CUDA GPU Programming

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CUDA

- Software ecosystem for NVIDIA GPUs
- Language for programming GPUs
  - C++ language extension
  - *.cu files
- NVCC compiler

```
> nvcc -o saxpy --generate-code arch=compute_80,code=sm_80 saxpy.cu
> ./saxpy
```

CUDA Syntax

```
__global__ void saxpy(float *x, float *y, float alpha) {
    int i = threadIdx.x;
    y[i] = alpha*x[i] + y[i];
}

int main() {
    ...
    saxpy<<<1, N>>>(x, y, alpha);
    ...
}
```

Possible Issues?

```
__global__ void saxpy(float *x, float *y, float alpha) {
    int i = threadIdx.x;
    y[i] = alpha*x[i] + y[i];
}

int main() {
    ...
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}
```

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__global__ void saxpy(float *x, float *y, float alpha) {
    int i = threadIdx.x;
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}

int main() {
    ...
    saxpy<<<1, N>>>(x, y, alpha);
    ...
}
```

What happens when:
- N > 1024?
- N > # device threads?

Multiple Blocks

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


...
int threadsPerBlock = 512;
int numBlocks = N/threadsPerBlock + (N % threadsPerBlock != 0);
saxpy<<<numBlocks, threadsPerBlock>>>(x, y, alpha, N);
```

Striding

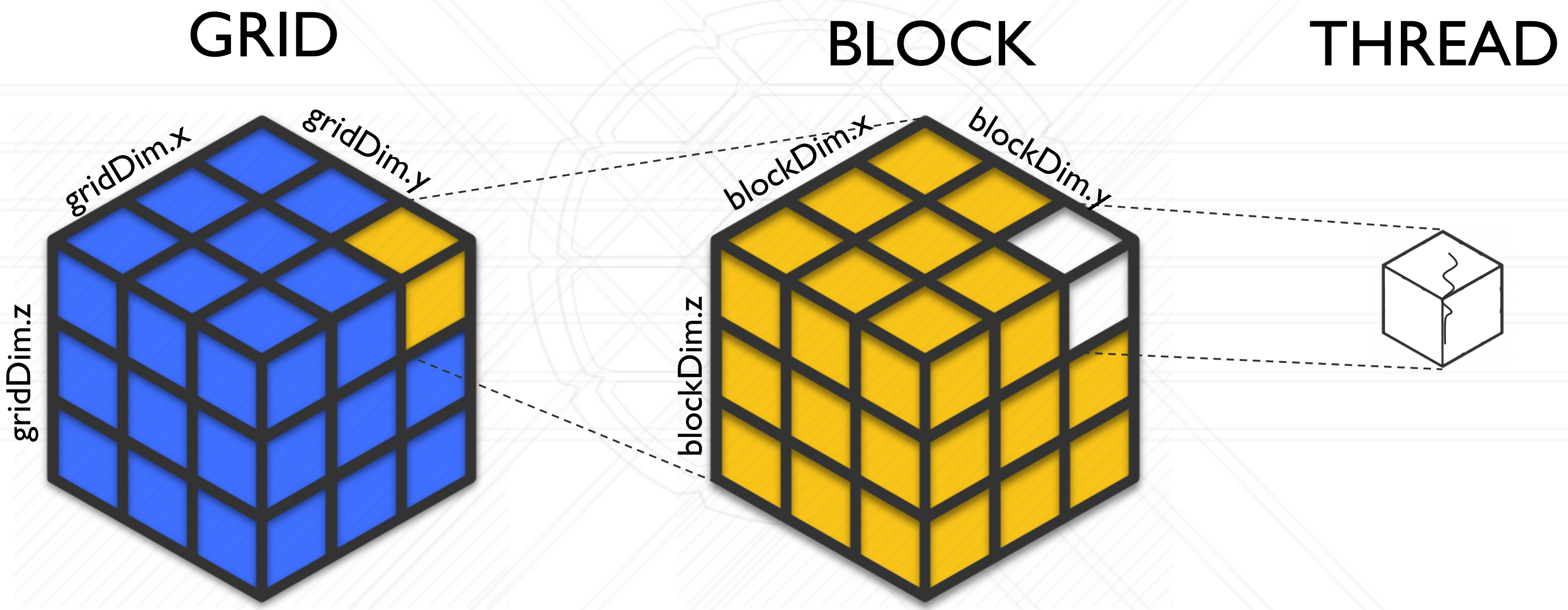
```
__global__ void saxpy(float *x, float *y, float alpha, int N) {
    int i0 = blockDim.x * blockIdx.x + threadIdx.x;
    int stride = blockDim.x * gridDim.x;

    for (int i = i0; i < N; i += stride)
        y[i] = alpha*x[i] + y[i];
}
```

Grid and Block Dimensions

- # of blocks and threads per block can be 3-vectors
- Useful for algorithms with 2d & 3d data layouts

Grid and Block Dimensions



Grid and Block Dimensions

```
dim3 threadsPerBlock(16, 16);
dim3 numBlocks(M/threadsPerBlock.x + (M % threadsPerBlock.x != 0),
               N/threadsPerBlock.y + (N % threadsPerBlock.y != 0));

matrixAdd<<<numBlocks, threadsPerBlock>>>(X, Y, alpha, M, N);
```

Grid and Block Dimensions

Each block is 16x16 threads.

```
dim3 threadsPerBlock(16, 16);
dim3 numBlocks(M/threadsPerBlock.x + (M % threadsPerBlock.x != 0),
               N/threadsPerBlock.y + (N % threadsPerBlock.y != 0));

matrixAdd<<<numBlocks, threadsPerBlock>>>(X, Y, alpha, M, N);
```

Grid and Block Dimensions

The grid is ⌈M/16⌉ x ⌈N/16⌉ blocks.

```
dim3 threadsPerBlock(16, 16);
dim3 numBlocks(M/threadsPerBlock.x + (M % threadsPerBlock.x != 0),
               N/threadsPerBlock.y + (N % threadsPerBlock.y != 0));

matrixAdd<<<numBlocks, threadsPerBlock>>>(X, Y, alpha, M, N);
```

Grid and Block Dimensions

```
__global__ void matrixAdd(float **X, float **Y, float alpha, int M, int N){
    int i = blockDim.x * blockIdx.x + threadIdx.x;
    int j = blockDim.y * blockIdx.y + threadIdx.y;

    if (i < M && j < N)
        Y[i][j] = alpha*X[i][j] + Y[i][j];
}
```

Questions?

