An Introduction to CUDA/OpenCL and Manycore Graphics Processors

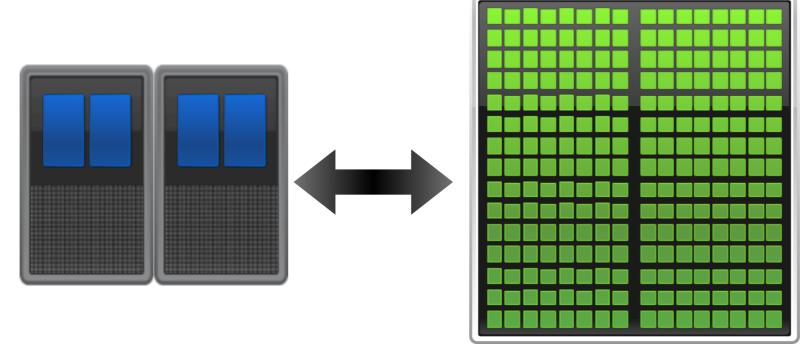
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Overview

- Terminology: Multicore, Manycore, SIMD
- The CUDA and OpenCL programming models
- Understanding how CUDA maps to NVIDIA GPUs
- Thrust

Heterogeneous Parallel Computing



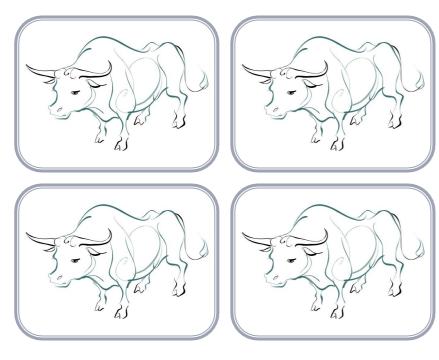
Multicore CPU

Fast Serial Processing

Manycore GPU

Scalable Parallel Processing

Multicore and Manycore



Multicore

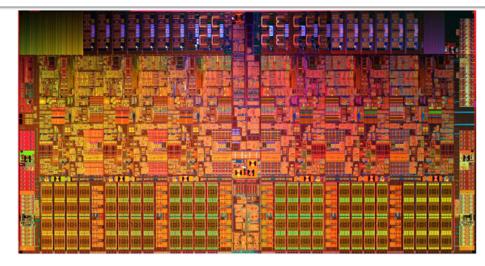


Manycore

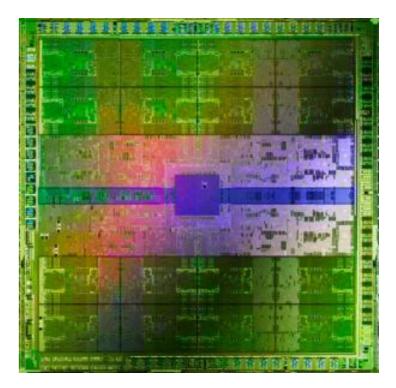
- Multicore: yoke of oxen
 - Each core optimized for executing a single thread
- Manycore: flock of chickens
 - Cores optimized for aggregate throughput, deemphasizing individual performance
- (apologies to Seymour Cray)

Multicore & Manycore, cont.

Specifications	Westmere-EP	Fermi (Tesla C2050)
Processing Elements	6 cores, 2 issue, 4 way SIMD @3.46 GHz	14 SMs, 2 issue, 16 way SIMD @1.15 GHz
Resident Strands/ Threads (max)	6 cores, 2 threads, 4 way SIMD: 48 strands	14 SMs, 48 SIMD vectors, 32 way SIMD: 21504 threads
SP GFLOP/s	166	1030
Memory Bandwidth	32 GB/s	144 GB/s
Register File	6 kB (?)	1.75 MB
Local Store/L1 Cache	192 kB	896 kB
L2 Cache	1536 kB	0.75 MB
L3 Cache	12 MB	-



Westmere-EP (32nm)

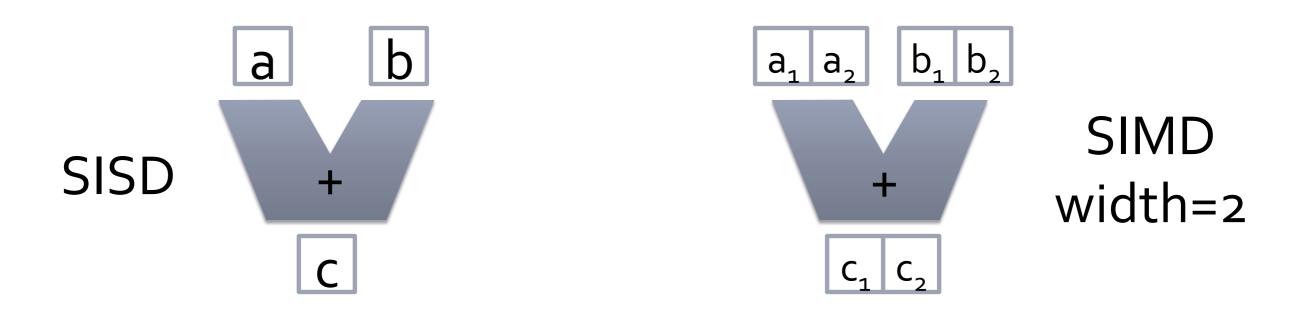


Fermi (40nm)

Why Heterogeneity?

