## Data-Parallel Thinking

### Today's theme

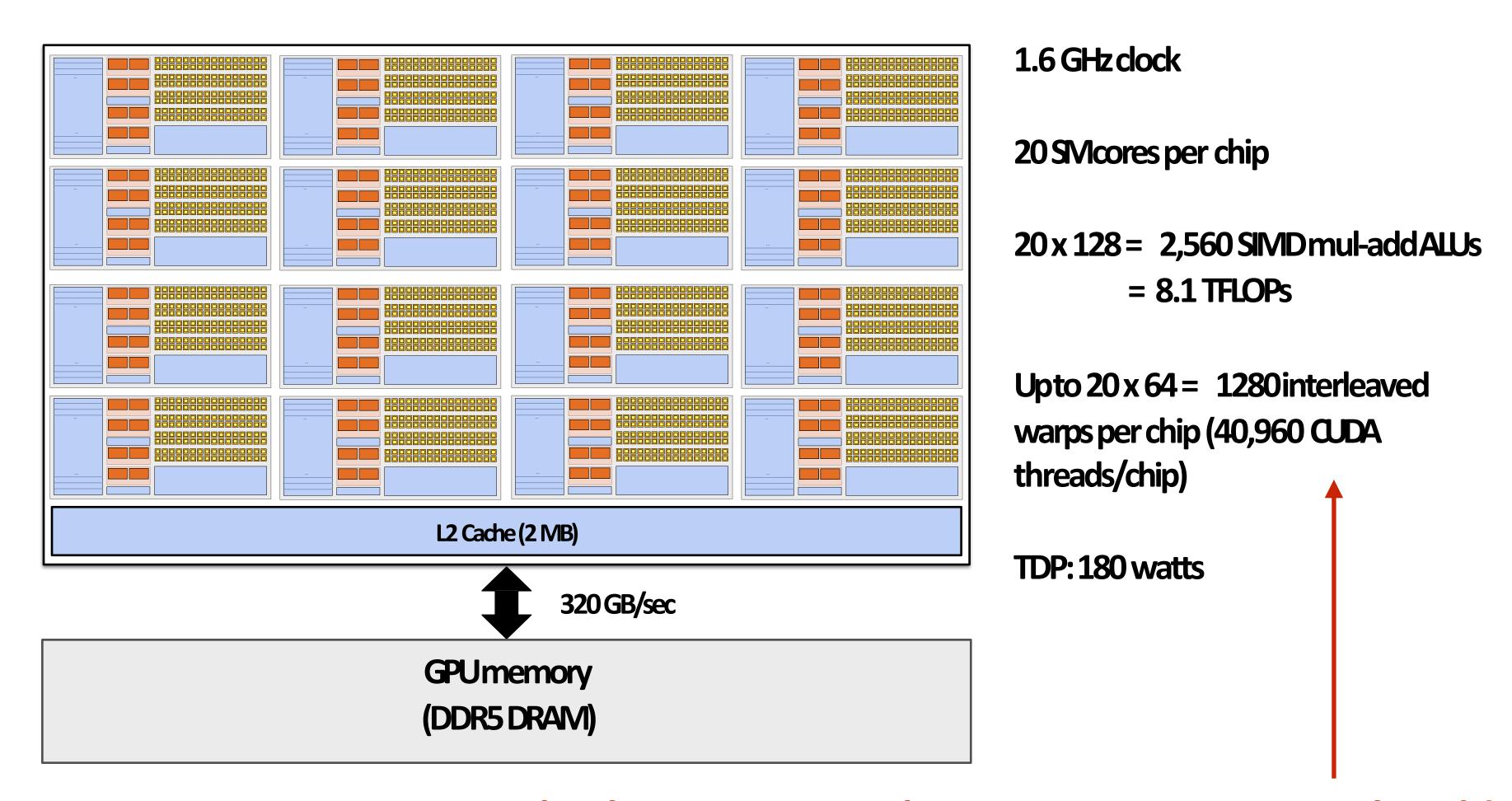
- Many of you are likely accustomed to thinking about parallel programming in terms of "what workers do"
- Today I would like you to think about describing algorithms in terms of operations on sequences of data
  - mapsort
  - filtergroupBy
  - fold / reducejoin
  - scan / segmented scan partition / flatten
- Main idea: high-performance implementations of these operations exist. So programs written in terms of these primitives can often run efficiently on a parallel machine

#### Motivation

Why must an application expose large amounts of parallelism?

- Utilize large numbers of cores
  - High core count machines
  - Many machines (e.g., cluster of machines in the cloud)
  - SIMD processing + multi-threaded cores require even more parallelism
  - GPU architectures require very large amounts of parallelism

### Recall: geometry of the GTX 1080 GPU



This chip can concurrently execute up to 40,960 CUDAthreads! (programs that do not expose significant amounts of parallelism will not run efficiently on GPUs!) \*

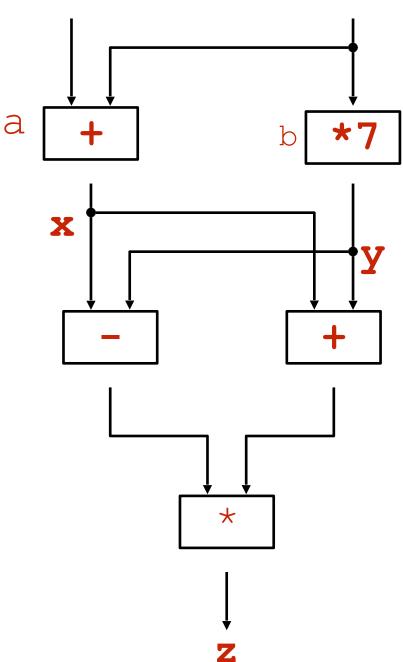
<sup>\*</sup>They need high arithmetic intensity as well.

#### Recall

 Key part of parallel programming is understanding when dependencies exist between operation

Lack of dependencies implies potential for parallel execution

```
x = a + b;
y = b * 7;
z = (x-y) * (x+y);
```



#### Data-parallel model

- Organize computation as operations on sequences of elements
  - e.g., perform same function on all elements of a sequence
- Historically: same operation on each element of an array
  - Matched capabilities SIMD supercomputers of 80's
  - Connection Machine (CM-1, CM-2): thousands of processors, one instruction decode unit
  - Early Cray supercomputers were vector processors
    - add(A, B, n)  $\leftarrow$  this was one instruction on vectors A, B of length n
- A well-known modern example: NumPy: C = A + B
   (A, B, and C are vectors of same length)

#### Key data type: sequences

- Ordered collection of elements
- For example, in a C++ like language:
   Sequence<T>
- e.g., Scala lists: List[T]
- In a functional language (like Haskell): seq T

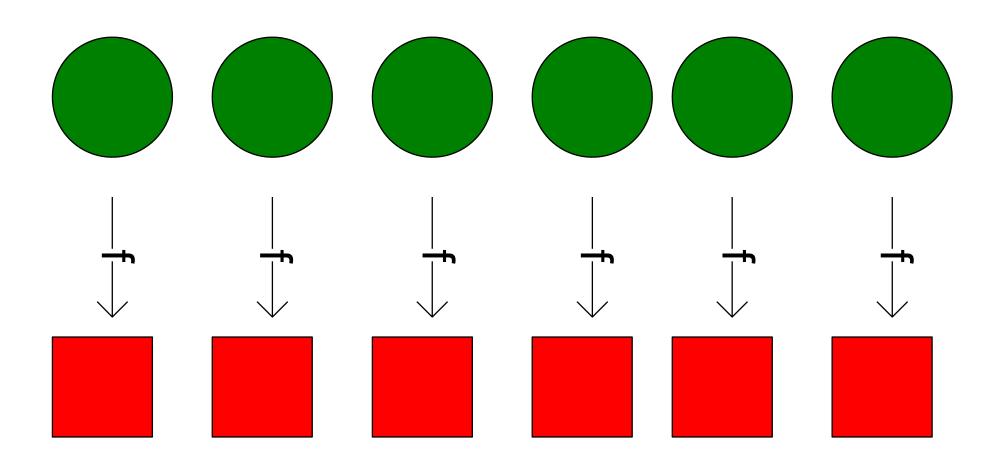
 Important: programs can only access elements of a sequence through specific operations

#### Map

- Higher order function (function that takes a function as an argument)
- Applies side-effect free unary function f:: a -> b to all elements
   of input sequence, to produce output sequence of the same length
- In a functional language (e.g., Haskell)

```
- map :: (a -> b) -> seq a -> seq b
```

