Heterogeneous computing with performance modelling

Performance modelling

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How do we measure performance?

Floprate (definition)

- The raw computing performance of a CPU or a GPU is usually measured in **Flops**. That is,

$$\mathit{Floprate} = \frac{\text{number of floating-point operations [Flop]}}{\text{time [s]}}.$$

- Usually the number of floating-point additions and multiplications the hardware can perform per second.
  - Additions and multiplications are usually faster (FMA).
  - Division and special functions are usually slower.

Floprate (theoretical peak floprate, double precision)

- A **theoretical peak floprate** can be calculated for each device.
- Quad-core Intel Skylake CPU:

$\sim$ 200 GFlops

- 14-core Intel Xeon Gold 6132 CPU:

$\sim$ 1200 GFlops

- Nvidia Tesla V100 GPU:

$\sim$ **7 000** GFlops

Floprate (theoretical speedup)

The Nvidia Tesla V100 GPU is **over 11 times faster** than the 14-core Intel Xeon CPU!

Floprate (single and half precision)

- The difference is even larger if we are willing to reduce the precision.
- Typical numbers (single precision):
  - Quad-core Intel Skylake CPU: $\sim$ 400 GFlops
  - 14-core Intel Xeon Gold 6132 CPU: $\sim$ 2 400 GFlops
  - Nvidia Tesla V100 GPU: $\sim$ 14 000 GFlops
- Typical numbers (half precision):
  - Quad-core Intel Skylake CPU: $\sim$ — GFlops
  - $2 \times$ Intel Xeon Gold 6132 CPU: $\sim$ — GFlops
  - Nvidia Tesla V100 GPU: $\sim$ **112 000** GFlops

Floprate (single and half precision, theoretical speedup)

The Nvidia Tesla V100 GPU is **over 90 times faster** than the 14-core Intel Xeon CPU!

AX example

- Lets perform a small experiments:

$$\alpha \in \mathbb{R}, \boldsymbol{x} \in \mathbb{R}^n,$$
$$\boldsymbol{x} \leftarrow \alpha \boldsymbol{x}$$

- The total number of flops is n. Total number of bytes moved is $16n$.
- CPU code would looks like this:

```
void ax(int n, double alpha, double *x)
{
    #pragma omp parallel for
    for (int i = 0; i < n; i++)
        x[i] = alpha * x[i];
}
```

- GPU code would looks like this:

```
__global__ void ax_kernel(int n, double alpha, double *x)
{
    int thread_id = blockIdx.x * blockDim.x + threadIdx.x;
    int thread_count = gridDim.x * blockDim.x;
    for (int i = thread_id; i < n; i += thread_count)
        x[i] = alpha * x[i];
}
```

AX example (actual performance)

- Quad-core Intel Skylake CPU ($\sim$ 200 GFlops):

```
$ OMP_NUM_THREADS=4 ./ax.cpu 500E6
Time = 0.291716 s
```

- 14-core Intel Xeon Gold 6132 CPU ($\sim$ 1 200 GFlops):

```
$ OMP_NUM_THREADS=14 srun .... ./ax.cpu 500E6
Time = 0.087790 s
```

- Nvidia Tesla V100 GPU ($\sim$ **7 000** GFlops):

```
$ srun .... ./ax.cuda 500E6
Time = 0.010582 s
```

AX example (actual speedup)

The V100 is over 8 times faster than the Xeon but ...

AX example (actual floprate)

- Quad-core Intel Skylake CPU ($\sim$ 200 GFlops):

```
$ OMP_NUM_THREADS=4 ./ax.cpu 500E6
Time = 0.291716 s
Floprate = 2 GFlops
```

- 14-core Intel Xeon Gold 6132 CPU ($\sim$ 1 200 GFlops):

```
$ OMP_NUM_THREADS=14 srun .... ./ax.cpu 500E6
Time = 0.087790 s
Floprate = 6 GFlops
```

- Nvidia Tesla V100 GPU ($\sim$ **7 000** GFlops):

```
$ srun .... ./ax.cuda 500E6
Time = 0.010582 s
Floprate = 47 GFlops
```

AX example (actual floprate)

The V100 is over 8 times faster than the Xeon but **we are using less than 1% of the peak floprate!**

Why?
What else could effect the performance?