Matrix Multiply

- Standard matrix multiply
- How can we parallelize?

```
for (i=0; i<M; i++)
    for (j=0; j<N; j++)
        for (k=0; k<P; k++)
            C[i][j] += A[i][k]*B[k][j];
```

Matrix Multiply

- C_{ij} can be computed independent of other values of C
- 2-D thread decomposition
- Thread (i, j) computes C_{ij}

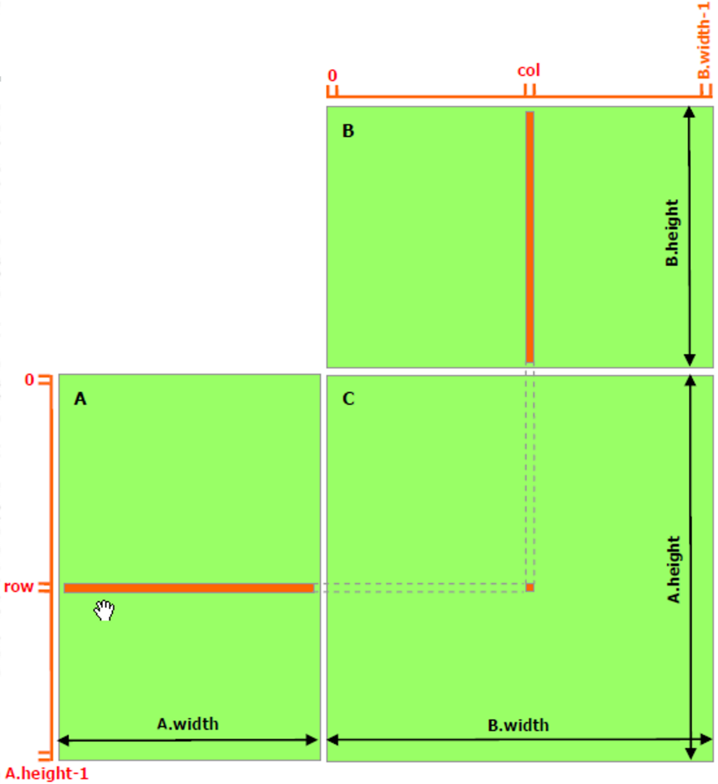


Image: https://docs.nvidia.com/cuda/cuda-c-programming-guide/index.html

Matrix Multiply

- Launch M x N threads
- Thread (i,j) computes C_{ij}

```
dim3 threadsPerBlock (BLOCK_SIZE, BLOCK_SIZE);
dim3 numBlocks(M/threadsPerBlock.x + (M%threadsPerBlock.x != 0),
               N/threadsPerBlock.y + (N%threadsPerBlock.y != 0));

matmul<<<numBlocks, threadsPerBlock>>>(C, A, B, M, P, N);
```

Matrix Multiply

```
__global__ void matmul(double *C, double *A, double *B, size_t M, size_t P,
size_t N) {

    int i = blockDim.x*blockIdx.x + threadIdx.x;
    int j = blockDim.y*blockIdx.y + threadIdx.y;

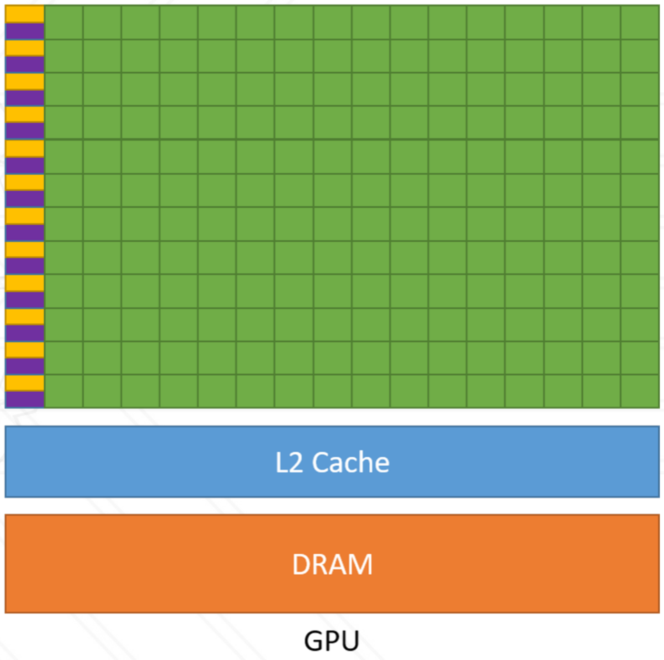
    if (i < M && j < N) {
        for (int k = 0; k < P; k++) {
            C[i*N+j] += A[i*P+k]*B[k*N+j];
        }
    }
}
```

Compute C_{ij}

Issues?

Issues?

- Poor data re-use
  - Every value of A & B is loaded from global memory



Issues?

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  - A is read N times
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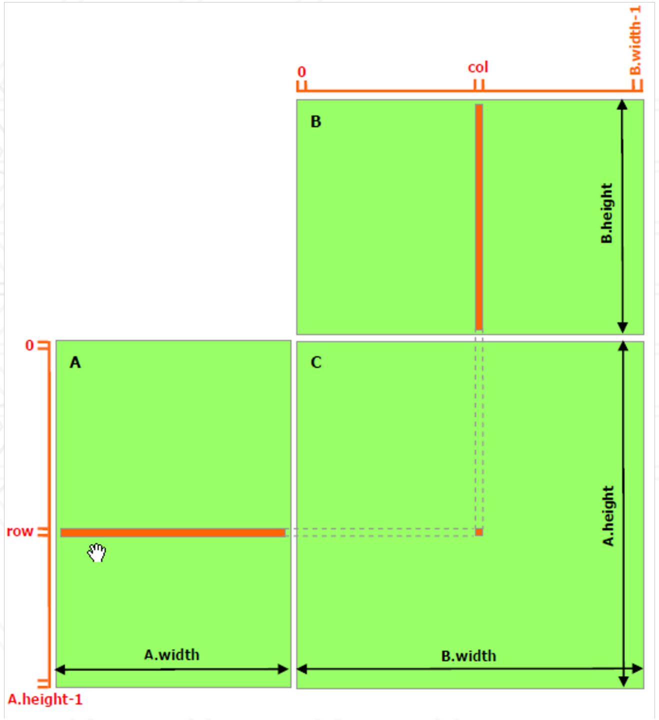
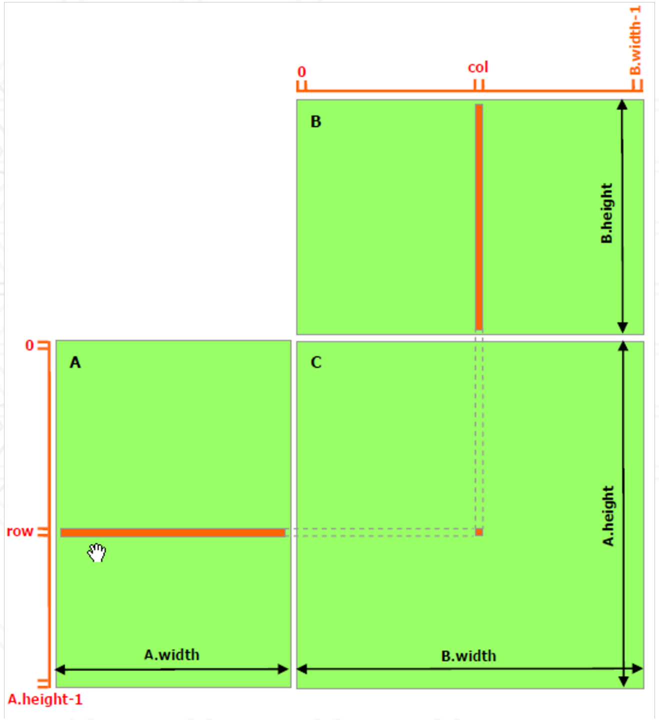