- Different goals produce different designs
 - Manycore assumes work load is highly parallel
 - Multicore must be good at everything, parallel or not
- Multicore: minimize latency experienced by 1 thread
 - lots of big on-chip caches
 - extremely sophisticated control
- Manycore: maximize throughput of all threads
 - lots of big ALUs
 - multithreading can hide latency ... so skip the big caches
 - simpler control, cost amortized over ALUs via SIMD

SIMD

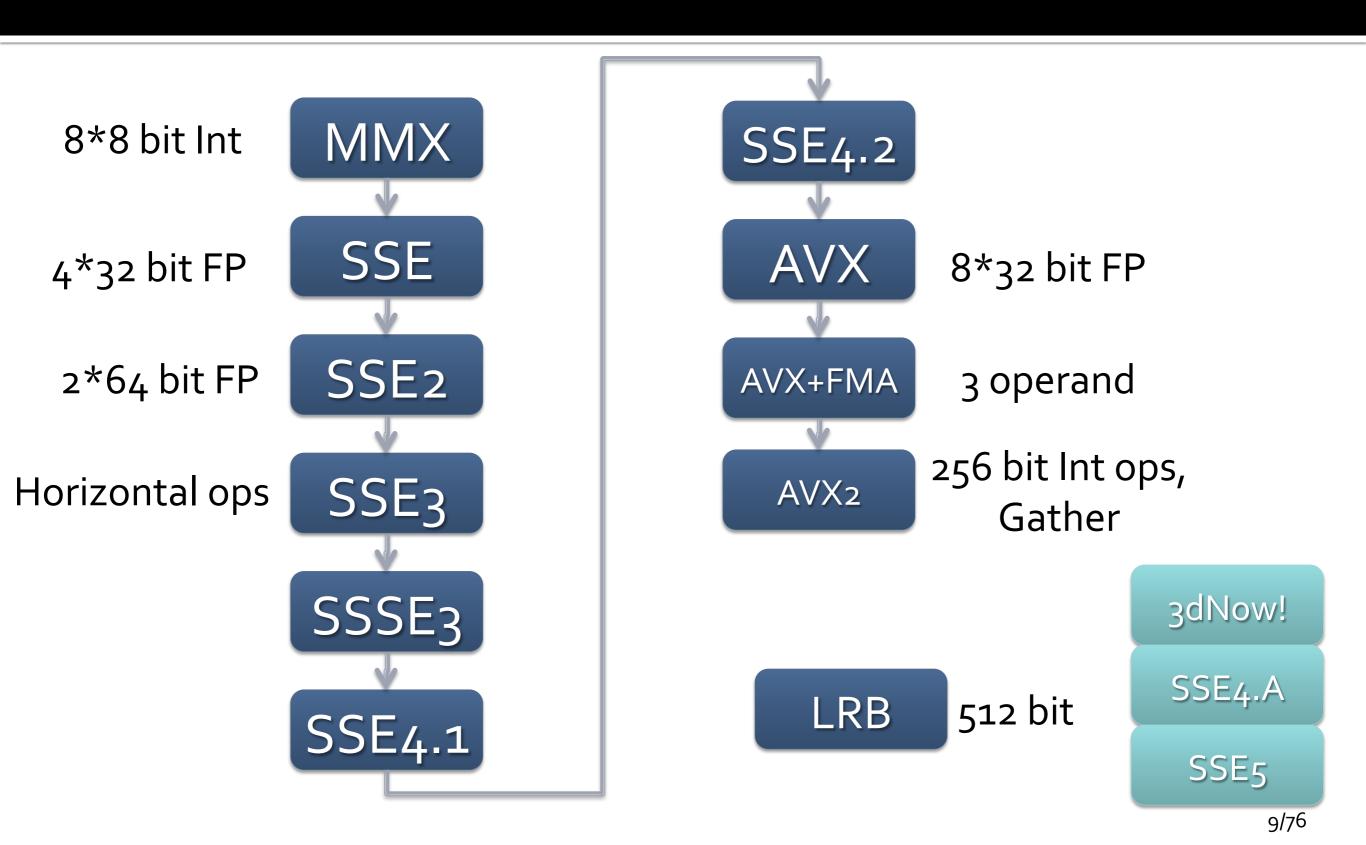


- Single Instruction Multiple Data architectures make use of data parallelism
- We care about SIMD because of area and power efficiency concerns
 - Amortize control overhead over SIMD width
- Parallelism exposed to programmer & compiler

SIMD: Neglected Parallelism

- OpenMP / Pthreads / MPI all neglect SIMD parallelism
- Because it is difficult for a compiler to exploit SIMD
- How do you deal with sparse data & branches?
 - Many languages (like C) are difficult to vectorize
- Most common solution:
 - Either forget about SIMD
 - Pray the autovectorizer likes you
 - Or instantiate intrinsics (assembly language)
 - Requires a new code version for every SIMD extension

A Brief History of x86 SIMD Extensions



What to do with SIMD?



4 way SIMD (SSE)

16 way SIMD (LRB)

- Neglecting SIMD is becoming more expensive
 - AVX: 8 way SIMD, Larrabee: 16 way SIMD,
 Nvidia: 32 way SIMD, ATI: 64 way SIMD
- This problem composes with thread level parallelism
- We need a programming model which addresses both problems

The CUDA Programming Model

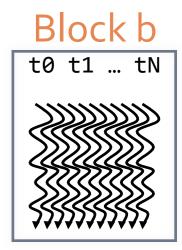
- CUDA is a programming model designed for:
 - Manycore architectures
 - Wide SIMD parallelism
 - Scalability
- CUDA provides:
 - A thread abstraction to deal with SIMD
 - Synchronization & data sharing between small groups of threads
- CUDA programs are written in C++ with minimal extensions
- OpenCL is inspired by CUDA, but HW & SW vendor neutral
 - Similar programming model, C only for device code

Hierarchy of Concurrent Threads

- Parallel kernels composed of many threads
 - all threads execute the same sequential program



- Threads are grouped into thread blocks
 - threads in the same block can cooperate



Threads/blocks have unique IDs

What is a CUDA Thread?

- Independent thread of execution
 - has its own program counter, variables (registers), processor state, etc.
 - no implication about how threads are scheduled

- CUDA threads might be physical threads
 - as mapped onto NVIDIA GPUs
- CUDA threads might be virtual threads
 - might pick 1 block = 1 physical thread on multicore CPU

What is a CUDA Thread Block?

