A CODELESS INTRODUCTION TO GPU PARALLELIZATION

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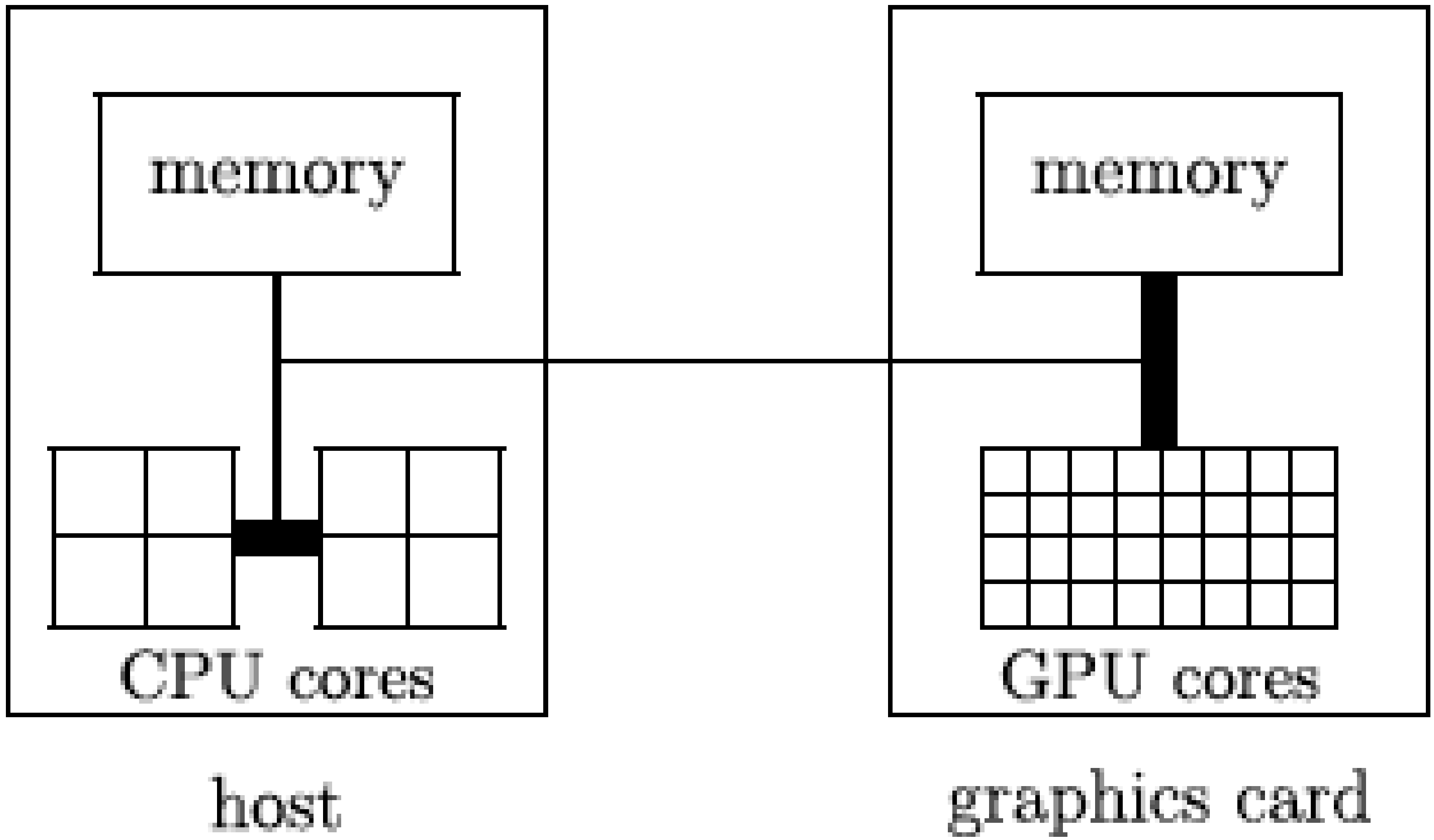
HOW THE CPU AND GPU WORK TOGETHER

A GPU can't run a whole computer on its own because it can't do control flow and it doesn't have access to all the system hardware.

In a GPU-capable computer, the CPU is the main processor, and the GPU is an optional hardware add-on.

The CPU is the "master" of the computer, and it can delegate its highest-throughput parallelizable arithmetic load to the GPU "minion".

Another analogy: the CPU uses the GPU in the same way that a human uses a hand-held calculator.


memory
memory
CPU cores
GPU cores
host
graphics card

GPUS AND PARALLELIZATION

Parallelization: Running different calculations simultaneously. It speeds up calculations dramatically, and GPUs are much better at it than CPUs.

Kernel: An instruction set executed on the GPU. (All others are executed on the CPU.)

In CUDA C, a kernel is any function prefixed with the keyword, **`__global__`**. (More on that in a later talk.)

REMINDER

There are several kinds of parallelization, all implemented differently:

1. CPU parallelization
2. GPU parallelization
3. parallel cloud computing
4. parallelization for openMP

I will only focus on GPU parallelization, which does not completely generalize to other kinds of parallelization.