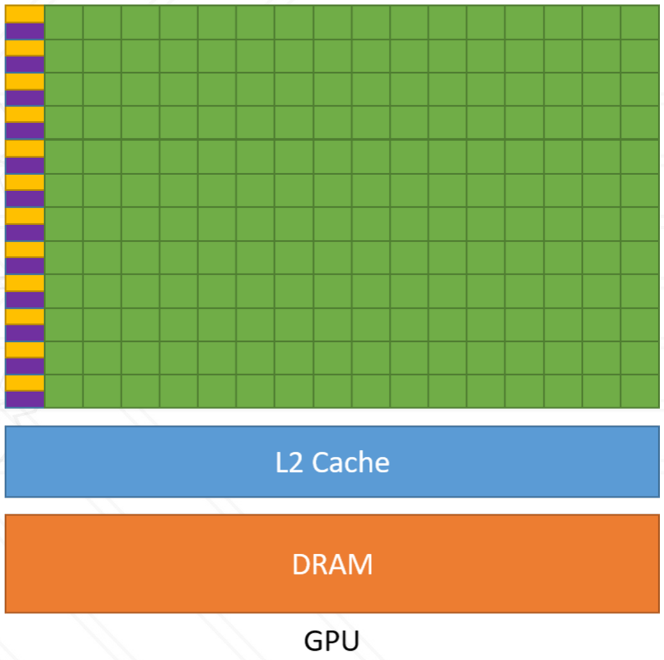
Issues?

- Poor data re-use
  - Every value of A & B is loaded from global memory
  - A is read N times
  - B is read M times
- How can we improve data re-use?

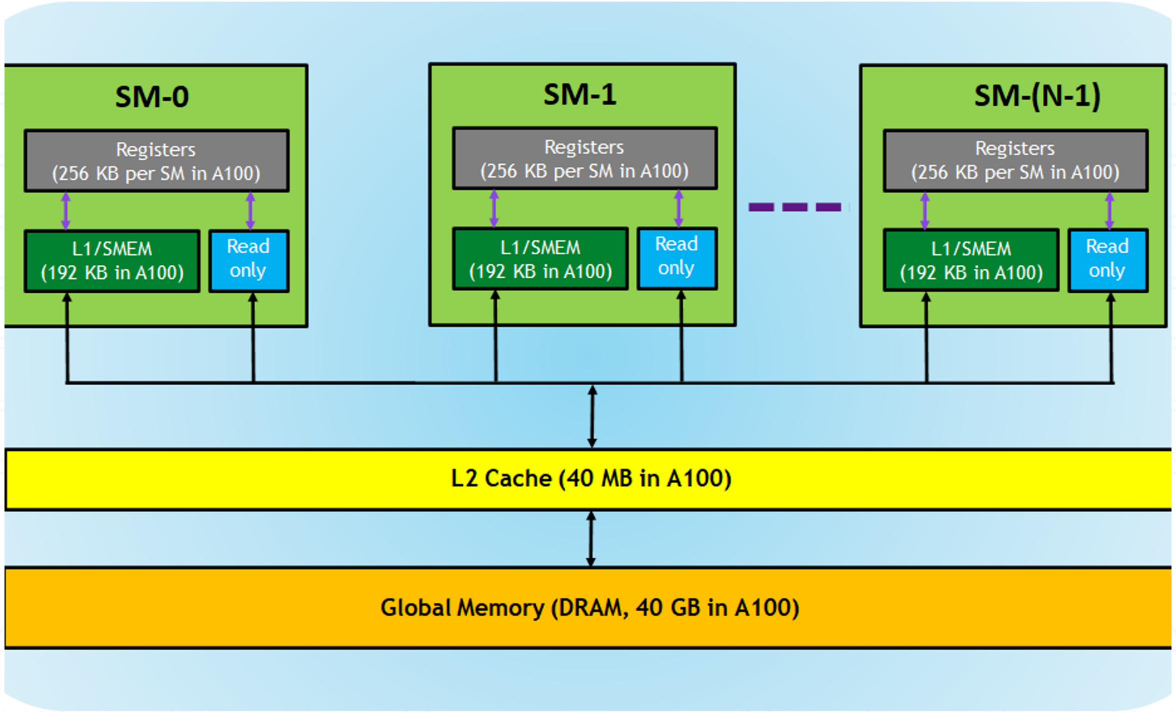


Shared Memory

- Local
  - thread only
- Shared
  - threads in block
- Global
  - all threads

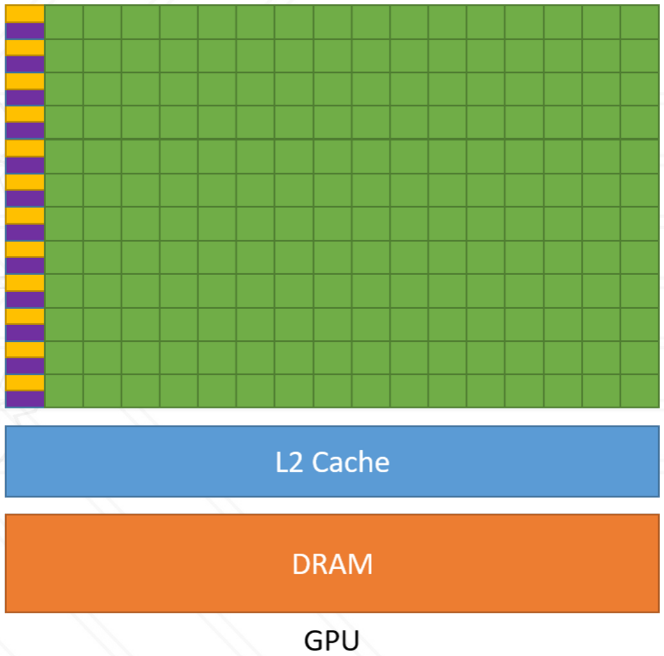


Shared Memory



Shared Memory

- `__shared__`
  - Denotes shared memory
- `__synchthreads()`
  - Synchronizes all threads in block



Reversing with Shared Memory

```
__global__ void reverse(int *vec) {
    __shared__ int sharedVec[N];

    int idx = threadIdx.x;
    int idxReversed = N - idx - 1;

    sharedVec[idx] = vec[idx];
    __syncthreads();
    vec[idx] = sharedVec[idxReversed];
}
```