- Thread block = a (data) parallel task
 - all blocks in kernel have the same entry point
 - but may execute any code they want

- Thread blocks of kernel must be independent tasks
 - program valid for any interleaving of block executions

CUDA Supports:

- Thread parallelism
 - each thread is an independent thread of execution
- Data parallelism
 - across threads in a block
 - across blocks in a kernel
- Task parallelism
 - different blocks are independent
 - independent kernels executing in separate streams

Synchronization

Threads within a block may synchronize with barriers

```
... Step 1 ...
__syncthreads();
... Step 2 ...
```

- Blocks coordinate via atomic memory operations
 - e.g., increment shared queue pointer with atomicInc()
- Implicit barrier between dependent kernels

```
vec_minus<<<nblocks, blksize>>>(a, b, c);

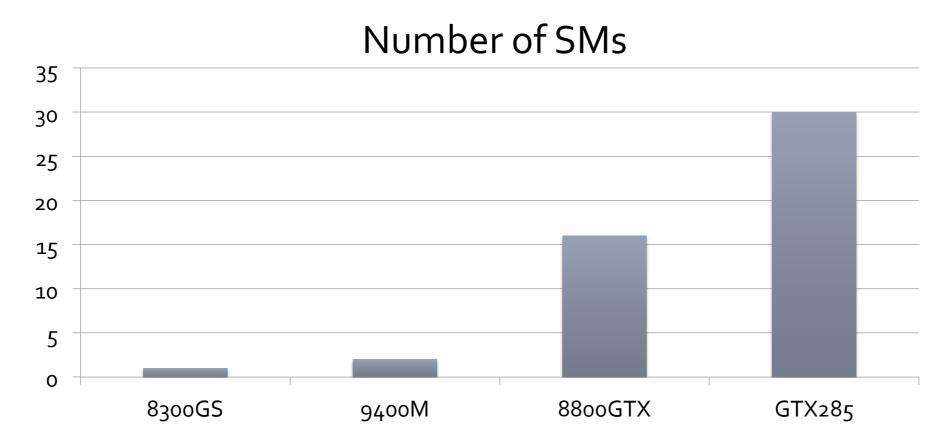
vec_dot<<<nblocks, blksize>>>(c, c);
```

Blocks must be independent

- Any possible interleaving of blocks should be valid
 - presumed to run to completion without pre-emption
 - can run in any order
 - can run concurrently OR sequentially
- Blocks may coordinate but not synchronize
 - shared queue pointer: OK
 - shared lock: BAD ... can easily deadlock
- Independence requirement gives scalability

Scalability

Manycore chips exist in a diverse set of configurations



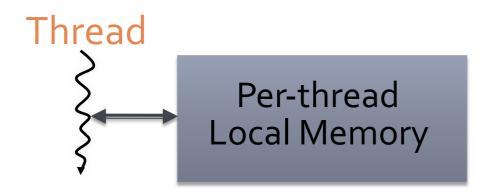
- CUDA allows one binary to target all these chips
- Thread blocks bring scalability!

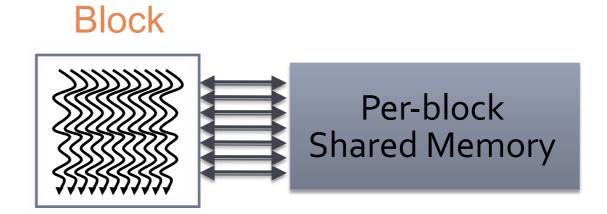
Hello World: Vector Addition

```
//Compute vector sum C=A+B
//Each thread performs one pairwise addition
_global__ void vecAdd(float* a, float* b, float* c) {
  int i = blockIdx.x * blockDim.x + threadIdx.x;
  c[i] = a[i] + b[i];
}

int main() {
  //Run N/256 blocks of 256 threads each
  vecAdd<<<<N/256, 256>>>(d_a, d_b, d_c);
}
```

Memory model





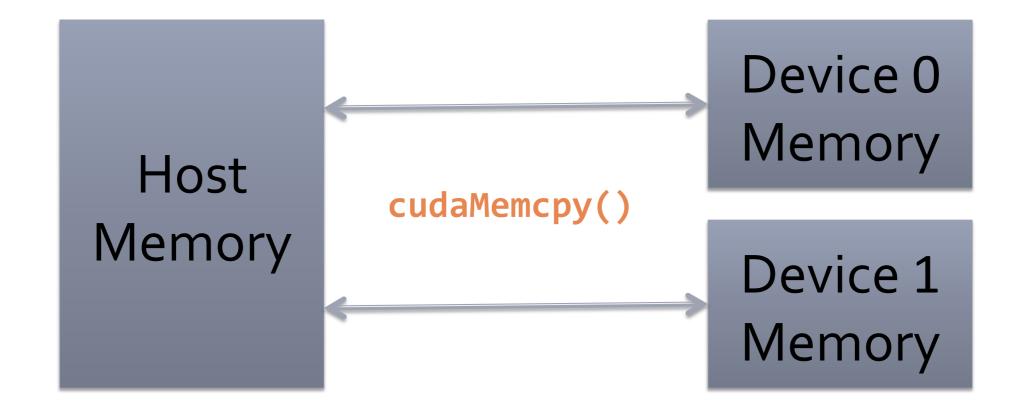
Memory model

Sequential Kernels

Kernel o

Per Device
Global
Memory

Memory model



Hello World: Managing Data

```
int main() {
  int N = 256 * 1024;
  float* h_a = malloc(sizeof(float) * N);
  //Similarly for h_b, h_c. Initialize h_a, h_b
  float *d_a, *d_b, *d_c;
  cudaMalloc(&d a, sizeof(float) * N);
  //Similarly for d b, d c
  cudaMemcpy(d_a, h_a, sizeof(float) * N, cudaMemcpyHostToDevice);
  //Similarly for d b
  //Run N/256 blocks of 256 threads each
  vecAdd<<<N/256, 256>>>(d_a, d_b, d_c);
  cudaMemcpy(h_c, d_c, sizeof(float) * N, cudaMemcpyDeviceToHost);
```

CUDA: Minimal extensions to C/C++

Declaration specifiers to indicate where things live

```
__global__ void KernelFunc(...); // kernel callable from host device__ void DeviceFunc(...); // function callable on device device__ int GlobalVar; // variable in device memory shared__ int SharedVar; // in per-block shared memory
```

