King Abdullah University of Science and Technology

KAUST

CS 380 - GPU and GPGPU Programming
Lecture 21: GPU Parallel Reduction

Markus Hadwiger, KAUST

Reading Assignment #8 (until Oct 28)

Read (required):

- Programming Massively Parallel Processors book, 4th edition
  Chapter 10: Reduction
- Optimizing Parallel Reduction in CUDA, Mark Harris,

https://developer.download.nvidia.com/assets/cuda/files/reduction.pdf

Read (optional):

- Faster Parallel Reductions on Kepler, Justin Luitjens

https://devblogs.nvidia.com/parallelforall/faster-parallel-reductions-kepler/

- CUDA Parallel Reduction implementation in CUDA SDK:

https://github.com/NVIDIA/cuda-samples/tree/master/Samples/2_Concepts_and_Techniques/reduction/

Next Lectures

Lecture 22: Mon, Oct 28

Lecture 23: Tue, Oct 29 (make-up lecture; 14:30 – 15:45)

Lecture 24: Thu, Oct 31

Lecture 25: Mon, Nov 4

Lecture 26: Tue, Nov 5 (make-up lecture; 14:30 – 15:45)

No lecture on Thu, Nov 7 !

GPU Reduction

- Parallel reduction is a basic parallel programming primitive; see reduction operation on a stream, e.g., in Brook for GPUs

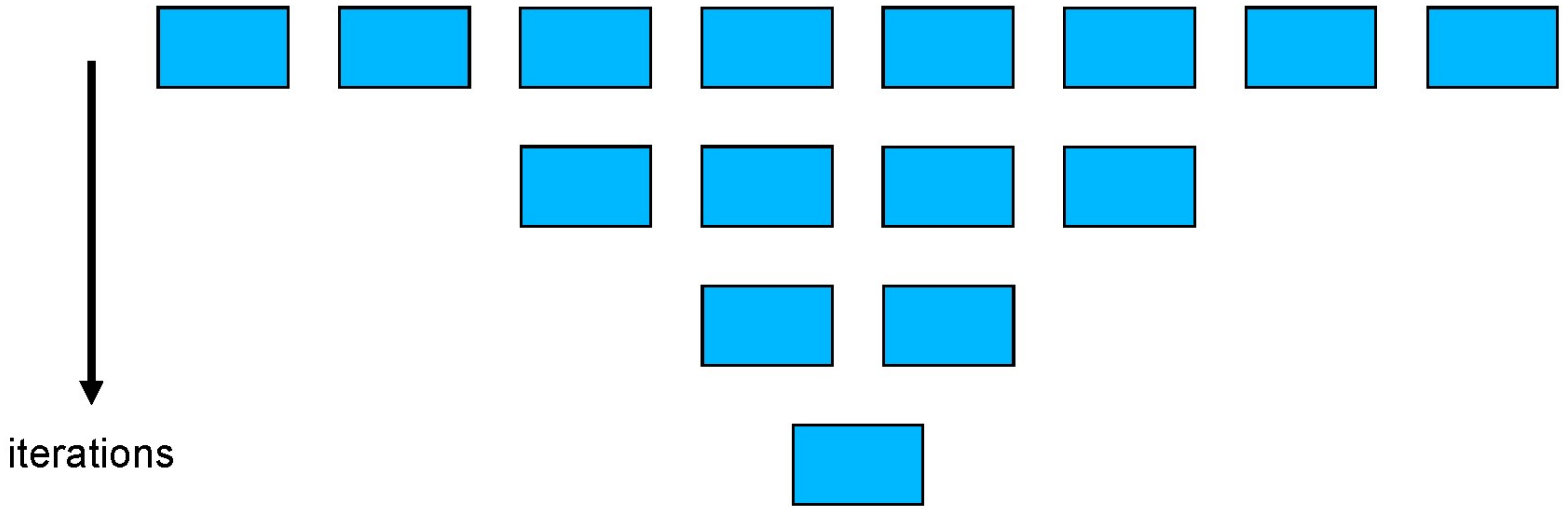
Example: Parallel Reduction

- **Given an array of values, "reduce" them to a single value in parallel**
- **Examples**
  - sum reduction: sum of all values in the array
  - Max reduction: maximum of all values in the array

- **Typical parallel implementation:**
  - Recursively halve # threads, add two values per thread
  - Takes log(n) steps for n elements, requires n/2 threads

Typical Parallel Programming Pattern

- **log(n) steps**



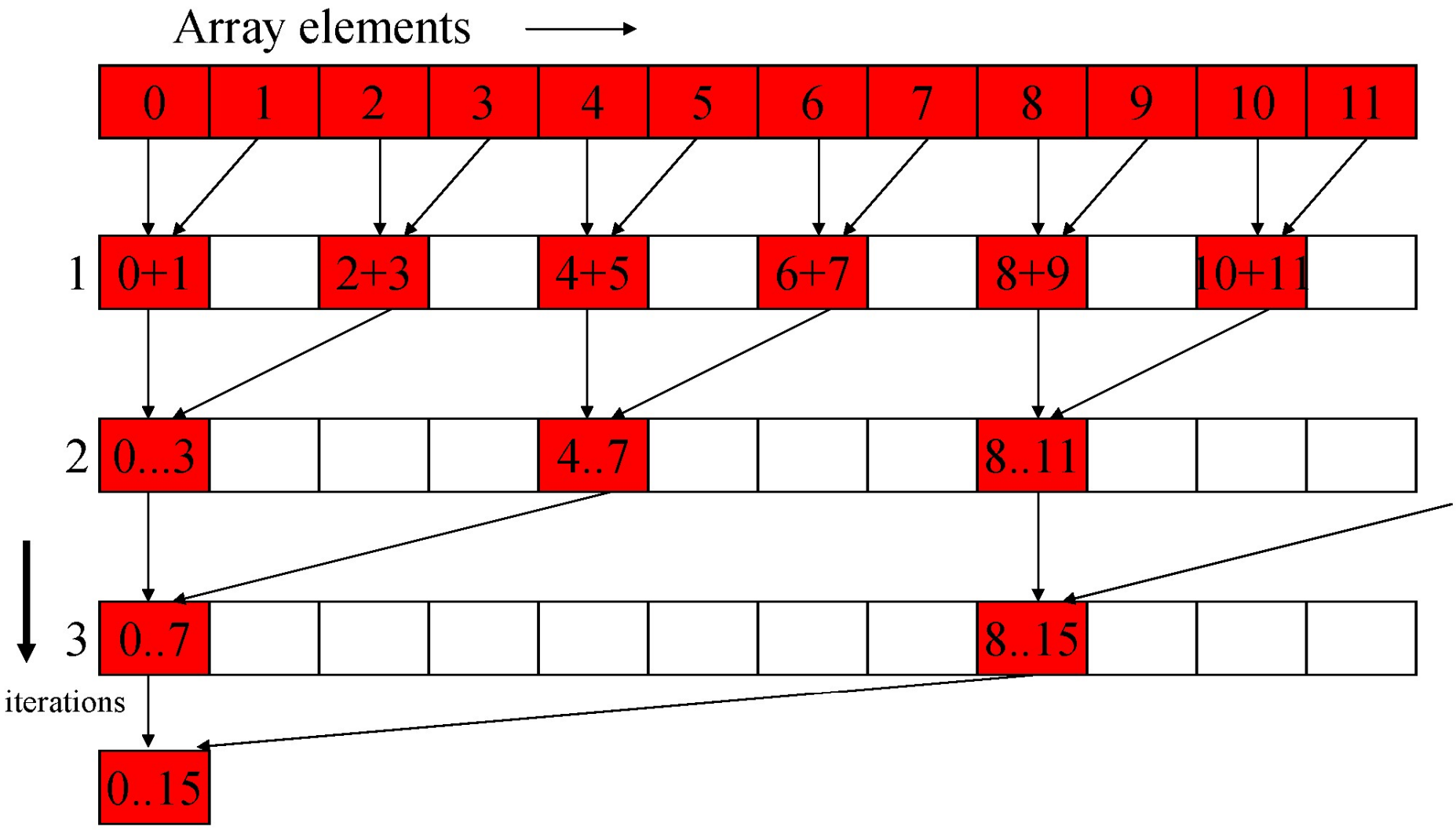
Helpful fact for counting nodes of full binary trees:
If there are N leaf nodes, there will be N-1 non-leaf nodes

Reduction – Version1

A Vector Reduction Example

- **Assume an in-place reduction using shared memory**
  - The original vector is in device global memory
  - The shared memory used to hold a partial sum vector
  - Each iteration brings the partial sum vector closer to the final sum
  - The final solution will be in element 0

