

HOW NOT TO PROGRAM YOUR GPUS.

BASED ON MY DISSERTATION WORK "LOAD BALANCING ON THE GPU"

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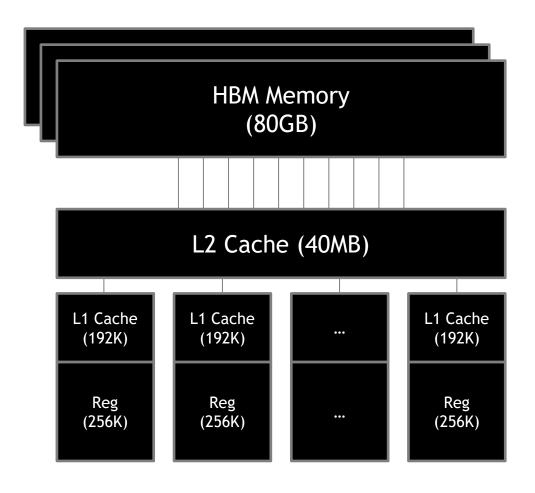
THE 3 PERSPECTIVES

- Programmability,
- Performance, and
- ... everything else

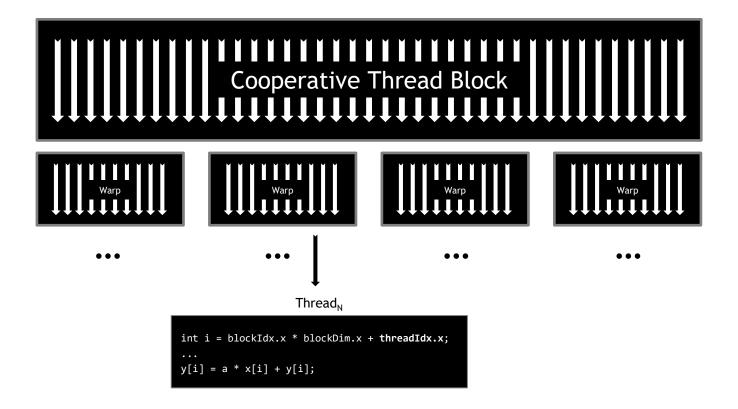
THE 3 PERSPECTIVES

- Programmability,
- Performance, and
- ... everything else (Software Engineering)

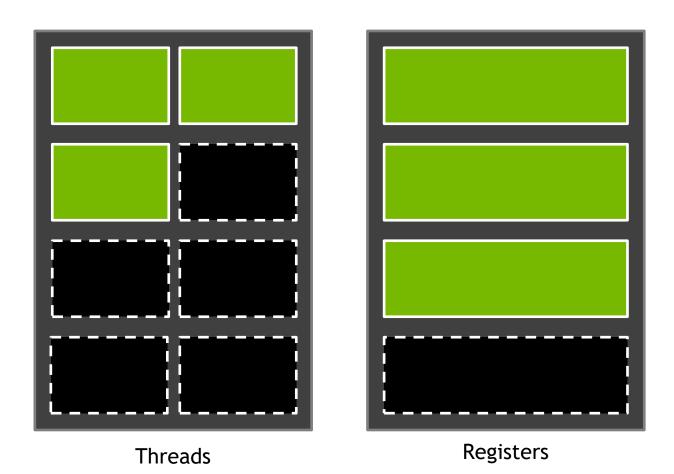
MEMORY SYSTEM

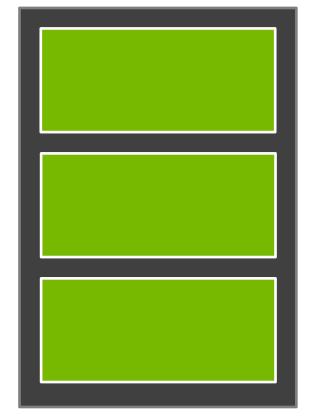


COMPUTE HIERARCHY



OCCUPANCY





Shared Memory

CONCURRENCY



"WHY CUDA PROGRAMMING IS THE WAY IT IS?"

Stephen Jones, CUDA Architect (NVIDIA)

It's all physics.

Memory system is everything.

Occupancy is the next big thing.

Concurrency is saving grace.

... and oversubscription is how we achieve it.

What does that look like? CUDA 101.

```
constexpr int N = 1<<20;</pre>
float* x; float* y;
cudaMalloc(&x, N * sizeof(float));
cudaMalloc(&y, N * sizeof(float));
cudaMemset(x, 1.0f, N * sizeof(float));
cudaMemset(y, 2.0f, N * sizeof(float));
constexpr int block size = 128;
int grid size = (N - block size + 1) / block size;
saxpy<<<grid_size, block_size>>>(N, 2.0f, x, y);
cudaFree(x); cudaFree(y);
```

```
constexpr int N = 1 << 20;
float* x; float* y;
cudaMalloc(&x, N * sizeof(float));
cudaMalloc(&y, N * sizeof(float));
cudaMemset(x, 1.0f, N * sizeof(float));
cudaMemset(y, 2.0f, N * sizeof(float));
constexpr int block size = 128;
int grid_size = (N - block_size + 1) / block_size;
saxpy<<<grid_size, block_size>>>(N, 2.0f, x, y);
cudaFree(x); cudaFree(y);
```

```
global__
void saxpy(const int N, const float a, const float *x, float *y) {
  int i = blockIdx.x * blockDim.x + threadIdx.x;
  if (i < N)
    y[i] = a * x[i] + y[i];</pre>
```

```
__global__
void saxpy(const int N, const float a, const float *x, float *y) {
  int i = blockIdx.x * blockDim.x + threadIdx.x;
  if (i < N)
    y[i] = a * x[i] + y[i];
}</pre>
```

```
__global__
void saxpy(const int N, const float a, const float *x, float *y) {
  int i = blockIdx.x * blockDim.x + threadIdx.x;
  if (i < N)
    y[i] = a * x[i] + y[i];
}</pre>
```

```
__global__
void saxpy(const int N, const float a, const float *x, float *y) {
  int i = blockIdx.x * blockDim.x + threadIdx.x;
  if (i < N)
    y[i] = a * x[i] + y[i];
}</pre>
```



This is great!
No. It's not.

PROBLEMS WITH THIS APPROACH.

Things crash when the grid stride exceeds the device limit.

Errors/Typos in calculating the grid stride (for example, ceil.)

There is no threads reuse, things are being created and destroyed.

You cannot debug by making the problem simpler: 1 thread, 1 block.

Readability (sequential saxpy is not written like the kernel code.)

```
constexpr int N = 1 << 20;
float* x; float* y;
cudaMalloc(&x, N * sizeof(float));
cudaMalloc(&y, N * sizeof(float));
cudaMemset(x, 1.0f, N * sizeof(float));
cudaMemset(y, 2.0f, N * sizeof(float));
constexpr int block size = 128;
int grid_size = (N - block_size + 1) / block_size;
                                                        Exceeds device limit.
saxpy<<<grid_size, block_size>>>(N, 2.0f, x, y);
```

cudaFree(x); cudaFree(y);

```
constexpr int N = 1 << 20;
float* x; float* y;
cudaMalloc(&x, N * sizeof(float));
cudaMalloc(&y, N * sizeof(float));
cudaMemset(x, 1.0f, N * sizeof(float));
cudaMemset(y, 2.0f, N * sizeof(float));
                                       Improper division.
constexpr int block size = 128;
int grid_size = (N - block_size + 1) / block_size;
saxpy<<<grid_size, block_size>>>(N, 2.0f, x, y);
cudaFree(x); cudaFree(y);
```

```
constexpr int N = 1 << 20;
float* x; float* y;
cudaMalloc(&x, N * sizeof(float));
cudaMalloc(&y, N * sizeof(float));
cudaMemset(x, 1.0f, N * sizeof(float));
cudaMemset(y, 2.0f, N * sizeof(float));
constexpr int block size = 128;
int grid_size = ceil_div(N, block_size);
                                             Improper division.
saxpy<<<grid_size, block_size>>>(N, 2.0f, x, y);
cudaFree(x); cudaFree(y);
```

```
constexpr int N = 1 << 20;
float* x; float* y;
cudaMalloc(&x, N * sizeof(float));
cudaMalloc(&y, N * sizeof(float));
cudaMemset(x, 1.0f, N * sizeof(float));
cudaMemset(y, 2.0f, N * sizeof(float));
constexpr int block size = 128;
int grid size = ceil div(N, block size);
saxpy<<<grid_size, block_size>>>(N, 2.0f, x, y);
          Correctness dependent on grid size.
cudaFree(x); cudaFree(y);
```

Correctness dependent on grid size.