In C++:



### Parallelizing map

 Since f:: a -> b is a function (side-effect free), then applying f to all elements of the sequence can be done in any order without changing the output of the program

 The implementation of map has flexibility to reorder/ parallelize processing of elements of sequence however it sees fit

```
map f s =
    partition sequence s into P smaller sequences for
    each subsequence s_i (in parallel)
        out_i = map f s_i
        out = concatenate out_i's
```

### Fold (fold left)

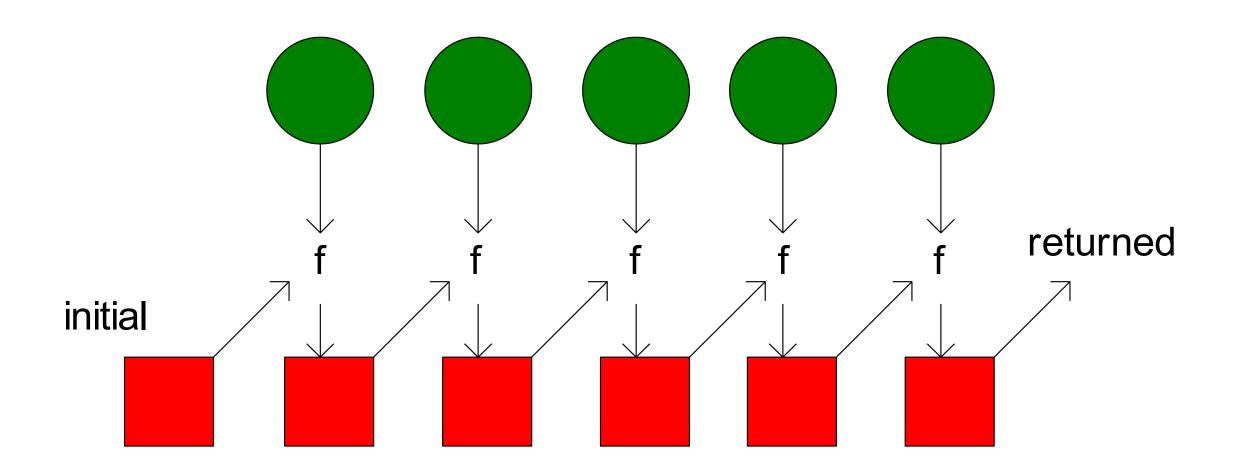
- Apply f to each element and an accumulated value
  - Seeded by initial value of type b

```
• f:: (b,a) -> b
```

fold :: b -> ((b,a) -> b) -> seq a -> b

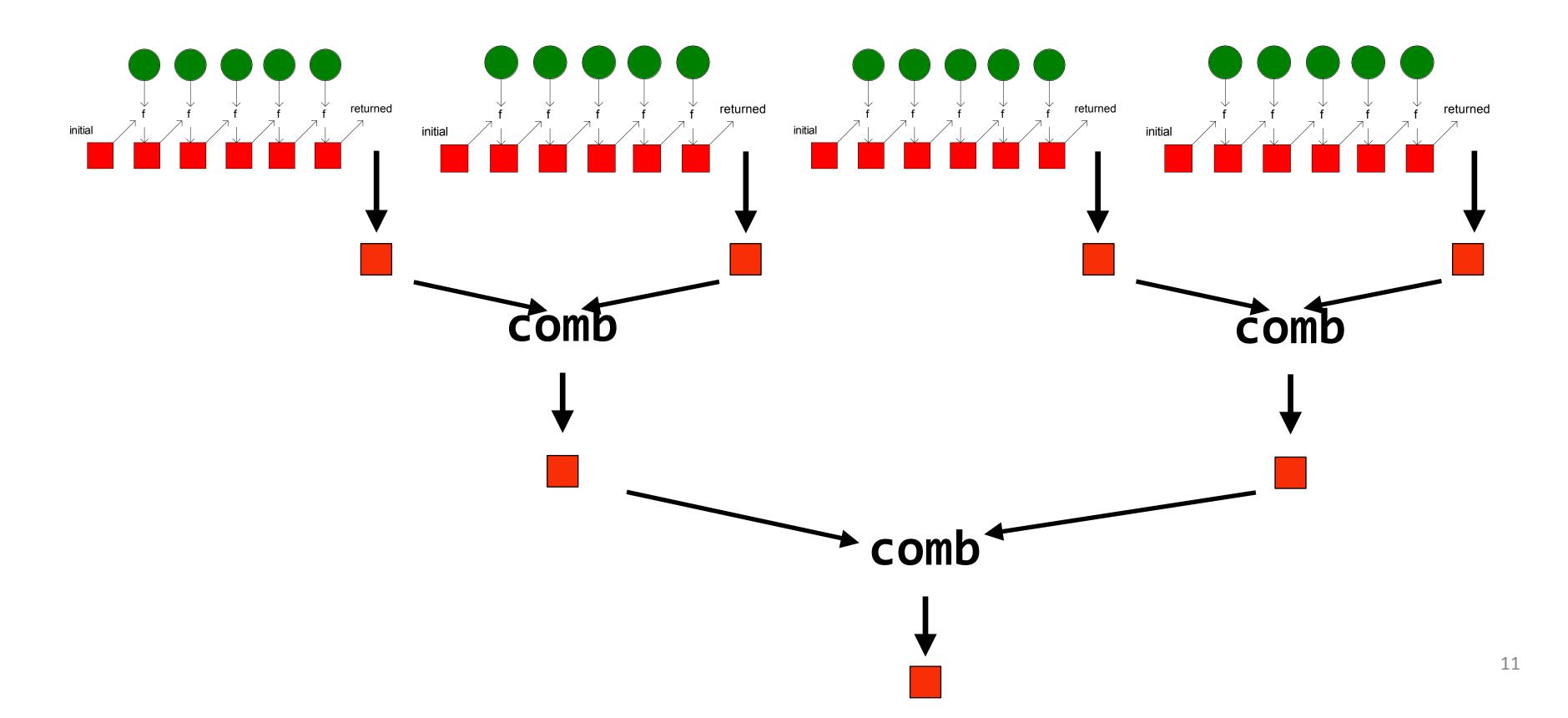
```
E.g., in Scala:
```

```
def foldLeft[A, B](init: B, f: (B, A) => B, l: List[A]): B
```



#### Parallel fold

- Apply f to each element and an accumulated value
  - Seeded by initial value of type b (identity for f and comb)
- f :: (b,a) -> b
- comb :: (b,b) -> b
- fold\_par :: b -> ((b,a) -> b) -> ((b,b)->b) ->seq a -> b



#### Scan

```
f :: (a,a) -> a (associative binary op)
scan :: a -> ((a,a) -> a) -> seq a -> seq a

scan_inclusive(float* in, float* out, int N) {
  out[0] = in[0];
  for (i=1; i<N; i++)
    out[i] = op(out[i-1], in[i-1]);
}</pre>
```

"Exclusive": the value of out[i] is the scan result for all elements up to, but excluding, in[i].