Vector Reduction



A Simple Implementation

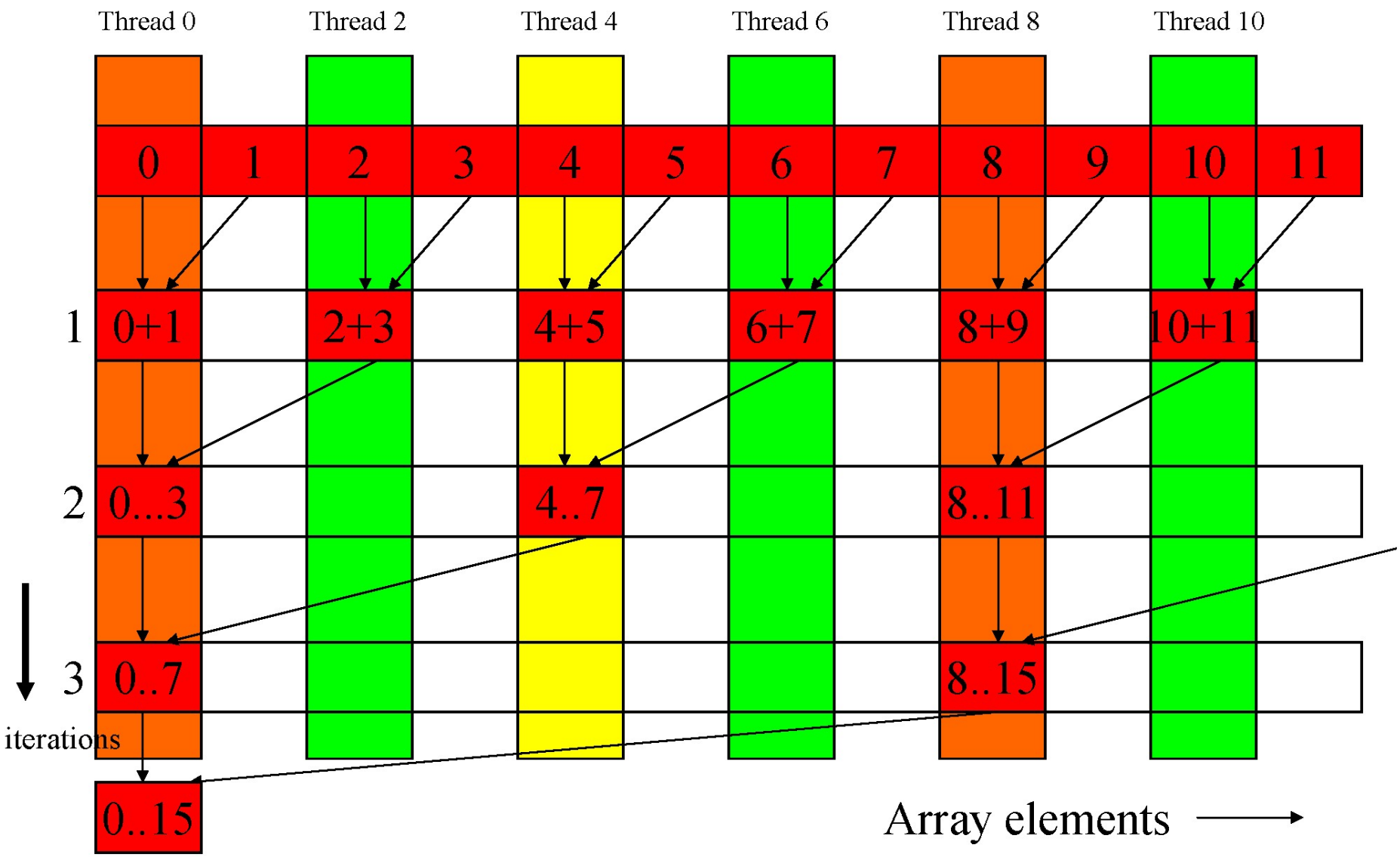
- **Assume we have already loaded array into**

```
__shared__ float partialSum[];

unsigned int t = threadIdx.x;

// loop log(n) times
for (unsigned int stride = 1;
     stride < blockDim.x;  stride *= 2)
{
  // make sure the sum of the previous iteration
  // is available
  __syncthreads();

  if (t % (2*stride) == 0)
     partialSum[t] += partialSum[t+stride];
}
```

Reduction #1: Interleaved Addressing


```
__global__ void reduce0(int *g_idata, int *g_odata) {
    extern __shared__ int sdata[];

    // each thread loads one element from global to shared mem
    unsigned int tid = threadIdx.x;
    unsigned int i = blockIdx.x*blockDim.x + threadIdx.x;
    sdata[tid] = g_idata[i];
    __syncthreads();

    // do reduction in shared mem
    for(unsigned int s=1; s < blockDim.x; s *= 2) {
        if (tid % (2*s) == 0) {
            sdata[tid] += sdata[tid + s];
        }
        __syncthreads();
    }

    // write result for this block to global mem
    if (tid == 0) g_odata[blockIdx.x] = sdata[0];
}
```

Vector Reduction with Branch Divergence



Some Observations

- **In each iterations, two control flow paths will be sequentially traversed for each warp**
  - Threads that perform addition and threads that do not
  - Threads that do not perform addition may cost extra cycles depending on the implementation of divergence

- **No more than half of threads will be executing at any time**
  - All odd index threads are disabled right from the beginning!
  - On average, less than ¼ of the threads will be activated for all warps over time.
  - After the 5^{th} iteration, entire warps in each block will be disabled, poor resource utilization but no divergence.
    - This can go on for a while, up to 4 more iterations (512/32=16= 2^4), where each iteration only has one thread activated until all warps retire

Short comings of the implementation

- **Assume we have already loaded array into**

```
__shared__ float partialSum[];

unsigned int t = threadIdx.x;
for (unsigned int stride = 1;
     stride < blockDim.x;  stride *= 2)
{
  __syncthreads();

  if (t % (2*stride) == 0)
    partialSum[t] += partialSum[t+stride];
}
```

BAD: Divergence due to interleaved branch decisions

BAD: Bank conflicts due to stride

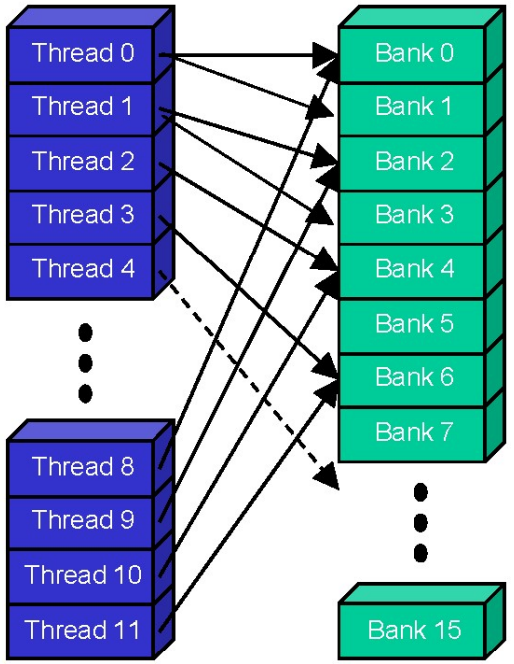
Reduction – Version2

Common Array Bank Conflict Patterns 1D

- **Each thread loads 2 elements into shared mem:**
  - 2-way-interleaved loads result in 2-way bank conflicts:

```
int tid = threadIdx.x;
shared[2*tid] = global[2*tid];
shared[2*tid+1] = global[2*tid+1];
```

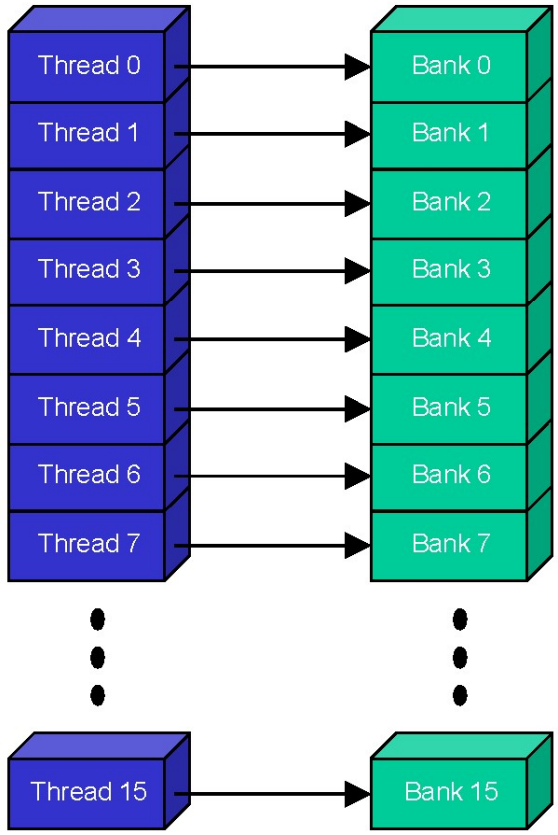
- **This makes sense for traditional CPU threads, locality in cache line usage and reduced sharing traffic.**
  - Not in shared memory usage where there is no cache line effects but banking effects



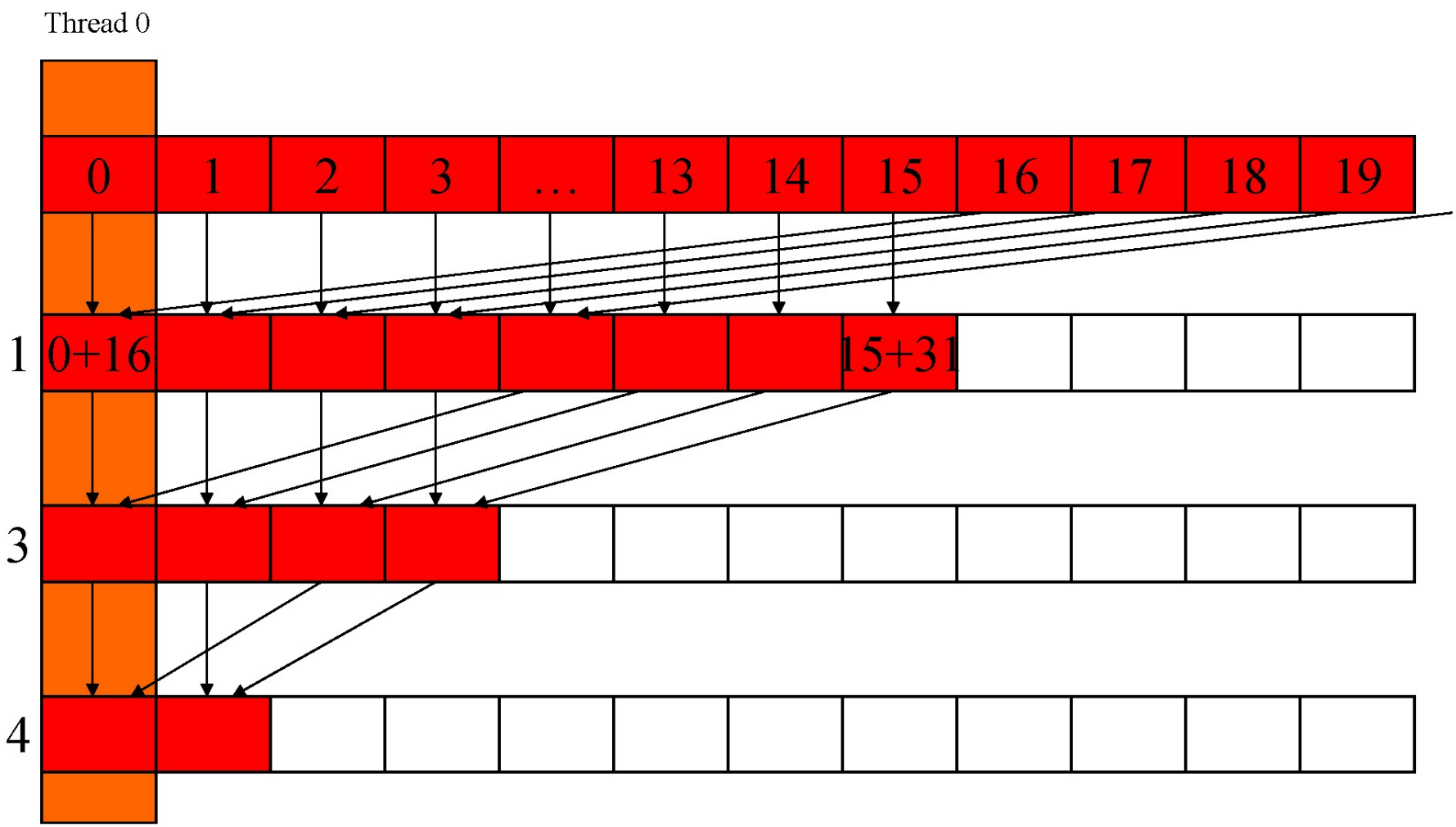
A Better Array Access Pattern

- **Each thread loads one element in every consecutive group of `blockDim` elements.**

```
shared[tid] = global[tid];
shared[tid + blockDim.x] =
  global[tid + blockDim.x];
```