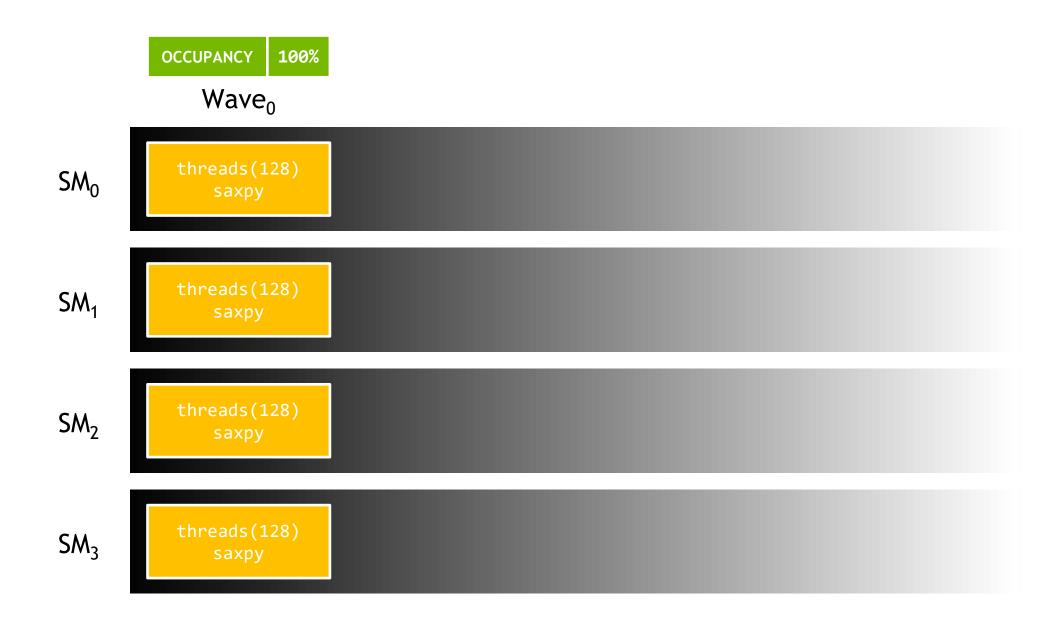
```
constexpr int N = 1 << 20;
float* x; float* y;
cudaMalloc(&x, N * sizeof(float));
cudaMalloc(&y, N * sizeof(float));
cudaMemset(x, 1.0f, N * sizeof(float));
cudaMemset(y, 2.0f, N * sizeof(float));
saxpy <<<1, 1>>>(N, 2.0f, x, y);
cudaFree(x); cudaFree(y);
```

WHAT THE GPU SEES.

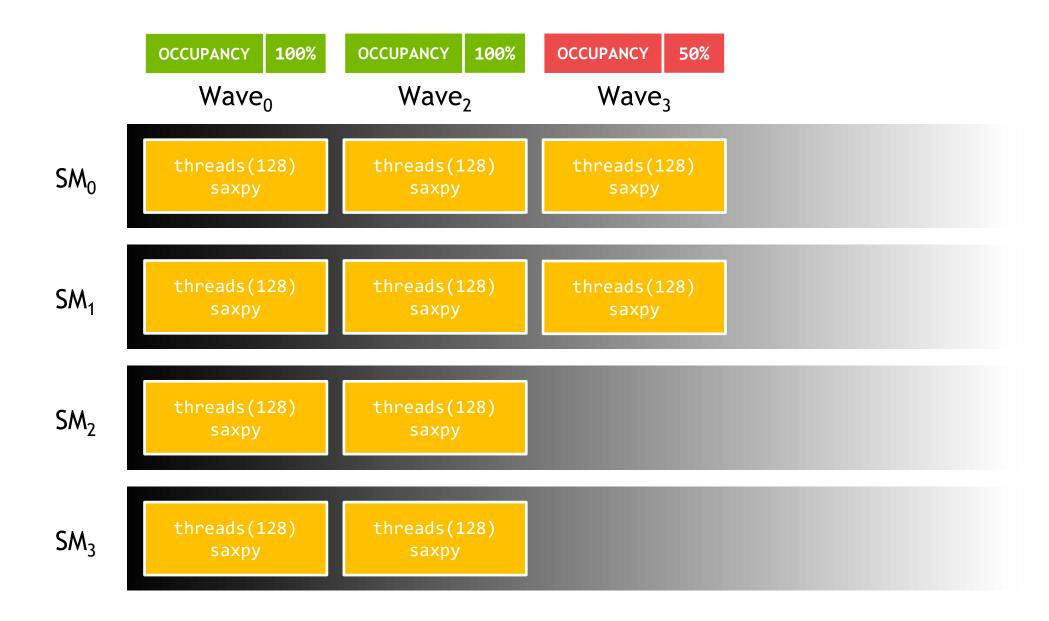
e.g.

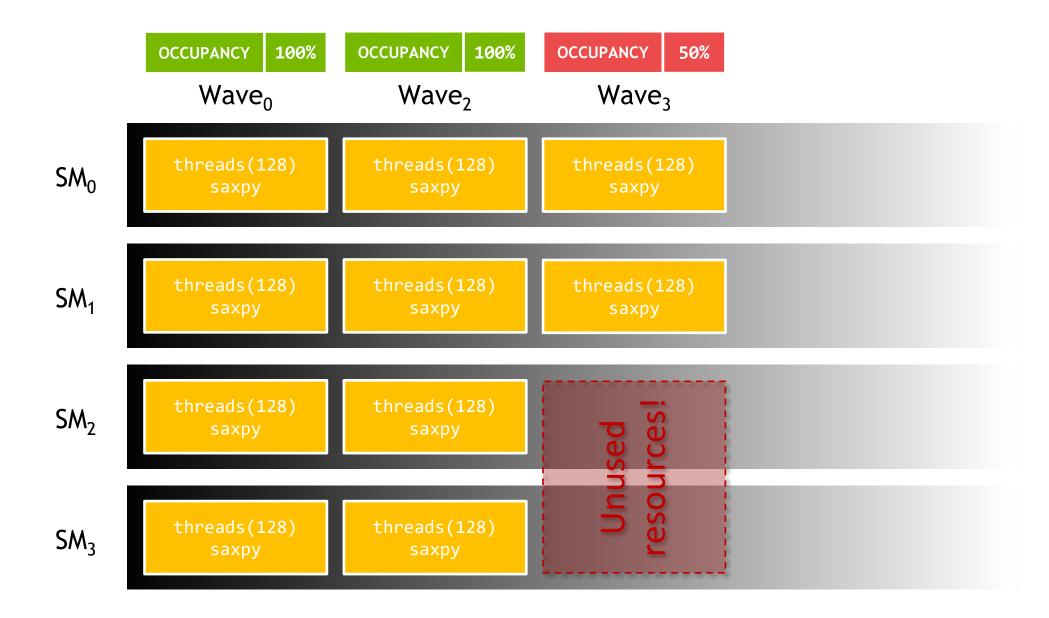
N = **4096** elements

Number of SMs = 4 (hypothetical GPU)









CUDA 201.

```
global__
void saxpy(const int N, const float a, const float *x, float *y) {
  int i = blockIdx.x * blockDim.x + threadIdx.x;
  if (i < N)
    y[i] = a * x[i] + y[i];</pre>
```