Memory throughput (definition)

- The memory performance of a CPU or a GPU is usually measured in terms of **memory throughput**. That is,

$$\text{Throughput} = \frac{\text{number of bytes moved [Byte]}}{\text{time [s]}}.$$

- Usually the bandwidth is measured between the CPU cores and the main memory; or the CUDA cores and the global memory.

Memory throughput (theoretical memory bandwidth)

- A **theoretical memory bandwidth** can be calculated for each device.
- Quad-core Intel Skylake CPU:

$\sim$ 35 GB/s

- 14-core Intel Xeon Gold 6132 CPU:

$\sim$ 100 GB/s

- Nvidia Tesla V100 GPU:

$\sim$ **900** GB/s

AX example (actual memory througput)

- Quad-core Intel Skylake CPU ($\sim$ 35 GB/s):

```
$ OMP_NUM_THREADS=4 ./ax.cpu 500E6
Time = 0.291716 s
Floprate = 2 GFlops
Memory throughput = 27 GB/s
```

- 14-core Intel Xeon Gold 6132 CPU ($\sim$ 100 GB/s):

```
$ OMP_NUM_THREADS=14 srun .... ./ax.cpu 500E6
Time = 0.087790 s
Floprate = 6 GFlops
Memory throughput = 91 GB/s
```

- Nvidia Tesla V100 GPU ($\sim$ **900** GB/s):

```
$ srun .... ./ax.cuda 500E6
Time = 0.010582 s
Floprate = 47 GFlops
Memory throughput = 756 GB/s
```

AX example (actual memory througput)

We are using between 77% and **91%** of the memory bandwidth!

AX example (profiler)

- We can use Nvidia's `nv-nsight-cu-cli` profiling tool to analyze the situation:

```
$ srun .... nv-nsight-cu-cli ./ax.cuda 500E6
....
---------------- -------------- --------------
Memory Frequency  cycle/usecond         875,84
SOL FB                        %          84,58
Elapsed Cycles            cycle     13 181 137
SM Frequency      cycle/nsecond           1,25
Memory [%]                    %          84,58
Duration                msecond          10,55
SOL L2                        %          31,21
SM Active Cycles          cycle  12 837 852,30
SM [%]                        %           3,34
SOL TEX                       %          15,21
```

AX example (profiler)

- The relevant fields are the following:

```
---------------- -------------- --------------
SOL FB                        %          84,58
Memory [%]                    %          84,58
SM [%]                        %           3,34
```

- `SOL FB` is related to global memory throughput and `Memory` is related to the occupancy rate of the memory subsystem.
- `SM` is related to the occupancy rate of the compute resources.
- Conclusion: **The CUDA cores are idling but the memory bus is busy**.

GEMM example

- Lets perform a second experiments:

$$\boldsymbol{A}, \boldsymbol{B} \in \mathbb{R}^{n \times n}$$
$$\boldsymbol{C} \leftarrow \boldsymbol{AB}, \boldsymbol{C} \in \mathbb{R}^{n \times n}$$

- A naive CPU code would looks like this:

```c
void gemm(int n, int ldA, int ldB, int ldC, double *A, double *B, double *
    C)
{
    for (int i = 0; i < n; i++) {        // columns
        for (int j = 0; j < n; j++) {    // rows
            double dot = 0.0;
            for (int k = 0; k < n; k++)
                dot += A[k*ldA+j] * B[i*ldB+k];
            C[i*ldC+j] = dot;
        }
    }
}
```

- Total number of flops is $2n^3$. Total number of bytes transferred is $16n^3 + 8n^2$ (this does not hold in practice).