Reversing with Shared Memory

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    __shared__ int sharedVec[N];

    int idx = threadIdx.x;
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}
```

Allocate N ints in block.

Reversing with Shared Memory

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__global__ void reverse(int *vec) {
    __shared__ int sharedVec[N];

    int idx = threadIdx.x;
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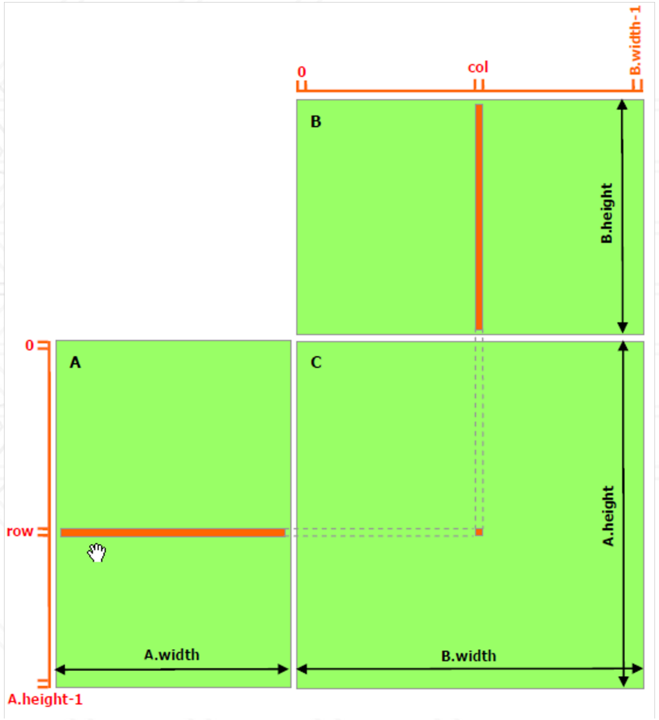
    sharedVec[idx] = vec[idx];
    __syncthreads();
    vec[idx] = sharedVec[idxReversed];
}
```

Allocate N ints in block.

Store into shared mem.
Synchronize.
Load from shared mem.

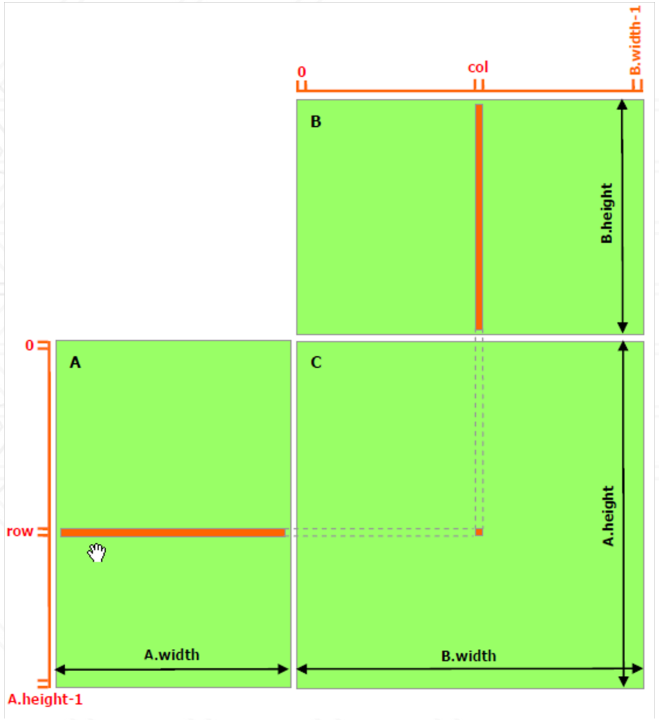
Matrix Multiply with Shared Memory

- How can we speed up matrix multiply with shared memory?



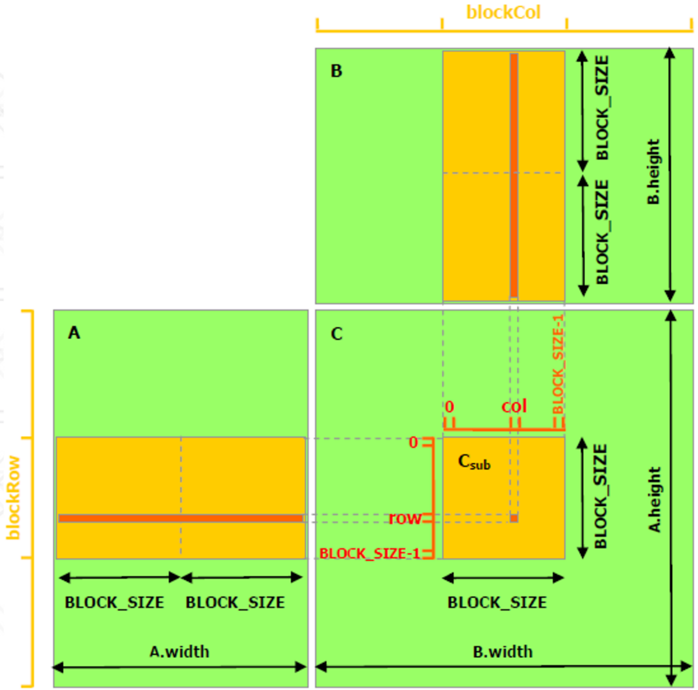
Matrix Multiply with Shared Memory

- Data Reuse
  - A is read N times
  - B is read M times



Matrix Multiply with Shared Memory

- Block computation
- Each block computes submatrix of C
- Save reused values in shared memory



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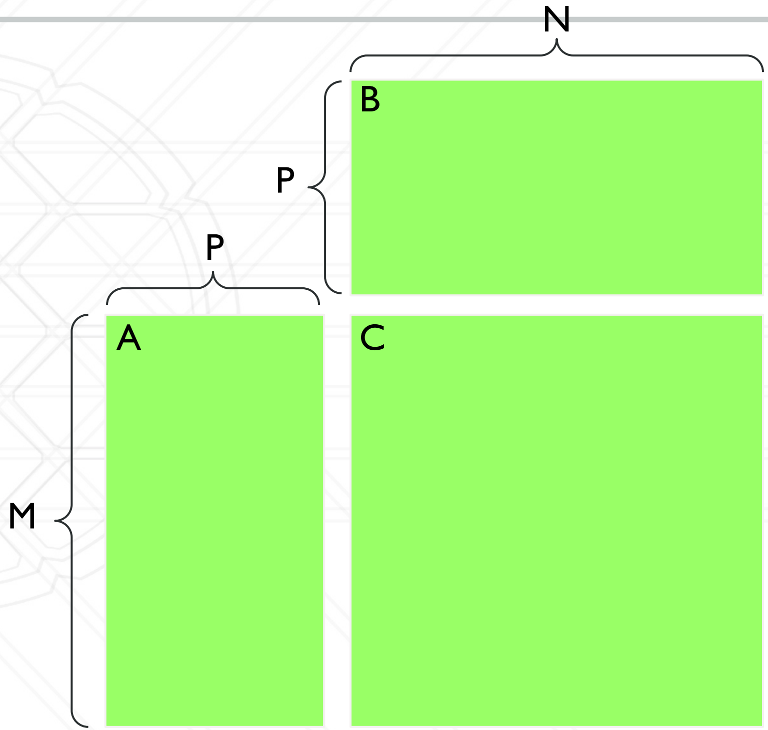
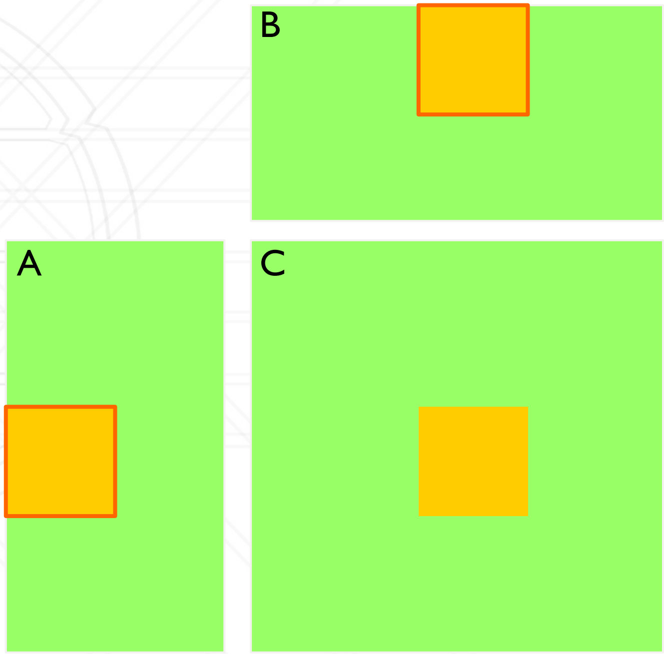
Matrix Multiply with Shared Memory