THE "GRID STRIDE" LOOP

THE "GRID STRIDE" LOOP

Thread 0

Grid Stride ----

THE "GRID STRIDE" LOOP

```
global
void saxpy(const int N, const float a, const float *x, float *y) {
  for (int i = blockIdx.x * blockDim.x + threadIdx.x;
       i < N;
       i += blockDim.x * gridDim.x) {
    y[i] = a * x[i] + y[i];
                                       Thread 0
            Thread 0
                     Grid Stride
```

"DATA PARALLEL" MODE

```
constexpr int block_size = 128;
int grid_size = ceil_div(N, block_size);
saxpy<<<grid_size, block_size>>>(N, 2.0f, x, y);
```

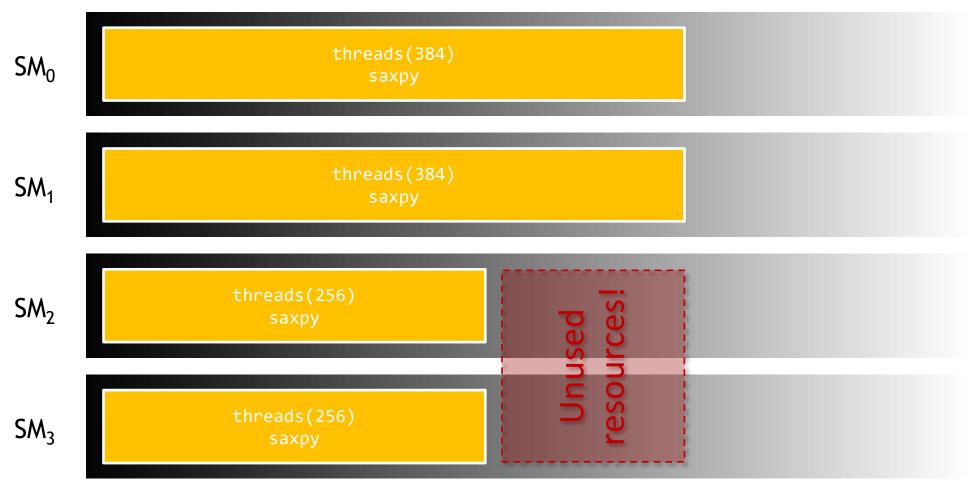
"DEBUG" MODE

```
constexpr int block_size = 128;
int grid_size = 1;
saxpy<<<grid_size, block_size>>>(N, 2.0f, x, y);
```

"..." MODE

```
constexpr int block_size = 128;
int grid_size = 2 * SMs;
saxpy<<<grid_size, block_size>>>(N, 2.0f, x, y);
```





LET'S ILLUSTRATE USING A <u>REAL</u> PROBLEM.

General Matrix-Multiplication (GEMM)



Α

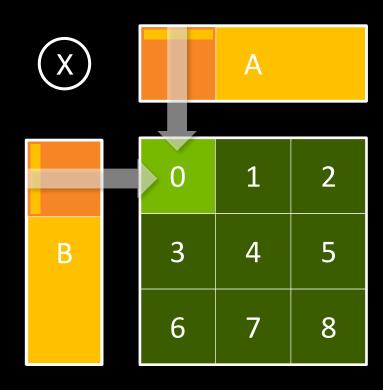


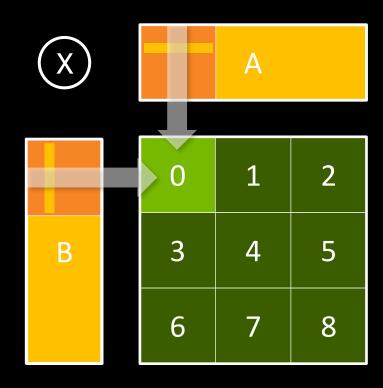
0	1	2
3	4	5
6	7	8

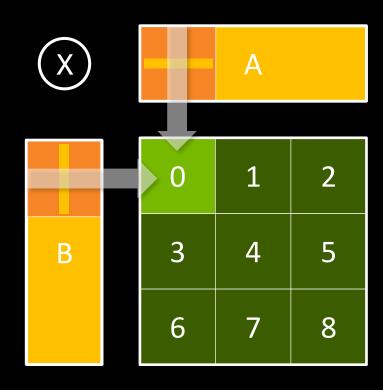
$$C = A \times B$$

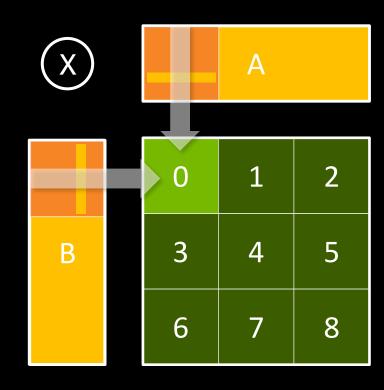
Fine-grained parallelism
Regular workload
Perfect for our memory systems
... but, how do we program it?

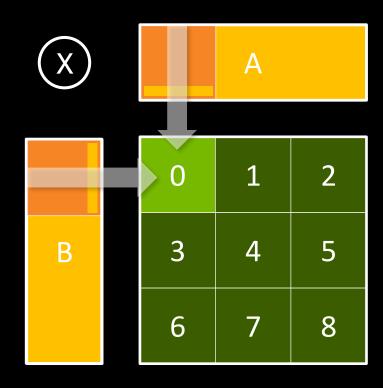
```
accumulator[BLK_M, BLK_K]
iters per tile = [k/BLK_K];
// One output tile per CTA.
fork CTA<sub>[x]</sub> in [[m/BLK_M] x [n/BLK_N]]
  // Perform MAC iterations for this tile.
  accumulator = mac_loop(x, 0, iters per tile);
  // Store accumulators to output tile.
  store_tile(C, x, accumulator);
join
```