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GEMM example (actual floprate)

- An optimized BLAS library was used to generate these results.
- Quad-core Intel Skylake CPU ($\sim$ 200 GFlops):

```
$ OMP_NUM_THREADS=4 ./gemm.cpu 5000
Runtime was 1.422 s.
Floprate was 176 GFlops.
```

- 14-core Intel Xeon Gold 6132 CPU ($\sim$ 1 200 GFlops)[1]:

```
$ OMP_NUM_THREADS=14 srun ..... ./gemm.cpu 5000
Runtime was 0.469 s.
Floprate was 533 GFlops
```

- Nvidia Tesla V100 GPU ($\sim$ **7 000** GFlops):

```
$ srun .... ./gemm.cuda 5000
Runtime was 0.041 s.
Floprate was 6077 GFlops
```

[1] I am using OpenBLAS (`fosscuda`). MKL would give better performance.

GEMM example (actual floprate)

We are using between 46% and **88%** of the peak floprate!

GEMM example (profiler)

- Let's see what the profiler says:

```
$ srun .... nv-nsight-cu-cli ./gemm.cuda 5000
....
---------------- -------------- --------------
Memory Frequency  cycle/usecond         878,08
SOL FB                        %          36,45
Elapsed Cycles            cycle     51 458 926
SM Frequency      cycle/nsecond           1,25
Memory [%]                    %          37,18
Duration                msecond          41,06
SOL L2                        %          23,69
SM Active Cycles          cycle  50 755 341,94
SM [%]                        %          98,31
SOL TEX                       %          37,68
```

GEMM example (profiler)

- The relevant fields:

```
---------------- -------------- --------------
SOL FB                        %          36,45
Memory [%]                    %          37,18
SM [%]                        %          98,31
```

- Conclusion: **The CUDA cores are busy but the memory bus is party idle**.

Arithmetical intensity

The two codes behave very differently...

Can we predict the behavior in advance?

Arithmetical intensity

- From now on, let's call
  - the former type of kernels (ax) **memory bound** and
  - the latter type of kernels (gemm) **compute bound**.
- That is,
  - the performance of a memory-bound code is limited by the available memory bandwidth and
  - the performance of a compute-bound code is limited by the instruction throughput.

Arithmetical intensity (definition)

- How do we know which kernels are memory bound and which are compute bound?
- We begin to answer this question by defining **arithmetical intensity**:

$$\text{Arithmetical intensity} = \frac{\text{number of floating-point operations [Flop]}}{\text{number of bytes moved [Byte]}}.$$

Arithmetical intensity (examples)

- Double precision AX has the arithmetical intensity of

$$\text{Arithmetical intensity}_{\text{AX,double}} = \frac{1\ \text{Flop}}{2 \cdot 8\ \text{Byte}} = \frac{1}{16}\ \text{Flop/Byte}.$$

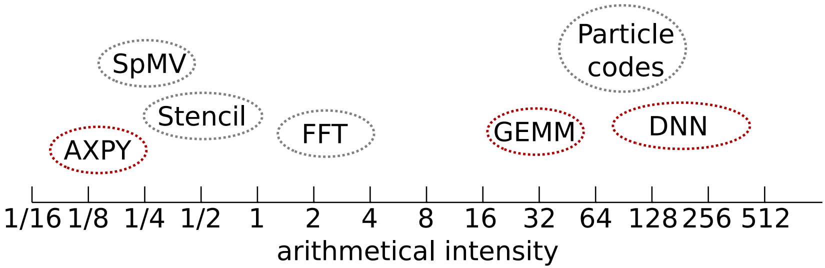
- Single precision AX has the arithmetical intensity of

$$\text{Arithmetical intensity}_{\text{AX,single}} = \frac{1\ \text{Flop}}{2 \cdot 4\ \text{Byte}} = \frac{1}{8}\ \text{Flop/Byte}.$$