### Parallel Scan

### Data-parallel scan

```
let A = [a_0, a_1, a_2, a_3, \dots, a_{n-1}]
```

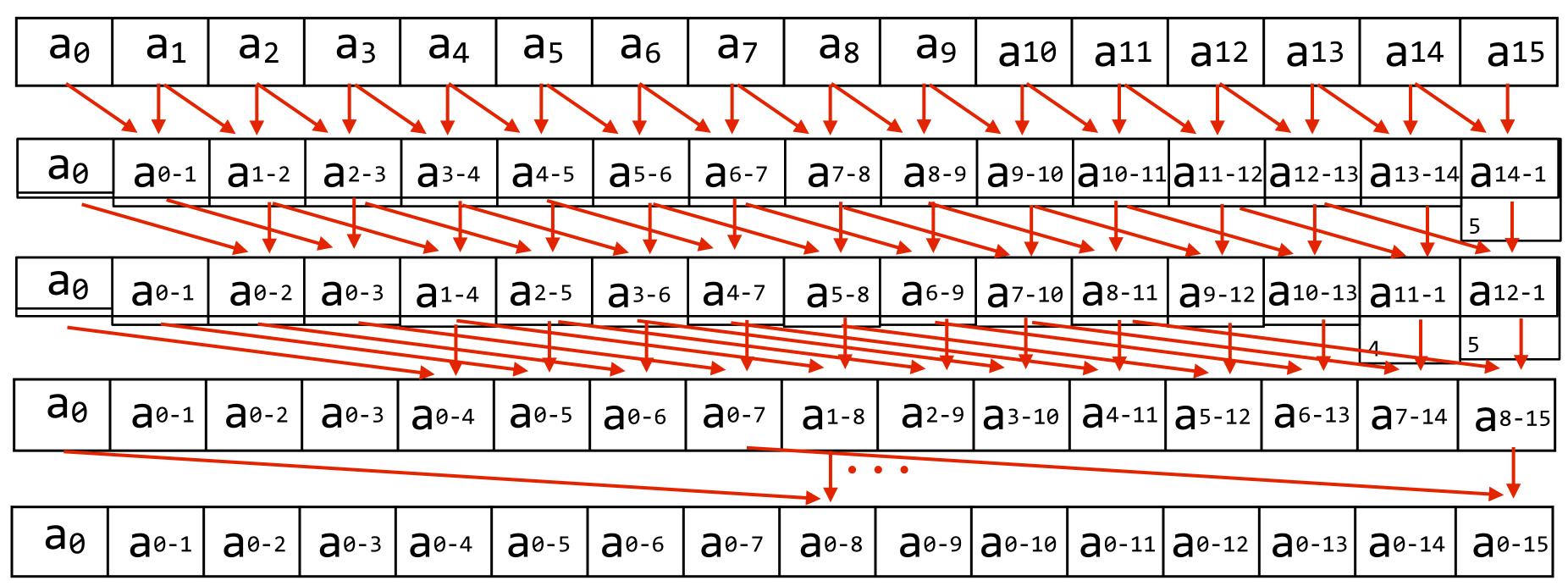
let  $\oplus$  be an associative binary operator with identity element I

```
scan_inclusive(\oplus, A) = [a_0, a_0 \oplus a_1, a_0 \oplus a_1 \oplus a_2, ...
scan_exclusive(\oplus, A) = [I, a_0, a_0 \oplus a_1, ...
```

If operator is +, then scan\_inclusive(+,A) is called "a prefix sum" prefix\_sum(A) =  $[a_0, a_0+a_1, a_0+a_1+a_2, ...$ 

### Data-parallel inclusive scan

(Subtract original vector to get exclusive scan result: not shown)



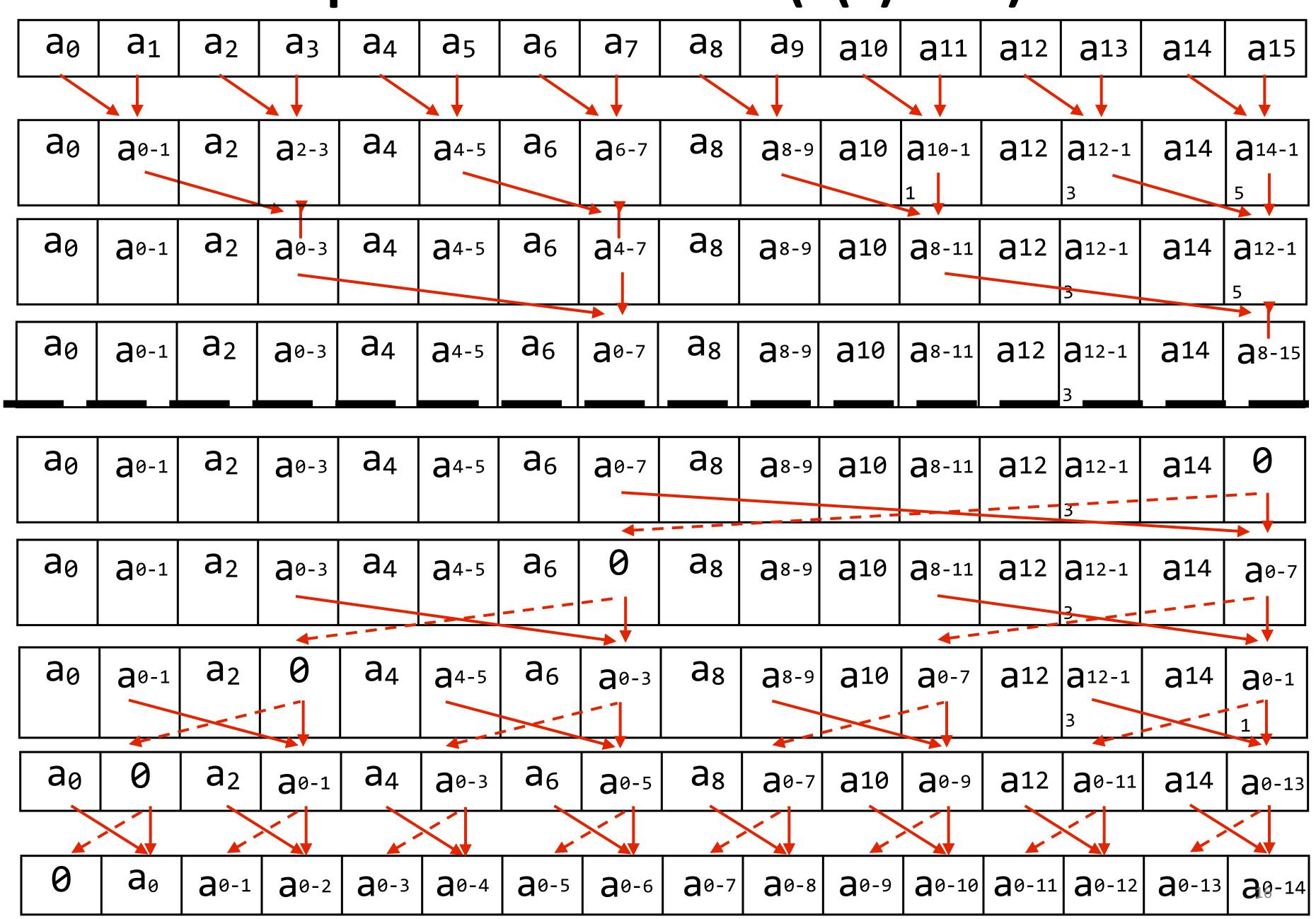
\*not showing all dependencies in last step

Work: O(Nlg N)

Inefficient compared to sequential algorithm!

Span: O(lg N)

#### Work-efficient parallel exclusive scan (O(N) work)



### Workefficient exclusive scan algorithm

```
(with \oplus = "+")
```

#### **Up-sweep:**

```
for d=0 to (\log_2 n - 1) do forall k=0 to n-1 by 2d+1 do a[k + 2d+1 - 1] = a[k + 2d - 1] + a[k + 2d+1 - 1]
```