- Compute C = AB + C



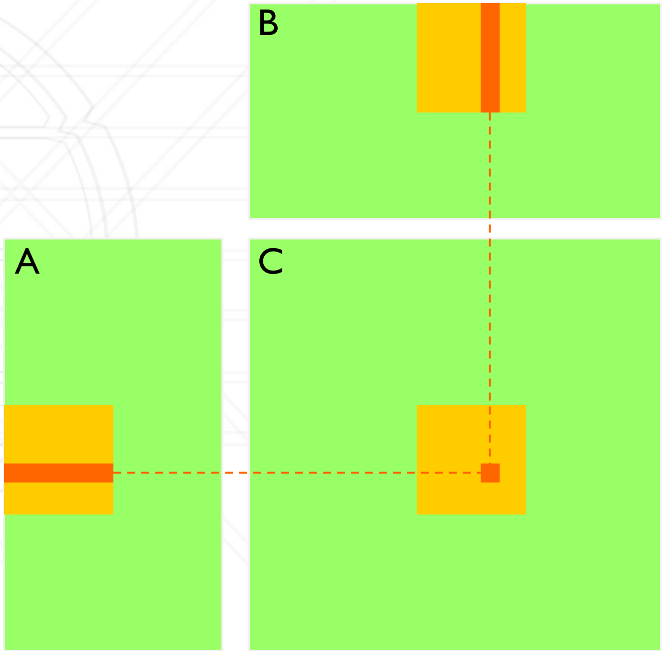
Matrix Multiply with Shared Memory

- Block (i, j) computes C_{ij} sub matrix
  - Save A & B submatrices into shared memory



Matrix Multiply with Shared Memory

- Block (i, j) computes C_{ij} sub matrix
  - Save A & B submatrices into shared memory
  - Accumulate partial dot product into C



Matrix Multiply with Shared Memory

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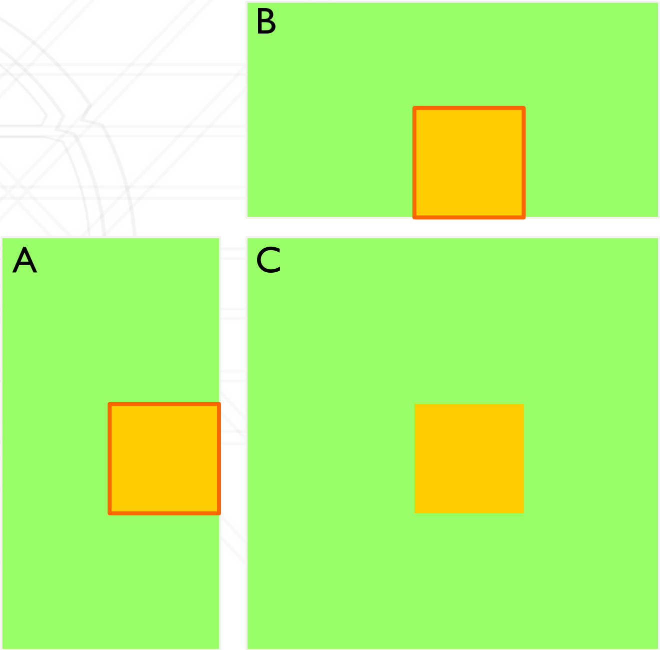
  - Save A & B submatrices into shared memory
  - Accumulate partial dot product into C



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- Block (i, j) computes C_{ij} sub matrix
  - Save A & B submatrices into shared memory
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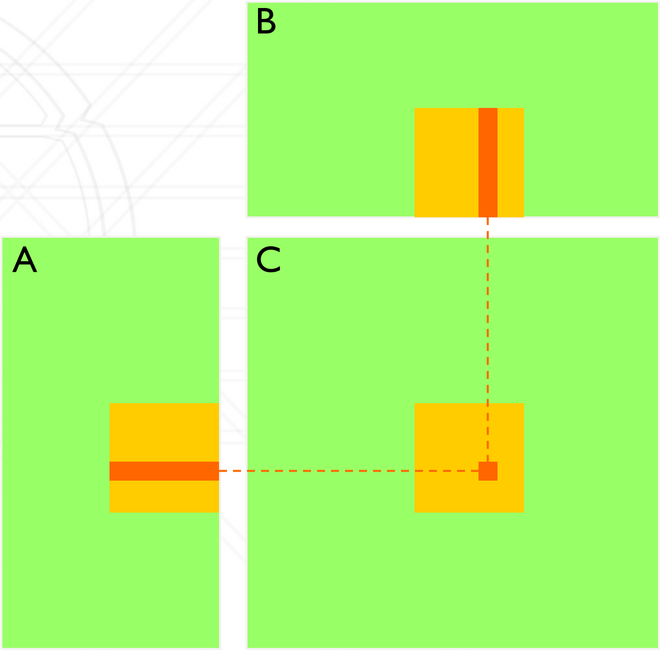
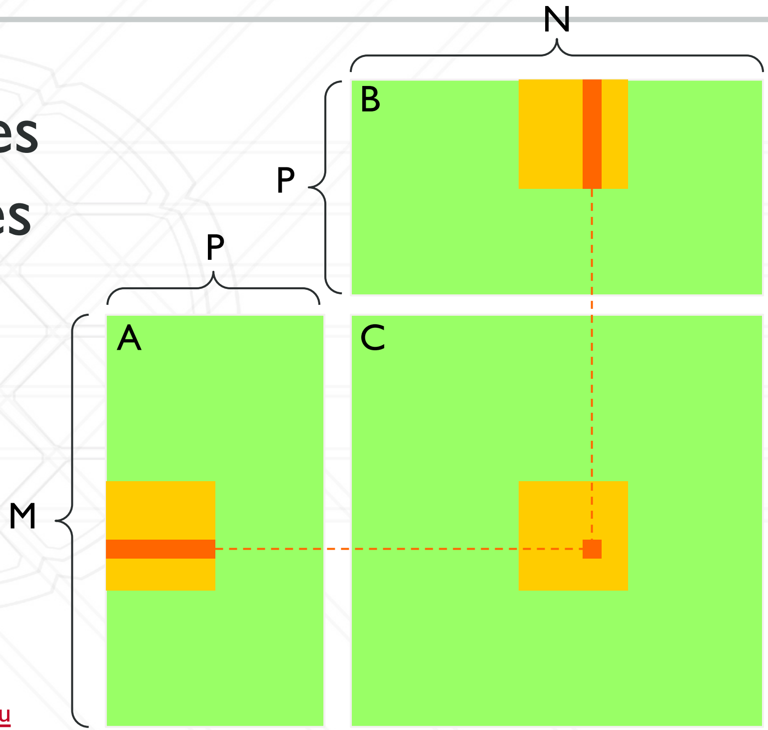