A better implementation



A better implementation

- **Assume we have already loaded array into**

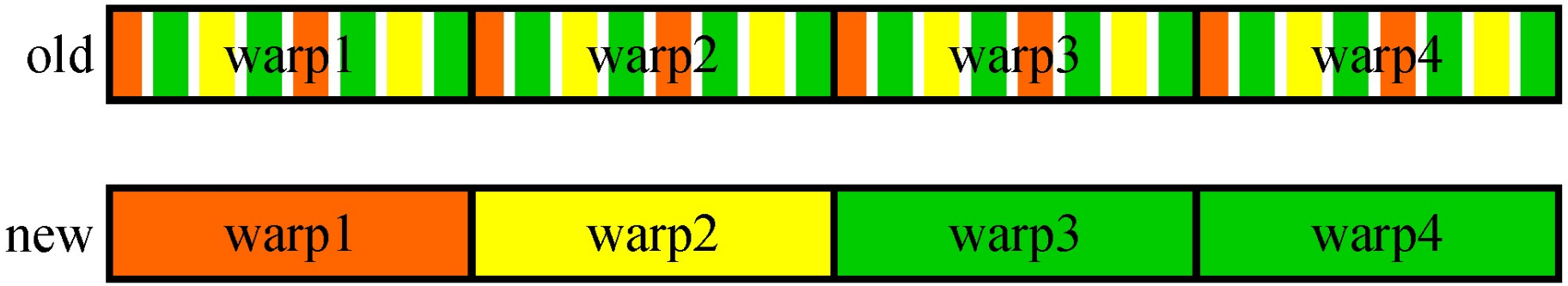
```
__shared__ float partialSum[];

unsigned int t = threadIdx.x;
for (unsigned int stride = blockDim.x;
     stride > 1;  stride >>=1)
{
  __syncthreads();
  if (t < stride)
     partialSum[t] += partialSum[t+stride];
}
```

if you want to fully retire warps, this should actually be:

```
if ( t < stride ) {
   partialSum[ t ] += partialSum[ t + stride ];
} else {
   break;
}
```

A better implementation

- **Only the last 5 iterations will have divergence**
- **Entire warps will be shut down as iterations progress**
  - For a 512-thread block, 4 iterations to shut down all but one warp in each block
  - Better resource utilization, will likely retire warps and thus blocks faster
- **Recall, no bank conflicts either**



Implicit Synchronization in a Warp

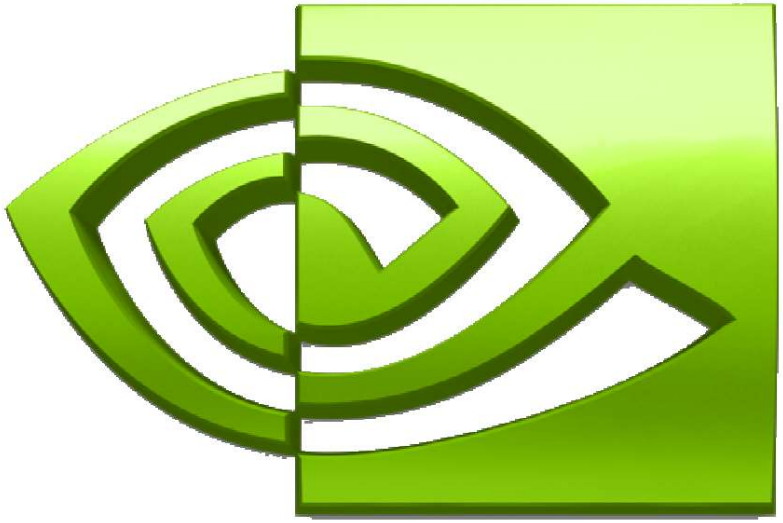
- **For last 6 loops only one warp active (i.e. tid's 0..31)**
  - Shared reads & writes SIMD synchronous within a warp
  - So skip `__syncthreads()` and unroll last 5 iterations

```
unsigned int tid = threadIdx.x
for (unsigned int d = n>>1; d
    __syncthreads();
    if (tid < d)
        shared[tid] += shared[
}
__syncthreads();
if (tid <= 32) {   // unroll last
    shared[tid] += shared[tid
    shared[tid] += shared[tid
    shared[tid] += shared[tid
    shared[tid] += shared[tid +
    shared[tid] += shared[tid + 2];
    shared[tid] += shared[tid + 1];
}
```

This would not work properly is warp size decreases; need __synchthreads() between each statement!
However, having ___synchthreads() in if statement is problematic.

now: `__syncwarp()`
or better: Cooperative Groups

Look at CUDA SDK reduction example and slides!



NVIDIA®

Optimizing Parallel Reduction in CUDA

Mark Harris
NVIDIA Developer Technology

Parallel Reduction

- Common and important data parallel primitive
- Easy to implement in CUDA
  - Harder to get it right
- Serves as a great optimization example
  - We'll walk step by step through 7 different versions
  - Demonstrates several important optimization strategies

```
template <unsigned int blockSize>
__global__ void reduce6(int *g_idata, int *g_odata, unsigned int n)
{
    extern __shared__ int sdata[];

    unsigned int tid = threadIdx.x;
    unsigned int i = blockIdx.x*(blockSize*2) + tid;
    unsigned int gridSize = blockSize*2*gridDim.x;
    sdata[tid] = 0;

    while (i < n) { sdata[tid] += g_idata[i] + g_idata[i+blockSize];  i += gridSize;  }
    __syncthreads();

    if (blockSize >= 512) { if (tid < 256) { sdata[tid] += sdata[tid + 256]; } __syncthreads(); }
    if (blockSize >= 256) { if (tid < 128) { sdata[tid] += sdata[tid + 128]; } __syncthreads(); }
    if (blockSize >= 128) { if (tid <  64) { sdata[tid] += sdata[tid +  64]; } __syncthreads(); }

    if (tid < 32) {
        if (blockSize >=  64) sdata[tid] += sdata[tid + 32];
        if (blockSize >=  32) sdata[tid] += sdata[tid + 16];
        if (blockSize >=  16) sdata[tid] += sdata[tid +  8];
        if (blockSize >=   8) sdata[tid] += sdata[tid +  4];
        if (blockSize >=   4) sdata[tid] += sdata[tid +  2];
        if (blockSize >=   2) sdata[tid] += sdata[tid +  1];
    }

    if (tid == 0) g_odata[blockIdx.x] = sdata[0];
}
```

Final Optimized Kernel

out-of-bounds check missing, see SDK code

be careful that shared variables are declared *volatile*! see SDK code

now also need __syncwarp() !!
see later slides

```
template <unsigned int blockSize>
__device__ void warpReduce(volatile int *sdata, unsigned int tid) {
    if (blockSize >=  64) sdata[tid] += sdata[tid + 32];
    if (blockSize >=  32) sdata[tid] += sdata[tid + 16];
    if (blockSize >=  16) sdata[tid] += sdata[tid +  8];
    if (blockSize >=   8) sdata[tid] += sdata[tid +  4];
    if (blockSize >=   4) sdata[tid] += sdata[tid +  2];
    if (blockSize >=   2) sdata[tid] += sdata[tid +  1];
}
template <unsigned int blockSize>
__global__ void reduce6(int *g_idata, int *g_odata, unsigned int n) {
    extern __shared__ int sdata[];
    unsigned int tid = threadIdx.x;
    unsigned int i = blockIdx.x*(blockSize*2) + tid;
    unsigned int gridSize = blockSize*2*gridDim.x;
    sdata[tid] = 0;

    while (i < n) { sdata[tid] += g_idata[i] + g_idata[i+blockSize];  i += gridSize;  }
    __syncthreads();

    if (blockSize >= 512) { if (tid < 256) { sdata[tid] += sdata[tid + 256]; } __syncthreads(); }
    if (blockSize >= 256) { if (tid < 128) { sdata[tid] += sdata[tid + 128]; } __syncthreads(); }
    if (blockSize >= 128) { if (tid <   64) { sdata[tid] += sdata[tid +   64]; } __syncthreads(); }

    if (tid < 32) warpReduce(sdata, tid);
    if (tid == 0) g_odata[blockIdx.x] = sdata[0];
}
```

now also need __syncwarp() !!
see later slides

Final Optimized Kernel

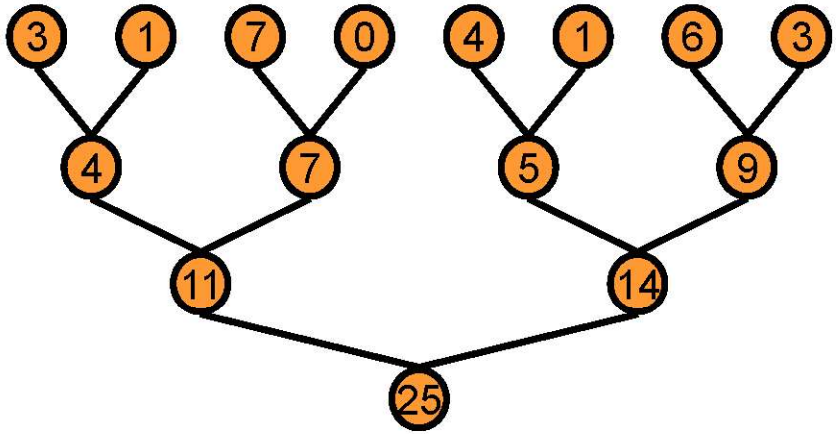
Invoking Template Kernels

- Don't we still need block size at compile time?
  - Nope, just a switch statement for 10 possible block sizes:

```
switch (threads)
    {
    case 512:
      reduce5<512><<< dimGrid, dimBlock, smemSize >>>(d_idata, d_odata); break;
    case 256:
      reduce5<256><<< dimGrid, dimBlock, smemSize >>>(d_idata, d_odata); break;
    case 128:
      reduce5<128><<< dimGrid, dimBlock, smemSize >>>(d_idata, d_odata); break;
    case 64:
      reduce5<  64><<< dimGrid, dimBlock, smemSize >>>(d_idata, d_odata); break;
    case 32:
      reduce5<  32><<< dimGrid, dimBlock, smemSize >>>(d_idata, d_odata); break;
    case 16:
      reduce5<  16><<< dimGrid, dimBlock, smemSize >>>(d_idata, d_odata); break;
    case  8:
      reduce5<   8><<< dimGrid, dimBlock, smemSize >>>(d_idata, d_odata); break;
    case  4:
      reduce5<   4><<< dimGrid, dimBlock, smemSize >>>(d_idata, d_odata); break;
    case  2:
      reduce5<   2><<< dimGrid, dimBlock, smemSize >>>(d_idata, d_odata); break;
    case  1:
      reduce5<   1><<< dimGrid, dimBlock, smemSize >>>(d_idata, d_odata); break;
    }
```