#### Down-sweep:

```
x[n-1] = 0

for d=(log_2n - 1) down to 0 do forall k=0 to n-1 by 2d+1

do

tmp = a[k + 2d - 1]

a[k + 2d - 1] = a[k + 2d+1 - 1]

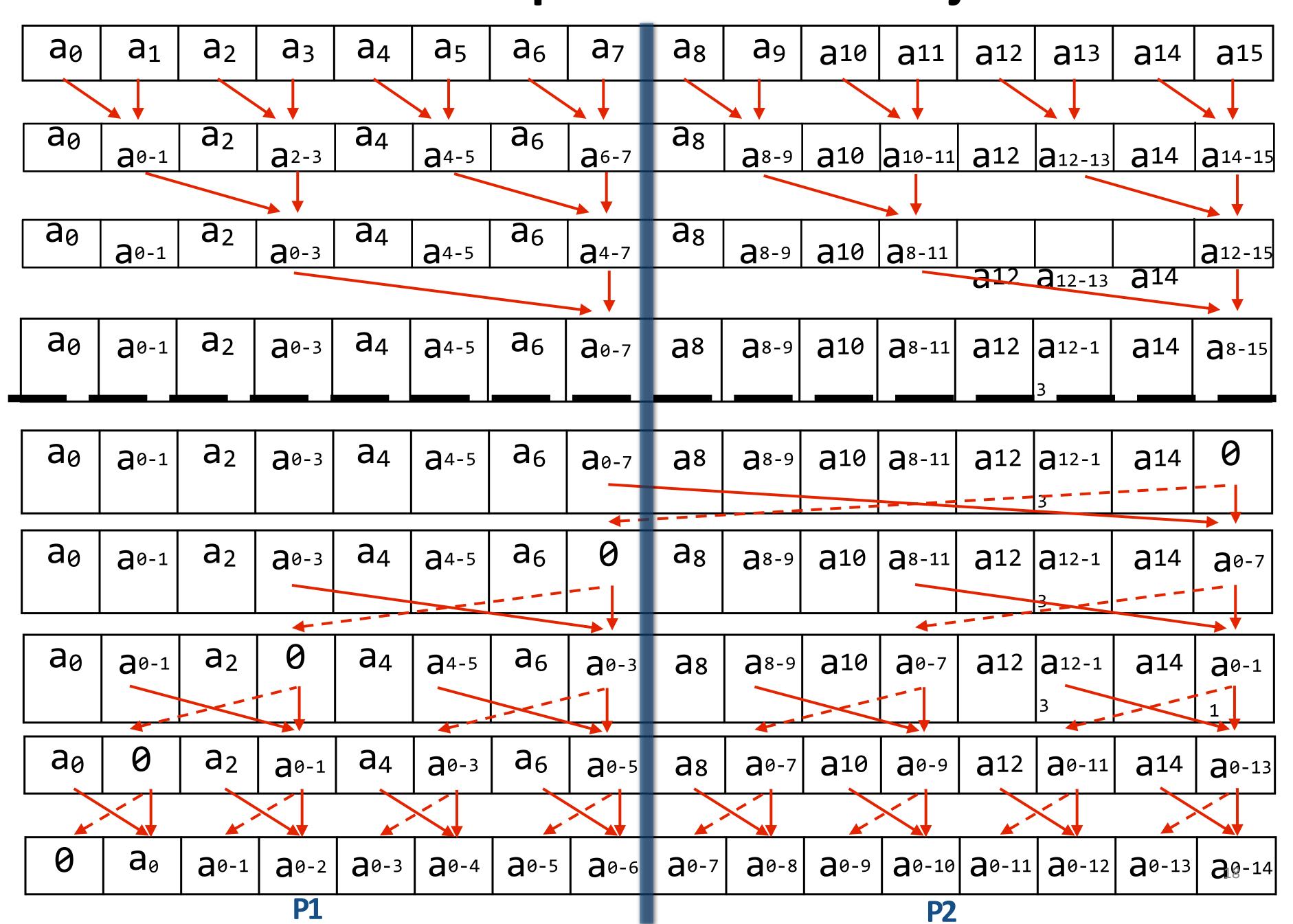
a[k + 2d+1 - 1] = tmp + a[k + 2d+1 - 1]
```

Work: O(N) (but what is the constant?)

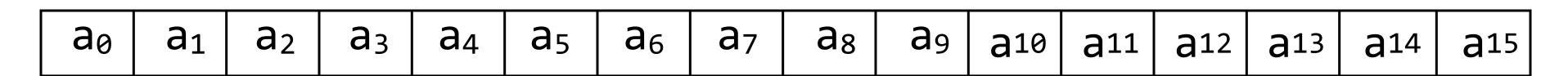
Span: O(lg N) (but what is the constant?)

Locality: ??

#### Now consider scan implementation on just two cores



#### Exclusive scan: two processor implementation



**P1** 

Sequential scan on elements [0-7]

Sequential scan on elements [8-15]

**P2** 

Let base =  $a_{0-7}$ 

Add base to elements  $a_8$  thru  $a_{8-11}$ 

Add base to elements  $a_{8-12}$  thru  $a_{8-15}$ 

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#### Work: O(N) (but constant is now only 1.5)

#### **Data-access:**

- Very high spatial locality (contiguous memory access)
- P1's access to  $a_8$  through  $a_{8-11}$  may be more costly on large core count 'NUNA' system, but on small-scale multi-core system the access cost is likely the same as from P2

#### Exclusive scan: CUDA implementation

Example: perform exclusive scan on 32-element array: SPMDprogram, assume 32-wide SIMDexecution

When s c an \_warp is run by a group of 32 CUDAthreads, each thread returns the

exclusive scan result for element idx

(also: upon completion ptr[] stores inclusive scan result)

CUDAthread

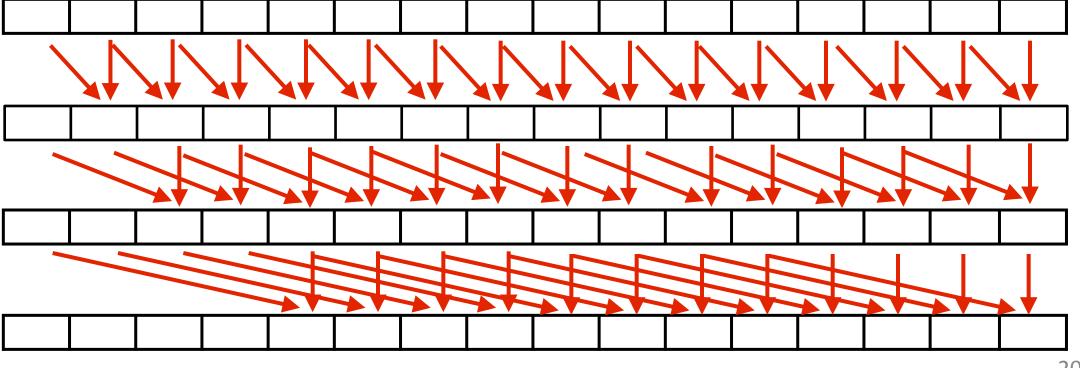
```
device _ int scan_warp(volatile int *ptr, const unsigned int idx)

const unsigned int lane = idx & 31; // index of thread in warp (0..31)

if (lane >= 1)    ptr[idx] = ptr[idx - 1] + ptr[idx];
if (lane >= 2)    ptr[idx] = ptr[idx - 2] + ptr[idx];
if (lane >= 4)    ptr[idx] = ptr[idx - 4] + ptr[idx];
if (lane >= 8)    ptr[idx] = ptr[idx - 8] + ptr[idx];
if (lane >= 16)    ptr[idx] = ptr[idx - 16] + ptr[idx);

return (lane > 0) ? ptr[idx-1] : 0;
```

Work:



2

#### Exclusive scan: CUDA implementation

**CUDA** thread index of caller

```
device __int scan_warp(volatile int *ptr, const unsigned int idx)
{
  const unsigned int lane = idx & 31; // index of thread in warp (0..31)

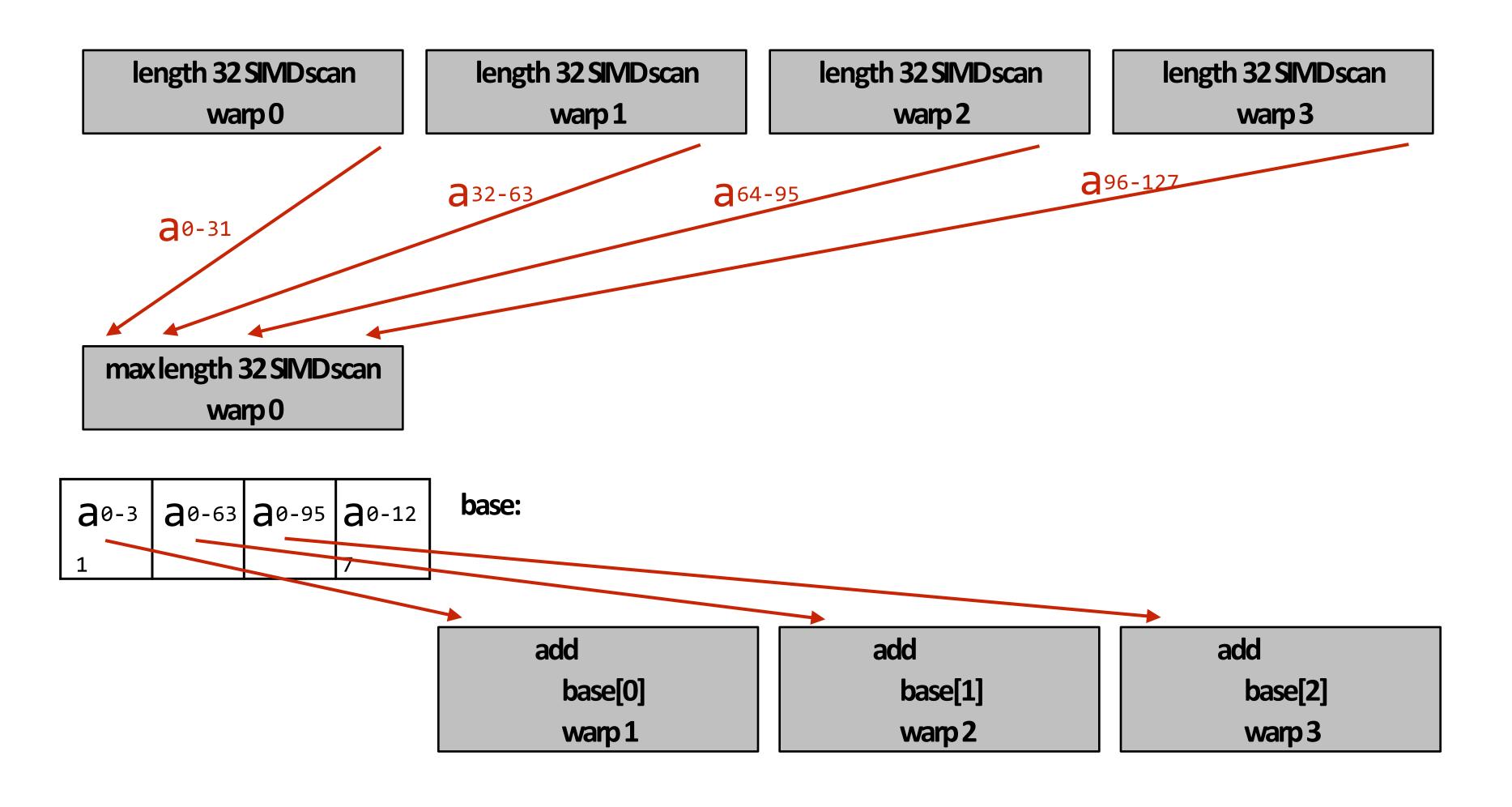
  if (lane >= 1)   ptr[idx] = ptr[idx - 1] + ptr[idx];
  if (lane >= 2)   ptr[idx] = ptr[idx - 2] + ptr[idx];
  if (lane >= 4)   ptr[idx] = ptr[idx - 4] + ptr[idx];
  if (lane >= 8)   ptr[idx] = ptr[idx - 8] + ptr[idx];
  if (lane >= 16)   ptr[idx] = ptr[idx - 16] + ptr[idx];
  return (lane > 0) ? ptr[idx-1] : 0;
}
```