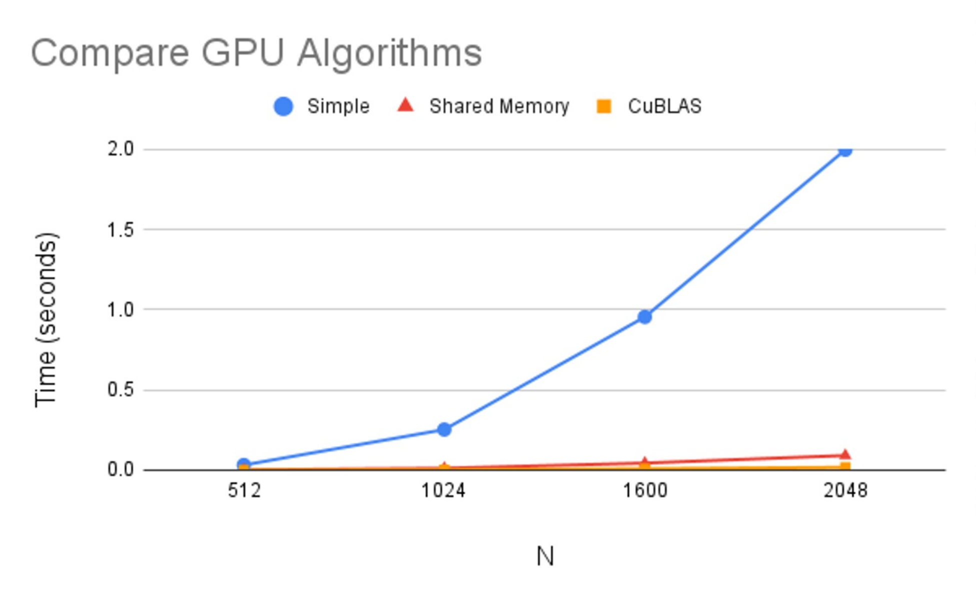
Matrix Multiply with Shared Memory

- A is read N / block_size times
- B is read M / block_size times
- Data reads from global memory are reduced by an order of the block size



Reference Implementation:
https://github.com/NVIDIA/cuda-samples/blob/master/Samples/matrixMul/matrixMul.cu

How much faster is it?



Algorithm	Time* (s)
Simple CPU	170.898
Simple GPU	1.997
Shared Memory	0.091
CuBLAS	0.017

A, B are 2048x2048

* on DeepThought2

Questions?

Profiling GPUs

- HPCToolkit + Hatchet
  - In addition to normal HPCToolkit commands
    - `hpcrun -e gpu=nvidia ...`
    - `hpcstruct <measurements_dir>`
- NSight
  - NVIDIA profiling suite

NSight

- nsys command to profile
  - `nsys profile -t cuda <executable> <args>`
  - Outputs .qdrep file
- View profile in NSight GUI
  - `nsys-ui report1.qdrep`

See https://docs.nvidia.com/nsight-systems/UserGuide/index.html

NSight

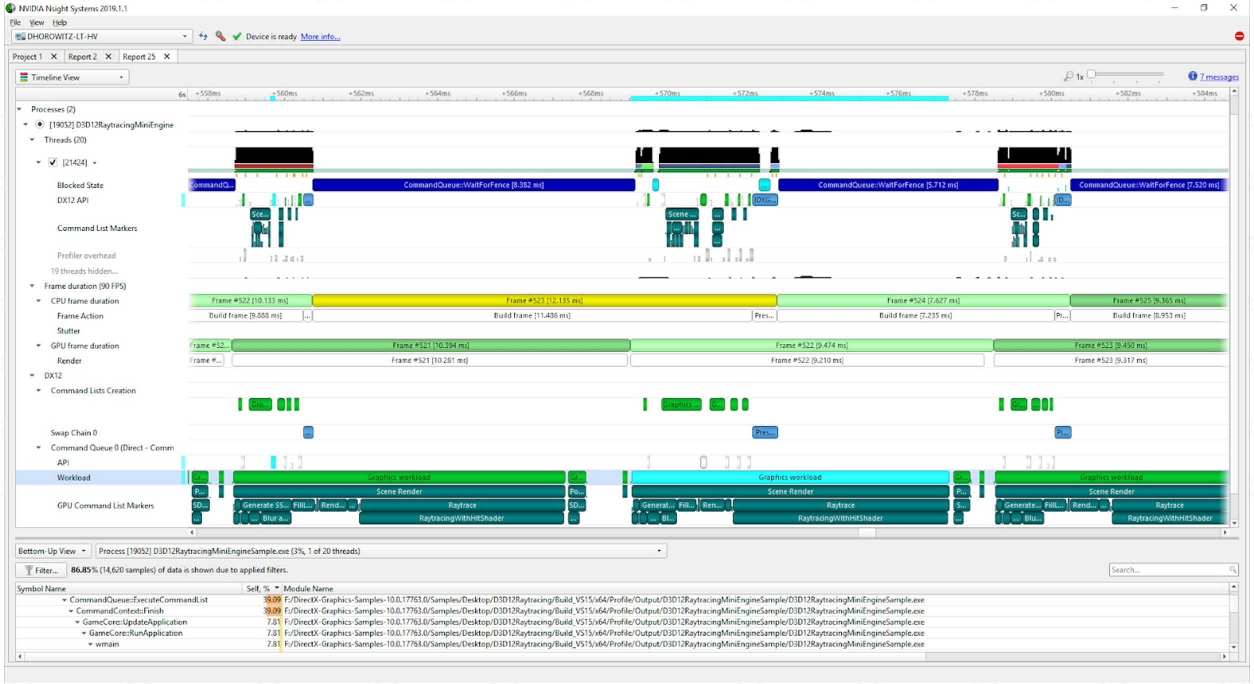


Image from https://developer.nvidia.com/blog/nvidia-tools-extension-api-nvtx-annotation-tool-for-profiling-code-in-python-and-c-c/