- Extend function invocation syntax for parallel kernel launch KernelFunc<<<500, 128>>>(...); // 500 blocks, 128 threads each
- Special variables for thread identification in kernels dim3 threadIdx; dim3 blockIdx; dim3 blockDim;
- Intrinsics that expose specific operations in kernel code __syncthreads(); // barrier synchronization

Using per-block shared memory

Variables shared across block

```
__shared__ int *begin, *end;
```

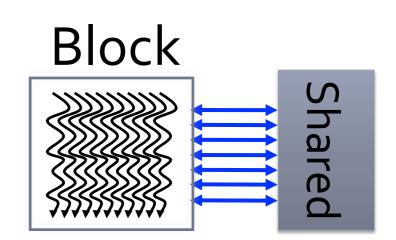
Scratchpad memory

```
__shared__ int scratch[BLOCKSIZE];
scratch[threadIdx.x] = begin[threadIdx.x];
// ... compute on scratch values ...
begin[threadIdx.x] = scratch[threadIdx.x];
```

Communicating values between threads

```
scratch[threadIdx.x] = begin[threadIdx.x];
__syncthreads();
int left = scratch[threadIdx.x - 1];
```

- Per-block shared memory is faster than L1 cache, slower than register file
- It is relatively small: register file is 2-4x larger



CUDA: Features available on GPU

Double and single precision (IEEE compliant)

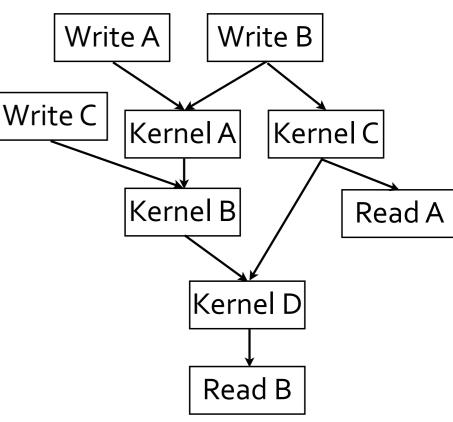
- Standard mathematical functions
 - sinf, powf, atanf, ceil, min, sqrtf, etc.
- Atomic memory operations
 - atomicAdd, atomicMin, atomicAnd, atomicCAS, etc.
- These work on both global and shared memory

CUDA: Runtime support

- Explicit memory allocation returns pointers to GPU memory
 - cudaMalloc(), cudaFree()
- Explicit memory copy for host ↔ device, device ↔ device
 - cudaMemcpy(), cudaMemcpy2D(), ...
- Texture management
 - cudaBindTexture(), cudaBindTextureToArray(), ...
- OpenGL & DirectX interoperability
 - cudaGLMapBufferObject(), cudaD3D9MapVertexBuffer(), ...

OpenCL

- OpenCL is supported by AMD {CPUs, GPUs} and Nvidia
 - Intel, Imagination Technologies (purveyor of GPUs for iPhone/OMAP/etc.) are also on board
- OpenCL's data parallel execution model mirrors CUDA,
 but with different terminology
- OpenCL has rich task parallelism model
 - Runtime walks a dependence DAG of kernels/memory transfers



CUDA and OpenCL correspondence

Thread Work-item Work-group Thread-block Global memory Global memory Constant memoryConstant memory Shared memory Local memory Local memory Private memory kernel function global function device functionno qualification needed __constant__ variable__constant variable device__ variableglobal variable

OpenCL and SIMD

- SIMD issues are handled separately by each runtime
- AMD GPU Runtime
 - Vectorize over 64-way SIMD, but not over 4/5-way VLIW
 - Use float4 vectors in your code
- AMD CPU Runtime
 - No vectorization
 - Use float4 vectors in your code (float8 when AVX appears?)
- Intel CPU Runtime
 - Vectorization optional, using float4/float8 vectors still good idea
- Nvidia GPU Runtime
 - Full vectorization, like CUDA
 - Prefers scalar code per work-item

Imperatives for Efficient CUDA Code

- Expose abundant fine-grained parallelism
 - need 1000's of threads for full utilization
- Maximize on-chip work
 - on-chip memory orders of magnitude faster
- Minimize execution divergence
 - SIMT execution of threads in 32-thread warps
- Minimize memory divergence
 - warp loads and consumes complete 128-byte cache line

Mapping CUDA to Nvidia GPUs

- CUDA is designed to be functionally forgiving
 - First priority: make things work. Second: get performance.
- However, to get good performance, one must understand how CUDA is mapped to Nvidia GPUs
- Threads: each thread is a SIMD vector lane
- Warps: A SIMD instruction acts on a "warp"
 - Warp width is 32 elements: LOGICAL SIMD width
- Thread blocks: Each thread block is scheduled onto an SM
 - Peak efficiency requires multiple thread blocks per SM

Mapping CUDA to a GPU, continued

- The GPU is very deeply pipelined to maximize throughput
- This means that performance depends on the number of thread blocks which can be allocated on a processor
- Therefore, resource usage costs performance:
 - More registers => Fewer thread blocks
 - More shared memory usage => Fewer thread blocks
- It is often worth trying to reduce register count in order to get more thread blocks to fit on the chip
 - For Fermi, target 20 registers or less per thread for full occupancy

Occupancy (Constants for Fermi)

- The Runtime tries to fit as many thread blocks simultaneously as possible on to an SM
 - The number of simultaneous thread blocks (B) is ≤ 8
- The number of warps per thread block (T) ≤ 32
- Each SM has scheduler space for 48 warps (W)
 - $B * T \le W = 48$
- The number of threads per warp (V) is 32
- B * T * V * Registers per thread ≤ 32768
- B * Shared memory (bytes) per block ≤ 49152/16384
 - Depending on Shared memory/L1 cache configuration
- Occupancy is reported as B * T / W

SIMD & Control Flow

- Nvidia GPU hardware handles control flow divergence and reconvergence
 - Write scalar SIMD code, the hardware schedules the SIMD execution
 - One caveat: __syncthreads() can't appear in a divergent path
 - This will cause programs to hang
 - Good performing code will try to keep the execution convergent within a warp
 - Warp divergence only costs because of a finite instruction cache