- Well-implemented double-precision GEMM has the arithmetical intensity of

$$\text{Arithmetical intensity}_{\text{GEMM,double}} = \sim 32\ \text{Flop/Byte}$$

Arithmetical intensity (more examples)



Arithmetical intensity (Deep Neural Networks)

- **Half precision numbers** from Nvidia:

Operation	**Arithmetical intensity**
Linear layer (4096 outputs, 1024 inputs, **batch size 512**)	**315** Flop/Byte
Linear layer (4096 outputs, 1024 inputs, batch size 1)	1 Flop/Byte
Max pooling with 3x3 window and unit stride	2.25 Flop/Byte
ReLU activation	0.25 Flop/Byte
Layer normalization	$<$ 10 Flop/Byte

Arithmetical intensity (Deep Neural Networks)

- Estimated **single precision** numbers:

Operation	**Arithmetical intensity**
Linear layer (4096 outputs, 1024 inputs, **batch size 512**)	**158** Flop/Byte
Linear layer (4096 outputs, 1024 inputs, batch size 1)	0.5 Flop/Byte
Max pooling with 3x3 window and unit stride	1.125 Flop/Byte
ReLU activation	0.125 Flop/Byte
Layer normalization	$<$ 5 Flop/Byte

Arithmetical intensity (what can we do with it?)

- Let's (loosely) define the total amount of **work** as

$$\text{Work} = \text{Flops} + \text{Transfers}.$$

- If we assume that floating-point and memory operations are more or less evenly distributed throughout the code, we can estimate the **execution time** with

$$\text{Time} = \max\left\{ \frac{\text{Flops}}{\text{Peak Floprate}}, \frac{\text{Transfers}}{\text{Bandwidth}} \right\}.$$

Arithmetical intensity (what can we do with it?)

- Now, since Performance = Flops / Time, we have

$$
\begin{aligned}
\textit{Performance} &= \frac{\text{Flops}}{\max\left\{\frac{\text{Flops}}{\text{Peak Floprate}}, \frac{\text{Transfers}}{\text{Bandwidth}}\right\}}. \\
&= \min\left\{\text{Peak Floprate}, \frac{\text{Flops}}{\text{Transfers}} \times \text{Bandwidth}\right\}.
\end{aligned}
$$

- Note that the right term is simply **the arithmetical intensity multiplied by the memory bandwidth!**

Arithmetical intensity (optimal intensity)

- An **optimal arithmetical intensity** can be calculated for each device:

$$\text{Optimal intensity} = \frac{\text{theoretical peak floprate}}{\text{theoretical memory bandwidth}}.$$

- In that case, we have

$$\begin{aligned}\text{Performance} &= \min\left\{\text{Peak Floprate}, \frac{\text{Peak Floprate}}{\text{Bandwidth}} \times \text{Bandwidth}\right\} \\ &= \text{Peak Floprate}.\end{aligned}$$

Arithmetical intensity (optimal intensity)

- If the arithmetical intensity is **smaller than** the optimal intensity, the kernel is **memory bound** and we have

$$\begin{aligned}\text{Performance} &= \frac{\text{Flops}}{\text{Transfers}} \times \text{Bandwidth} \\ &\leq \text{Peak Floprate.}\end{aligned}$$

- If the arithmetical intensity is **larger than** the optimal intensity, the kernel is **compute bound** and we have

$$\text{Performance} = \text{Peak Floprate.}$$

Arithmetical intensity (optimal intensity, double precision)