Parallel Reduction

- Tree-based approach used within each thread block



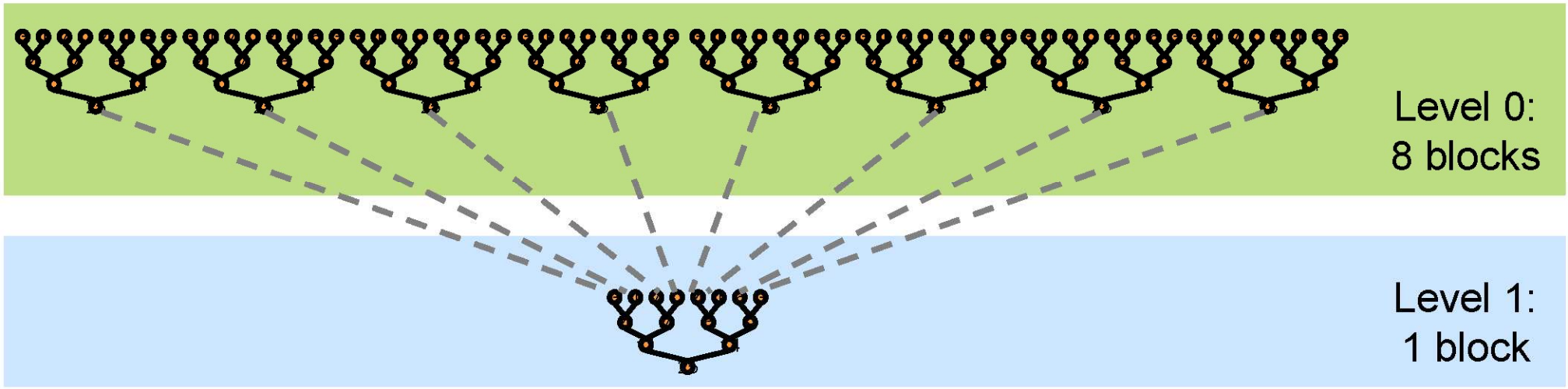
- Need to be able to use multiple thread blocks
  - To process very large arrays
  - To keep all multiprocessors on the GPU busy
  - Each thread block reduces a portion of the array
- But how do we communicate partial results between thread blocks?

Problem: Global Synchronization

- If we could synchronize across all thread blocks, could easily reduce very large arrays, right?
  - Global sync after each block produces its result
  - Once all blocks reach sync, continue recursively
- But CUDA has no global synchronization. Why?
  - Expensive to build in hardware for GPUs with high processor count
  - Would force programmer to run fewer blocks (no more than # multiprocessors * # resident blocks / multiprocessor) to avoid deadlock, which may reduce overall efficiency
- Solution: decompose into multiple kernels
  - Kernel launch serves as a global synchronization point
  - Kernel launch has negligible HW overhead, low SW overhead

Solution: Kernel Decomposition

- Avoid global sync by decomposing computation into multiple kernel invocations



- In the case of reductions, code for all levels is the same
  - Recursive kernel invocation

Performance for 4M element reduction

	Time (2^{22} ints)	Bandwidth	Step Speedup	Cumulative Speedup
Kernel 1: interleaved addressing with divergent branching	8.054 ms	2.083 GB/s		
Kernel 2: interleaved addressing with bank conflicts	3.456 ms	4.854 GB/s	2.33x	2.33x
Kernel 3: sequential addressing	1.722 ms	9.741 GB/s	2.01x	4.68x
Kernel 4: first add during global load	0.965 ms	17.377 GB/s	1.78x	8.34x
Kernel 5: unroll last warp	0.536 ms	31.289 GB/s	1.8x	15.01x
Kernel 6: completely unrolled	0.381 ms	43.996 GB/s	1.41x	21.16x
Kernel 7: multiple elements per thread	0.268 ms	62.671 GB/s	1.42x	30.04x

Kernel 7 on 32M elements: 73 GB/s!

And More...

1. On Volta and newer (Ampere, ...),
   reduction in shared memory must use
   warp synchronization! `__syncwarp()` or Cooperative Groups

2. Last optimization step for parallel reduction:

Do not use shared memory for last 5 steps, but use

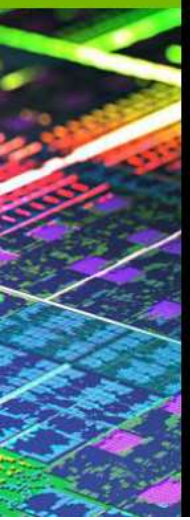
warp shuffle instructions

EXAMPLE: REDUCTION VIA SHARED MEMORY

__syncwarp

Re-converge threads and perform memory fence

```
v += shmem[tid+16]; __syncwarp();
shmem[tid] = v;     __syncwarp();
v += shmem[tid+8];  __syncwarp();
shmem[tid] = v;     __syncwarp();
v += shmem[tid+4];  __syncwarp();
shmem[tid] = v;     __syncwarp();
v += shmem[tid+2];  __syncwarp();
shmem[tid] = v;     __syncwarp();
v += shmem[tid+1];  __syncwarp();
shmem[tid] = v;
```

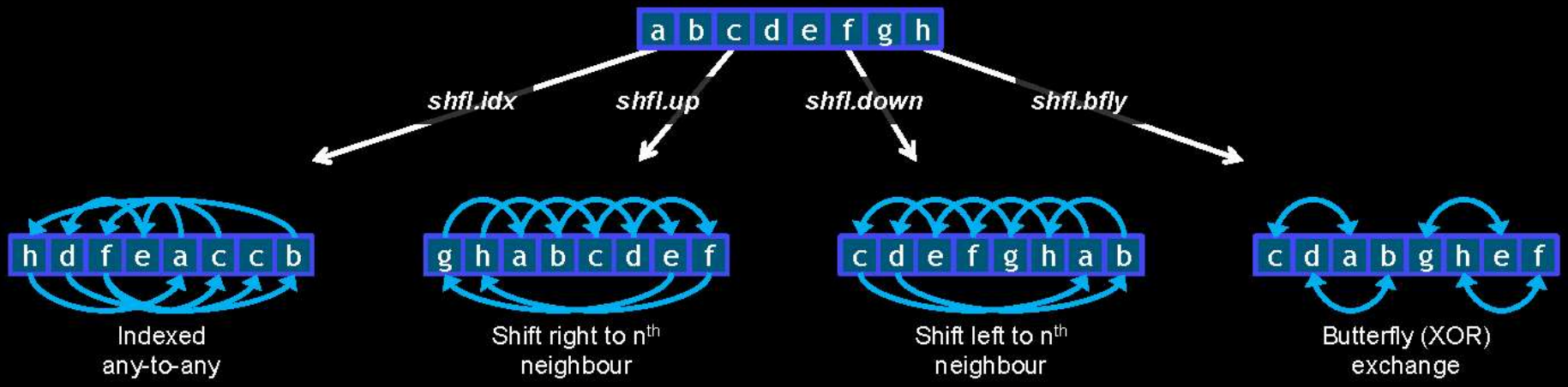


Shuffle (SHFL)

- Instruction to exchange data in a warp
- Threads can “read” other threads’ registers
- No shared memory is needed
- It is available starting from SM 3.0

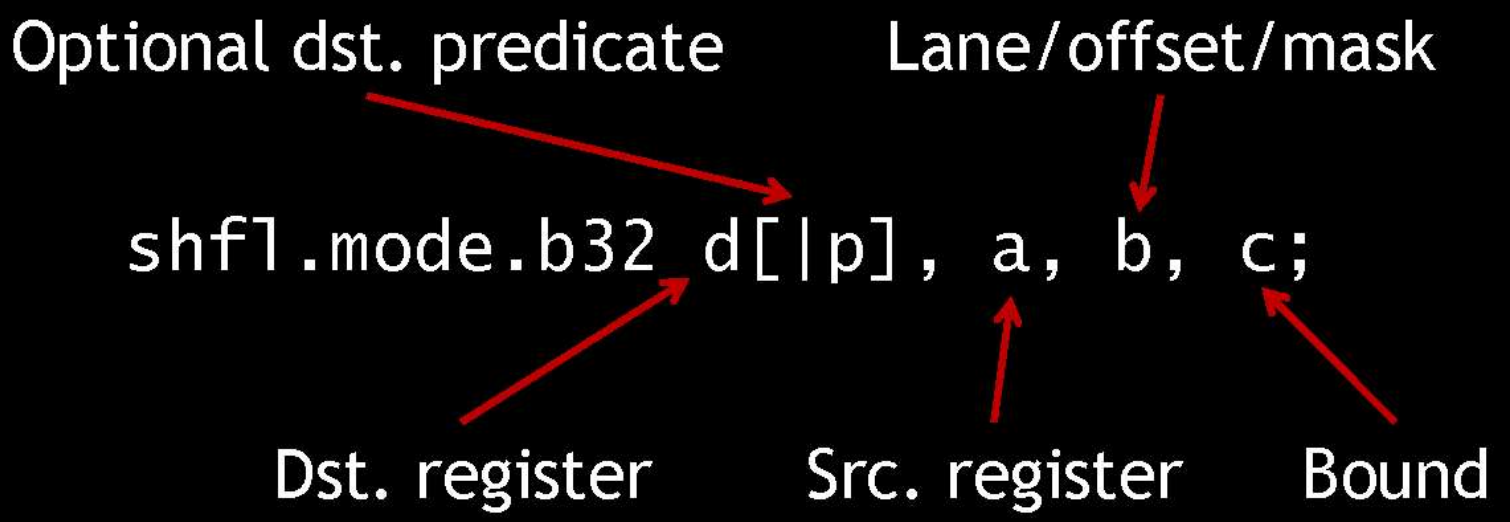
Variants

- 4 variants (idx, up, down, bfly):



Now: Use _sync variants / shuffle in cooperative thread groups!