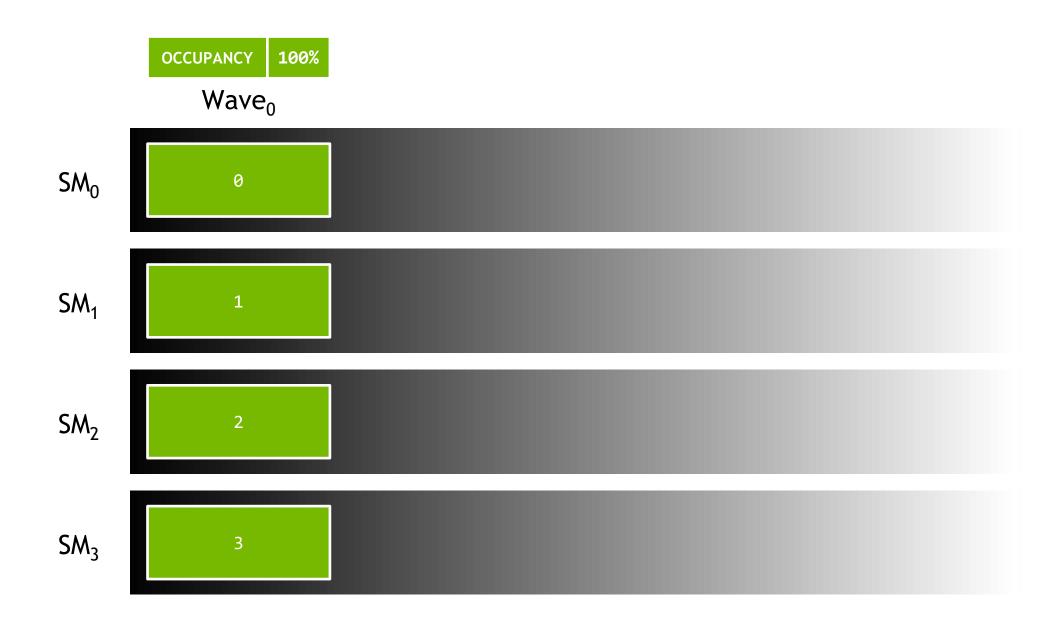






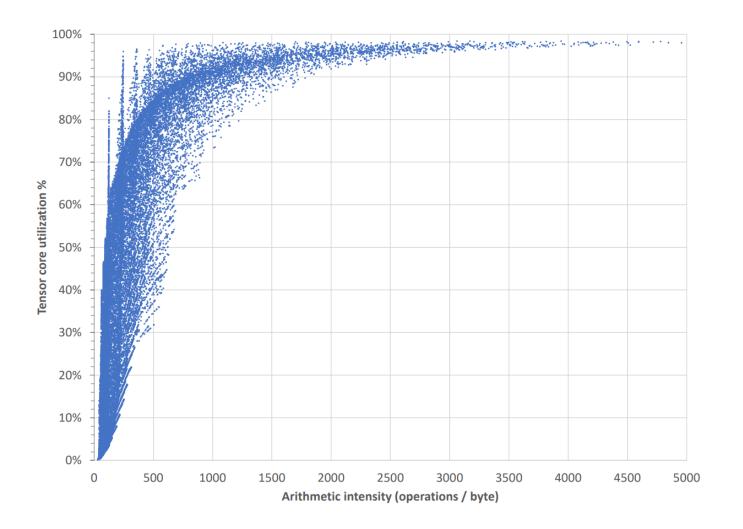








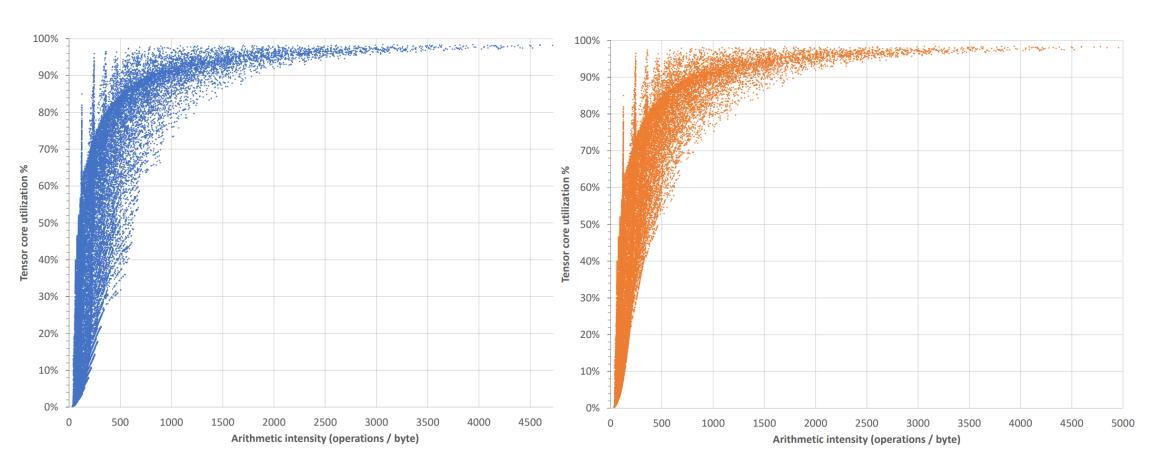




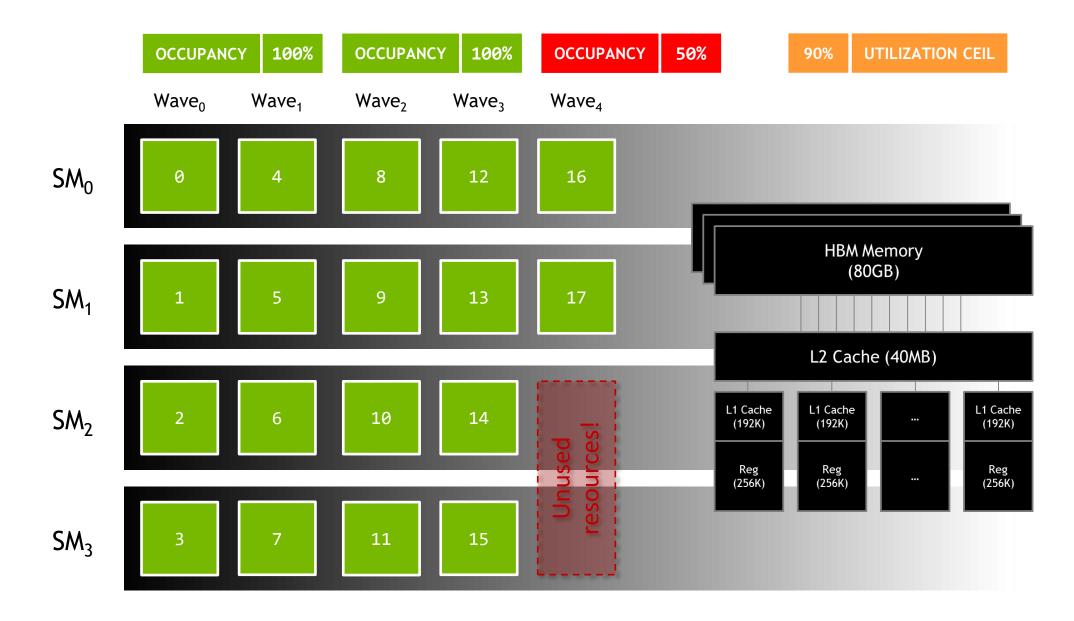
DATA-PARALLEL HGEMM.

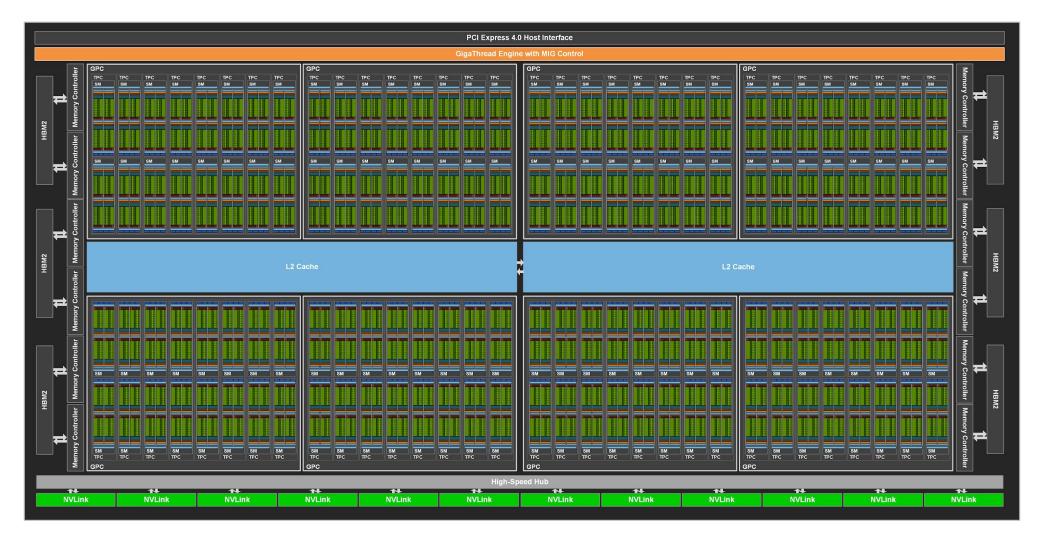






DATA-PARALLEL HGEMM W/ MORE TILE SIZES.