- Quad-core Intel Skylake CPU:

$$\sim 5.7 \text{ Flop/Byte}$$

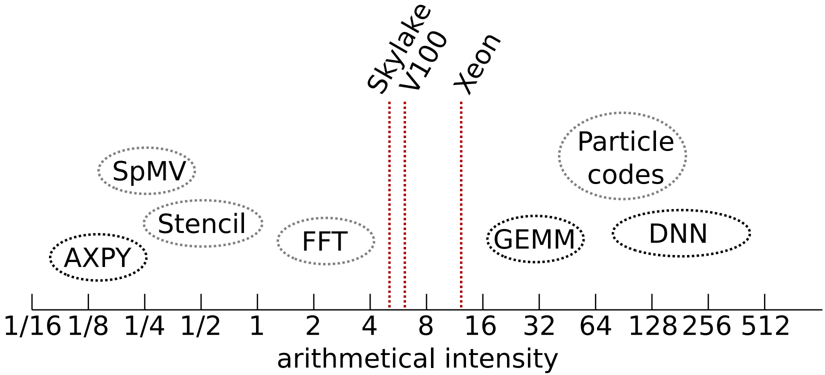
- 14-core Intel Xeon Gold 6132 CPU:

$$\sim 12 \text{ Flop/Byte}$$

- Nvidia Tesla V100 GPU:

$$\sim 7.7 \text{ Flop/Byte}$$

Arithmetical intensity (optimal intensity, double precision)



Arithmetical intensity (optimal intensity, single precision)

- Quad-core Intel Skylake CPU:

$$\sim 11.4 \text{ Flop/Byte}$$

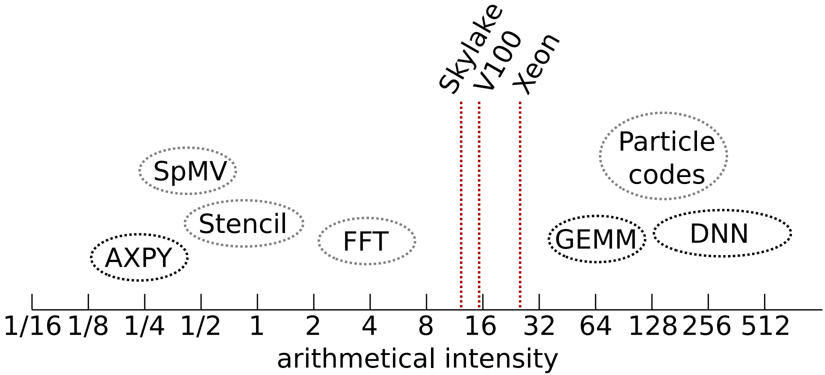
- 14-core Intel Xeon Gold 6132 CPU:

$$\sim 24 \text{ Flop/Byte}$$

- Nvidia Tesla V100 GPU:

$$\sim 15.6 \text{ Flop/Byte}$$

Arithmetical intensity (optimal intensity, double precision)



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Arithmetical intensity (optimal intensity, half precision)

- Quad-core Intel Skylake CPU:

  — Flop/Byte

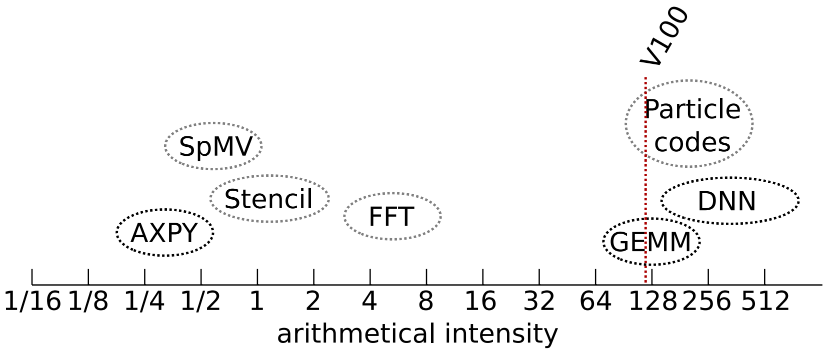
- 14-core Intel Xeon Gold 6132 CPU:

  — Flop/Byte

- Nvidia Tesla V100 GPU:

  $\sim$ **124** Flop/Byte

Arithmetical intensity (optimal intensity, half precision)