#### Work: N Ig(N)

Work-efficient formulation of scan is not beneficial in this context because it results in low SIMD utilization. It would require more than 2x the number of instructions as the implementation above!

### Building scan on larger array

Example: 128-element scan using four-warp thread block



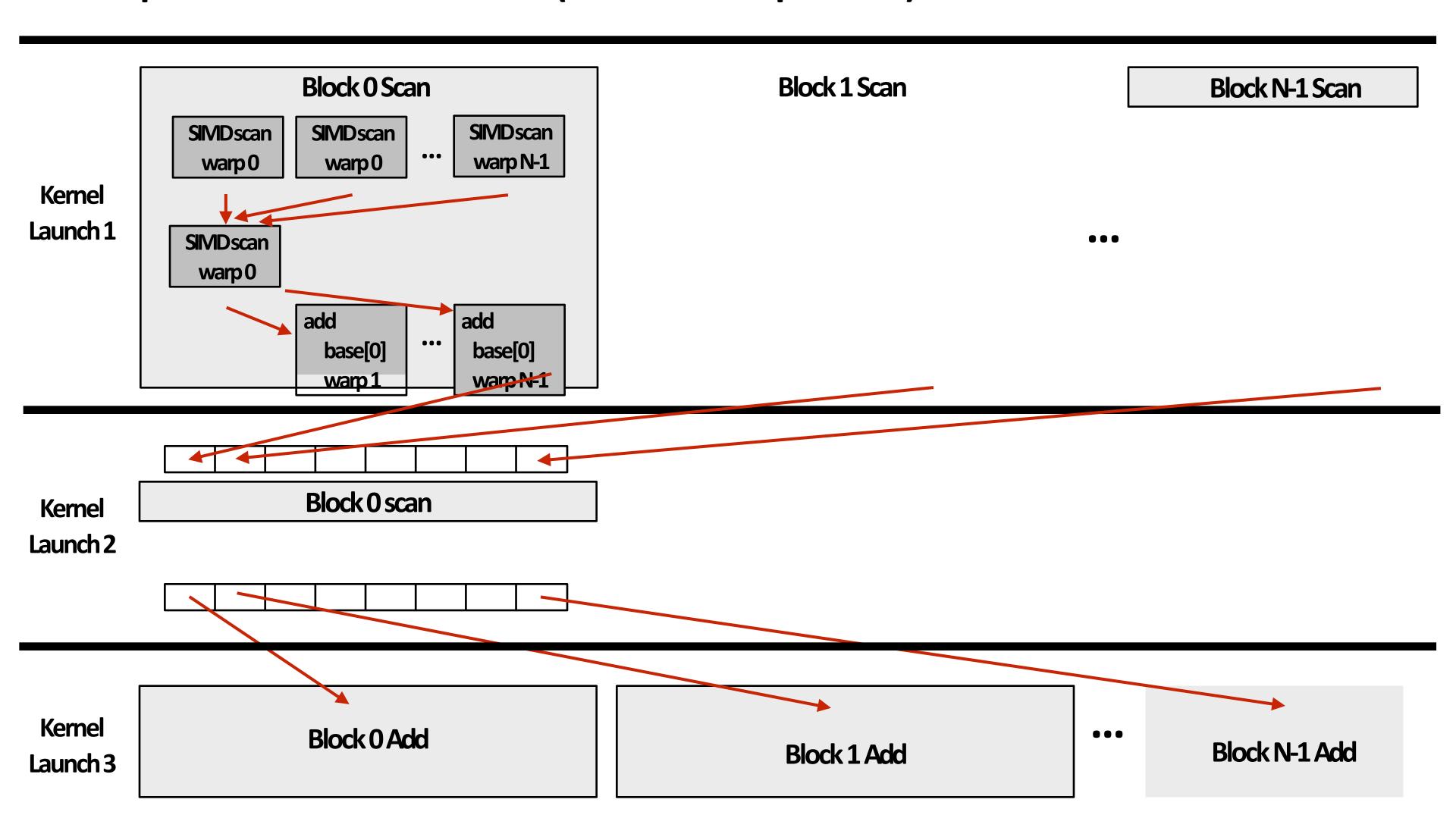
#### Multi-threaded, CUDA implementation

#### Example: cooperating threads in a CUDA thread block perform scan

**CUDA** thread Code assumes length of array given by ptr is same as number of threads per block. index of caller \_\_device\_\_ void scan\_block(volatile int \*ptr, const unsigned int idx)
{ const unsigned int lane = idx & 31; // index of thread in warp (0..31) const unsigned int warp\_id = idx >> 5; // warp index in block int val = scan\_warp(ptr, idx); // Step 1. per-warp partial scan // (Performed by all threads in block, // with threads in same warp communicating // through shared memory buffer 'ptr') if (lane == 31) ptr[warp\_id] = ptr[idx]; // Step 2. thread 31 in each warp copies syncthreads(); // partial-scan bases in per-block // shared mem if (warp\_id == 0) scan\_warp(ptr, idx); // Step 3. scan to accumulate bases syncthreads(); // (only performed by warp 0) if (warp\_id > 0) // Step 4. apply bases to elements all // (performed by all threads symathremat(); ptr[warp\_id-1]; in block) ptr[idx] = val;

### Building a larger scan

Example: one million element scan (1024 elements per block)



#### Scan implementation

#### Parallelism

- Scan algorithm features O(N) parallel work
- But efficient implementations only leverage as much parallelism as required to make good utilization of the machine
  - Goal is to reduce work and reduce communication/synchronization

#### Locality

- Multi-level implementation to match memory hierarchy
   (CUDA example: per-block implementation carried out in local memory)
- Heterogeneity in algorithm: different strategy for performing scan at different levels of the machine
  - CUDA example: different algorithm for intra-warp scan than inter-thread scan
  - Low-core count CPU example: based largely on sequential scan

### Parallel Segmented Scan

### Segmented scan

- Common problem: operating on sequence of sequences
- Examples:
  - For each vertex in a graph:
    - For each edge incoming to vertex:
  - For each particle in simulation
    - For each particle within cutoff radius
- For each document in a collection
- For each word in document
- There are two levels of parallelism in the problem that a programmer might want to exploit
- But its irregular: the size of edge lists, particle neighbor lists, words per document, etc, may be very different from vertex to vertex (or particle to particle)