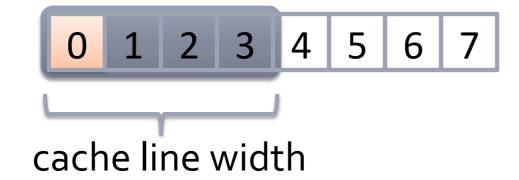
Memory, Memory, Memory



- Lots of processors, only one socket
- Memory concerns dominate performance tuning

Memory is SIMD too

Virtually all processors have SIMD memory subsystems



- This has two effects:
 - Sparse access wastes bandwidth



2 words used, 8 words loaded: 1/4 effective bandwidth

Unaligned access wastes bandwidth

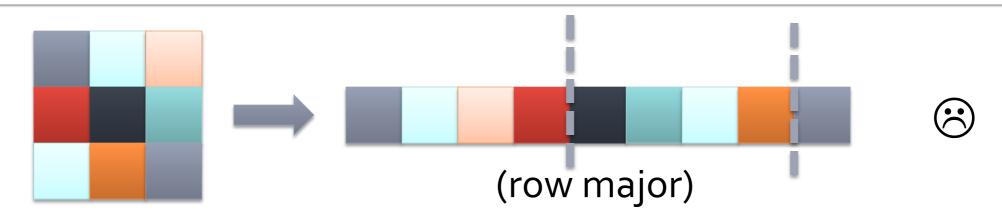


4 words used, 8 words loaded: 1/2 effective bandwidth

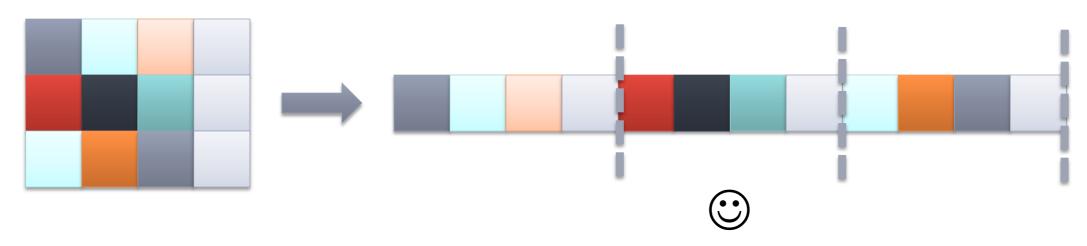
Coalescing

- GPUs and CPUs both perform memory transactions at a larger granularity than the program requests ("cache line")
- GPUs have a "coalescer", which examines memory requests dynamically and coalesces them
- To use bandwidth effectively, when threads load, they should:
 - Present a set of unit strided loads (dense accesses)
 - Keep sets of loads aligned to vector boundaries

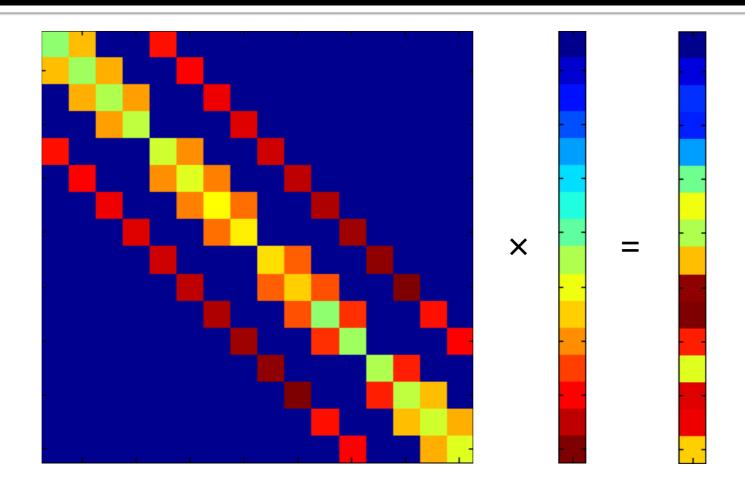
Data Structure Padding



- Multidimensional arrays are usually stored as monolithic vectors in memory
- Care should be taken to assure aligned memory accesses for the necessary access pattern

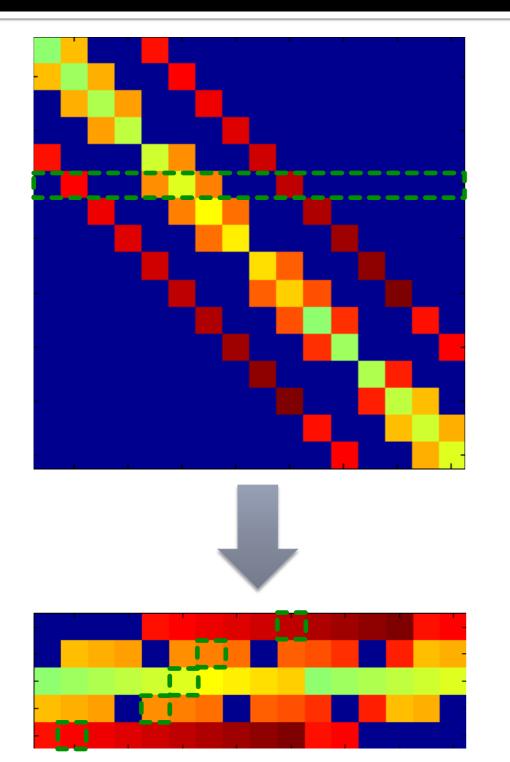


Sparse Matrix Vector Multiply



- Problem: Sparse Matrix Vector Multiplication
- How should we represent the matrix?
 - Can we take advantage of any structure in this matrix?