Instruction (PTX)



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Reduce

- Code

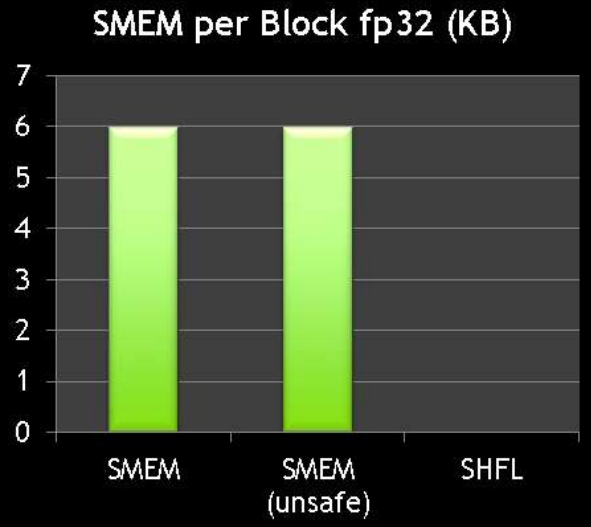
```
// Threads want to reduce the value in x.

float x = …;

#pragma unroll
for(int mask = WARP_SIZE / 2 ; mask > 0 ; mask >>= 1)
    x += __shfl_xor(x, mask);

// The x variable of laneid 0 contains the reduction.
```

- Performance
  - Launch 26 blocks of 1024 threads
  - Run the reduction 4096 times



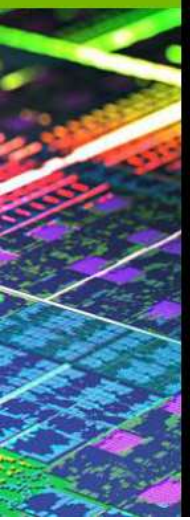
Shuffle: Tips and Tricks

Julien Demouth, NVIDIA

Glossary

Safer with cooperative thread groups!

- Warp
  - ~~Implicitly synchronized~~ group of threads (32 on current HW)
- Warp ID (`warpid`)
  - Identifier of the warp in a block: `threadIdx.x / 32`
- Lane ID (`laneid`)
  - Coordinate of the thread in a warp: `threadIdx.x % 32`
  - Special register (available from PTX): `%laneid`



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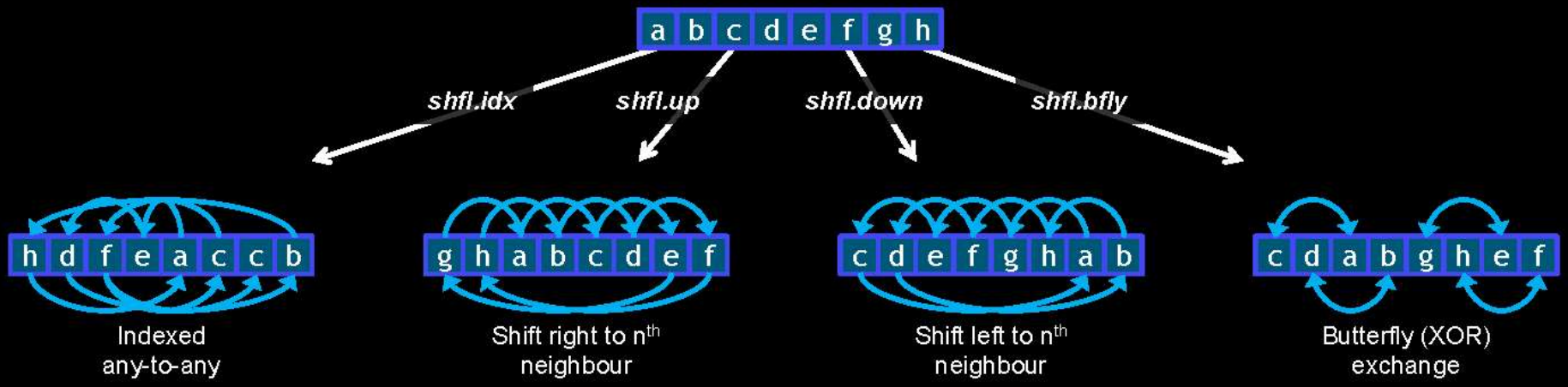

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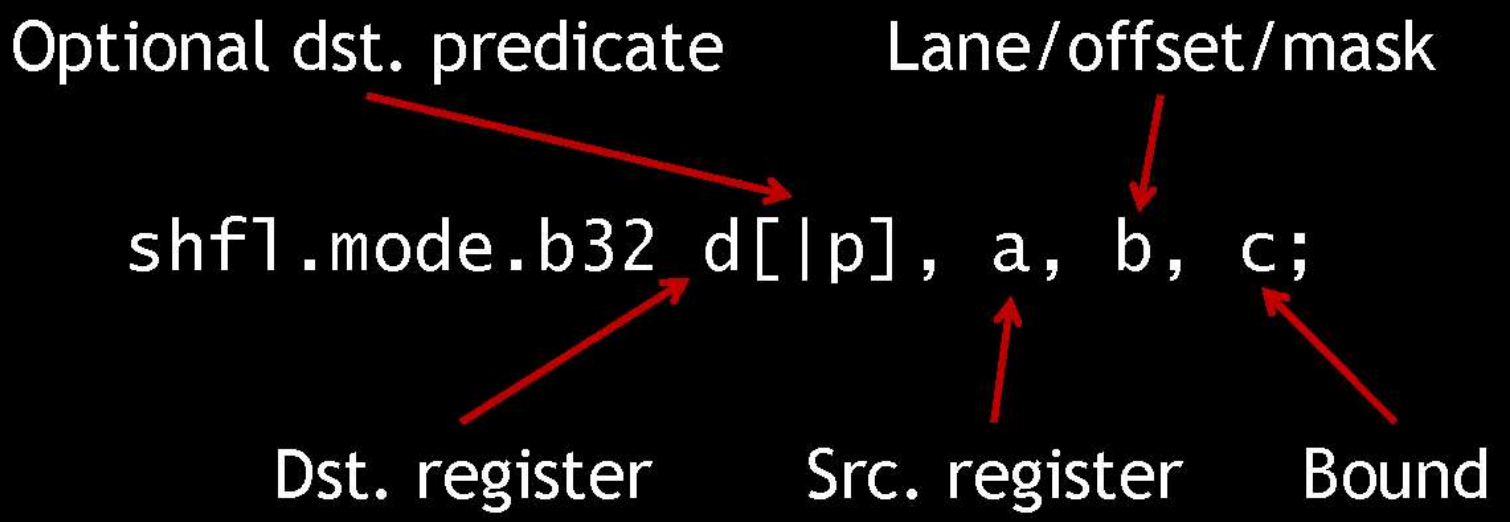

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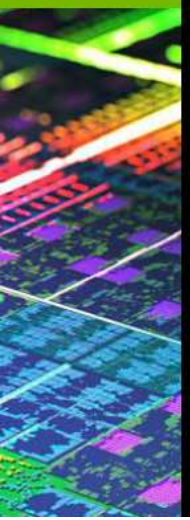


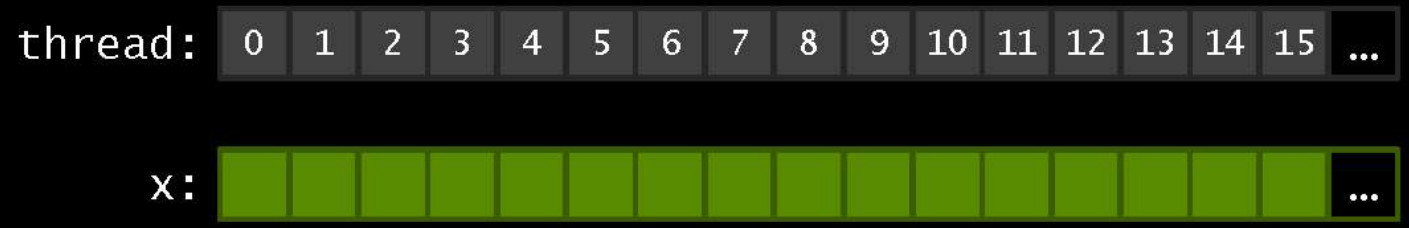
Implement SHFL for 64b Numbers

```
__device__ __inline__ double shfl(double x, int lane)
{
    // Split the double number into 2 32b registers.
    int lo, hi;
    asm volatile( "mov.b32 {%0,%1}, %2;" : "=r"(lo), "=r"(hi) : "d"(x));

    // Shuffle the two 32b registers.
    lo = __shfl(lo, lane);
    hi = __shfl(hi, lane);

    // Recreate the 64b number.
    asm volatile( "mov.b64 %0, {%1,%2};" : "=d(x)" : "r"(lo), "r"(hi));

    return x;
}
```

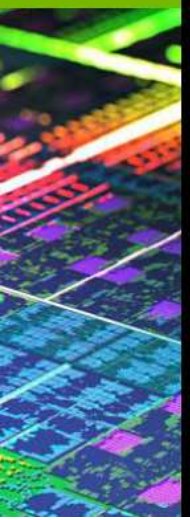
- Generic SHFL: https://github.com/BryanCatanzaro/generics

Performance Experiment

- One element per thread



- Each thread takes its right neighbor



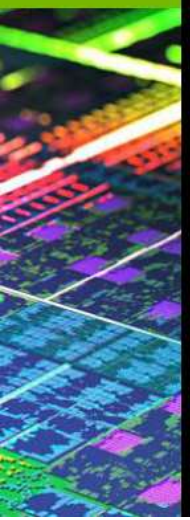
Performance Experiment

- We run the following test on a K20

```
T x = input[tidx];
for(int i = 0 ; i < 4096 ; ++i)
    x = get_right_neighbor(x);
output[tidx] = x;
```

- We launch 26 blocks of 1024 threads
  - On K20, we have 13 SMs
  - We need 2048 threads per SM to have 100% of occupancy

- We time different variants of that kernel



Performance Experiment

- Shared memory (SMEM)

```
smem[threadIdx.x] = smem[32*warpid + ((laneid+1) % 32)];

__syncthreads();
```