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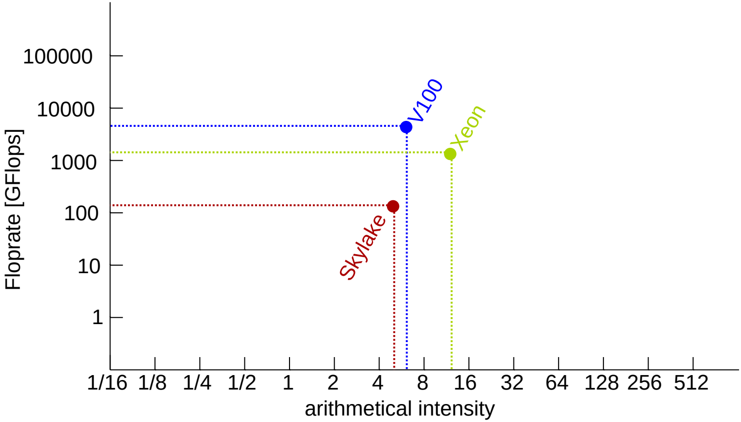
Roofline model

- We could plot both the **peak floprate** and the **optimal arithmetical intensity** to a same figure:



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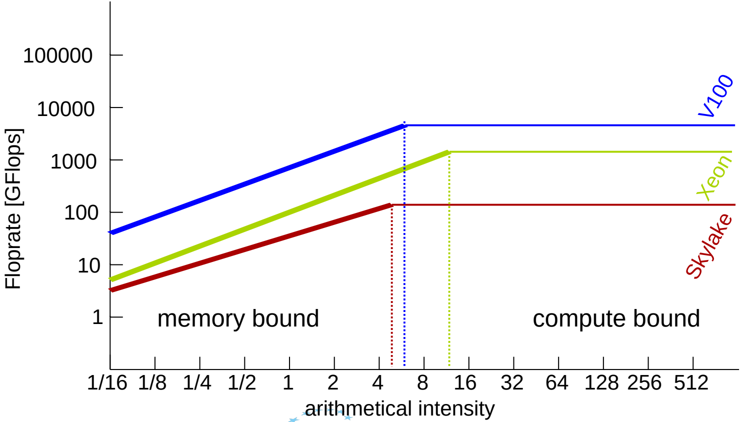
Roofline model (model)

- By including the function

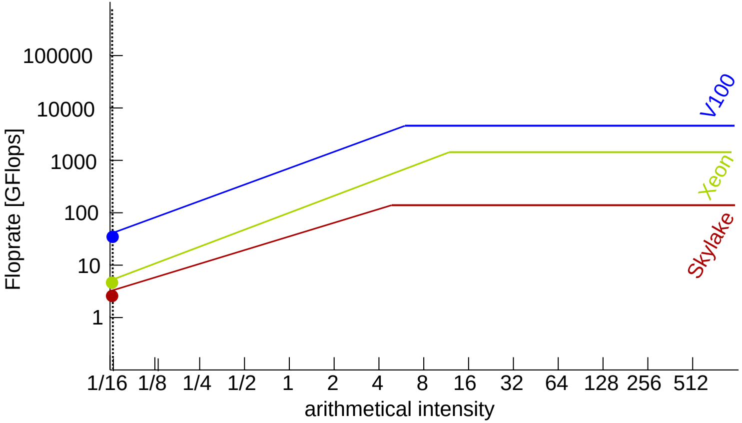
$$Performance = \min\left\{\text{Peak Floprate}, \frac{\text{Flops}}{\text{Transfers}} \times \text{Bandwidth}\right\}$$

to the plot, we get the following **"roofline"**:



Roofline model (AX kernel)

- By including Arithmetical intensity$_{\text{AX,double}}$ to the figure, we see that the measured floprate is actually quite close to the value predicted by the model:



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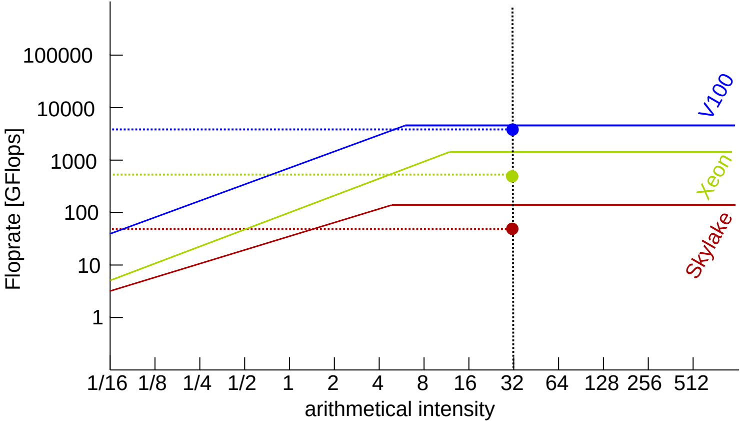
Roofline model (GEMM kernel)

- The same applies to Arithmetical intensity$_{\text{GEMM,double}}$:



Arithmetical intensity (caches and shared memory)

- When calculated naively, the double precision GEMM has the arithmetical intensity of

$$\text{Arithmetical intensity}_{\text{GEMM,double}} = \frac{2n^3}{16n^3 + 8n^2} \text{ Flop/Byte}$$
$$= \sim \frac{1}{8} \text{ Flop/Byte}$$

- Why is the real number

$$\text{Arithmetical intensity}_{\text{GEMM,double}} = \sim 32 \text{ Flop/Byte?}$$

Arithmetical intensity (caches and shared memory)

- When implemented naively, we compute each entry separately:

$$\boldsymbol{A}, \boldsymbol{B} \in \mathbb{R}^{n \times n}, (\boldsymbol{AB})_{i,j} = \sum_{k=1}^{n} a_{ik} b_{kj} \quad \left(\frac{n^2 \cdot 2n}{8n^2(2n+1)} \text{ Flop/Byte} \right)$$

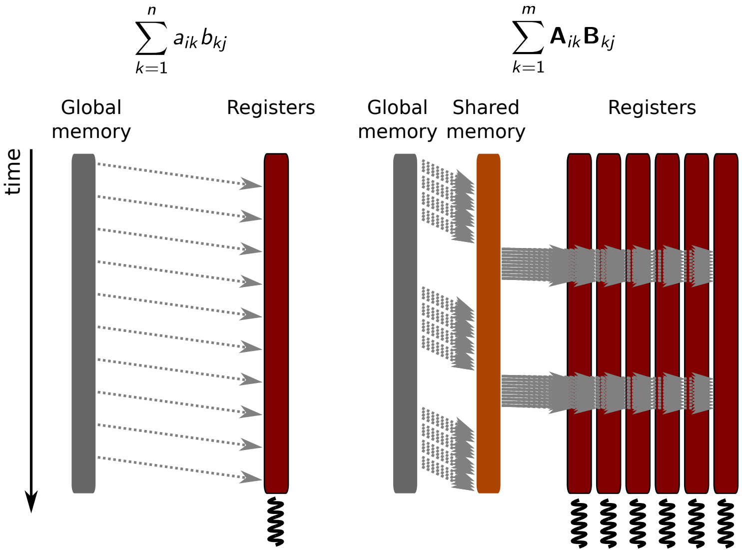
- However, we can also do the following:

$$\left(\begin{bmatrix} \boldsymbol{A}_{11} & \dots & \boldsymbol{A}_{1m} \\ \vdots & \ddots & \vdots \\ \boldsymbol{A}_{m1} & \dots & \boldsymbol{A}_{mm} \end{bmatrix} \begin{bmatrix} \boldsymbol{B}_{11} & \dots & \boldsymbol{B}_{1m} \\ \vdots & \ddots & \vdots \\ \boldsymbol{B}_{m1} & \dots & \boldsymbol{B}_{mm} \end{bmatrix} \right)_{i,j} = \sum_{k=1}^{m} \boldsymbol{A}_{ik} \boldsymbol{B}_{kj}$$