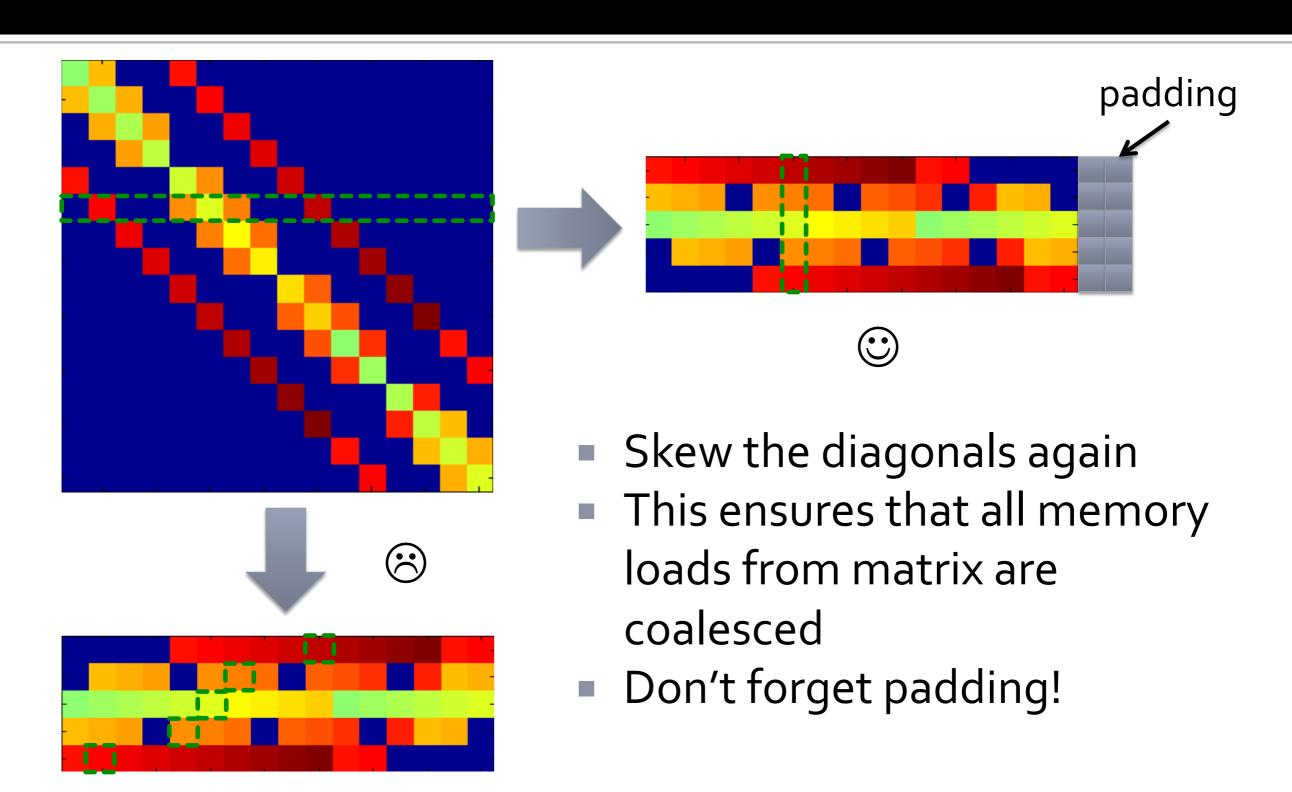
Diagonal representation



- Since this matrix has nonzeros only on diagonals, let's project the diagonals into vectors
- Sparse representation becomes dense
- Launch a thread per row
- Are we done?

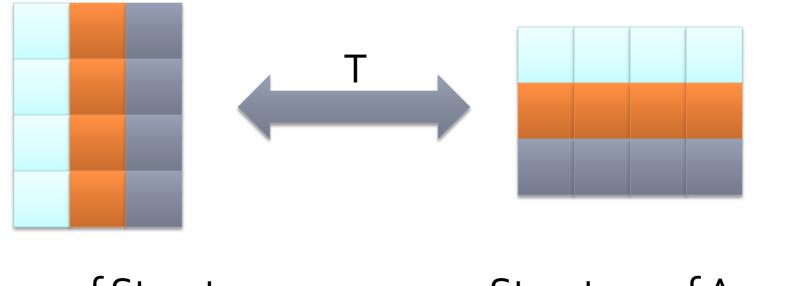
 The straightforward diagonal projection is not aligned

Optimized Diagonal Representation



SoA, AoS

 Different data access patterns may also require transposing data structures



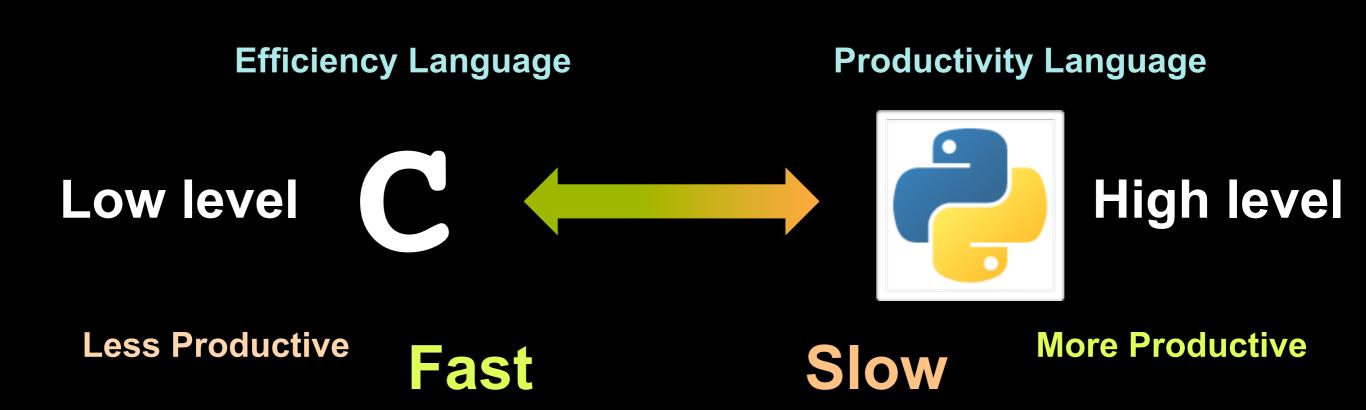
Array of Structs Structure of Arrays

- The cost of a transpose on the data structure is often much less than the cost of uncoalesced memory accesses
- Use shared memory to handle block transposes

Certainties: Death and Taxes



- Productivity is often in tension with efficiency
 - This is often called the "abstraction tax"



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The Concrete Tax



- Parallel programming also gives us a "concrete tax"
 - How many of you have tried to write ... which is faster than a vendor supplied library?