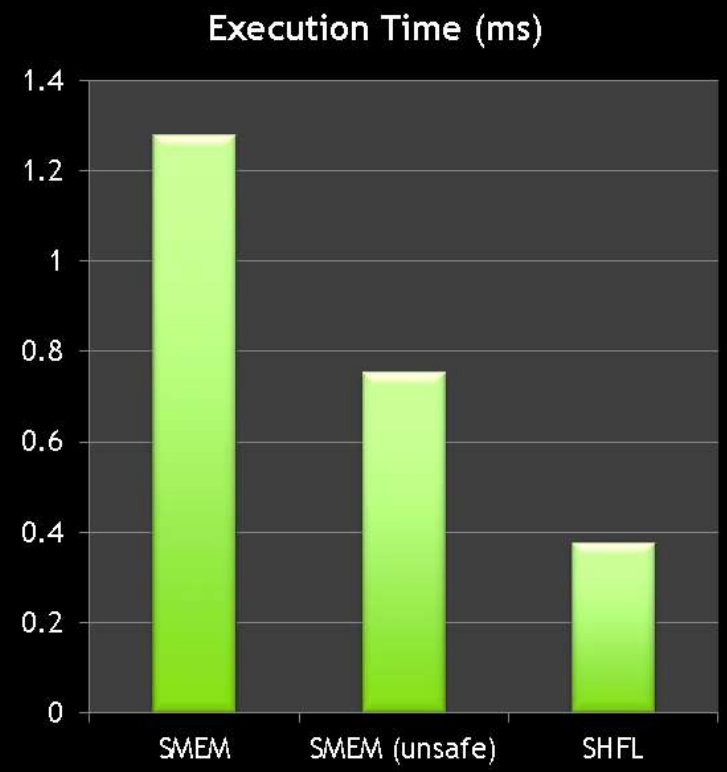
- Shuffle (SHFL)

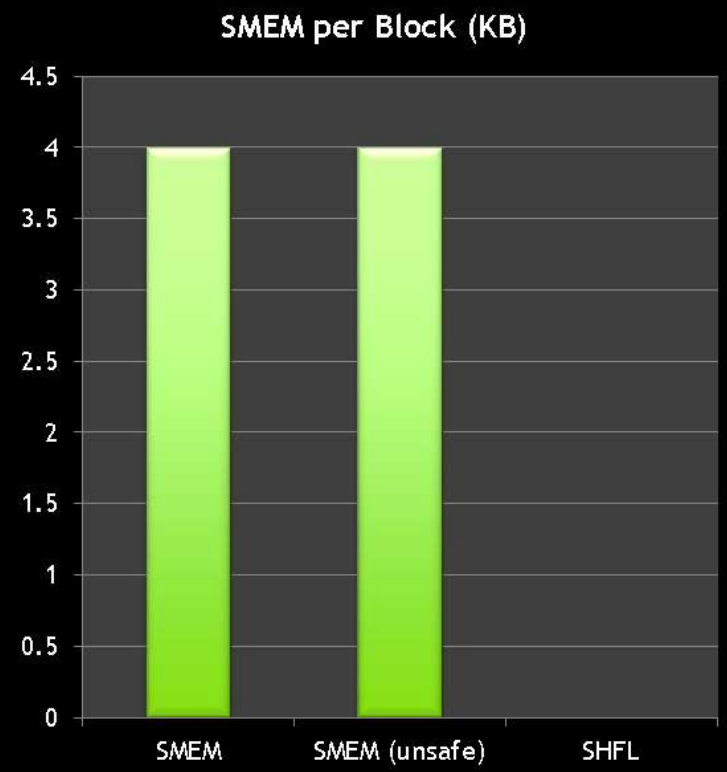
```
x = __shfl(x, (laneid+1) % 32);
```

- Shared memory without __syncthreads + volatile (*unsafe*)

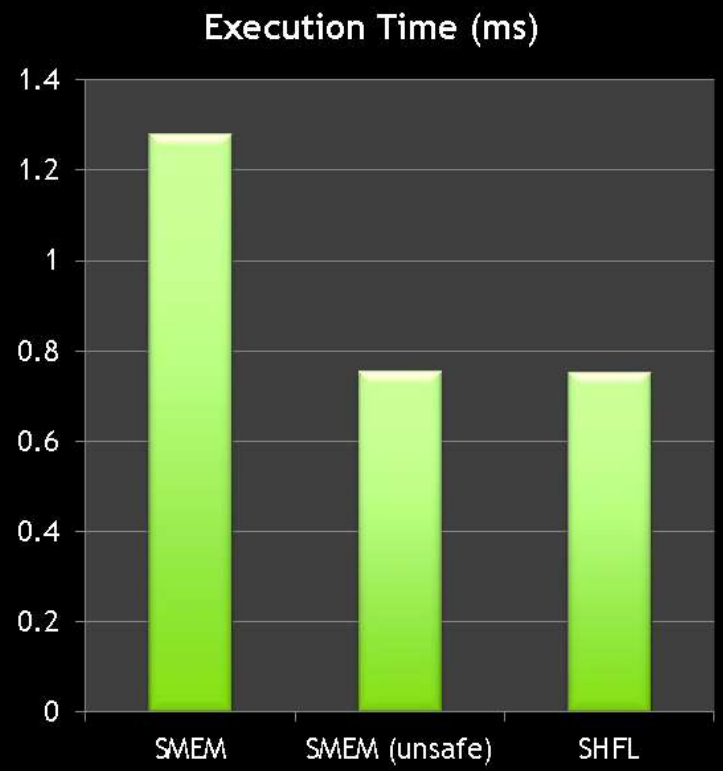
```
__shared__ volatile T *smem = ...;

smem[threadIdx.x] = smem[32*warpid + ((laneid+1) % 32)];
```

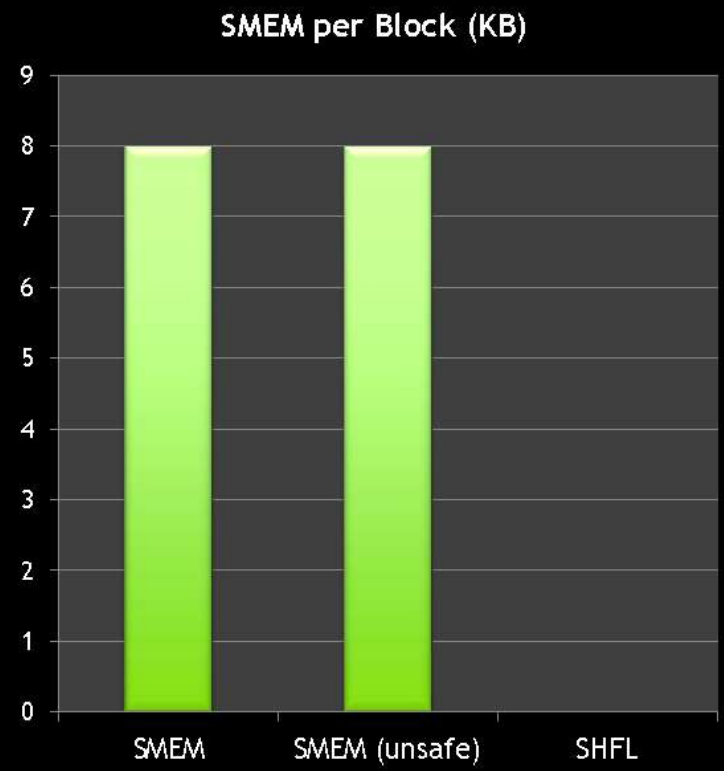
Performance Experiment (fp32)

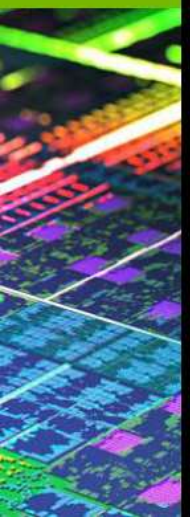




Performance Experiment (fp64)

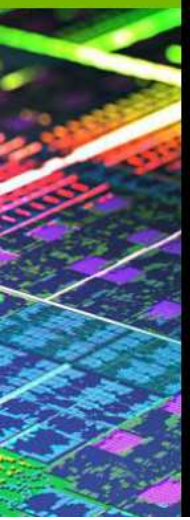






Performance Experiment

- Always faster than shared memory
- Much safer than using no __syncthreads (and volatile)
  - And never slower
- Does not require shared memory
  - Useful when occupancy is limited by SMEM usage



Broadcast

Now: Use cooperative thread groups!

- All threads read from a single lane

```
x = __shfl(x, 0); // All the threads read x from laneid 0.
```

- More complex example

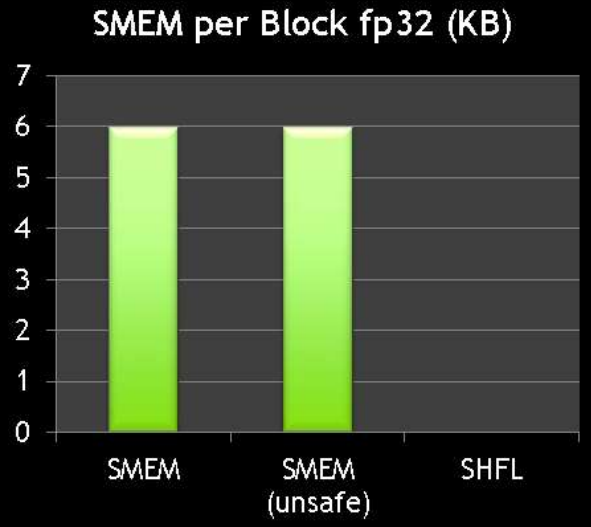
```
// All threads evaluate a predicate.
int predicate = ...;

// All threads vote.
unsigned vote = __ballot(predicate);

// All threads get x from the "last" lane which evaluated the predicate to true.
if(vote)
    x = __shfl(x, __bfind(vote));


// __bind(unsigned i): Find the most significant bit in a 32/64 number (PTX).
__bfind(&b, i) { asm volatile("bfind.u32 %0, %1;" : "=r"(b) : "r"(i)); }
```

Reduce

- Code

```
// Threads want to reduce the value in x.

float x = …;

#pragma unroll
for(int mask = WARP_SIZE / 2 ; mask > 0 ; mask >>= 1)
    x += __shfl_xor(x, mask);

// The x variable of laneid 0 contains the reduction.
```

- Performance
  - Launch 26 blocks of 1024 threads
  - Run the reduction 4096 times