Arithmetical intensity (caches and shared memory)

- If the blocks $\boldsymbol{A}_{ik}$ and $\boldsymbol{B}_{kj}$ are small enough, they can be fitted into CPU caches or SMP's shared memory.
- Each block is loaded only once and then **shared among the thread block**!
- The matrix-matrix multiplication $\boldsymbol{A}_{ik}\boldsymbol{B}_{kj}$ can therefore be performed with minimal global memory communications.
- Only the global memory transfers are counted in the analysis
  $\implies$ the denominator decreases
  $\implies$ the arithmetical intensity increases
  $\implies$ higher performance on modern CPUs and GPUs.

Arithmetical intensity (caches and shared memory)



PCI-E bandwidth (AX example)

- In the earlier example, the necessary **data already resided in the global memory** when the timer was started:

```
struct timespec ts_start;
clock_gettime(CLOCK_MONOTONIC, &ts_start);

dim3 threads = 256;
dim3 blocks = max(1, min(256, n/threads.x));
ax_kernel<<<blocks, threads>>>(n, alpha, d_y);

cudaDeviceSynchronize();

struct timespec ts_stop;
clock_gettime(CLOCK_MONOTONIC, &ts_stop);
```

- Outcome:

```
$ srun .... ./ax.cuda 500E6
Time = 0.010582 s
Floprate = 47 GFlops
Memory throughput = 756 GB/s
```

PCI-E bandwidth (AX example)

- Let's change that:

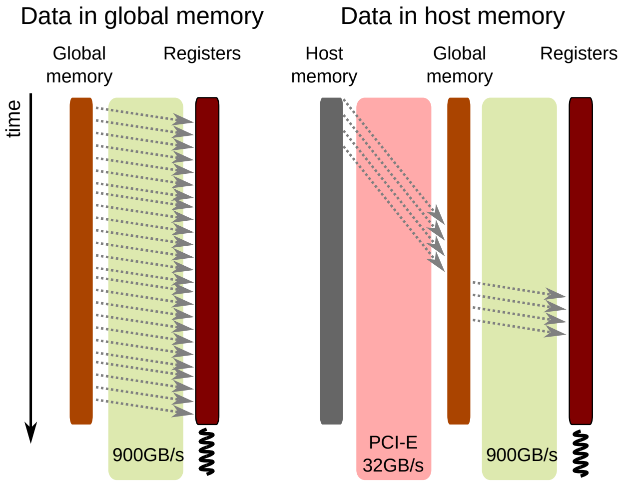
```
struct timespec ts_start;
clock_gettime(CLOCK_MONOTONIC, &ts_start);

cudaMemcpy(d_y, y, n*sizeof(double), cudaMemcpyHostToDevice);

dim3 threads = 256;
dim3 blocks = max(1, min(256, n/threads.x));
ax_kernel<<<blocks, threads>>>(n, alpha, d_y);

cudaMemcpy(y, d_y, n*sizeof(double), cudaMemcpyDeviceToHost);

struct timespec ts_stop;
clock_gettime(CLOCK_MONOTONIC, &ts_stop);
```

- Outcome:

```
Time = 1.652748 s
Floprate = 0.3 GFlops
Memory throughput = 5 GB/s
```

PCI-E bandwidth (bandwidth)

- We must remember that the data must be transferred over the PCI-E bus:



PCI-E bandwidth (roofline model)

- We must recalibrate the roofline model for PCI-E 3.0:

$$\mathit{Performance} = \min\left\{\text{Peak Floprate}, \frac{\text{Flops}}{\text{Transfers}} \times 32\ \text{BG/s.}\right\}$$

- The rooline plot is going to look very different: