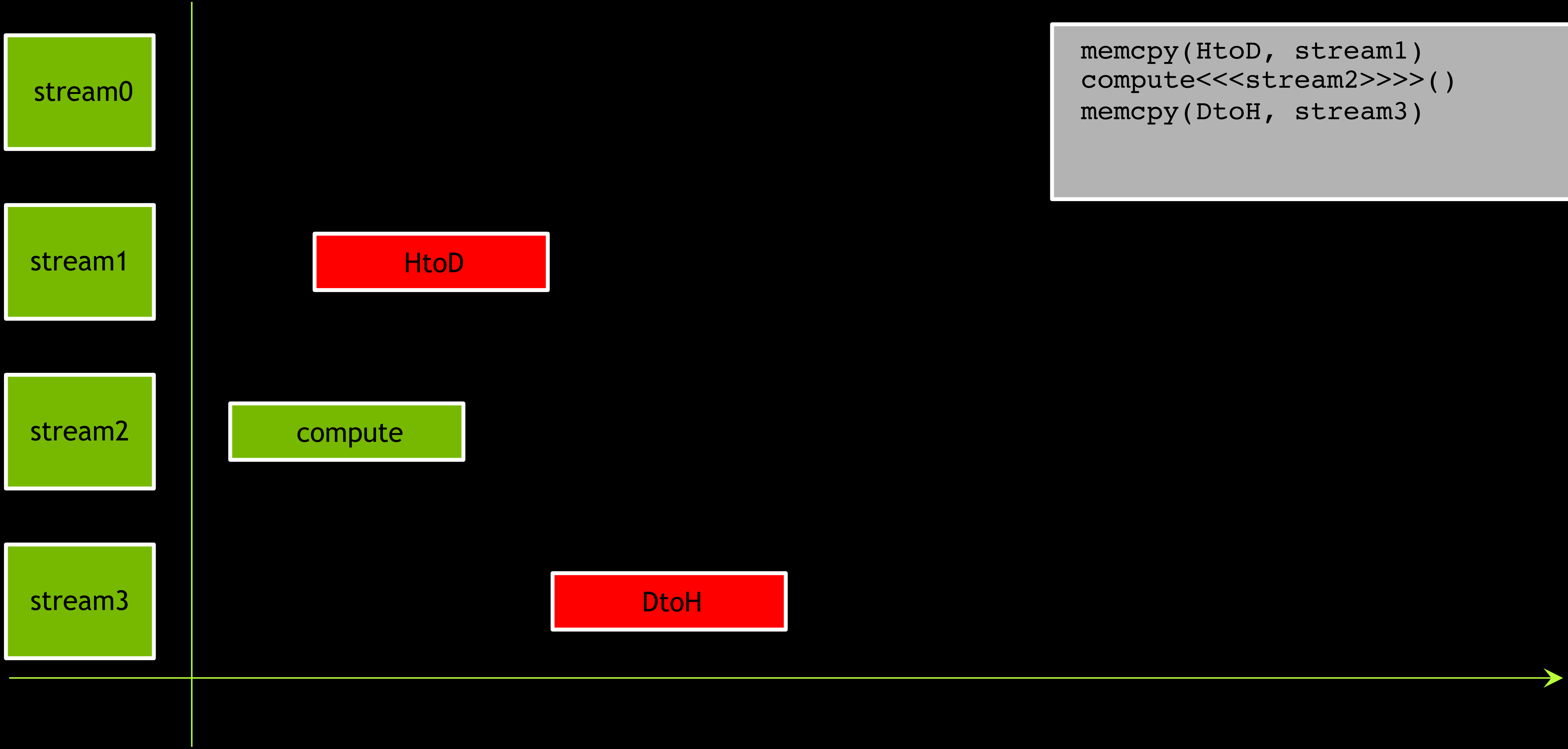
Recall that operations in non-default streams have no guaranteed order, therefore…

```
memcpy(HtoD, stream1)
compute<<<stream2>>>>()
memcpy(DtoH, stream3)
```



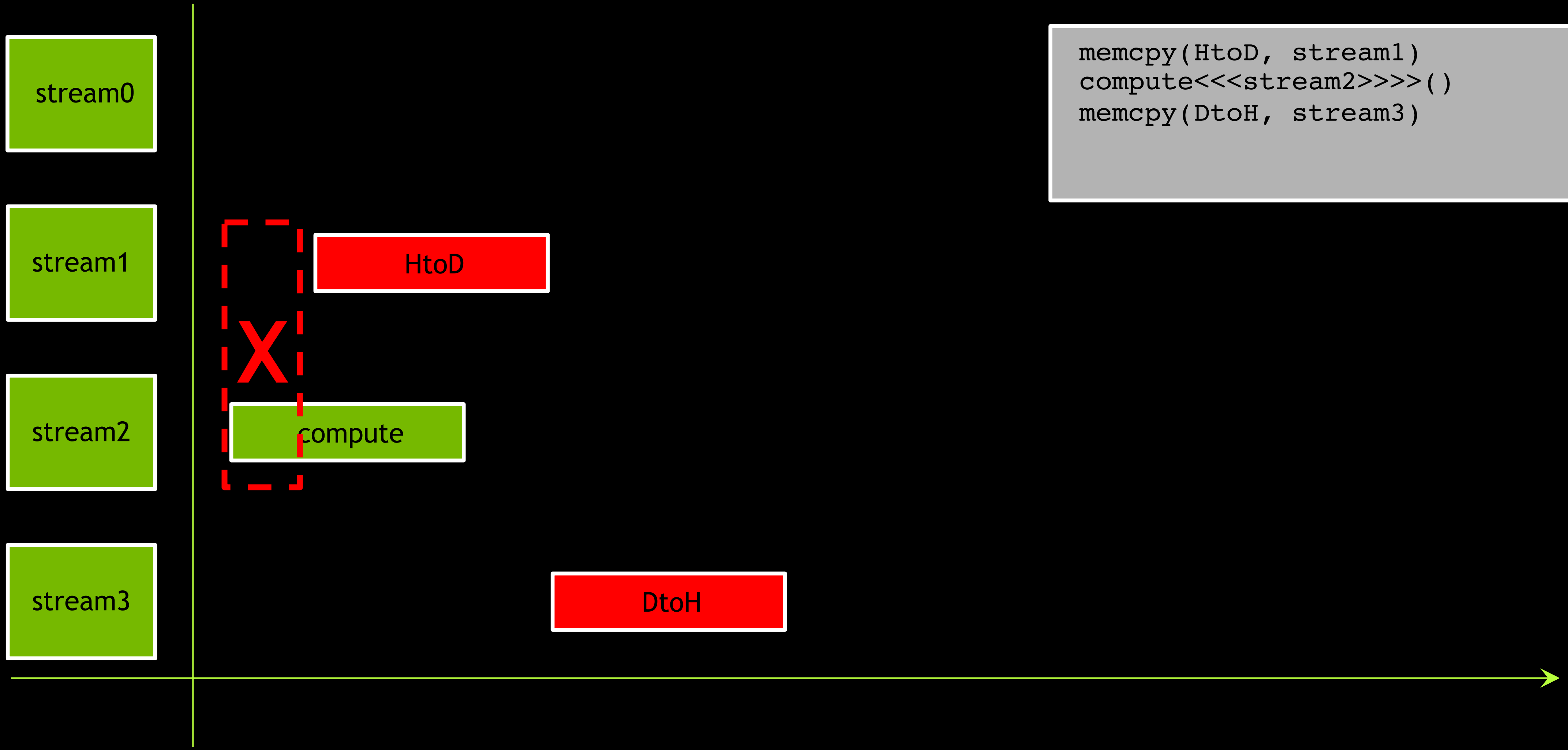
…something like this could occur

```
memcpy(HtoD, stream1)
compute<<<stream2>>>>()
memcpy(DtoH, stream3)
```

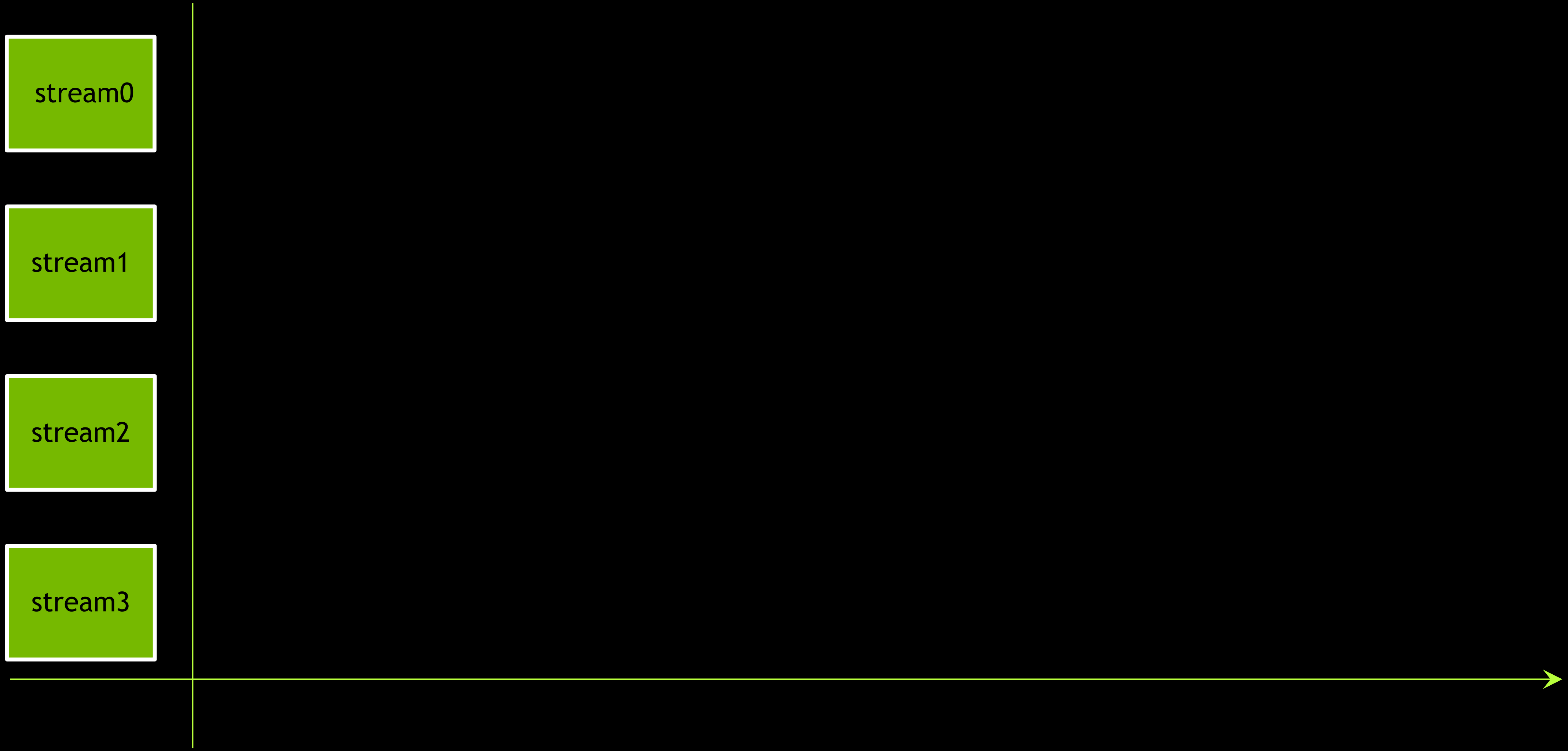


…and compute might begin before the data it needs is present on the GPU

```
memcpy(HtoD, stream1)
compute<<<stream2>>>>()
memcpy(DtoH, stream3)
```



Another naïve approach might be to issue them all in the same non-default stream, to guarantee data/compute order