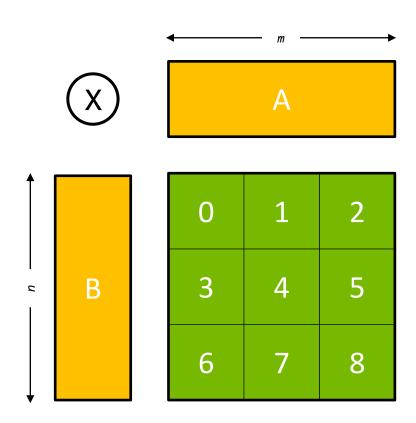
NVIDIA GA100 (128 SMs)

CUDA 201.5

"Work-centric approach" & Programmability

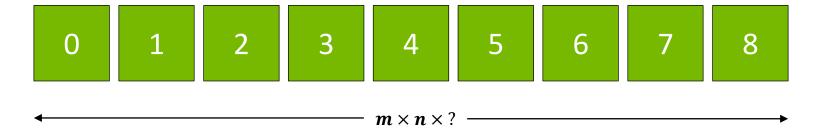
Consider scheduling as a first-class citizen when programming your GPUs.

THE WORK-CENTRIC GEMM.

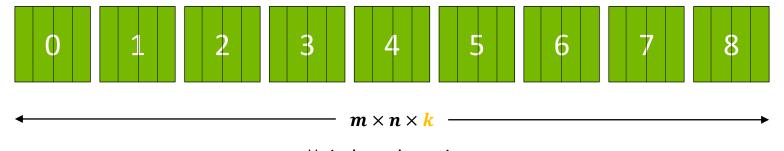


Data-parallel approach, work scheduled: $m \times n$

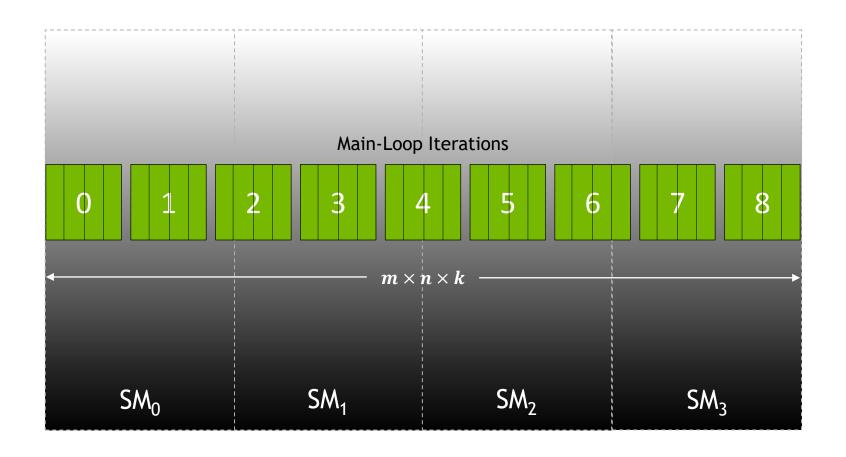
THE WORK-CENTRIC GEMM.

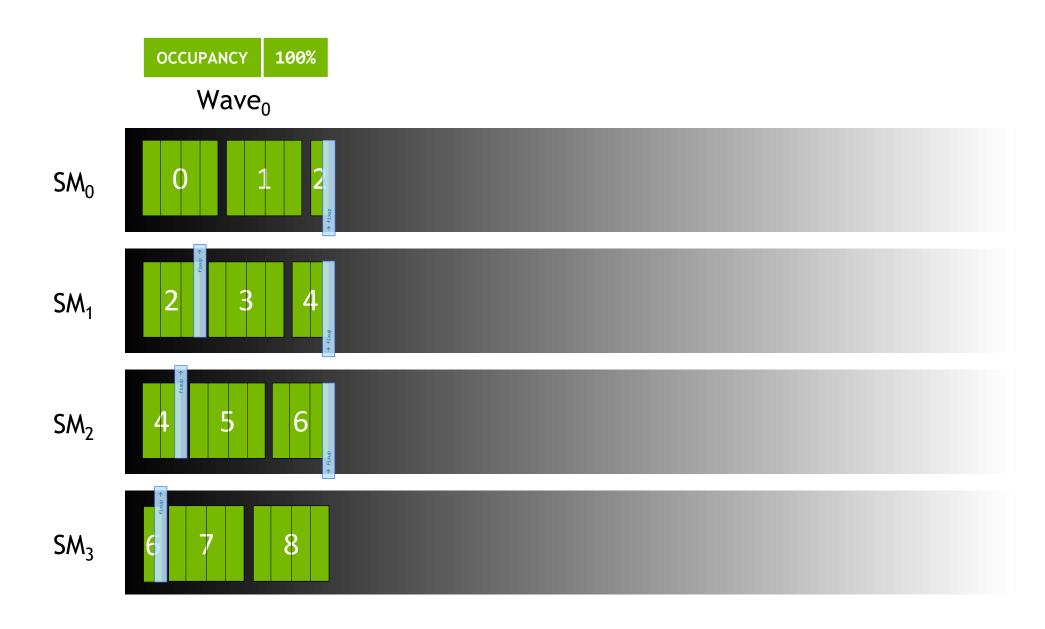


THE WORK-CENTRIC GEMM.



The Work-Centric GEMM.





```
__global__ gemm(...) {
   // The Stream-K work-processing loop
   while (cta_itr < cta_last_itr) {</pre>
        // The standard tile-based GEMM main loop
       accum = gemm_tile(tile_id, cta_itr - tile_first_itr, tile_stop_itr - tile_first_itr);
       if (!started_tile && !finished_tile) {
            // Carry-out partial sums
       } else {
           if (started_tile && !finished_tile) {
               // Carry-in sets of partial sums
            // Produce final output tile
            eplilogue(accum, tile_id);
```

```
__global__ gemm(...) {
   // The Stream-K work-processing loop
   while (cta_itr < cta_last_itr) {</pre>
        // The standard tile-based GEMM main loop
        accum = gemm_tile(tile_id, cta_itr - tile_first_itr, tile_stop_itr - tile_first_itr);
        if (!started_tile && !finished_tile) {
            // Carry-out partial sums
        } else {
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               // Carry-in sets of partial sums
            // Produce final output tile
            eplilogue(accum, tile_id);
```

"DEBUG" MODE

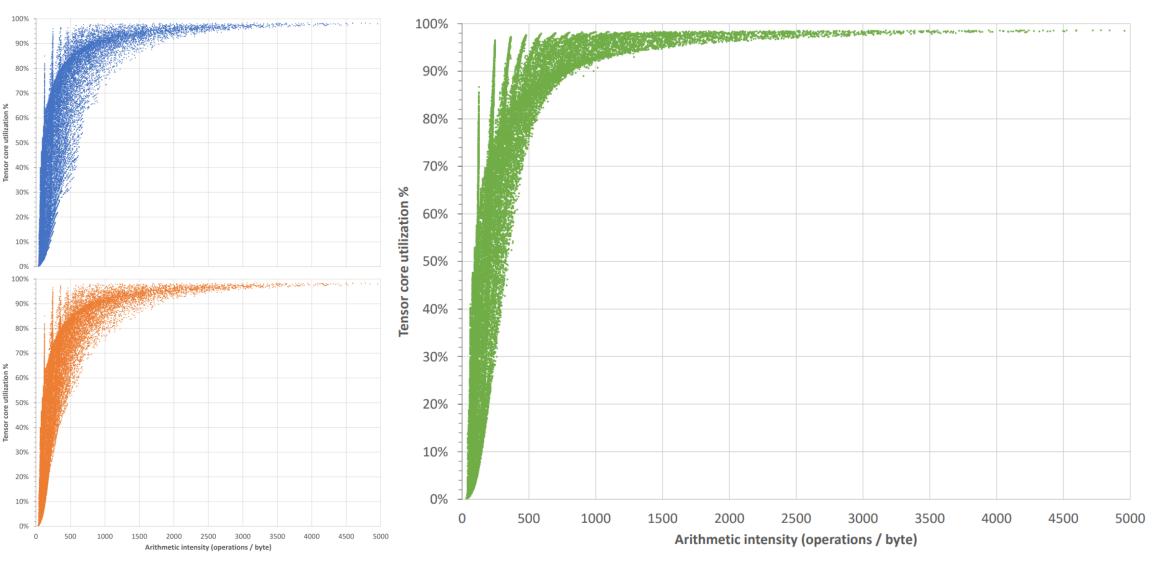
```
constexpr int block_size = 128;
int grid_size = 1;
gemm<<<grid_size, block_size>>>(...);
```

"100% UTILIZATION" MODE

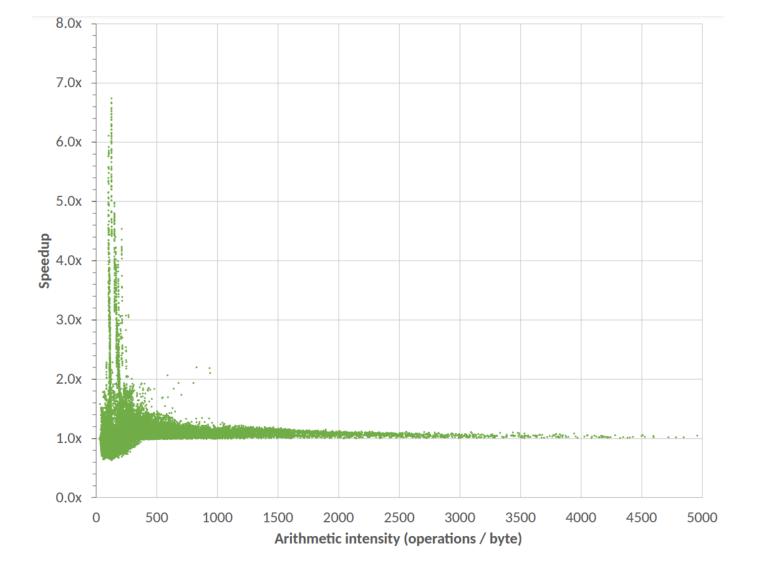
```
constexpr int block_size = 128;
int grid_size = 2 * SMs;
gemm<<<grid_size, block_size>>>(...);
```

"DATA PARALLEL" MODE

```
constexpr int block_size = 128;
int grid_size = num_output_tiles;
gemm<<<grid_size, block_size>>>(...);
```



WORK-CENTRIC HGEMM.



SPEED-UP COMPARED TO CUBLAS.

Generic Programming In CUDA/C++ (1) Lifting

```
__global__
void saxpy(const int N, const float a, const float *x, float *y) {
  for (auto i : ranges::grid_stride_range(0, N)) {
    y[i] = a * x[i] + y[i];
  }
}
```

```
__global__
void saxpy(const int N, const float a, const float *x, float *y) {
  for (auto i : ranges::grid_stride_range(0, N)) {
    y[i] = a * x[i] + y[i];
  }
}
```

```
__global__
void saxpy(const int N, const float a, const float *x, float *y) {
  for (auto i : ranges::grid_stride_range(0, N)) {
    y[i] = a * x[i] + y[i];
  }
}
```

```
__global__
void saxpy(const int N, const float a, const float *x, float *y) {
  for (auto i : ranges::grid_stride_range(0, N)) {
    y[i] = a * x[i] + y[i];
  }
}
```

```
__global__
void saxpy(const int N, const float a, const float *x, float *y) {
  for (auto i : ranges::grid_stride_range(0, N)) {
    y[i] = a * x[i] + y[i];
  }
}
```

```
template <typename T>
   _device__ _forceinline__ step_range_t<T>
   grid_stride_range(T begin, T end) {
   begin += blockIdx.x * blockDim.x + threadIdx.x;
   return range(begin, end).step(blockDim.x * gridDim.x);
}
```

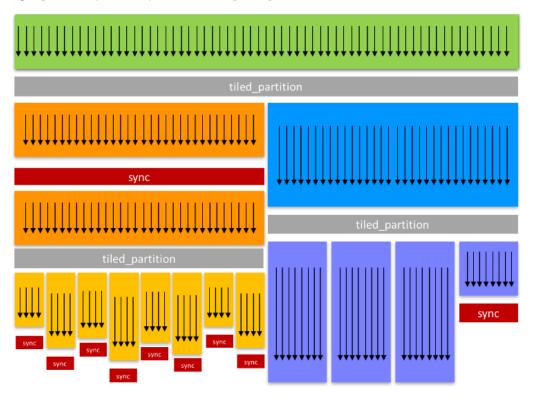
```
template <typename T>
   _device__ _forceinline__ step_range_t<T>
   grid_stride_range(T begin, T end) {
   begin += blockIdx.x * blockDim.x + threadIdx.x;
   return range(begin, end).step(blockDim.x * gridDim.x);
}
```

```
__global__
void saxpy(const int N, const float a, const float *x, float *y) {
  for (auto i : ranges::grid_stride_range(0, N)) {
    y[i] = a * x[i] + y[i];
  }
}
```

Cooperative Groups: Flexible CUDA Thread Programming

By Mark Harris and Kyrylo Perelygin

Tags: Algorithms, Cooperative Groups, CUDA, Parallel Programming



```
/// Loading an integer from global into shared memory
__global__ void kernel(int *globalInput) {
    shared int x;
   thread block g = this thread block();
   // Choose a leader in the thread block
   if (g.thread rank() == 0) {
        // load from global into shared for
        // all threads to work with
       x = (*globalInput);
    // After loading data into shared memory,
    // you want to synchronize if all threads
    // in your thread block need to see it
   g.sync(); // equivalent to syncthreads();
```

Generic Programming In CUDA/C++

(2) Specialization

```
__global__
template<typename type_t, typename size_t>
void saxpy(const size_t N, const type_t a, const type_t *x, type_t *y) {
  for (auto i : ranges::grid_stride_range(0, N)) {
    y[i] = a * x[i] + y[i];
  }
}
```

```
saxpy<float, int><<<grid_size, block_size>>>(N, 2.0f, x, y);
```

```
__global__
void saxpy(const int N, const float a, const float *x, float *y) {
  for (auto i : ranges::grid_stride_range(0, N)) {
    y[i] = a * x[i] + y[i];
  }
}
```

Generic Programming In C++20

(3) Concepts

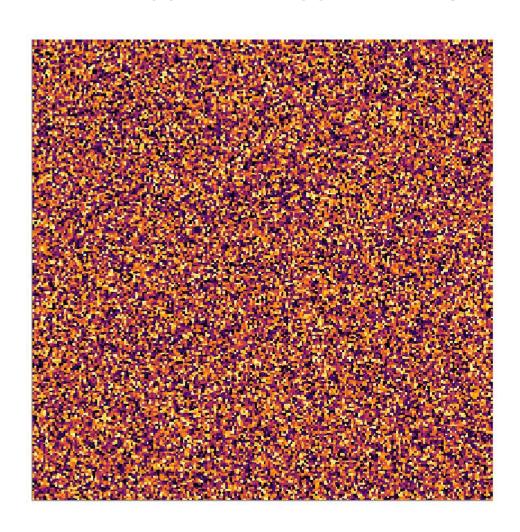
```
__global___
template<typename type_t, typename size_t>
void saxpy(const size_t N, const type_t a, const type_t *x, type_t *y) {
  for (auto i : ranges::grid_stride_range(0, N)) {
    y[i] = a * x[i] + y[i];
  }
    Valid?
}
```

WHY DOES IT MATTER?

- Study existing works.
- "Lift" away unnecessary requirements.
- Repeat the process until we have found generic algorithm.
- Express specializations (types, processes, etc.)
- Catalog requirements (concepts.)

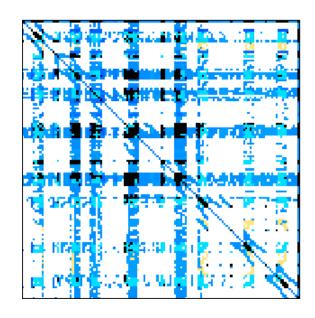
Generic programming is an instrumental process in developing abstractions.

WHAT WE HAVE LOOKED AT SO FAR.

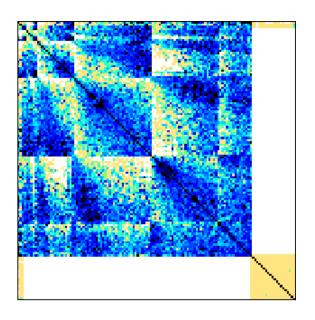


Regular problem. Memory system's heaven. We solved the problem (100% utilization)

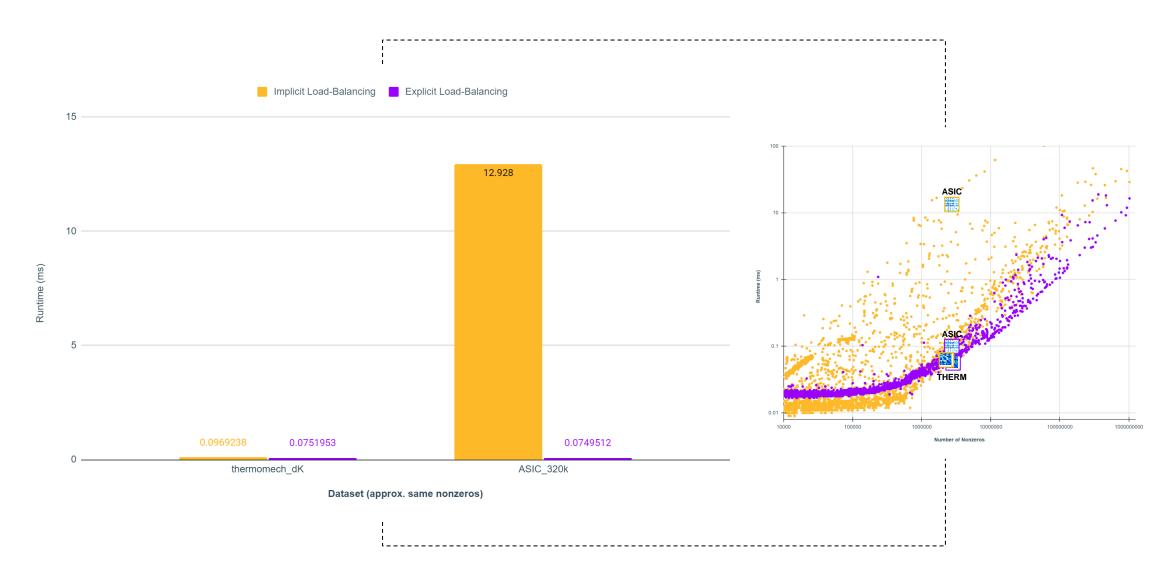
BUT WHAT IF... WORLD ISN'T ALL NICE.



ASIC_320K **Circuit Simulation** 2,635,364 nonzeros



Thermomech_dK Temperature & Deformation 2,846,228 nonzeros



```
Coordinat
    BLOCK
                                                                      If (CubDebug(error = cudaDeviceGetAttribute(Smax dim x, cudaDevAttrBasGridDimX, device ordinal))) break;
     RowOff
                                                                     int num_segment_fixup_tiles - cub::DivideAndRoundUp(num_merge_tiles, segment_fixup_tile_size);
     Offse
                                                                                                                               Load-balance
     Coordi
                                                                        segment fixup am occupancy,
                                                                                                                              configurations
                                                                        segment fixup kernel,
                                                                                                                            and fix-up step
                                                                        CUM_MIN(num_merge_tiles, max_dim_x),
                                                                         cub::DivideAndRoundRofeum merce tiles, man
                                                                        CUB_MIN(now segment fixup tiles, max dim x),
                                                                        cub::DivideAndRoundUp(num segment fixup tiles, max dim x),
                                                                     allocation_sizes[1] = num_merge_tiles * sizeof(KeyWaluePairT); // bytes needed for block carry-out pairs allocation_sizes[2] = (num_merge_tiles + 1) * sizeof(CoordinateT); // bytes needed for tile starting coordinates
                                                                     If (CubDebug(error - AliasTemporaries(d temp storage, temp storage bytes, allocations, allocation sizes))) break;
                                                                      If (d temp storage -- MULL)
                                                                      int search grid size - cub::DivideAndRoundUp(num merge tiles + 1, search block size)
                                                                        If (debug synchronous) Cublog("Invoking spmv search kernel<<Xd, Xd, 0, X11d>>>()\n",
```

```
num_merge_tiles)
                     if (threadIdx.x == 0)
                         scan_item.key = -1;
                                                                                                           SpMV kernel +
                     #pragma unroll
                     for (int ITEM = 0; ITEM < ITEMS PER THREAD; ++ITEM)
                                                                                                           work-oriented
                         if (scan_segment[ITEM].key < tile_num_rows)</pre>
                                                                                                           load-balancing
                             if (scan_item.key == scan_segment[ITEM].key)
                                 scan_segment[ITEM].value = scan_item.value + scan_segment[ITEM].
                             if (HAS ALPHA)
                                 scan_segment[ITEM].value *= spmv_params.alpha;
                              if (HAS_BETA)
                                 scan_segment[ITEM].value += addend;
                              spmv params.d_vector_y[tile_start_coord.x + scan_segment[ITEM].key] = scan_segment[ITEM].value;
                  return tile_carry;
   OffsetT row end offset = s tile row end offsets[thread current coord.x];
   if (tile nonzero indices[thread current coord.v] < row end offset)
     running total += nonzero;
     scan_segment[ITEM].value = running_total;
     scan_segment[ITEM].key - tile_num_rows;
      ++thread_current_coord.y;
     scan_segment[ITEM].value = running_total;
     scan_segment[ITEM].key = thread_current_coord.x;
      ++thread_current_coord.x;
KeyValuePairT tile_carry;
scan item.value - running total;
scan_item.key = thread_current_coord.x;
```

```
#pragma unroll
for (int ITEM = 0; ITEM < ITEMS_PER_THREAD; ++ITEM)</pre>
   OffsetT nonzero_idx
                             = CUB_MIN(tile_nonzero_indices[thread_current_coord.y], spmv_params.num_nonzeros - 1);
   OffsetT column idx
                             = wd column indices[nonzero idx];
   ValueT value
                              = wd_values[nonzero_idx];
   ValueT vector_value
                             = wd_vector_x[column_idx];
   ValueT nonzero
                              = value * vector_value;
                                                                                     Equates to the actual
   OffsetT row_end_offset
                              = s_tile_row_end_offsets[thread_current_coord.x];
                                                                                     computation the user
   if (tile_nonzero_indices[thread_current_coord.y] < row_end_offset)</pre>
                                                                                              wants to do:
                                                                                                    y = Ax
       // Move down (accumulate)
       running_total += nonzero;
       scan_segment[ITEM].value
                                 = running_total;
       scan_segment[ITEM].key
                                 = tile_num_rows;
       ++thread_current_coord.y;
       scan_segment[ITEM].value
                                 = running_total;
       scan_segment[ITEM].key
                                 = thread_current_coord.x;
       running_total
                                 = 0.0;
       ++thread_current_coord.x;
```

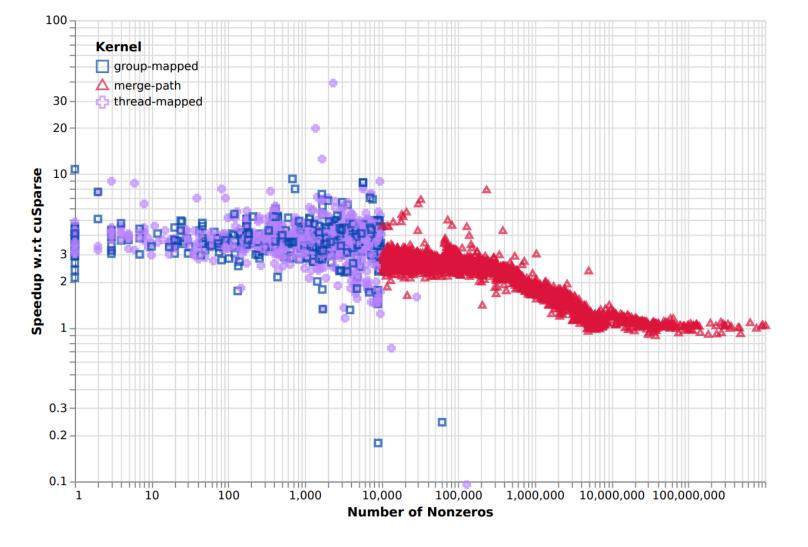
(1) GITHUB.COM/NVIDIA/CUB

```
_global__ void spmv(const csr_t* A, const float *x, float *y) {
using namespace loops;
auto config = setup<schedule::merge path>(
     A->offsets, A->rows, A->nnz);
float temp = 0.0f;
// loop over all assigned tiles
for (auto m : tile::range(config)) {
  // loop over all assigned atoms per tile
  for (auto k : atom::range(config))
    temp += A->values[k] * x[A->indices[k]];
 y[m] = temp;
  temp = 0.0f;
```

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 y[m] = temp;
  temp = 0.0f;
```

```
// return the range of tiles to process
device step range t<tile size t> tiles() const {
    return loops::grid stride range(tile size t(0),
                                    tile traits t::size());
// return the range of atoms to process
__device__ auto atoms(const tile_size_t& tid) const {
    return loops::range(tile_traits_t::begin()[tid],
                        tile_traits_t::begin()[tid + 1]);
```



LOAD BALANCING ABSTRACTED: SPMV

Everything else.

You'll be tempted to write your own "heterogeneous" array (CPU/GPU). Don't.

CUDA error reporting is terrible. Good luck.

Spend a few days learning Nsight (System and Compute).

Don't write your own binary search.

```
constexpr int N = 1<<20;</pre>
float* x; float* y;
cudaMalloc(&x, N * sizeof(float));
cudaMalloc(&y, N * sizeof(float));
cudaMemset(x, 1.0f, N * sizeof(float));
cudaMemset(y, 2.0f, N * sizeof(float));
constexpr int block size = 128;
int grid_size = (N - block_size + 1) / block_size;
saxpy<<<grid_size, block_size>>>(N, 2.0f, x, y);
                             You are going to forget
cudaFree(x); cudaFree(y);
                              to free the memory.
```

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Don't write your own binary search.

```
device host
int binary_search(int* array, int x, int low, int high) {
  while (low <= high) {</pre>
    int mid = (low + high) / 2;
    if (array[mid] == x)
      return mid;
    if (array[mid] < x)</pre>
      low = mid + 1;
    else
      high = mid - \overline{1};
  return -1;
```

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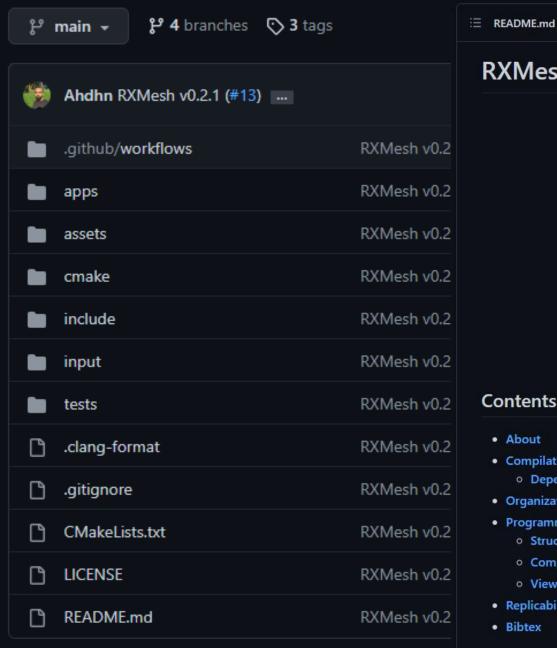
```
device host
int binary_search(int* array, int x, int low, int high) {
  while (low <= high) {</pre>
    int mid = low + (high - low) / 2;
    if (array[mid] == x)
      return mid;
    if (array[mid] < x)</pre>
      low = mid + 1;
    else
      high = mid - \overline{1};
  return -1;
```

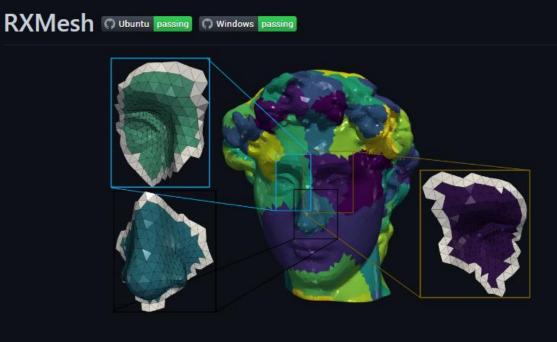
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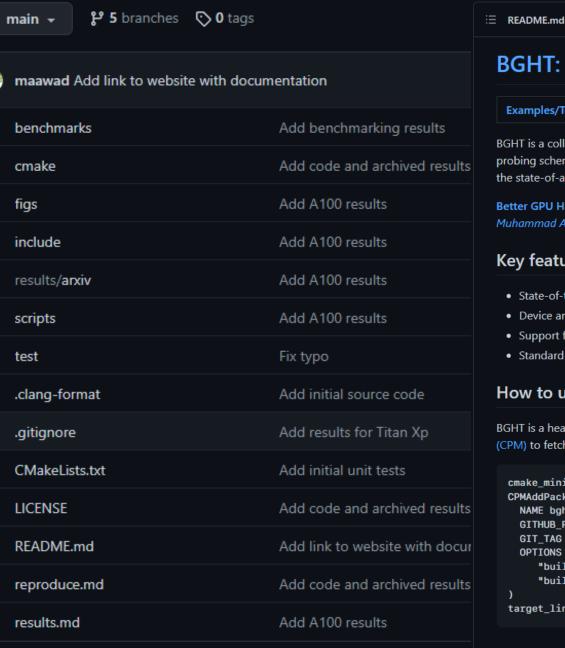
Don't write your own binary search.





Contents

- About
- Compilation
- Dependencies
- Organization
- Programming Model Structures
 - Computation
 - Viewer
- Replicability
- Bibtex



BGHT: Better GPU Hash Tables

Examples/Tests Benchmarks Results

BGHT is a collection of high-performance static GPU hash tables. BGHT contains hash tables that use three different probing schemes 1) bucketed cuckoo, 2) power-of-two, 3) iceberg hashing. Our bucketed static cuckoo hash table is the state-of-art static hash table. For more information, please check our paper:

Better GPU Hash Tables

Muhammad A. Awad, Saman Ashkiani, Serban D. Porumbescu, Martín Farach-Colton, and John D. Owens

Key features

- State-of-the-art static GPU hash tables
- Device and host side APIs
- Support for different types of keys and values
- Standard-like APIs

How to use

BGHT is a header-only library. To use the library, you can add it as a submodule or use CMake Package Manager (CPM) to fetch the library into your CMake-based project (complete example).

```
cmake_minimum_required(VERSION 3.8 FATAL_ERROR)
CPMAddPackage(
  NAME bght
  GITHUB_REPOSITORY owensgroup/BGHT
  GIT_TAG main
  OPTIONS
     "build tests OFF"
     "build benchmarks OFF"
target_link_libraries(my_library PRIVATE bght)
```

https://github.com/neoblizz/neoblizz/wiki

CUDA 301.

Solve Multi-GPUs and Multi-Node.

CUDA 301.

Solve Multi-GPUs and Multi-Node.

You got this.

THANK YOU ALL!

John D. Owens

Serban D. Porumbescu

Jason Lowe-Power, Soheil Ghiasi, Venkatesh Akella

Stephen Jones, Michael Garland, Duane Merrill, Cris Cecka

Sean Treichler, Aamer Jaleel

Owensgroup lab students!