FFT SGEMM

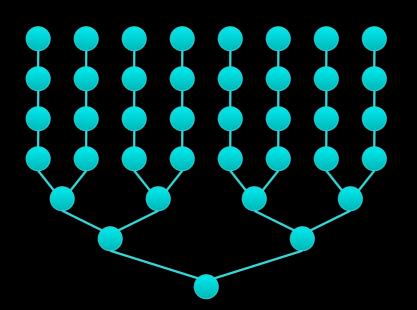
Sort Scan Reduce

- Divergent Parallel Architectures means performance portability is increasingly elusive
- Low-level programming models tie you to a particular piece of hardware
- And if you're like me, often make your code slow
 - My SGEMM isn't as good as NVIDIA's

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The Concrete Tax: A Case Study

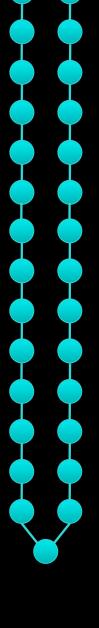




Wide Parallel
Reduction
(good for GPU)

Narrow Parallel Reduction (good for CPU)

- OpenCL experiment on CPU and GPU
- Two optimized reductions, one for CPU, one for GPU
- Running GPU code on CPU:
 - 40X performance loss compared to CPU optimized code
- Running CPU on GPU:
 - ~100X performance loss compared to GPU optimized code
- Concrete code led to overspecialization



Abstraction, cont.



- Reduction is one of the simplest parallel computations
- Performance differentials are even starker as complexity increases
- There's a need for abstractions at many levels
 - Primitive computations (BLAS, Data-parallel primitives)
 - Domain-specific languages
- These abstractions make parallel programming more efficient and more productive

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- A C++ template library for CUDA
 - Mimics the C++ STL
- Containers
 - On host and device
- Algorithms
 - Sorting, reduction, scan, etc.

Diving In



```
#include <thrust/host vector.h>
#include <thrust/device vector.h>
#include <thrust/sort.h>
#include <cstdlib>
int main(void)
    // generate 32M random numbers on the host
    thrust::host vector<int> h vec(32 << 20);</pre>
    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 (846M keys per sec on GeForce GTX 480)
    thrust::sort(d_vec.begin(), d_vec.end());
    // transfer data back to host
    thrust::copy(d_vec.begin(), d_vec.end(), h_vec.begin());
    return 0;
```

Objectives



- Programmer productivity
 - Build complex applications quickly
- Encourage generic programming
 - Leverage parallel primitives
- High performance
 - Efficient mapping to hardware

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Containers



- Concise and readable code
 - Avoids common memory management errors

```
// 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;
// write device values from the host
d \ vec[0] = 13;
d vec[1] = 27;
// read device values from the host
std::cout << "sum: " << d vec[0] + d vec[1] <<
std::endl;
```

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Iterators



Pair of iterators defines a range

```
// allocate device memory
device vector<int> d vec(10);
// declare iterator variables
device vector<int>::iterator begin =
d vec.begin();
device vector<int>::iterator end = d vec.end();
device vector<int>::iterator middle = begin + 5;
// sum first and second halves
int sum half1 = reduce(begin, middle);
int sum half2 = reduce(middle, end);
// empty range
int empty = reduce(begin, begin);
```

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Iterators



Iterators act like pointers

```
// declare iterator variables
device vector<int>::iterator begin = d vec.begin();
device vector<int>::iterator end = d vec.end();
// pointer arithmetic
begin++;
// dereference device iterators from the host
int a = *begin;
int b = begin[3];
// compute size of range [begin,end)
int size = end - begin;
```

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Iterators



- Encode memory location
 - Automatic algorithm selection

```
// initialize random values on host
host_vector<int> h_vec(100);
generate(h_vec.begin(), h_vec.end(), rand);

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

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

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

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Algorithms



- Elementwise operations
 - for each, transform, gather, scatter ...
- Reductions
 - reduce, inner product, reduce by key ...
- Prefix-Sums
 - inclusive_scan, inclusive_scan_by_key...
- Sorting
 - sort, stable_sort, sort_by_key ...

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Algorithms



Standard operators

```
// allocate memory
device_vector<int> A(10);
device_vector<int> B(10);
device_vector<int> C(10);

// transform A + B -> C
transform(A.begin(), A.end(), B.begin(), C.begin(), plus<int>());

// transform A - B -> C
transform(A.begin(), A.end(), B.begin(), C.begin(), minus<int>());

// multiply reduction
int product = reduce(A.begin(), A.end(), 1, multiplies<int>());
```

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Algorithms



Standard data types

```
// allocate device memory
device_vector<int> i_vec = ...
device_vector<float> f_vec = ...

// sum of integers
int i_sum = reduce(i_vec.begin(), i_vec.end());

// sum of floats
float f_sum = reduce(f_vec.begin(),
f_vec.end());
```

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Custom Types & 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 function object or 'functor'
negate float2 func;
// negate vectors
transform(input.begin(), input.end(), output.begin(), func);
```

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Custom Types & Operators



```
// compare x component of two float2 structures
struct compare float2
     host device
   bool operator()(float2 a, float2 b)
       return a.x < b.x;</pre>
// declare storage
device vector<float2> vec = ...
// create comparison functor
compare float2 comp;
// sort elements by x component
sort(vec.begin(), vec.end(), comp);
```