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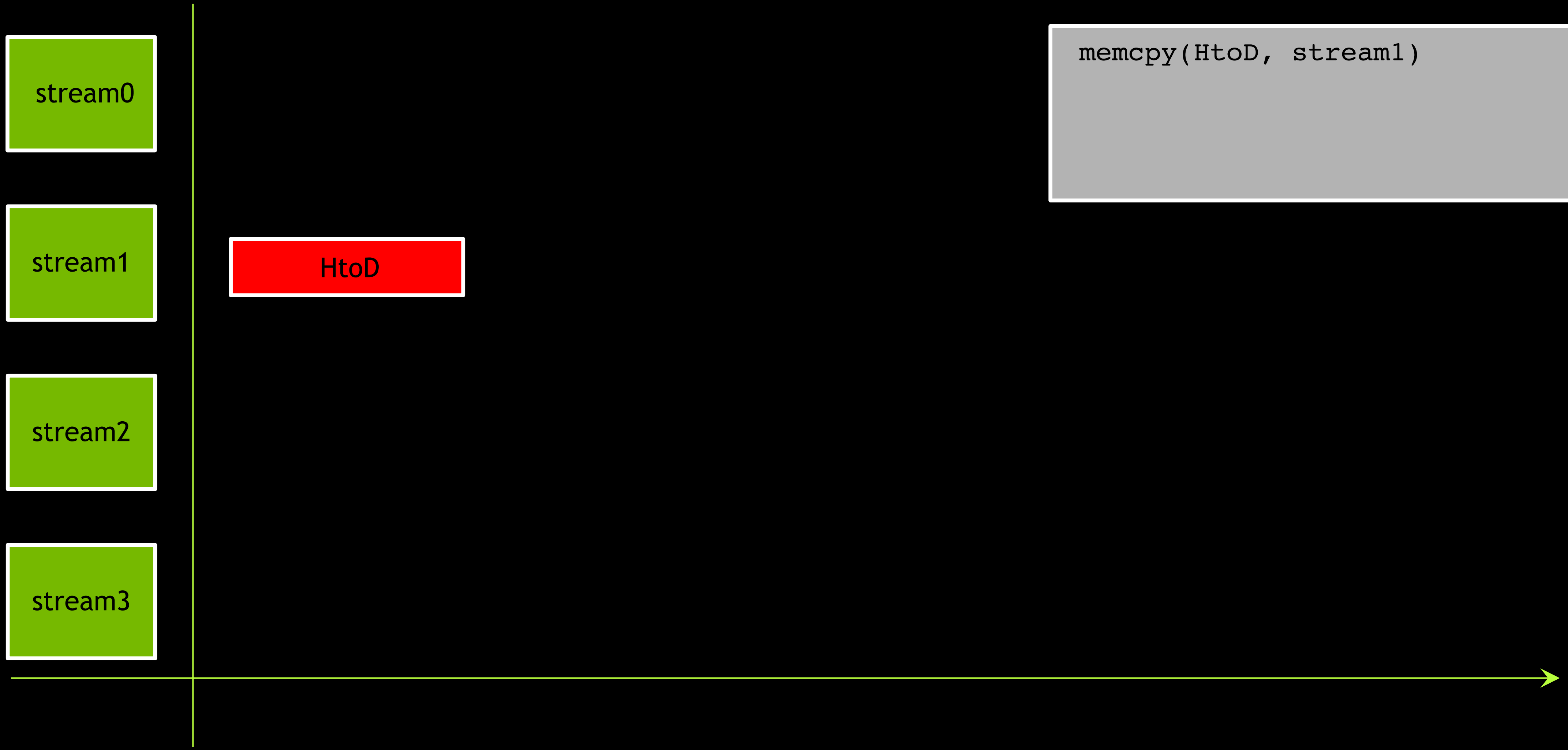
```
memcpy(HtoD, stream1)
```



Another naïve approach might be to issue them all in the same non-default stream, to guarantee data/compute order

```
memcpy(HtoD, stream1)
compute<<<stream1>>>()
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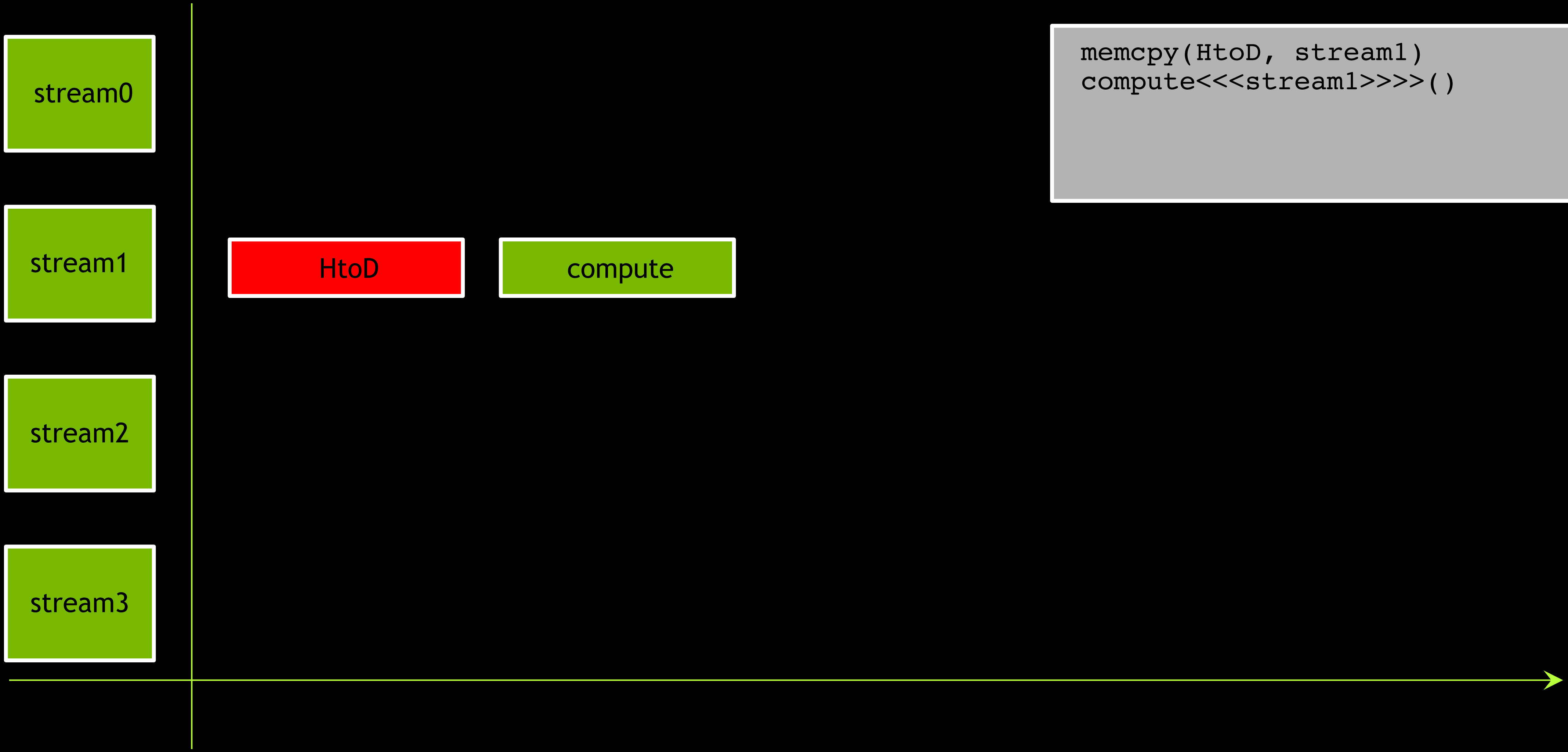

Another naïve approach might be to issue them all in the same non-default stream, to guarantee data/compute order

```
memcpy(HtoD, stream1)
compute<<<stream1>>>>()
memcpy(DtoH, stream1)
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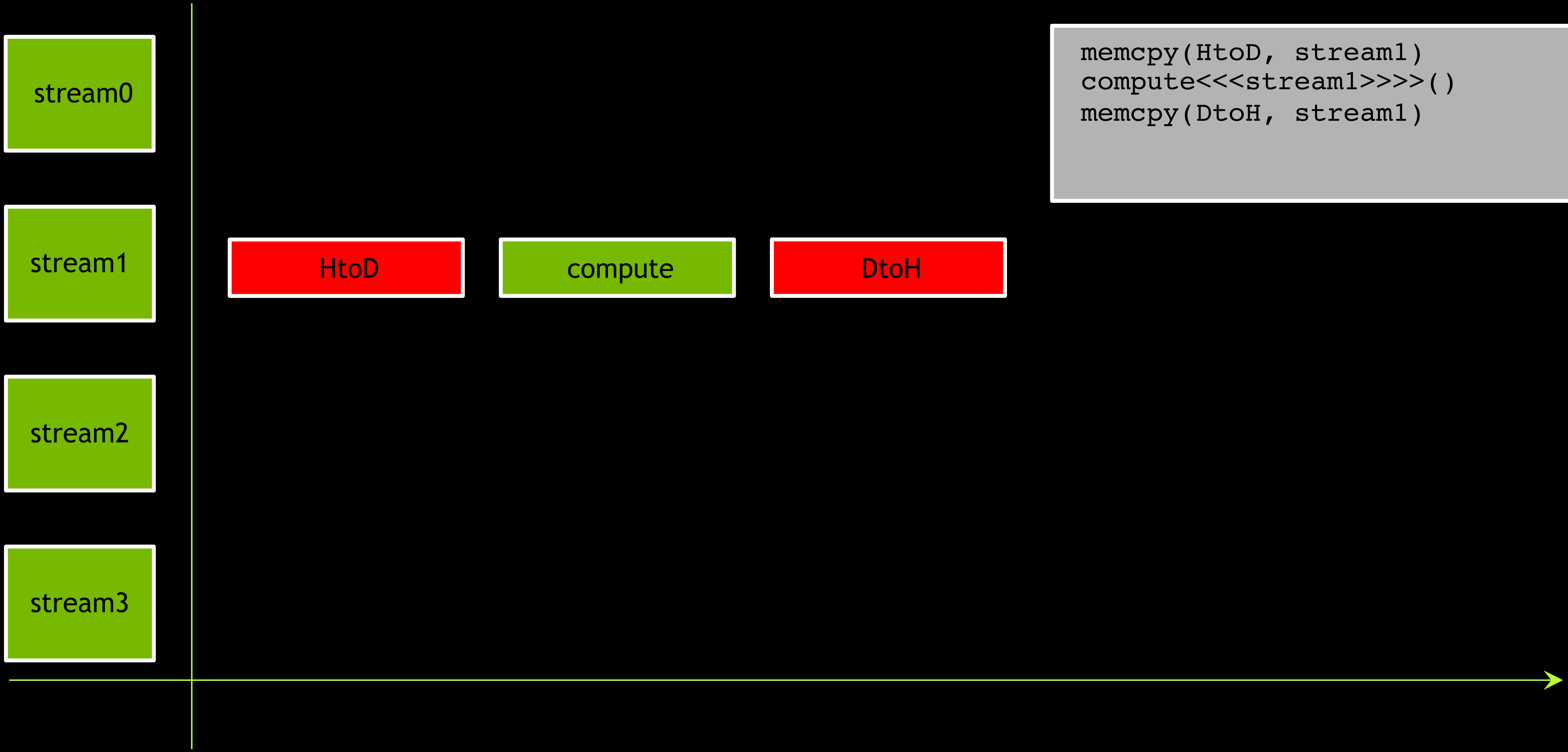
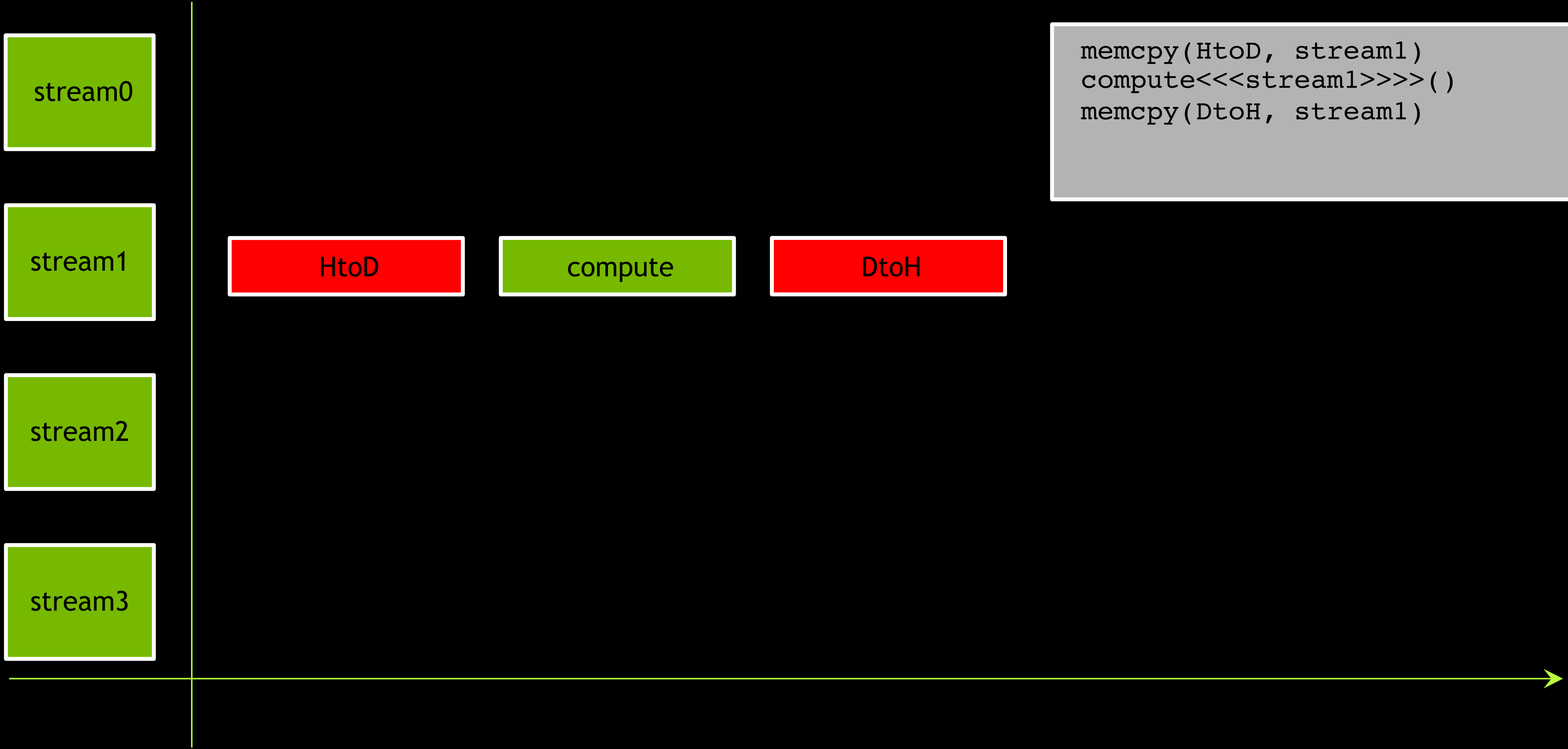
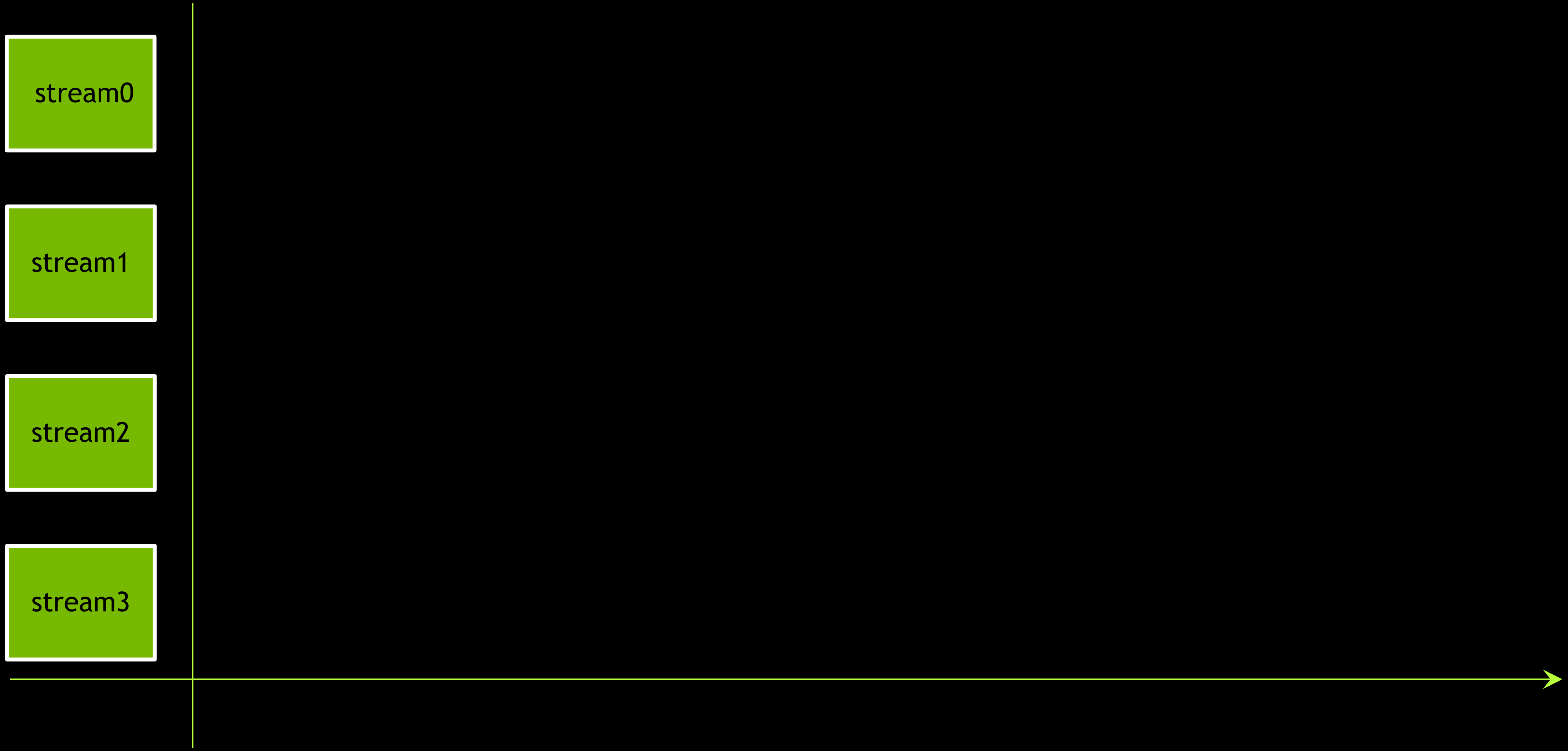


However, this results in the same behavior as using the default stream: no overlap

```
memcpy(HtoD, stream1)
compute<<<stream1>>>>()
memcpy(DtoH, stream1)
```

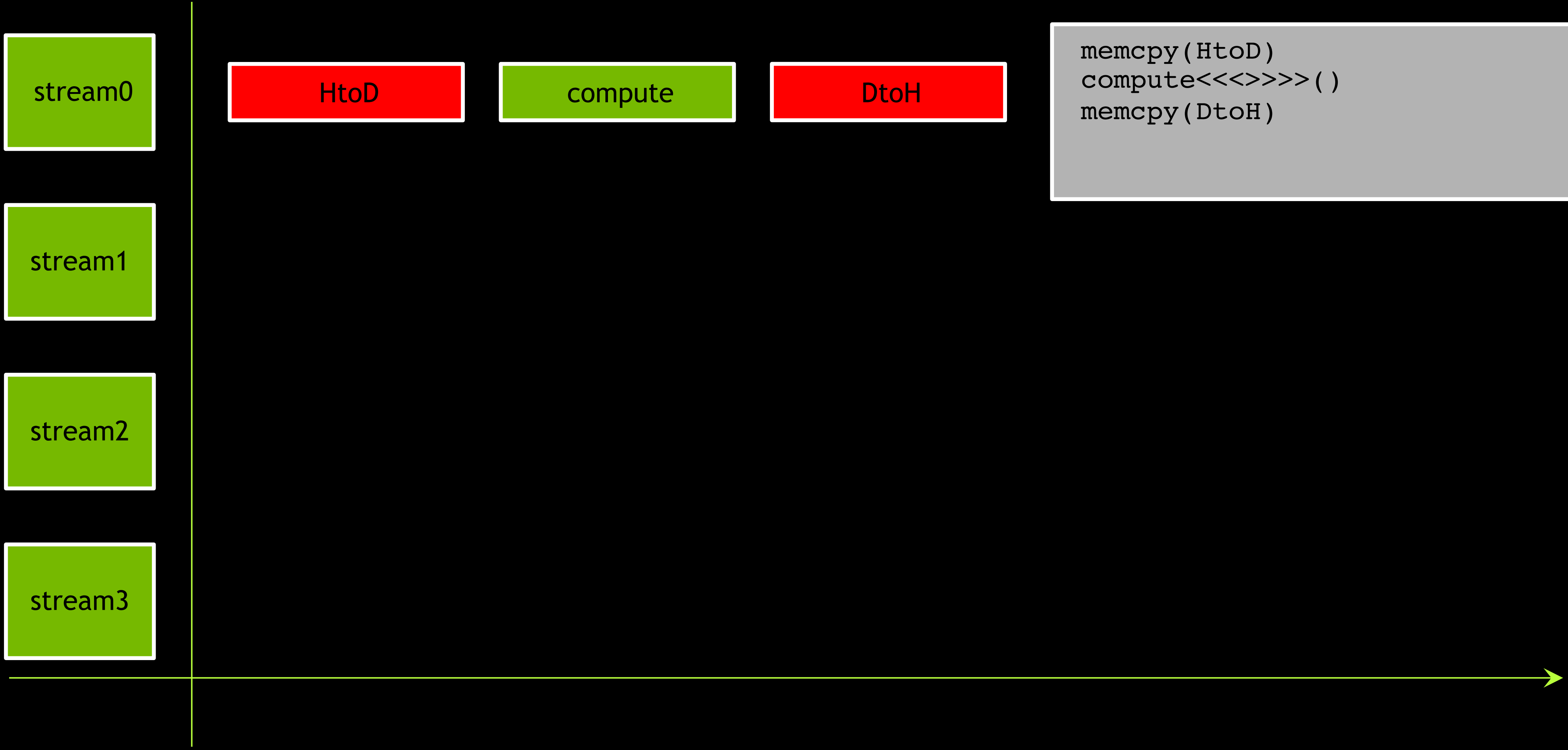


Consider if we were to take the existing program…

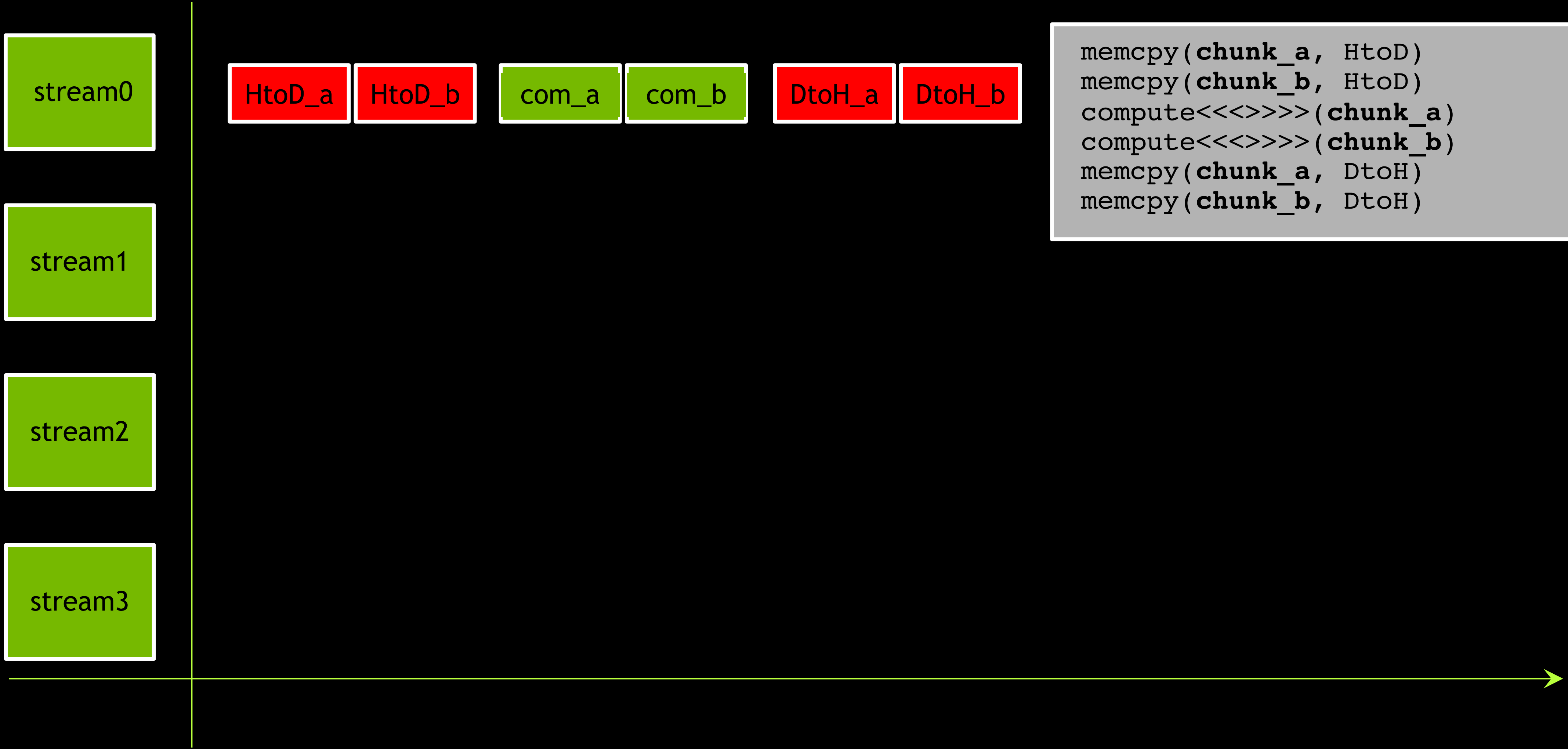


Consider if we were to take the existing program…

```
memcpy(HtoD)
compute<<<>>>()
memcpy(DtoH)
```

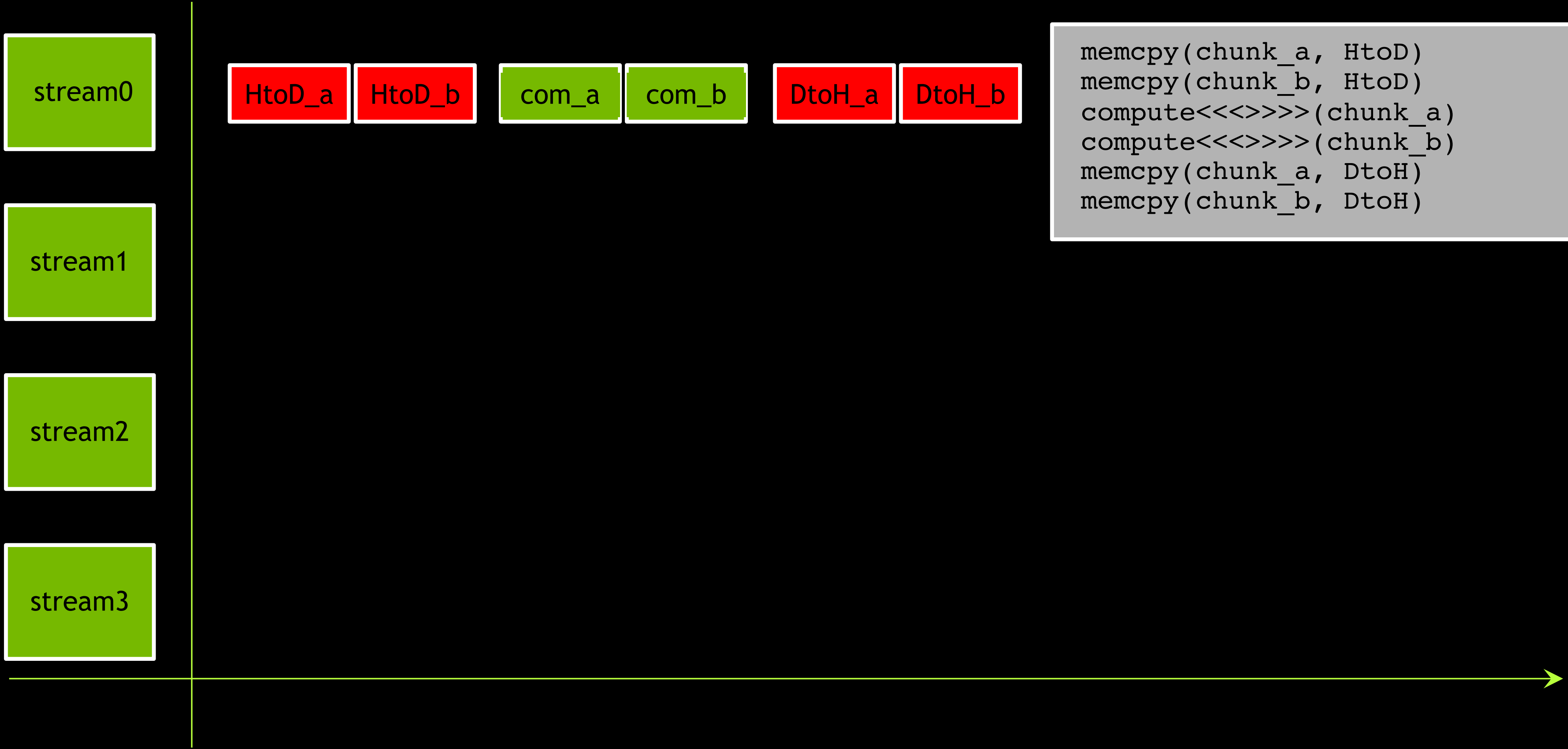


...and split the data into 2 **chunks**




```
memcpy(chunk_a, HtoD)
memcpy(chunk_b, HtoD)
compute<<<>>>(chunk_a)
compute<<<>>>(chunk_b)
memcpy(chunk_a, DtoH)
memcpy(chunk_b, DtoH)
```

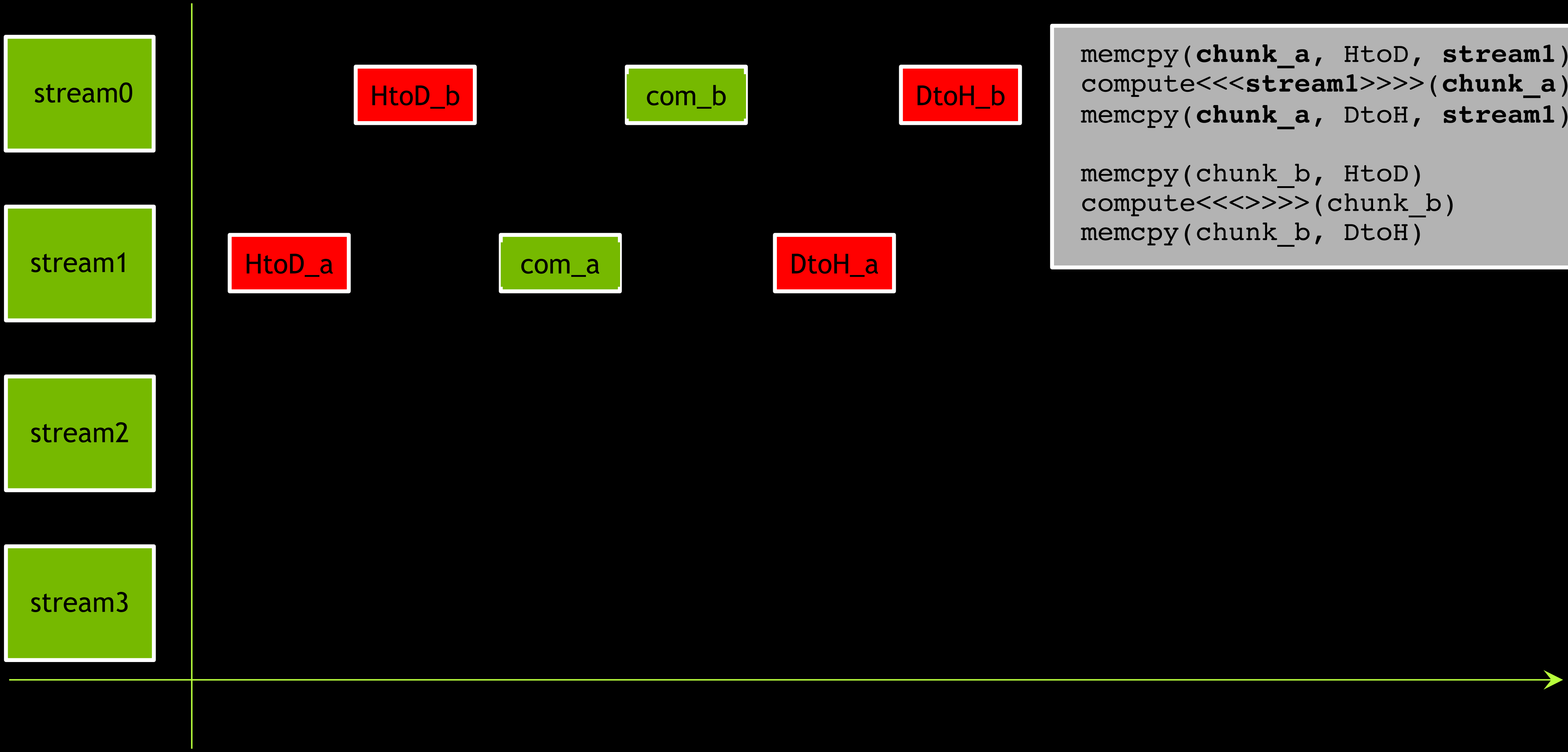
If we now move all operations for each chunk into their own separate non-default stream…




```
memcpy(chunk_a, HtoD)
memcpy(chunk_b, HtoD)
compute<<<>>>(chunk_a)
compute<<<>>>(chunk_b)
memcpy(chunk_a, DtoH)
memcpy(chunk_b, DtoH)
```

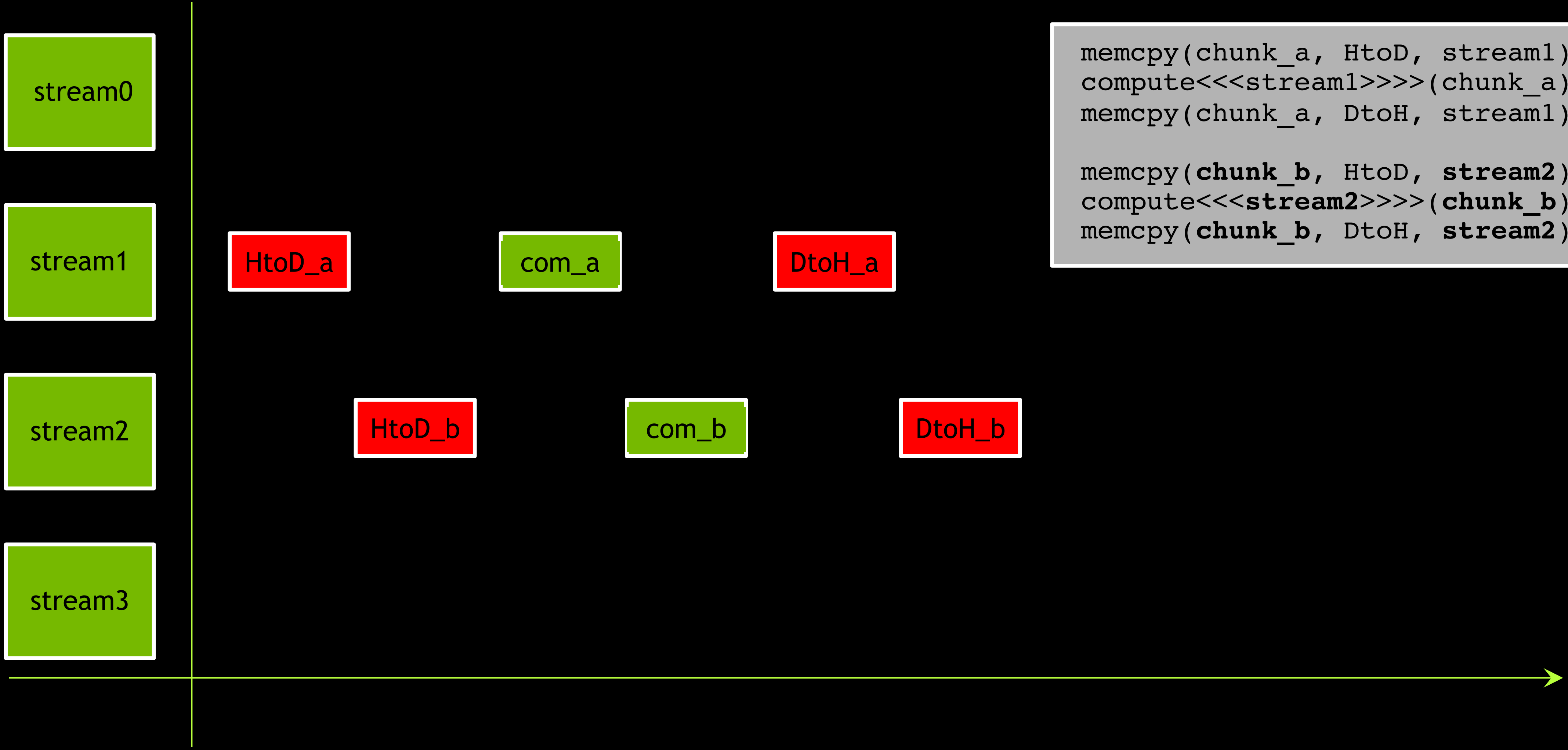
If we now move all operations for each chunk into their own separate non-default stream…

```
memcpy(chunk_a, HtoD, stream1)
compute<<<stream1>>>>(chunk_a)
memcpy(chunk_a, DtoH, stream1)

memcpy(chunk_b, HtoD)
compute<<<>>>>(chunk_b)
memcpy(chunk_b, DtoH)
```