### Segmented scan

- Generalization of scan
- Simultaneously perform scans on arbitrary contiguous partitions of input collection

```
let A = [[1,2],[6],[1,2,3,4]]
let ⊕ = +
segmented_scan_exclusive(⊕,A) = [[0,1], [0], [0,1,3,6]]
```

#### Assume a simple "start-flag" representation of nested sequences:

```
A = [[1,2,3],[4,5,6,7,8]]
flag: 1 0 0 1 0 0 0
data: 1 2 3 4 5 6 7 8
```

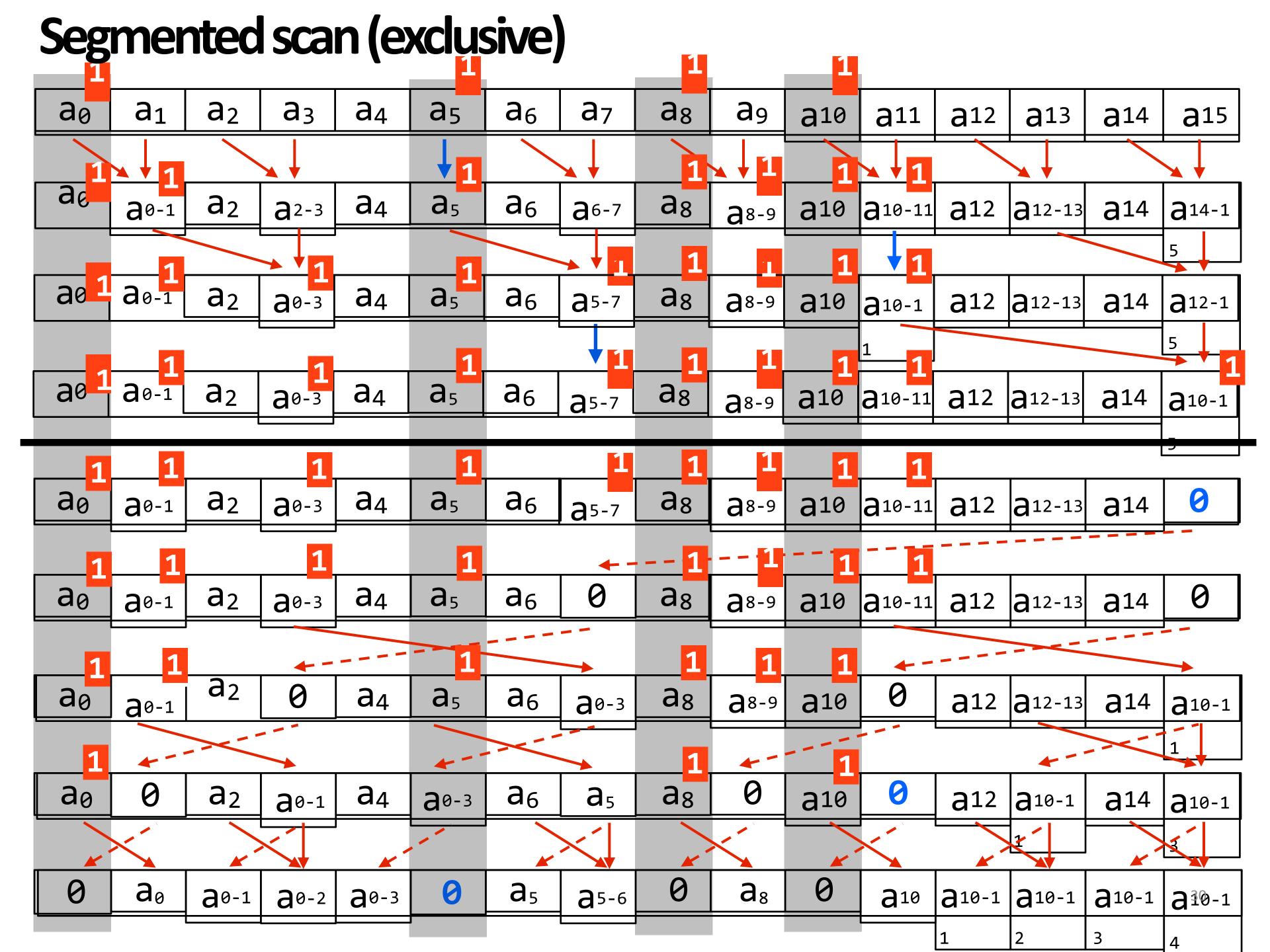
### Work-efficient segmented scan

(with  $\oplus$  = "+")

#### **Up-sweep:**

```
for d=0 to (log<sub>2</sub>n - 1) do:
    forall k=0 to n-1 by 2d+1 do:
        if flag[k + 2d+1 - 1] == 0:
             data[k + 2d+1 - 1] = data[k + 2d - 1] + data[k + 2d+1 - 1]
        flag[k + 2d+1 - 1] = flag[k + 2d - 1] || flag[k + 2d+1 - 1]
```

#### Down-sweep:



### Sparse matrix multiplication example

$$\begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ \vdots \\ y_{n-1} \end{bmatrix} = \begin{bmatrix} 3 & 0 & 1 & \cdots & 0 \\ 0 & 2 & 0 & \cdots & 0 \\ 0 & 0 & 4 & \cdots & 0 \\ \vdots \\ 0 & 2 & 6 & \cdots & 8 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_{n-1} \end{bmatrix}$$

- Most values in matrix are zero
  - Note: easy parallelization by parallelizing the different per-row dot products
  - But different amounts of work per row (complicates wide SIMD execution)
- Example sparse storage format: compressed sparse row

```
values = [ [3,1], [2], [4], ..., [2,6,8] ]
cols = [ [0,2], [1], [2], ..., ]
row_starts = [0, 2, 3, 4, ... ]
```

### Sparse matrix multiplication with scan

$$\begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 3 & 0 & 1 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 0 & 2 & 6 & 8 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

- 1. Map over all non-zero values: products[i] = values[i] \* x[cols[i]] products =  $[3x_0, x_2, 2x_1, 4x_2, 2x_1, 6x_2, 8x_3]$
- 2. Create flags vector from row\_starts: flags = [1,0,1,1,0,0]
- 3. Perform inclusive segmented-scan on (products, flags) using addition operator  $[3x_0, 3x_0+x_2, 2x_1, 4x_2, 2x_1, 2x_1+6x_2, 2x_1+6x_2+8x_2]$
- 4. Take last element in each segment:

$$y = [3x_0+x_2, 2x_1, 4x_2, 2x_1+6x_2+8x_2]$$

### Scan/segmented scan summary

#### Scan

- Theory: parallelism in problem is linear in number of elements
- Practice: exploit locality, use only as much parallelism as necessary to fill the machine's execution resources
  - Great example of applying different strategies at different levels of the machine

#### Segmented scan

- Express computation and operate on irregular data structures (e.g., list of lists) in a regular, data parallel way

#### More operations

#### Group by key

- Seq (key, T) —> Seq (key, Seq T)
- Similar to: sort sequence by key, the performing segmented scan operations on segments with same key