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Interoperability



Convert iterators 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!
```

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Recap

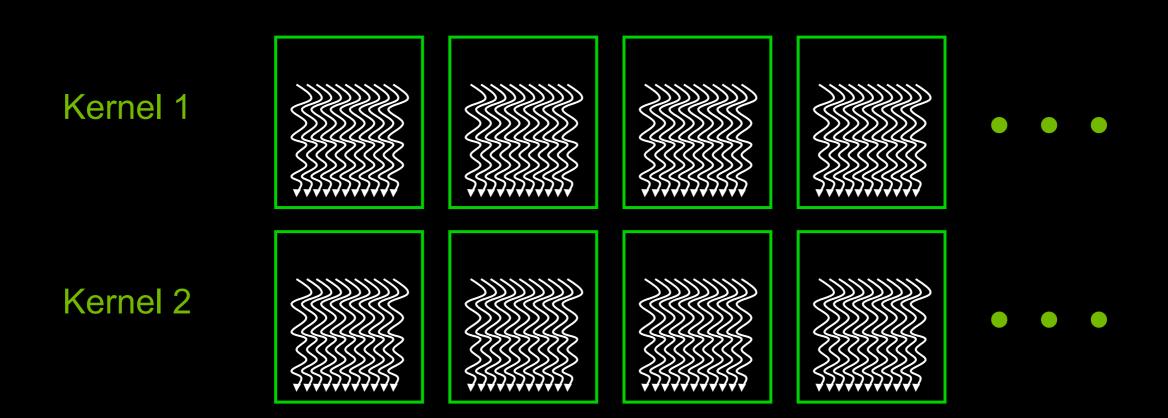


- Containers manage memory
 - Help avoid common errors
- Iterators define ranges
 - Know where data lives
- Algorithms act on ranges
 - Support general types and operators

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- CUDA is explicit
 - Programmer's responsibility to schedule resources.
 - Decompose algorithm into kernels
 - Decompose kernels into blocks
 - Decompose blocks into threads



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SAXPY in CUDA

```
__global__
void SAXPY(int n, float a, float * x, float * y)
{
    int i = blockDim.x * blockIdx.x + threadIdx.x;

    if (i < n)
        y[i] = a * x[i] + y[i];
}
SAXPY <<< n/256, 256 >>> (n, a, x, y);
```

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SAXPY in CUDA

```
global_
void SAXPY(int n, float a, float * x, float * y)
{
    int i = blockDim.x * blockIdx.x + threadIdx.x;

    if (i < n)
        y[i] = a * x[i] + y[i];
}

SAXPY <<< n/256, 256 >>>(n, a, x, y);
```



SAXPY in Thrust

```
// C++ functor replaces global function
struct saxpy
   float a;
   saxpy(float _a) : a(_a) {}
    host device
   float operator()(float x, float y)
       return a * x + y;
};
transform(x.begin(), x.end(), y.begin(), y.begin(),
  saxpv(a)):
```

Implicitly Parallel



- Algorithms expose lots of fine-grained parallelism
 - Generally expose O(N) independent threads of execution
 - Minimal constraints on implementation details
- Programmer identifies opportunities for parallelism
 - Thrust determines explicit decomposition onto hardware
- Finding parallelism in sequential code is hard
 - Mapping parallel computations onto hardware is easier

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Consider a serial reduction

```
// sum reduction
int sum = 0;
for(i = 0; i < n; ++i)
   sum += v[i];</pre>
```



Consider a serial reduction

```
// product reduction
int product = 1;
for(i = 0; i < n; ++i)
  product *= v[i];</pre>
```

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Consider a serial reduction

```
// max reduction
int max = 0;
for(i = 0; i < n; ++i)
   max = std::max(max,v[i]);</pre>
```

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Compare to low-level CUDA

```
int sum = 0;
for(i = 0; i < n; ++i)
  sum += v[i];</pre>
```

```
global
void block sum(const float *input,
               float *per block results,
               const size t n)
           shared float sdata[];
  extern
 unsigned int i = blockIdx.x *
   blockDim.x + threadIdx.x;
  // load input into shared memory
  float x = 0;
 if(i < n)
   x = input[i];
```

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Leveraging Parallel Primitives



Use sort liberally

data type	std::sort	tbb::parallel_sort	thrust::sort
char	25.1	68.3	3532.2
short	15.1	46.8	1741.6
int	10.6	35.1	804.8
long	10.3	34.5	291.4
float	8.7	28.4	819.8
double	8.5	28.2	358.9

Intel Core i7 950

NVIDIA GeForce 480

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Input-Sensitive Optimizations





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Leveraging Parallel Primitives



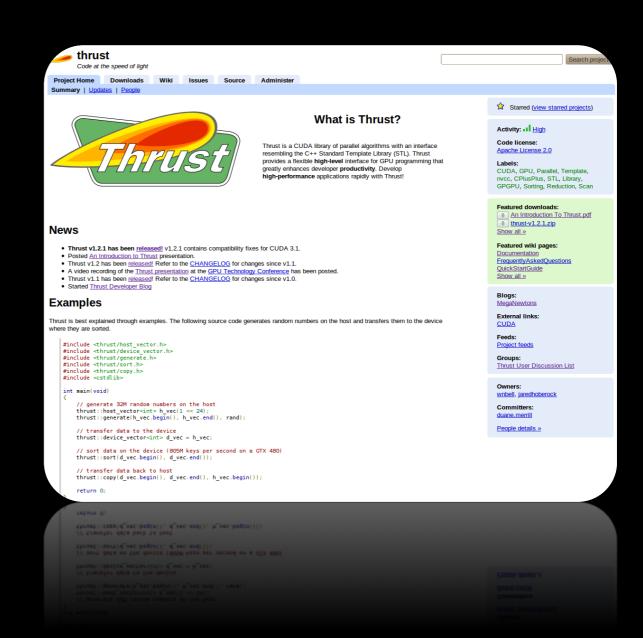
- Combine sort with reduce by key
 - Keyed reduction
 - Bring like items together, collapse
 - Poor man's MapReduce
- Can often be faster than custom solutions
 - I wrote an image histogram routine in CUDA
 - Bit-level optimizations and shared memory atomics
 - Was 2x slower than thrust::sort + thrust::reduce by key

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Thrust on Google Code



- Quick Start Guide
- Examples
- Documentation
- Mailing list (thrust-users)



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Summary

- Manycore processors provide useful parallelism
- Programming models like CUDA and OpenCL enable productive parallel programming
- They abstract SIMD, making it easy to use wide SIMD vectors
- CUDA and OpenCL encourages SIMD friendly, highly scalable algorithm design and implementation
- Thrust is a productive C++ library for CUDA development

Questions?

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