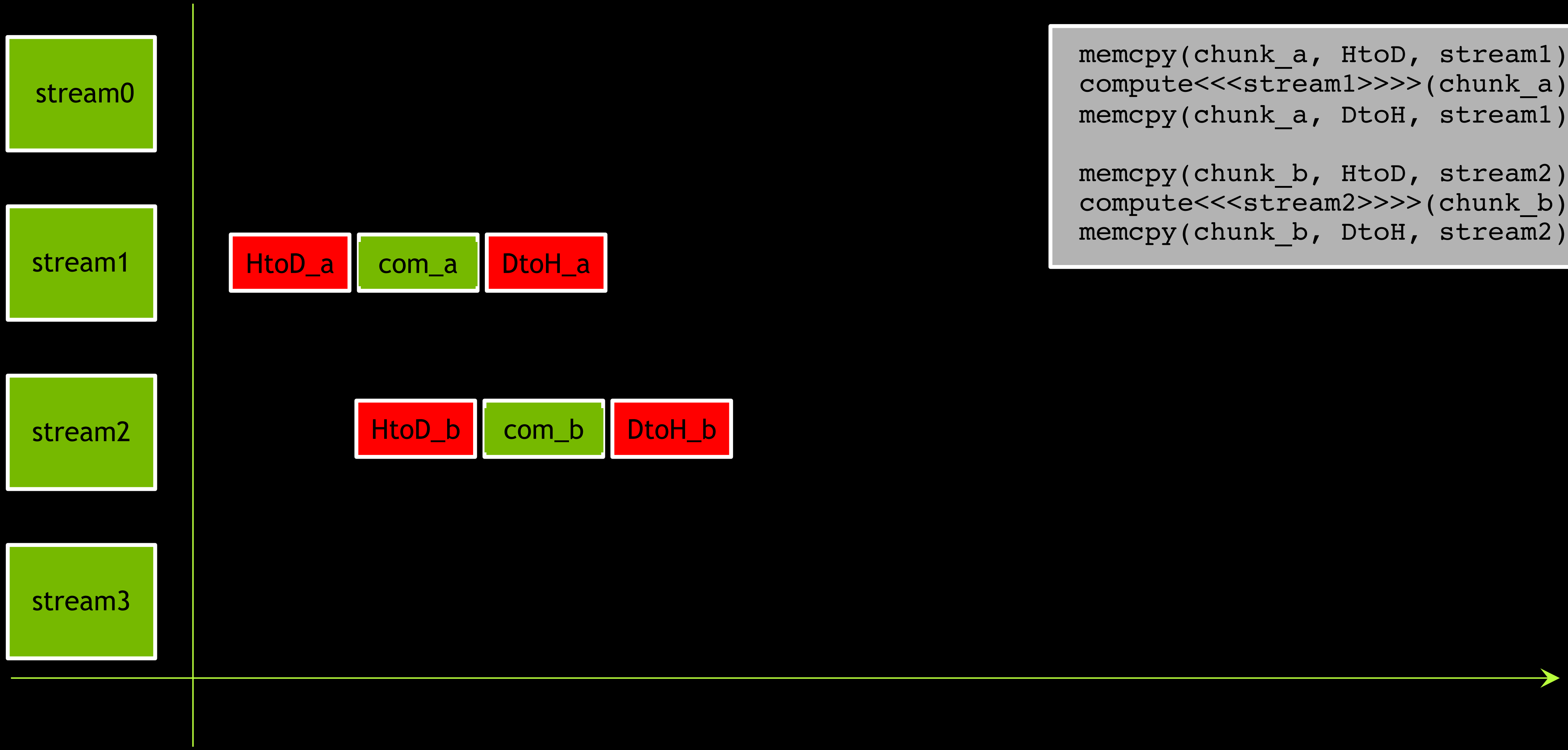
If we now move all operations for each chunk into their own separate non-default stream…

```
memcpy(chunk_a, HtoD, stream1)
compute<<<stream1>>>>(chunk_a)
memcpy(chunk_a, DtoH, stream1)

memcpy(chunk_b, HtoD, stream2)
compute<<<stream2>>>>(chunk_b)
memcpy(chunk_b, DtoH, stream2)
```



…data/compute order is maintained, and, we can achieve some overlap

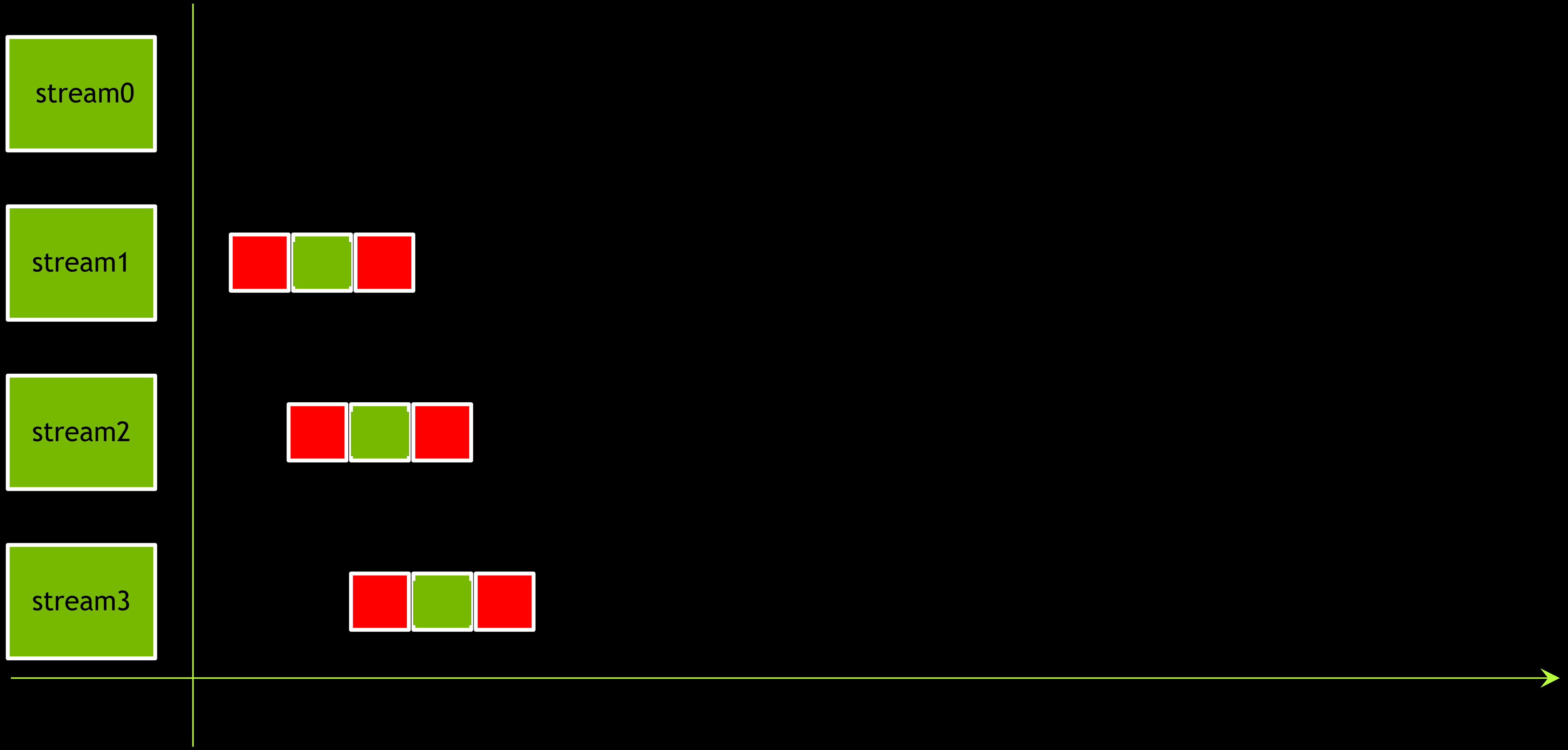
```
memcpy(chunk_a, HtoD, stream1)
compute<<<stream1>>>>(chunk_a)
memcpy(chunk_a, DtoH, stream1)

memcpy(chunk_b, HtoD, stream2)
compute<<<stream2>>>>(chunk_b)
memcpy(chunk_b, DtoH, stream2)
```



…data/compute order is maintained, and,
we can achieve some overlap

```
memcpy(chunk_a, HtoD, stream1)
compute<<<stream1>>>>(chunk_a)
memcpy(chunk_a, DtoH, stream1)

memcpy(chunk_b, HtoD, stream2)
compute<<<stream2>>>>(chunk_b)
memcpy(chunk_b, DtoH, stream2)
```

Hypothetically, the number of chunks could be increased for perhaps even better overlap



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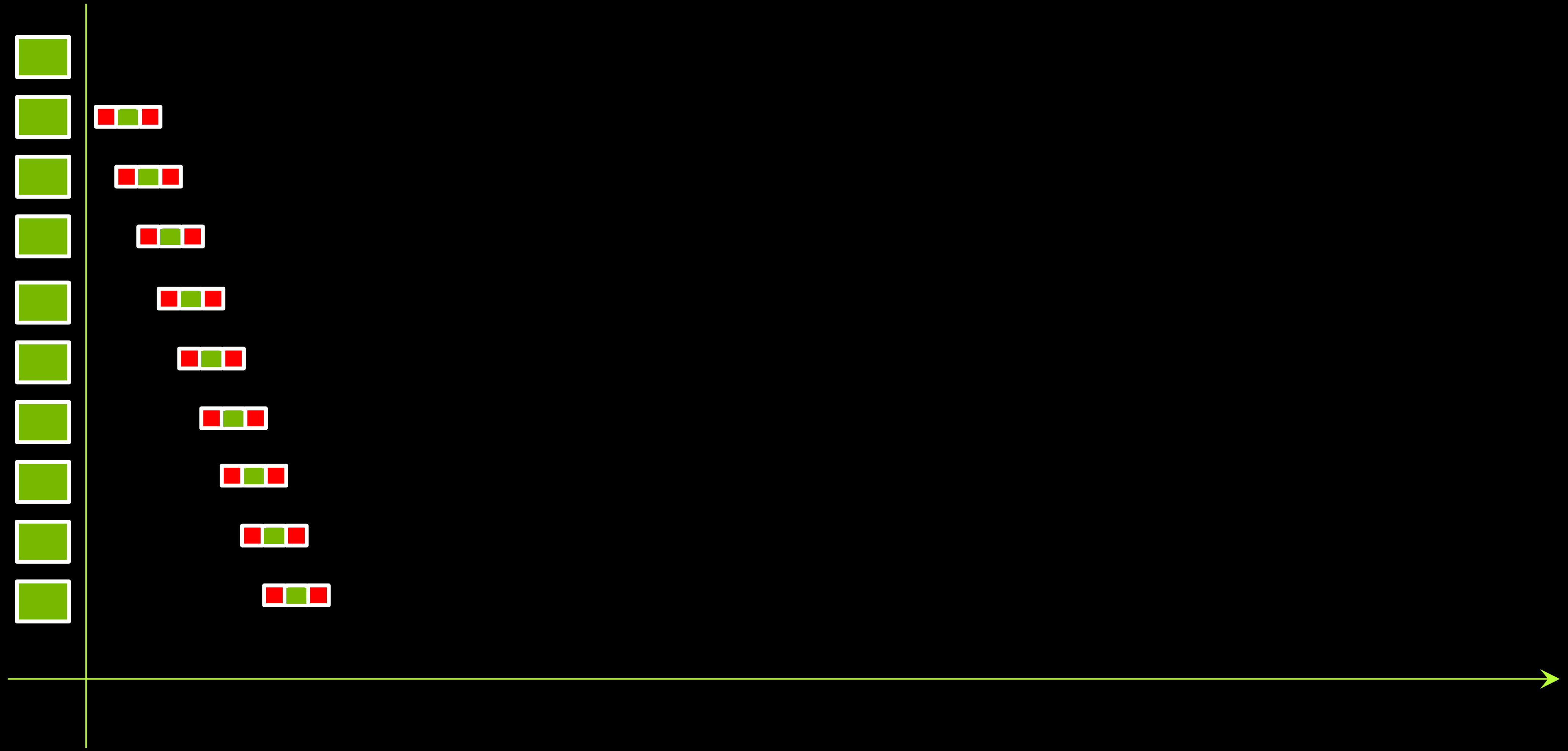
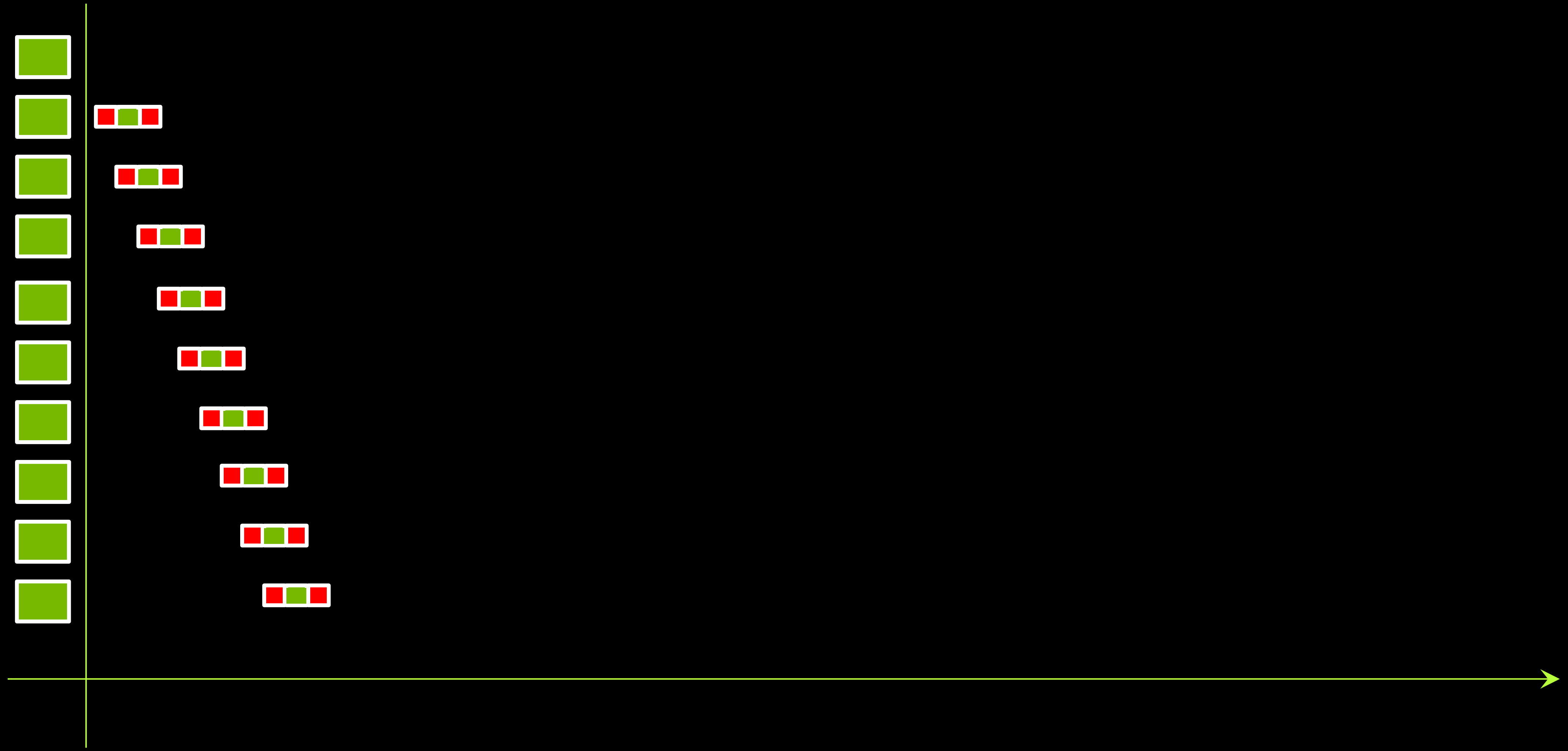


The ideal chunking is best learned by observing program performance



COPY/COMPUTE OVERLAP INDEXING

When chunking data to use in multiple streams, indexing can be tricky

Let’s look at a couple examples of how it can be done

We will start by allocating the data needed for all chunks, here a small size to make the example clear

0	1	2	3	4	5	6	7	8	9

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```
cudaMallocHost(&data_cpu, N)
```

N	10	10

0	1	2	3	4	5	6	7	8	9
0	1	2	3	4	5	6	7	8	9

Of course we would allocate for the GPU as well, but here we will only present one image of the data

```
cudaMallocHost(&data_cpu, N)
cudaMalloc(&data_gpu, N)
```

N	10	10

0	1	2	3	4	5	6	7	8	9

Of course we would allocate for the GPU as well, but here we will only present one image of the data

```
cudaMallocHost(&data_cpu, N)
```

N	10	10

0	1	2	3	4	5	6	7	8	9

Next, we will define the number of streams, and loop to create and collect them in an array

N	10	10

0	1	2	3	4	5	6	7	8	9

Next, we will define the number of streams, and loop to create and collect them in an array

```
num_streams = 2
// for stream_i in num_streams
     cudaStreamCreate(stream)
     streams[stream_i] = stream
```

N	10	10
num_streams	2	2

0	1	2	3	4	5	6	7	8	9

The size of each chunk of data will depend on the number of data entries and the number of streams

N	10	10
num_streams	2	2

0 1 2 3 4 5 6 7 8 9

The size of each chunk of data will depend on the number of data entries and the number of streams

```
chunk_size = N / num_streams
```

N	10	10
num_streams	2	2
chunk_size	N/num_streams	5

0	1	2	3	4	5	6	7	8	9

Each stream will need to handle one chunk of data. We need to calculate its index into the whole data set

N	10	10
num_streams	2	2
chunk_size	N/num_streams	5

0 1 2 3 4 5 6 7 8 9

To do this we will range over the number of streams, starting at 0...

```
// for stream_i in num_streams
```

N	10	10
num_streams	2	2
chunk_size	N/num_streams	5
stream_i	0	0

0 1 2 3 4 5 6 7 8 9

...and multiply by chunk size

```
// for stream_i in num_streams
     lower = chunk_size*stream_i
```

N	10	10
num_streams	2	2
chunk_size	N/num_streams	5
stream_i	0	0
lower	chunk_size*stream_i	0

0	1	2	3	4	5	6	7	8	9

Starting at the **lower** index and utilizing a chunk size worth of data will give us the stream's data within all data

```
// for stream_i in num_streams
    lower = chunk_size*stream_i
```

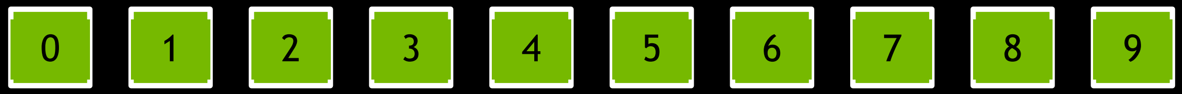
N	10	10
num_streams	2	2
chunk_size	N/num_streams	5
stream_i	0	0
lower	chunk_size*stream_i	0

0	1	2	3	4	5	6	7	8	9

This method will work for each stream_i

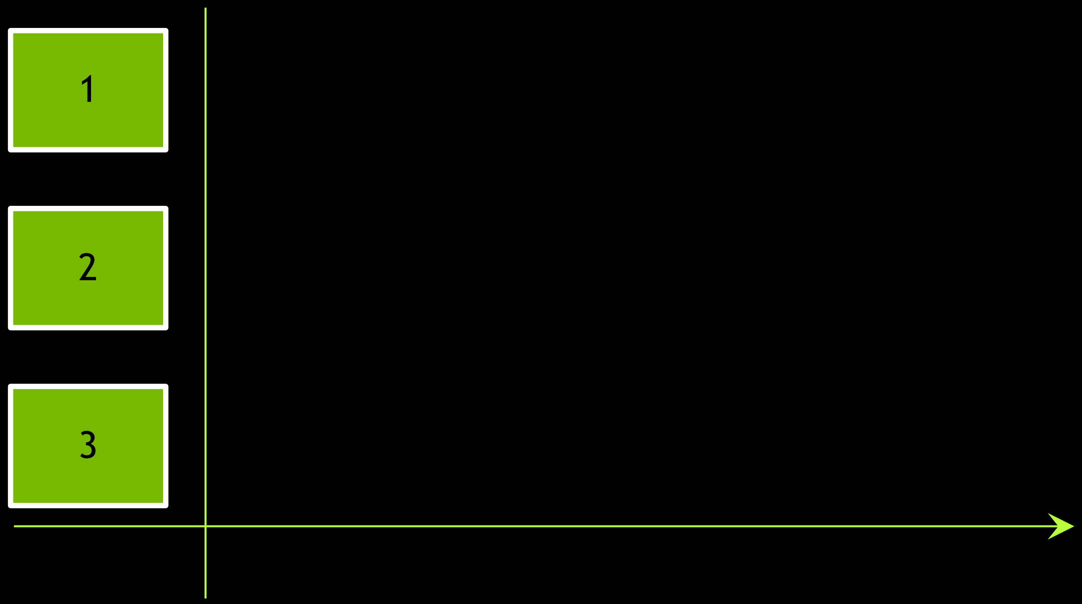
```
// for stream_i in num_streams
     lower = chunk_size*stream_i
```

N	10	10
num_streams	2	2
chunk_size	N/num_streams	5
stream_i	1	1
lower	chunk_size*stream_i	5

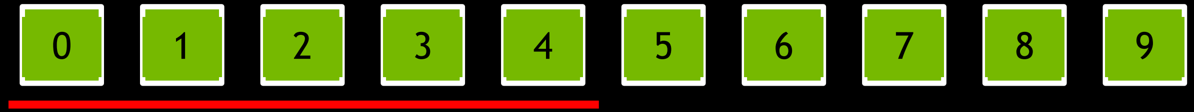


Having calculated these values, we can now perform non-default stream HtoD memory copies...

```
cudaMemcpyAsync(
    data_cpu+lower,
    data_gpu+lower,
    sizeof(uint64_t)*chunk_size,
    cudaMemcpyHostToDevice,
    streams[stream_i]
)
```



N	10	10
num_streams	2	2
chunk_size	N/num_streams	5
stream_i	0	0
lower	chunk_size*stream_i	0



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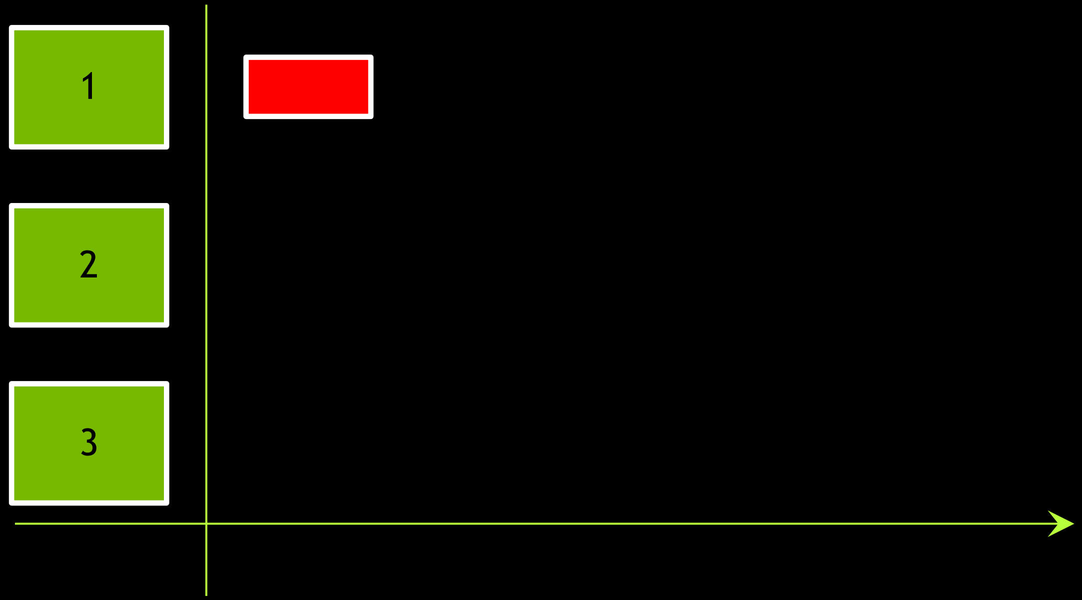
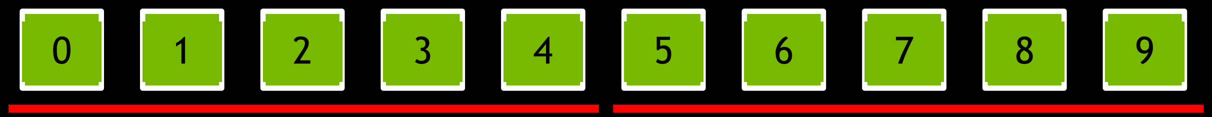


N	10	10
num_streams	2	2
chunk_size	N/num_streams	5
stream_i	0	0
lower	chunk_size*stream_i	0



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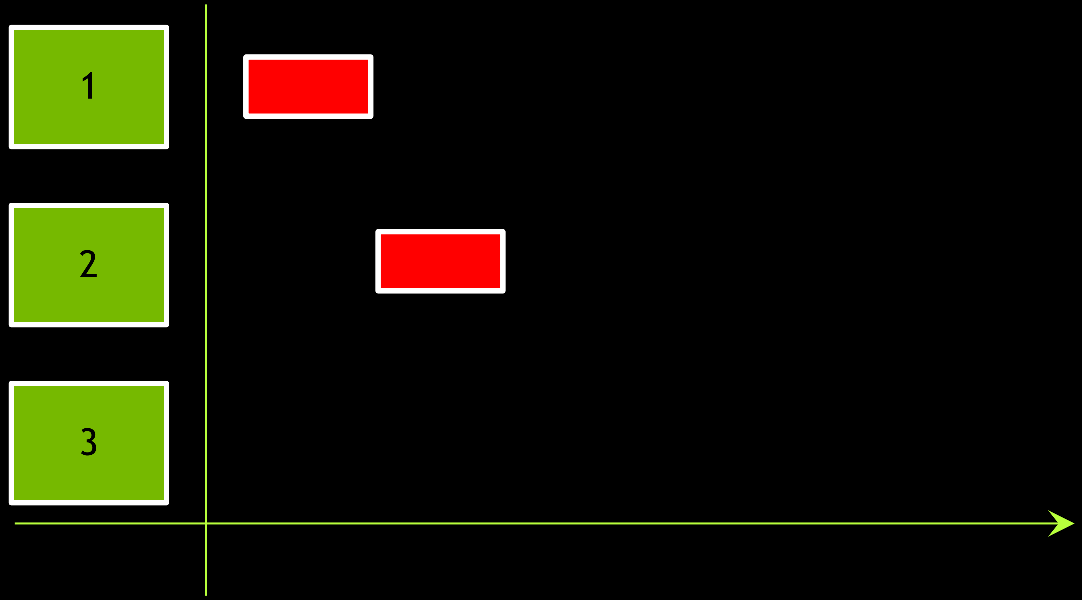
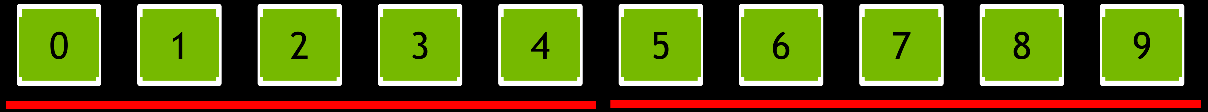
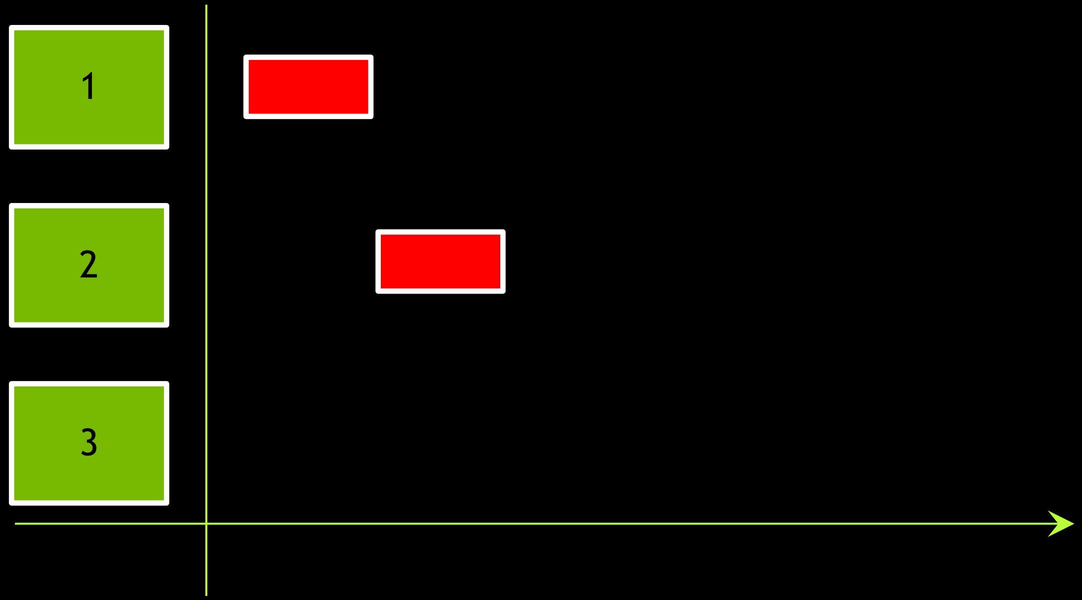


N	10	10
num_streams	2	2
chunk_size	N/num_streams	5
stream_i	1	1
lower	chunk_size*stream_i	5



...non-default stream kernel launches...

```
kernel
<<<G, B, 0,streams[stream_i]>>>(
     data_gpu + lower,
     chunk_size
)
```



N	10	10
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chunk_size	N/num_streams	5
stream_i	0	0
lower	chunk_size*stream_i	0

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kernel
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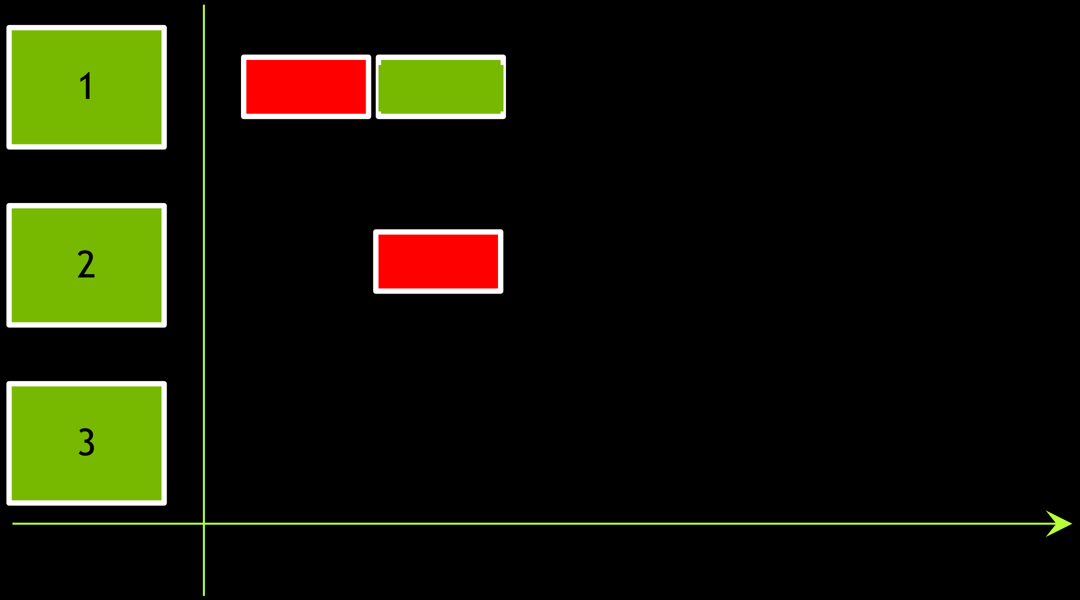

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num_streams	2	2
chunk_size	N/num_streams	5
stream_i	0	0
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<<<G, B, 0,streams[stream_i]>>>(
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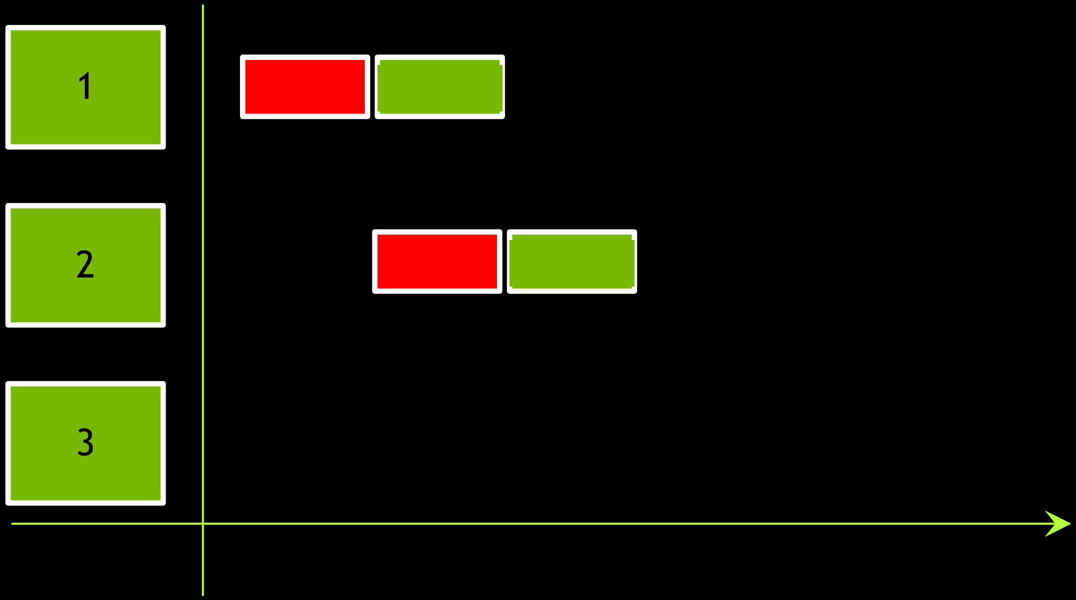

N	10	10
num_streams	2	2
chunk_size	N/num_streams	5
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lower	chunk_size*stream_i	5

…and non-default stream DtoH memory copies

```
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)
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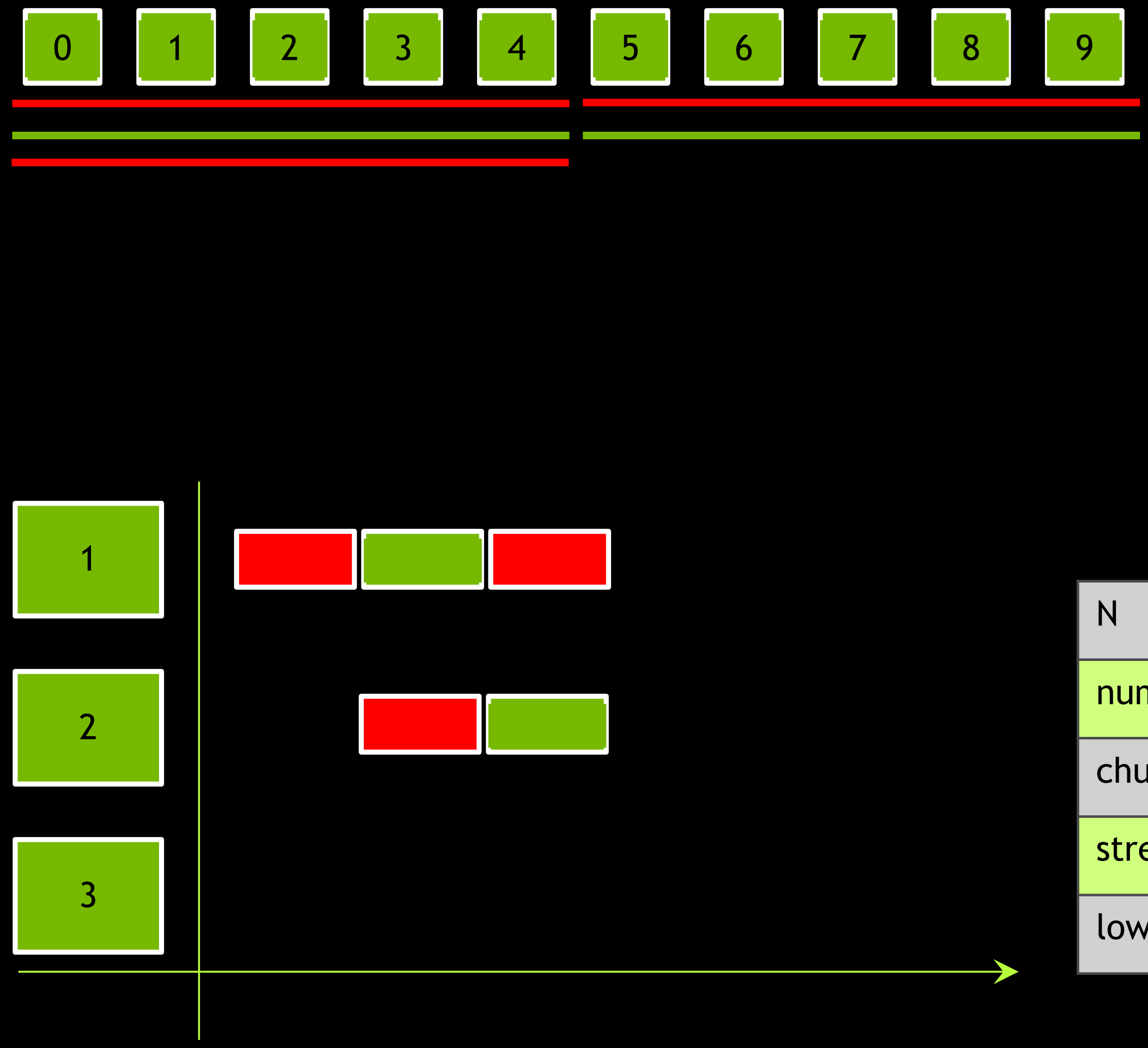
N	10	10
num_streams	2	2
chunk_size	N/num_streams	5
stream_i	0	0
lower	chunk_size*stream_i	0