#### Filter

Remove elements from sequence that do not match predicate

# Example: create grid of particles data structure on large parallel machine (e.g., a GPU)

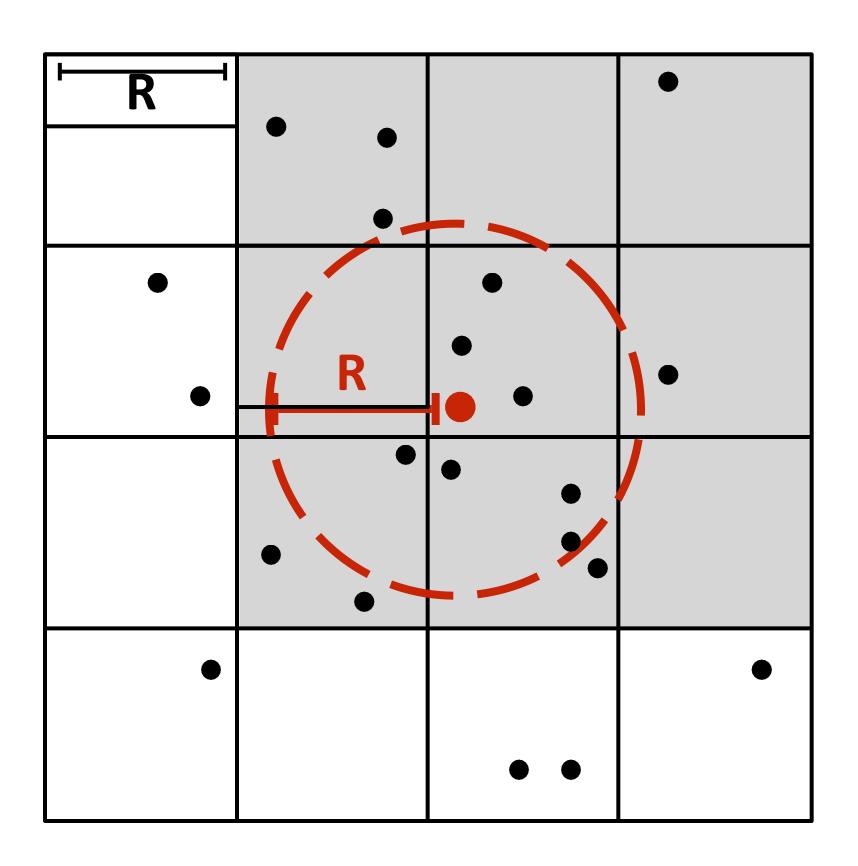
- Problem: place 1Mpoint particles in a 16-cell uniform grid based on 2D position
  - Parallel data structure manipulation problem: build a 2D array of lists
- Recall: Upto 2048 CUDAthreads per SM core on a GTX 1080 GPU (20 SM cores)

0	1	2	3
3 • 4 5•	5	1 6 4 • 2•	7
8	9	10	11
12	13	14	<b>15</b>

Cell id	Count	Particle id
	•	10
0	0	
1	0	
2	0	
3	0	
4	2	3, 5
5	0	
6	3	1, 2, 4
7	0	
8	0	
9	1	0
10	0	
11	0	
12	0	
13	0	
14	0	
15	0	

#### Commonuse of this structure: N-body problems

- Acommon operation is to compute interactions with neighboring particles
- Example: given a particle, find all particles within radius R
  - Organize particles by placing them in grid with cells of size R
  - Only need to inspect particles in surrounding grid cells



### Solution 1: parallelize over cells

- One possible answer is to decompose work by cells: for each cell, independently compute what particles are within it (eliminates contention because no synchronization is required)
  - Insufficient parallelism: only 16 parallel tasks, but need thousands of independent tasks to efficiently utilize GPU)
  - Work inefficient: performs 16 times more particle-in-cell computations than sequential algorithm

### Solution 2: parallelize over particles

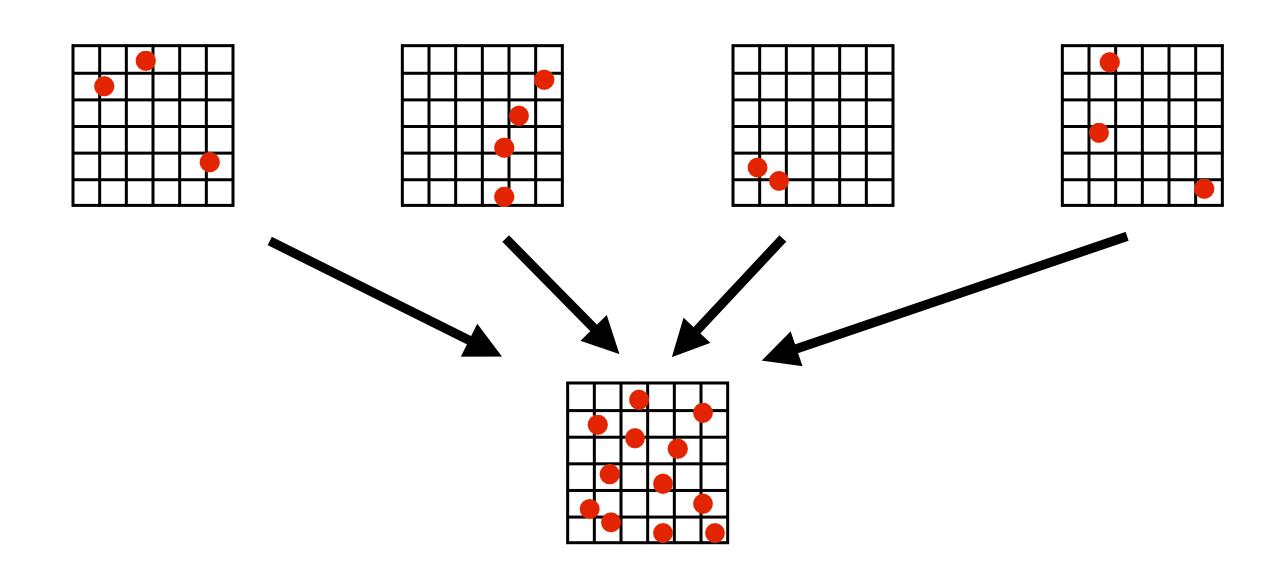
- Another answer: assign one particle to each CUDA thread. Thread computes cell containing particle, then atomically updates per cell list.
  - Massive contention: thousands of threads contending for access to update single shared data structure

# Solution 3: use finer-granularity locks

- Alleviate contention for single global lock by using percell locks
  - Assuming uniform distribution of particles in 2D space...
     ~16x less contention than solution 2

### Solution 4: compute partial results + merge

- Yet another answer: generate N "partial" grids in parallel, then
  - Example: create N thread blocks (at least as many thread blocks as SM cores)
  - All threads in thread block update same grid
    - Enables faster synchronization: contention reduced by factor of N and cost of synchronization is lower because it is performed on block-local variables (in CUDA shared memory)
  - Requires extra work: merging the N grids at the end of the computation
  - Requires extra memory footprint: Store N grids of lists, rather than 1



#### Solution 5: data-parallel approach

#### Step 1: map

compute cell containing each particle (parallel over input particles)

 particle\_index:
 0
 1
 2
 3
 4
 5

 9
 6
 6
 4
 6
 4

 grid\_cell:
 -</td

#### Step 2: sort results by cell (particle index array permuted based on sort)

particle\_index:

grid\_cell:

	5	1	2		
4	4	6	6	6	9

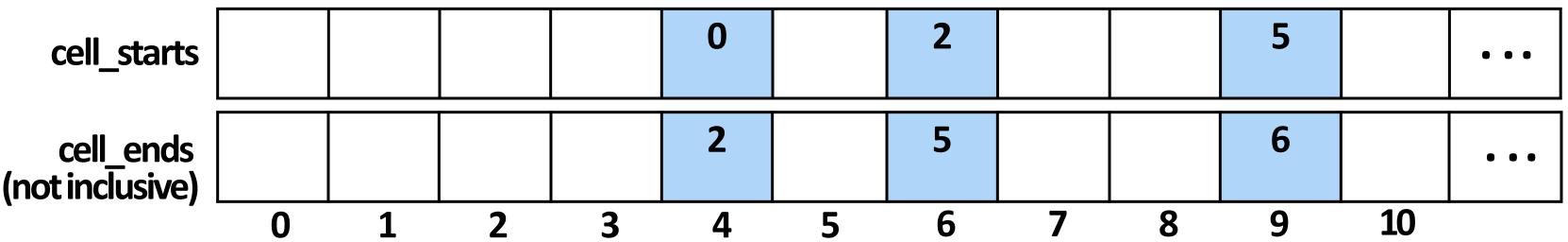
#### Step 3: find start/end of each cell (parallel over particle\_index elements)

```
particle_cell = grid_cell[index];
if (index == 0)
    cell_starts[particle_cell] = index;
else if (particle_cell != grid_cell[index-1]) {
    cell_starts[particle_cell] = index;
    cell_ends[grid_cell[index-1]] = index;
}
if (index == numParticles-1) // special case for last cell
    cell_ends[particle_cell] = index+1;
```

0	1	2	3
3• 4 5•	5	1 6 4 •	7
8	9• 0	10	11
12	13	14	15

This solution maintains a large amount of parallelism and removes the need for fine-grained synchronization... at cost of a sort and extra passes over the data (extra BW)

This code is run for each element of the particle\_index array. (each invocation has a unique valid of 'index')



## Another example: parallel histogram

Consider compute a histogram for a large sequence of values

 Create a massively parallel implementation of histogram given only map() and sort() on sequences

# Another example: parallel histogram (part 1)

```
void compute_bin(float* input, int* bin_ids) {
  bin_ids[idx] = f(input[idx]);
void find_starts(int* bin_ids, int* starts) {
  if (idx == 0 || bin_ids[idx] != bin_ids[idx-1])
    starts[bin_ids[idx]] = idx;
float input[N];
int sorted_bin_idx[N];
    bin_starts[NUM_BINS]; // initialized to -1
int
// map f onto input to get bin ids of all elements
launch<<<N>>>compute_bin(input, bin_ids);
// find starting point of each bin in sorted list
sort(N, bin_ids, sorted_bin_ids);
launch<<<N>>>find_starts(sorted_bin_ids, bin_starts);
```

# Another example: parallel histogram

```
void bin_sizes(int* bin_starts, int* histogram_bins, int num_items, int num_bins) {
if (bin_starts[idx] == -1) {
                              // no items in this bin
    histogram bins[idx] = 0;
} else {
   // find start of next bin in order to determined size of current bin
   // Tricky edge case: if the next bin is empty, then must search forward to find
    the next non-empty bin
    int next idx = idx+1;
    while(next_idx < num_bins && bin_starts[next_idx] == -1)</pre>
       id++;
    if (next_idx < num_bins)</pre>
       histogram_bins[idx] = bin_starts[next_idx] - bin_starts[idx];
    else
       histogram_bins[idx] = num_items - bin_starts[idx];
launch<<<NUM_BINS>>>bin_sizes(bin_starts, histogram_bins, N, NUM_BINS);
```

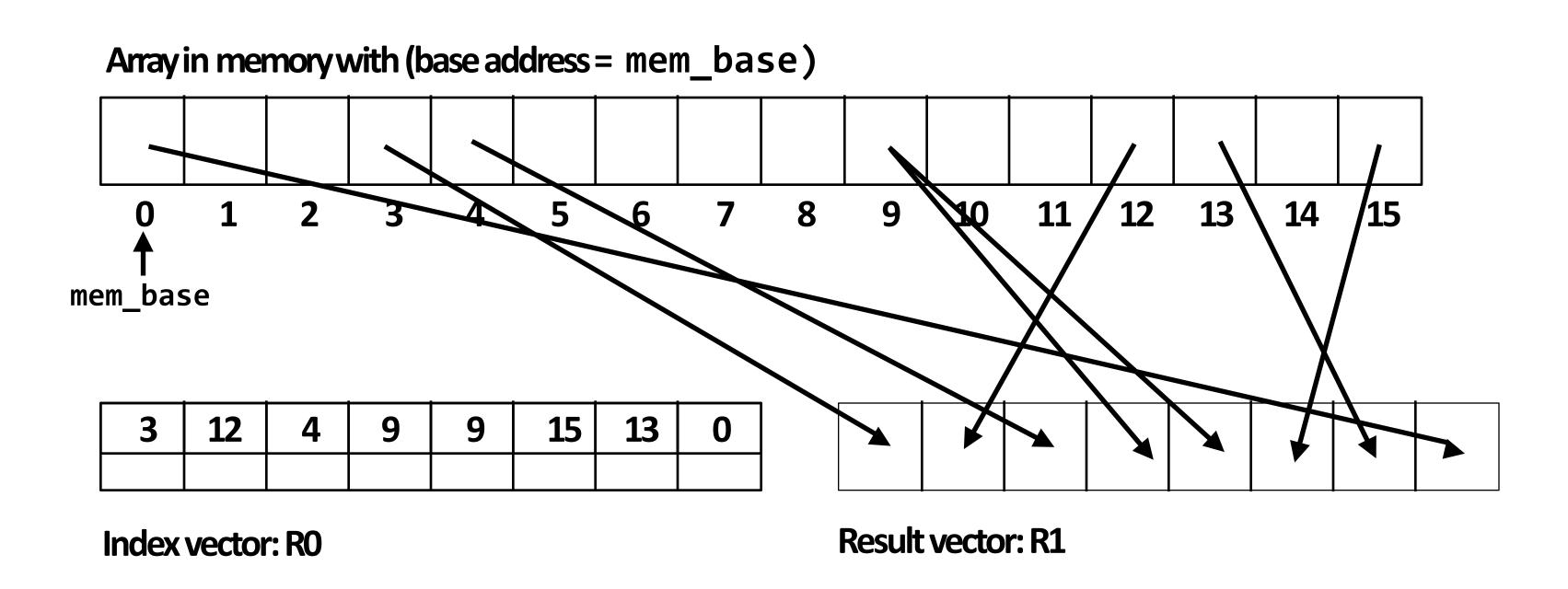
## Scatter/gather operations on sequences

- gather(index, input, output)
  - output[i] = input[index[i]]

- scatter(index, input, output)
  - output[index[i]] = input[i]

#### **Gather instruction**

gather(R1, R0, mem\_base); "Gatherfrom buffermem\_base into R1 according to indices specified by RO."



Gather supported with AVX2 in 2013
But AVX2 does not support SIMD scatter (must implement as scalar loop)
Scatter instruction exists in AVX512

Hardware supported gather/scatter does exist on GPUs. (still an expensive operation compared to load/store of contiguous vector)

# Turning scatter into sort/gather

- scatter(index, input, output)
  - output[index[i]] = input[i]

 Assume elements of index are unique and all elements references in index (scatter is a permutation)

```
temp = sort input sequence by values in index sequence
output[i] = temp[i]
```

# Turning scatter with atomic sort/map/scan

```
for all elements in sequence
  atomicOp(output[index[i]], input[i])
```

Assume elements in index are not unique, so synchronization is required for atomicity!

Sort input sequence according to values in index sequence

```
[0, 0, 0, 1, 1, 2]
[input[2] input[4], input[5], input[0], input[1], input[3]]
,
```

Compute starts of each range of the same index number

```
[1, 0, 0, 1, 0, 1]
```

Segmented scan (using 'op') each range

```
[op(op(input[2], input[4]), input[5]), op(input[0], input[1]), input[3])
```

### Summary

- Data parallel thinking:
  - Implementing algorithms in terms of simple (often widely parallelizable, efficiently implemented) operations on large data collections
- Turn irregular parallelism into regular parallelism

- Turn fine-grained synchronization into coarse (barrier) synchronization
- But most solutions require multiple passes over data
  - bandwidth hungry!

### Summary

Data parallel primitives are basis for many parallel/distributed

systems today

**CUDA's Thrust Library** 





 $map(f: T \Rightarrow U)$  $RDD[T] \Rightarrow RDD[U]$  $filter(f: T \Rightarrow Bool)$  $RDD[T] \Rightarrow RDD[T]$  $flatMap(f: T \Rightarrow Seq[U])$  $RDD[T] \Rightarrow RDD[U]$ sample(fraction : Float)  $RDD[T] \Rightarrow RDD[T]$  (Deterministic sampling)  $RDD[(K, V)] \Rightarrow RDD[(K, Seq[V])]$ groupByKey()  $RDD[(K, V)] \Rightarrow RDD[(K, V)]$  $reduceByKey(f : (V, V) \Rightarrow V)$  $(RDD[T], RDD[T]) \Rightarrow RDD[T]$ **Transformations** union()  $(RDD[(K, V)], RDD[(K, W)]) \Rightarrow RDD[(K, (V, W))]$ join()  $(RDD[(K, V)], RDD[(K, W)]) \Rightarrow RDD[(K, (Seq[V], Seq[W]))]$ cogroup() crossProduct()  $(RDD[T], RDD[U]) \Rightarrow RDD[(T, U)]$  $mapValues(f : V \Rightarrow W)$  $RDD[(K, V)] \Rightarrow RDD[(K, W)]$  (Preserves partitioning) sort(c : Comparator[K])  $RDD[(K, V)] \Rightarrow RDD[(K, V)]$ partitionBy(p:Partitioner[K])  $RDD[(K, V)] \Rightarrow RDD[(K, V)]$ 

▼ Iterators **Fancy Iterators** Iterator Tags **Iterator Tag Classes ▼** Algorithms Searching ▼ Binary Search **Vectorized Searches ▼** Copying Gathering Scattering Reductions Counting Comparisons **Extrema Transformed Reductions** Logical **Predicates** Merging ▼ Reordering **Partitioning Stream Compaction** ▼ Prefix Sums **Segmented Prefix Sums Transformed Prefix Sums Set Operations** 

Sorting