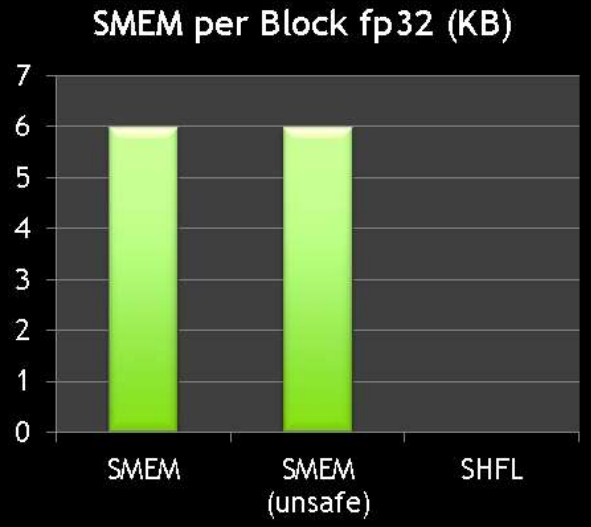


Scan

- Code

```
#pragma unroll
for( int offset = 1 ; offset < 32 ; offset <<= 1 )
{
    float y = __shfl_up(x, offset);
    if(laneid() >= offset)
        x += y;
}
```

- Performance
  - Launch 26 blocks of 1024 threads
  - Run the reduction 4096 times

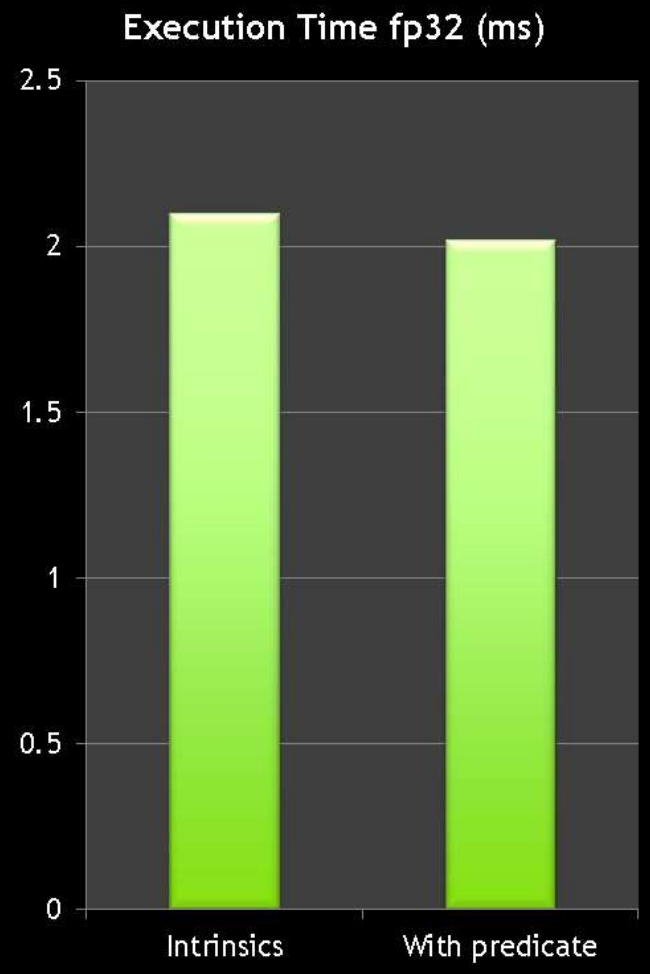


Scan

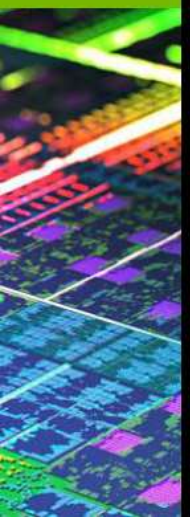
- Use the predicate from SHFL

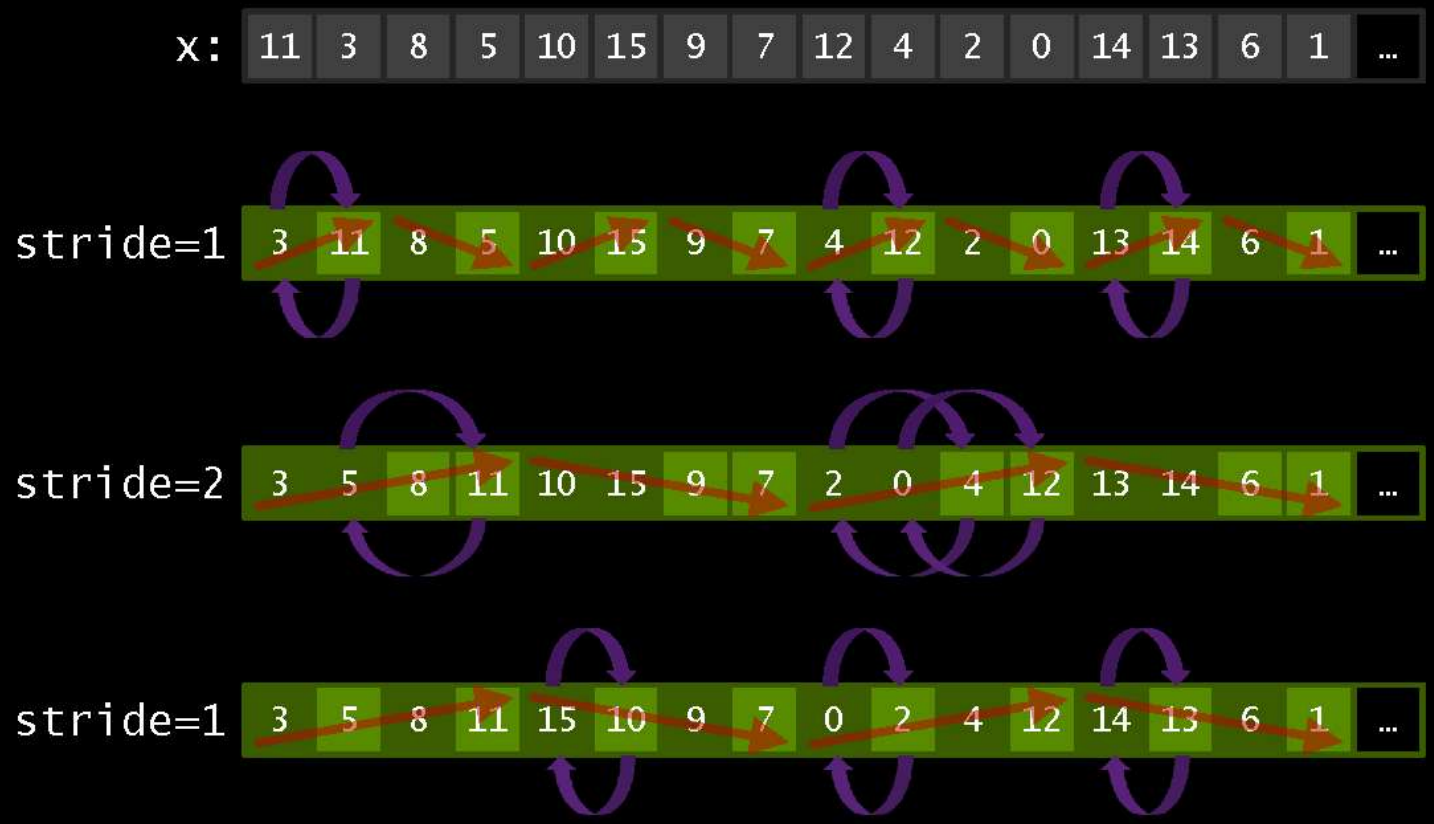
```
#pragma unroll
for( int offset = 1 ; offset < 32 ; offset <<= 1 )
{
    asm volatile( "{"
          "  .reg .f32 r0;"
          "  .reg .pred p;"
          "  shfl.up.b32 r0|p, %0, %1, 0x0;"
          "  @p add.f32 r0, r0, %0;"
          "  mov.f32 %0, r0;"
          "}" : "+f"(x) : "r"(offset));
}
```