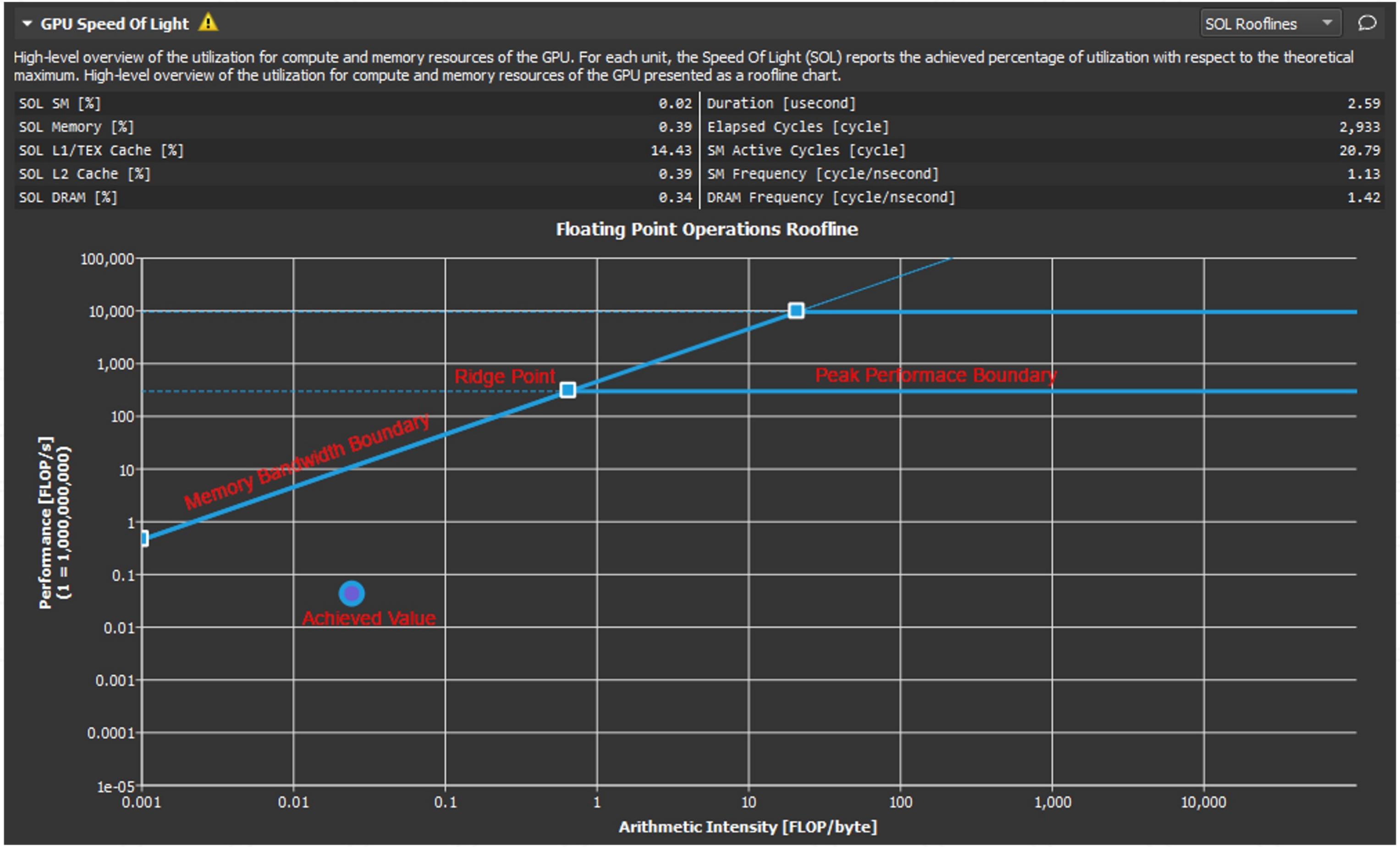


Image from https://docs.nvidia.com/nsight-compute/ProfilingGuide/index.html#roofline-charts

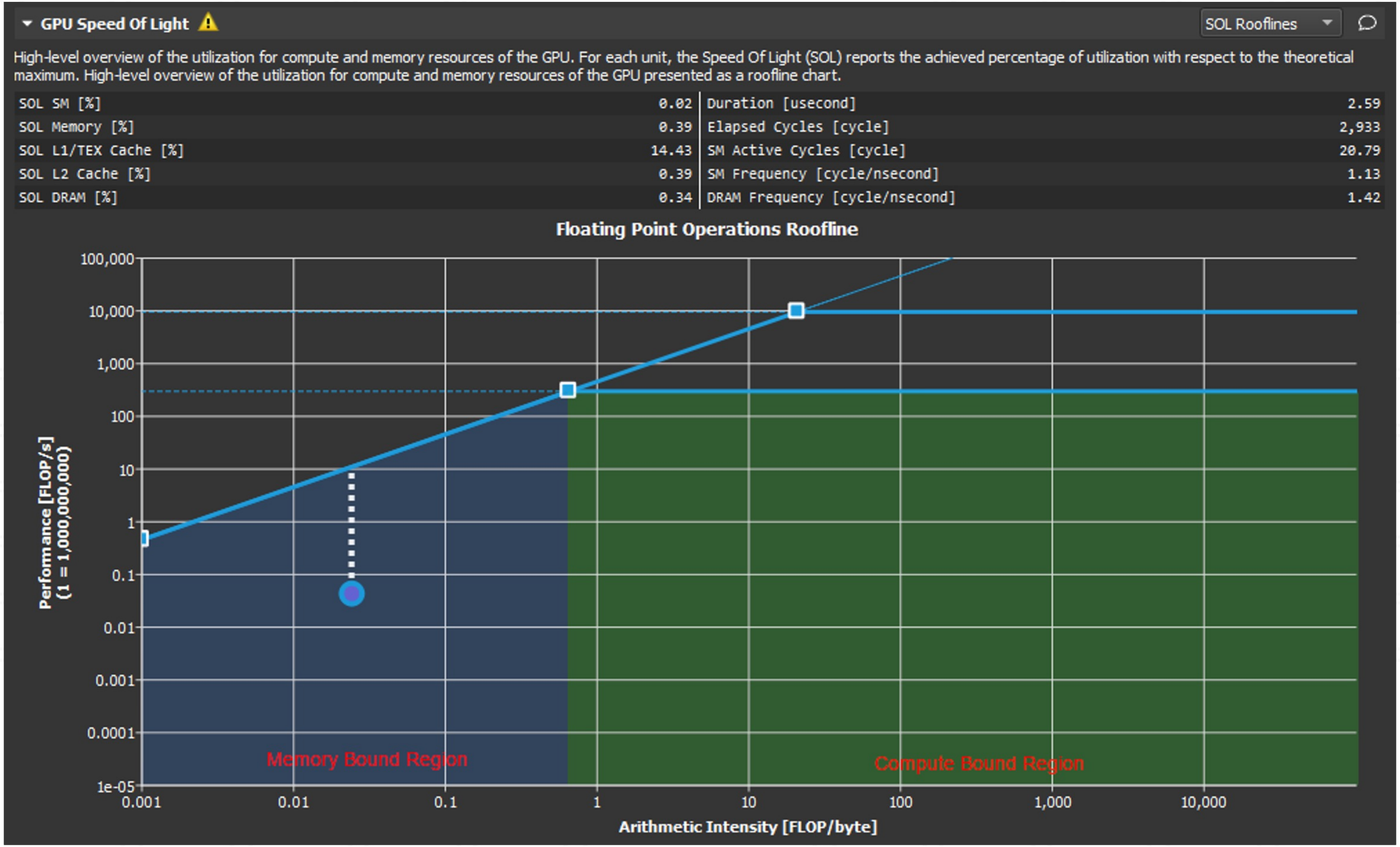


Image from https://docs.nvidia.com/nsight-compute/ProfilingGuide/index.html#roofline-charts