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chunk_size	N/num_streams	5
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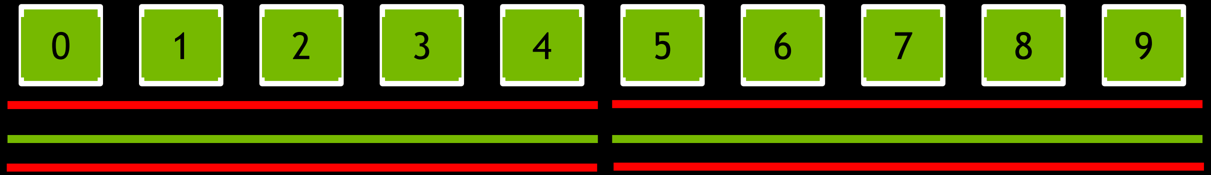

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    data_gpu + lower,
    sizeof(uint64_t)*chunk_size,
    cudaMemcpyHostToDevice,
    streams[stream_i]
)
```
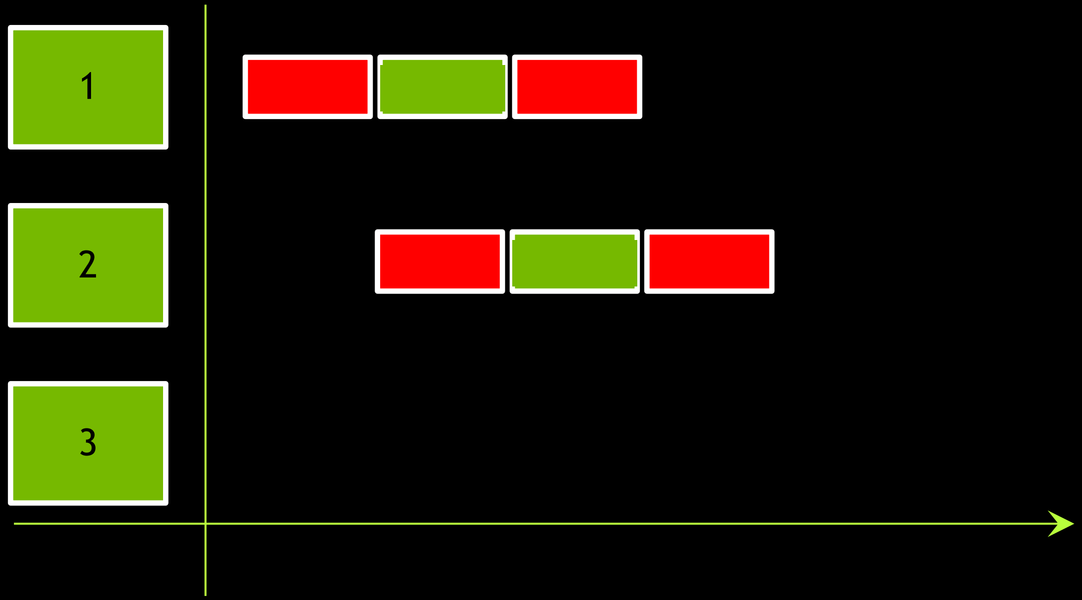



N	10	10
num_streams	2	2
chunk_size	N/num_streams	5
stream_i	1	1
lower	chunk_size*stream_i	5

0	1	2	3	4	5	6	7	8	9

For this example, N was evenly divided by number of streams

N	10	10
num_streams	2	2
chunk_size	N/num_streams	5
stream_i	0	0
lower	chunk_size*stream_i	0

0 1 2 3 4 5 6 7 8 9

But what if this is not the case?

N	10	10
num_streams	3	3
chunk_size	N/num_streams	?
stream_i	0	0
lower	chunk_size*stream_i	?

0	1	2	3	4	5	6	7	8	9

Dividing two ints will result in an int, rounded down if necessary, as in this case

N	10	10
num_streams	3	3
chunk_size	N/num_streams	3
stream_i	0	0
lower	chunk_size*stream_i	0

0 1 2 3 4 5 6 7 8 9

Now as we iterate through the streams to get lower, and then apply chunk size...

N	10	10
num_streams	3	3
chunk_size	N/num_streams	3
stream_i	0	0
lower	chunk_size*stream_i	0

0 1 2 3 4 5 6 7 8 9

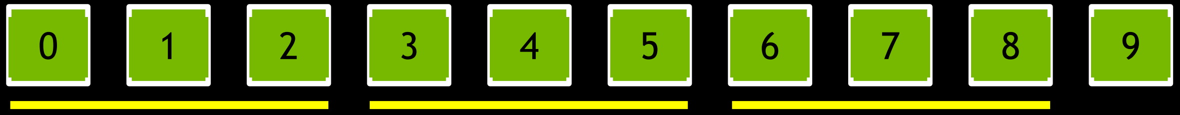
Now as we iterate through the streams to get lower, and then apply chunk size...

N	10	10
num_streams	3	3
chunk_size	N/num_streams	3
stream_i	0	0
lower	chunk_size*stream_i	0

0	1	2	3	4	5	6	7	8	9

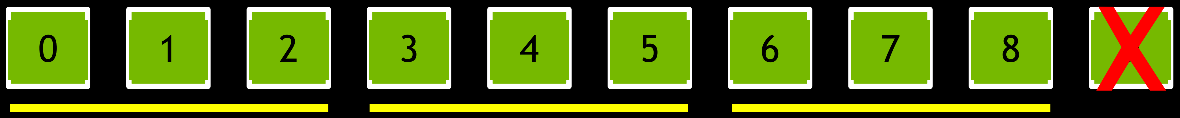
Now as we iterate through the streams to get lower, and then apply chunk size...

N	10	10
num_streams	3	3
chunk_size	N/num_streams	3
stream_i	1	1
lower	chunk_size*stream_i	3



Now as we iterate through the streams to get lower, and then apply chunk size...

N	10	10
num_streams	3	3
chunk_size	N/num_streams	3
stream_i	2	2
lower	chunk_size*stream_i	6



...we fail to access all values in the data

N	10	10
num_streams	3	3
chunk_size	N/num_streams	3
stream_i	-	-
lower	chunk_size*stream_i	-

0	1	2	3	4	5	6	7	8	9

To fix this we use round-up division to calculate chunk size

N	10	10
num_streams	3	3
chunk_size	ceil_div(N/num_streams)	4
stream_i	0	0
lower	chunk_size*stream_i	0

0 1 2 3 4 5 6 7 8 9

Now as we iterate...

N	10	10
num_streams	3	3
chunk_size	ceil_div(N/num_streams)	4
stream_i	0	0
lower	chunk_size*stream_i	0

0	1	2	3	4	5	6	7	8	9

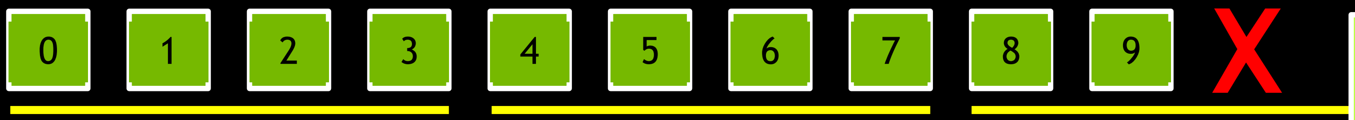
Now as we iterate...

N	10	10
num_streams	3	3
chunk_size	ceil_div(N/num_streams)	4
stream_i	0	0
lower	chunk_size*stream_i	0

0	1	2	3	4	5	6	7	8	9

Now as we iterate…

N	10	10
num_streams	3	3
chunk_size	ceil_div(N/num_streams)	4
stream_i	1	1
lower	chunk_size*stream_i	4



We actually access all data, but we have a new problem: chunk size is too large for our last chunk of data

N	10	10
num_streams	3	3
chunk_size	ceil_div(N/num_streams)	4
stream_i	2	2
lower	chunk_size*stream_i	8

0	1	2	3	4	5	6	7	8	9

If, however, we calculate an **upper** index for each chunk that is bound by N...

```
upper = min(lower+chunk_size, N)
```

N	10	10
num_streams	3	3
chunk_size	ceil_div(N/num_streams)	4
stream_i	0	0
lower	chunk_size*stream_i	0
upper	min(lower + chunk_size, N)	4

0 1 2 3 4 5 6 7 8 9

And then calculate a chunk **width** using **upper** and **lower**…

```
width = upper - lower
```

N	10	10
num_streams	3	3
chunk_size	ceil_div(N/num_streams)	4
stream_i	0	0
lower	chunk_size*stream_i	0
upper	min(lower + chunk_size, N)	4
width	upper - lower	4

...now when we iterate using width instead of chunk size...

N	10	10
num_streams	3	3
chunk_size	ceil_div(N/num_streams)	4
stream_i	0	0
lower	chunk_size*stream_i	0
upper	min(lower + chunk_size, N)	4
width	upper - lower	4

0 1 2 3 4 5 6 7 8 9

...now when we iterate using width instead of chunk size...

N	10	10
num_streams	3	3
chunk_size	ceil_div(N/num_streams)	4
stream_i	0	0
lower	chunk_size*stream_i	0
upper	min(lower + chunk_size, N)	4
width	upper - lower	4

0 1 2 3 4 5 6 7 8 9

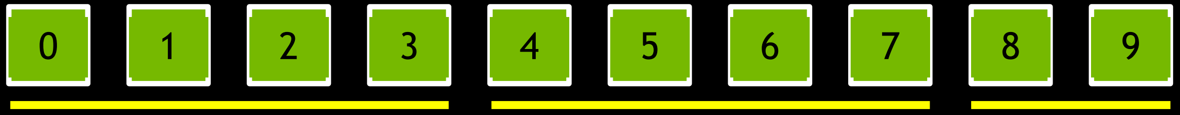
…now when we iterate using width instead of chunk size…

N	10	10
num_streams	3	3
chunk_size	ceil_div(N/num_streams)	4
stream_i	0	1
lower	chunk_size*stream_i	4
upper	min(lower + chunk_size, N)	8
width	upper - lower	4

0 1 2 3 4 5 6 7 8 9

...now when we iterate using width instead of chunk size...

N	10	10
num_streams	3	3
chunk_size	ceil_div(N/num_streams)	4
stream_i	0	2
lower	chunk_size*stream_i	8
upper	min(lower + chunk_size, N)	10
width	upper - lower	2



…we fit the data perfectly, no matter its size or the number of streams

N	10	10
num_streams	3	3
chunk_size	ceil_div(N/num_streams)	4
stream_i	0	2
lower	chunk_size*stream_i	8
upper	min(lower + chunk_size, N)	10
width	upper - lower	2

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