- Use CUB:
  https://nvlabs.github.com/cub

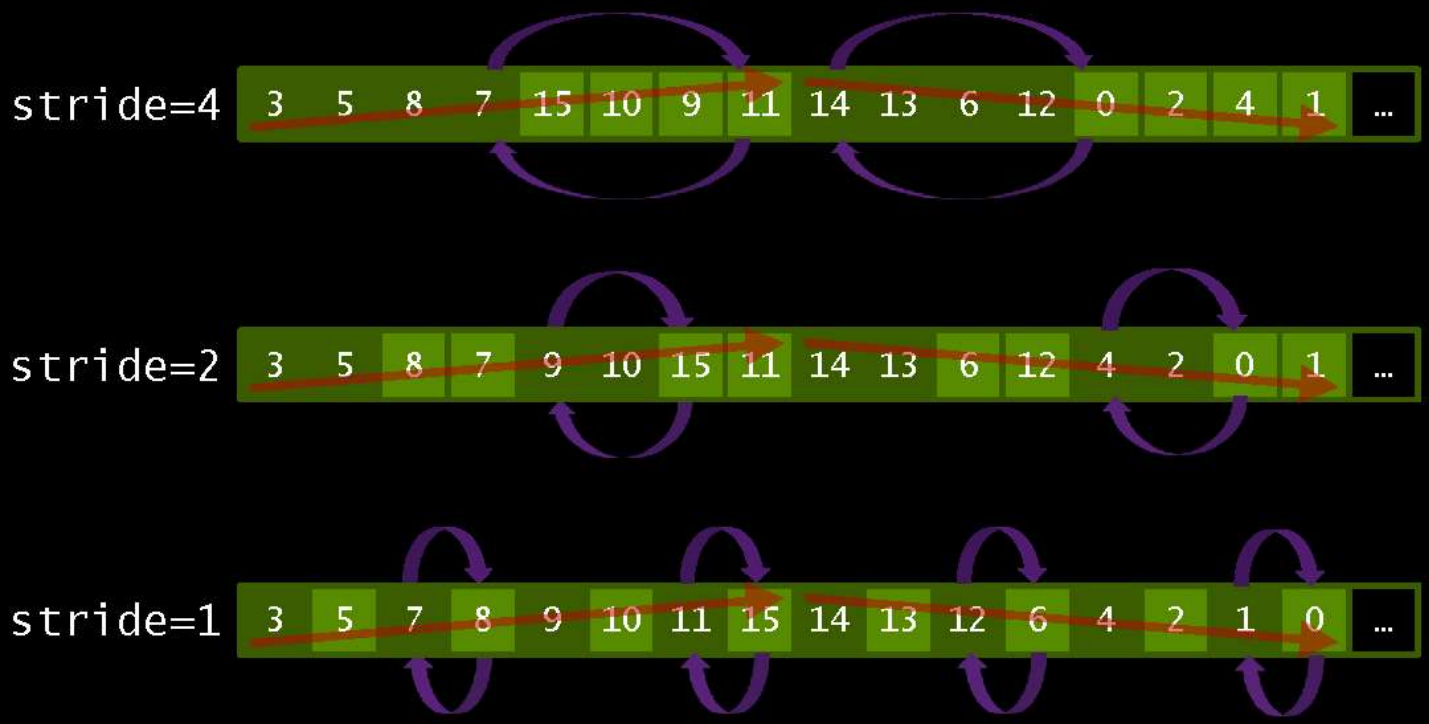


Bitonic Sort



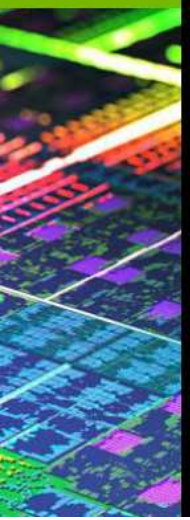


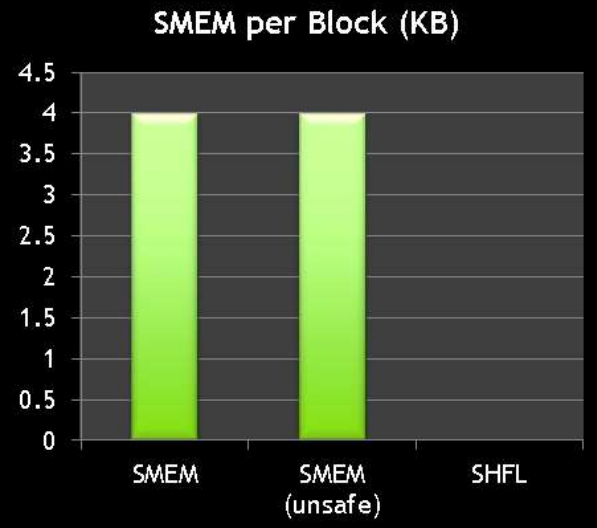
Bitonic Sort



Bitonic Sort

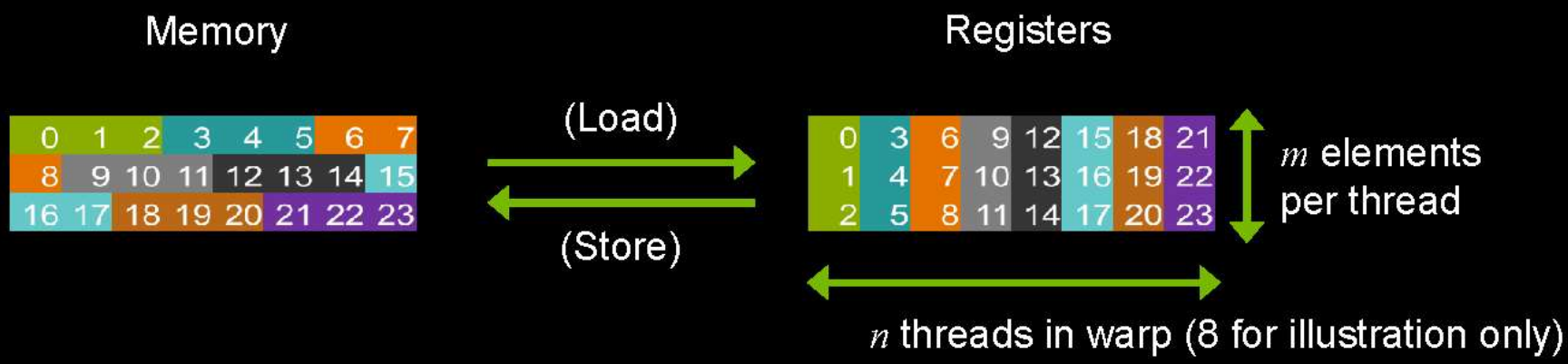
```
int swap(int x, int mask, int dir)
{
     int y = __shfl_xor(x, mask);
     return x < y == dir ? y : x;
}

x = swap(x, 0x01, bfe(laneid, 1) ^ bfe(laneid, 0)); //  2
x = swap(x, 0x02, bfe(laneid, 2) ^ bfe(laneid, 1)); //  4
x = swap(x, 0x01, bfe(laneid, 2) ^ bfe(laneid, 0));
x = swap(x, 0x04, bfe(laneid, 3) ^ bfe(laneid, 2)); //  8
x = swap(x, 0x02, bfe(laneid, 3) ^ bfe(laneid, 1));
x = swap(x, 0x01, bfe(laneid, 3) ^ bfe(laneid, 0));
x = swap(x, 0x08, bfe(laneid, 4) ^ bfe(laneid, 3)); // 16
x = swap(x, 0x04, bfe(laneid, 4) ^ bfe(laneid, 2));
x = swap(x, 0x02, bfe(laneid, 4) ^ bfe(laneid, 1));
x = swap(x, 0x01, bfe(laneid, 4) ^ bfe(laneid, 0));
x = swap(x, 0x10,                  bfe(laneid, 4)); // 32
x = swap(x, 0x08,                  bfe(laneid, 3));
x = swap(x, 0x04,                  bfe(laneid, 2));
x = swap(x, 0x02,                  bfe(laneid, 1));
x = swap(x, 0x01,                  bfe(laneid, 0));

// int bfe(int i, int k): Extract k-th bit from i

// PTX: bfe dst, src, start, len (see p.81, ptx_isa_3.1)
```





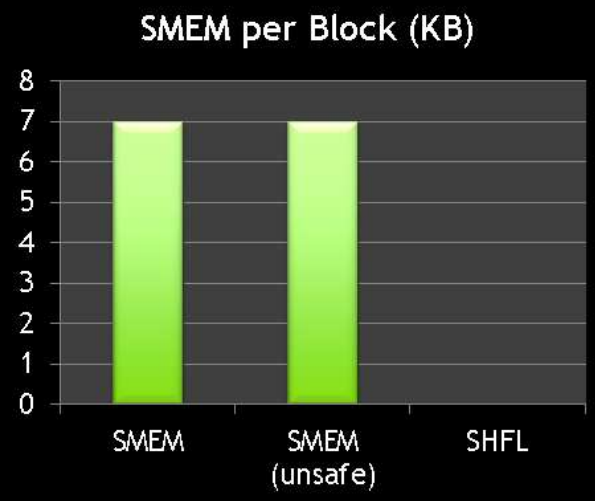
Transpose

- When threads load or store arrays of structures, transposes enable fully coalesced memory operations
- *e.g.* when loading, have the warp perform coalesced loads, then transpose to send the data to the appropriate thread



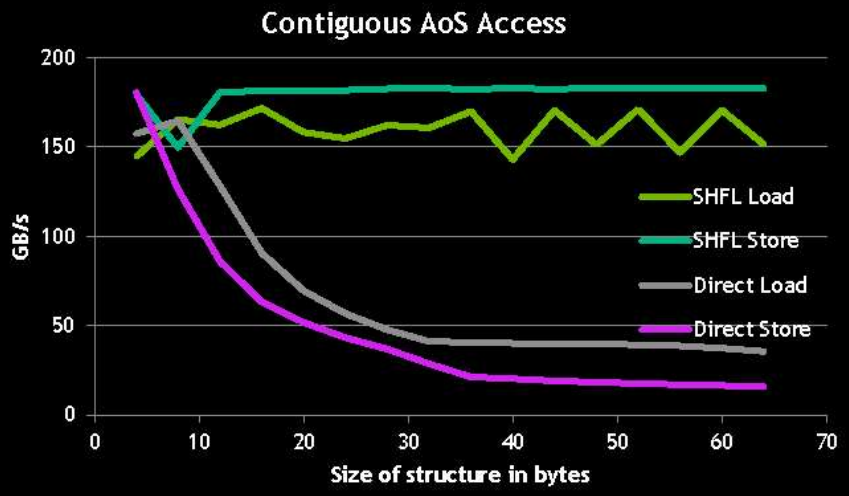
Transpose

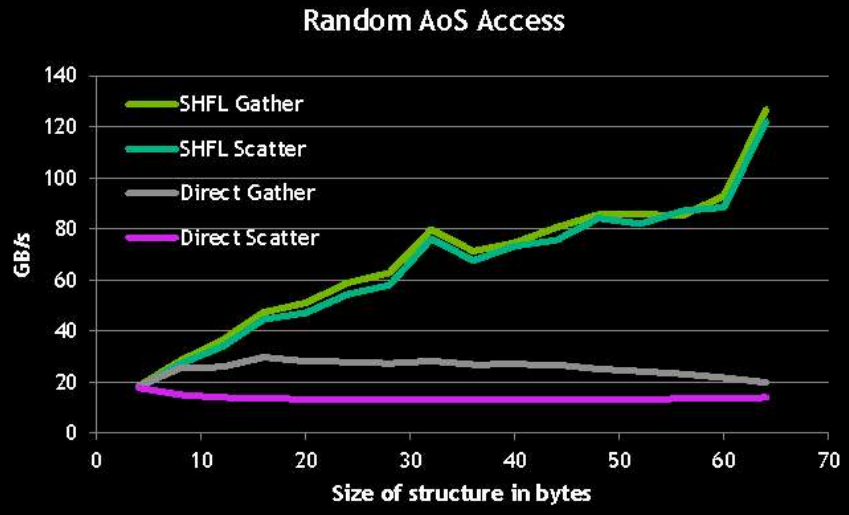
- You can use SMEM to implement this transpose, or you can use SHFL
- Code:
  http://github.com/bryancatanzaro/trove
- Performance
  - Launch 104 blocks of 256 threads
  - Run the transpose 4096 times

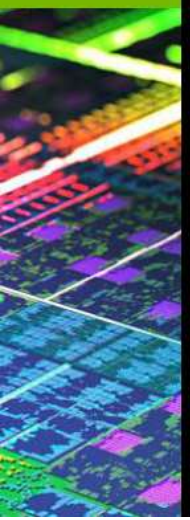


Array of Structures Access via Transpose

- Transpose speeds access to arrays of structures
- High-level interface: `coalesced_ptr<T>`
  - Just dereference like any pointer
  - Up to 6x faster than direct compiler generated access







Conclusion

- SHFL is available for SM >= SM 3.0
- It is always faster than “safe” shared memory
- It is never slower than “unsafe” shared memory
- It can be used in many different algorithms

Thank you.