Streams

- Kernels execute in streams
- Stream is passed to kernel invocation
- Streams can execute concurrently

```
cudaStream_t stream;
...
kernel<<<grid, block, 0, stream>>>(x, b);
```

More info
https://developer.download.nvidia.com/CUDA/training/StreamsAndConcurrencyWebinar.pdf

Streams

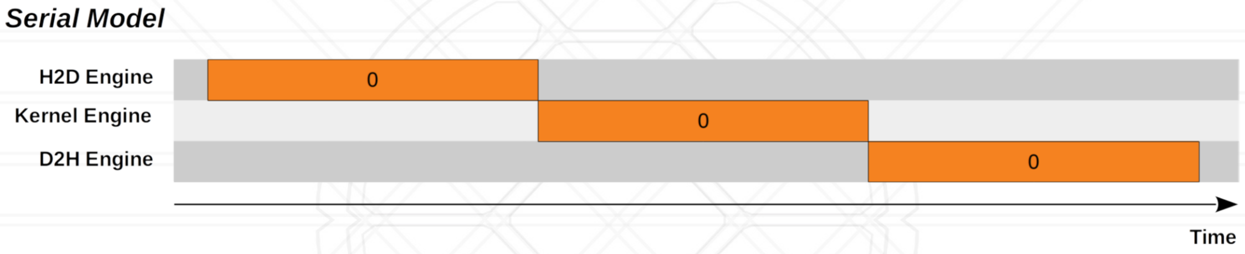


Image from https://leimao.github.io/blog/CUDA-Stream/

Streams

```
cudaStream_t stream[nStreams];
for (int i = 0; i < nStreams; i++) {
   cudaStreamCreate(&stream[i]);
}
```

Create some streams

Streams

```
cudaStream_t stream[nStreams];
for (int i = 0; i < nStreams; i++) {
   cudaStreamCreate(&stream[i]);
}

for (int i = 0; i < nStreams; i ++){
   int offset = i * streamSize;
   cudaMemcpyAsync(&d_a[offset], &a[offset], streamBytes, cudaMemcpyHostToDevice, stream[i]);

   kernel<<<streamSize/blockSize, blockSize, 0, stream[i]>>>(d_a, offset);

   cudaMemcpyAsync(&a[offset], &d_a[offset], streamBytes, cudaMemcpyDeviceToHost, stream[i]);
}
```

Launch all streams at once

Streams

```
cudaStream_t stream[nStreams];
for (int i = 0; i < nStreams; i++) {
   cudaStreamCreate(&stream[i]);
}

for (int i = 0; i < nStreams; i ++){
   int offset = i * streamSize;
   cudaMemcpyAsync(&d_a[offset], &a[offset], streamBytes, cudaMemcpyHostToDevice, stream[i]);

   kernel<<<streamSize/blockSize, blockSize, 0, stream[i]>>>(d_a, offset);

   cudaMemcpyAsync(&a[offset], &d_a[offset], streamBytes, cudaMemcpyDeviceToHost, stream[i]);
}

for (int i = 0; i < nStreams; i++) {
   cudaStreamDestroy(stream[i]);
}
```

Cleanup streams

Streams

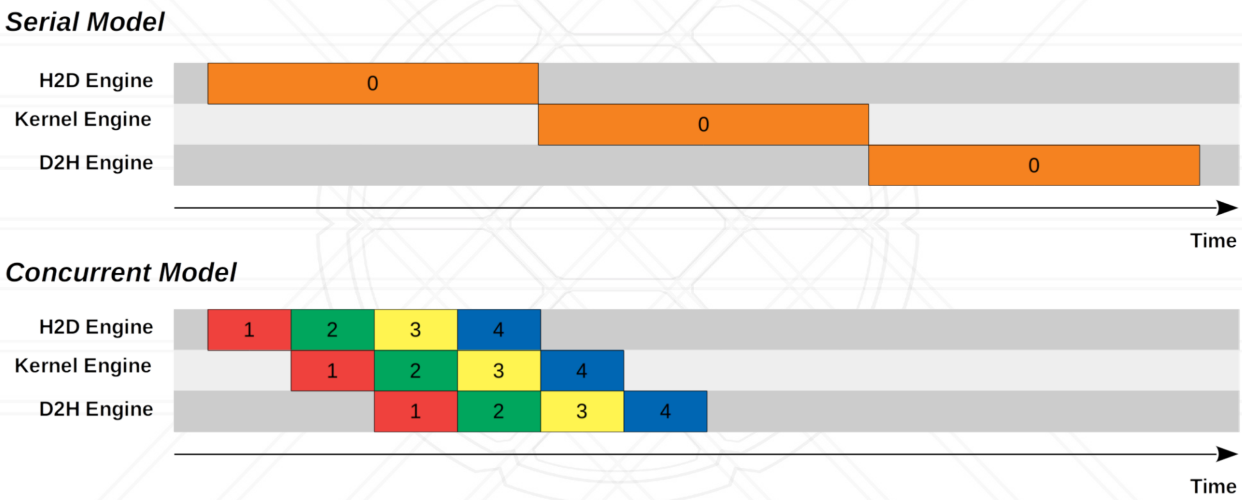


Image from https://leimao.github.io/blog/CUDA-Stream/

Unified Memory

- Data is on both GPU and CPU
- GPU takes care of synchronization
- Incurs small overhead

```
void sortfile(FILE *fp, int N) {
    char *data;
    cudaMallocManaged(&data, N);

    fread(data, 1, N, fp);
    qsort<<<...>>>(data, N, 1, compare);
    cudaDeviceSynchronize();

    … use data on CPU …
    cudaFree(data);
}
```

More info https://developer.nvidia.com/blog/unified-memory-cuda-beginners/

Higher Level GPU Programming

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- Linear Algebra
  - CuBLAS, MAGMA, CUTLASS, Eigen, CuSPARSE, …

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  - CuFFT, ArrayFire, …
- Deep Learning
  - CuDNN, TensorRT, …
- Graphics
  - OpenCV, FFmpeg, OpenGL, …
- Algorithms and Data Structures
  - Thrust, Raja, Kokkos, OpenACC, OpenMP, ...

Big Picture

- When to use GPUs?

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    - Data parallel tasks & lots of data
    - Performance/$$$ and time-to-solution

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- What software/algorithm to use?

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- When to use GPUs?
  - Data parallel tasks & lots of data
  - Performance/$$$ and time-to-solution
- What software/algorithm to use?
  - Performance critical
    - Native languages
  - Development time & maintainability
    - higher level APIs

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