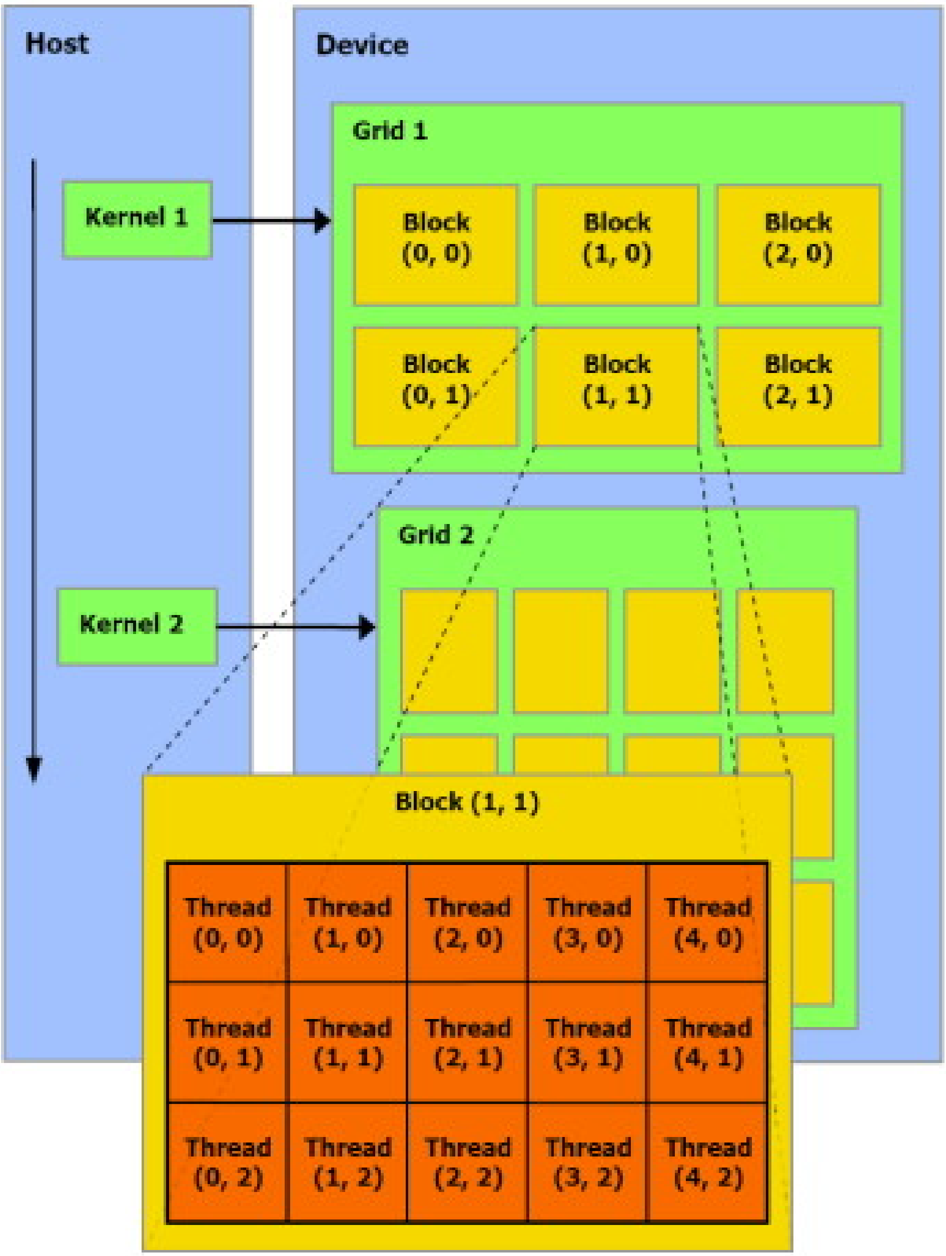
IMPLEMENTING PARALLELIZATION ON THE GPU IN PRACTICE

1. The CPU sends a kernel (instruction set) to the GPU.
2. For every time the CPU sends a kernel, the GPU executes the kernel multiple times simultaneously (in **PARALLEL**). Each such execution of the kernel is called a **thread**.

ORGANIZATION OF THREADS

Grid: The collection of all the threads that are spawned when the CPU sends a kernel to the GPU.

Block: A collection of threads within a grid that share memory.


Host
Device
Grid 1
Kernel 1
Block (0, 0)
Block (1, 0)
Block (2, 0)
Block (0, 1)
Block (1, 1)
Block (2, 1)
Grid 2
Kernel 2
Block (1, 1)
Thread (0, 0)
Thread (1, 0)
Thread (2, 0)
Thread (3, 0)
Thread (4, 0)
Thread (0, 1)
Thread (1, 1)
Thread (2, 1)
Thread (3, 1)
Thread (4, 1)
Thread (0, 2)
Thread (1, 2)
Thread (2, 2)
Thread (3, 2)
Thread (4, 2)

IMPORTANT REMARKS:

- With one grid per kernel, GRIDS are executed SEQUENTIALLY.
- Blocks within the same grid are executed SIMULTANEOUSLY (unless otherwise specified).
- Threads within the same grid are executed SIMULTANEOUSLY (unless otherwise specified), whether they share a block or not.

NOTE: PARALLELIZATION HAS TWO EQUIVALENT DEFINITIONS

1. Running different calculations simultaneously.
2. Breaking up a calculation into grids, then into blocks, and then into threads.

When I say "parallelization" in practice, I will most likely be referring to definition 2.

WHEN TO PARALLELIZE

Calculations you want to parallelize:

- Repeated floating point arithmetic procedures that can all be done simultaneously.
- Anything that can be broken down into or framed as such.

Calculations you don't want to parallelize:

- Inherently sequential calculations, such as recursions.
- Control flow: if-then statements, etc.
- CPU system routines, such as printing to the console.

EXAMPLES OF EASILY PARALLELIZABLE ALGORITHMS

Linear algebraic algorithms are particularly amenable to GPU computing because they involve a high volume of simple arithmetic.

I will showcase:

1. vector addition
2. the pairwise (cascading) sum
3. matrix multiplication
4. the QR factorization

VECTOR ADDITION

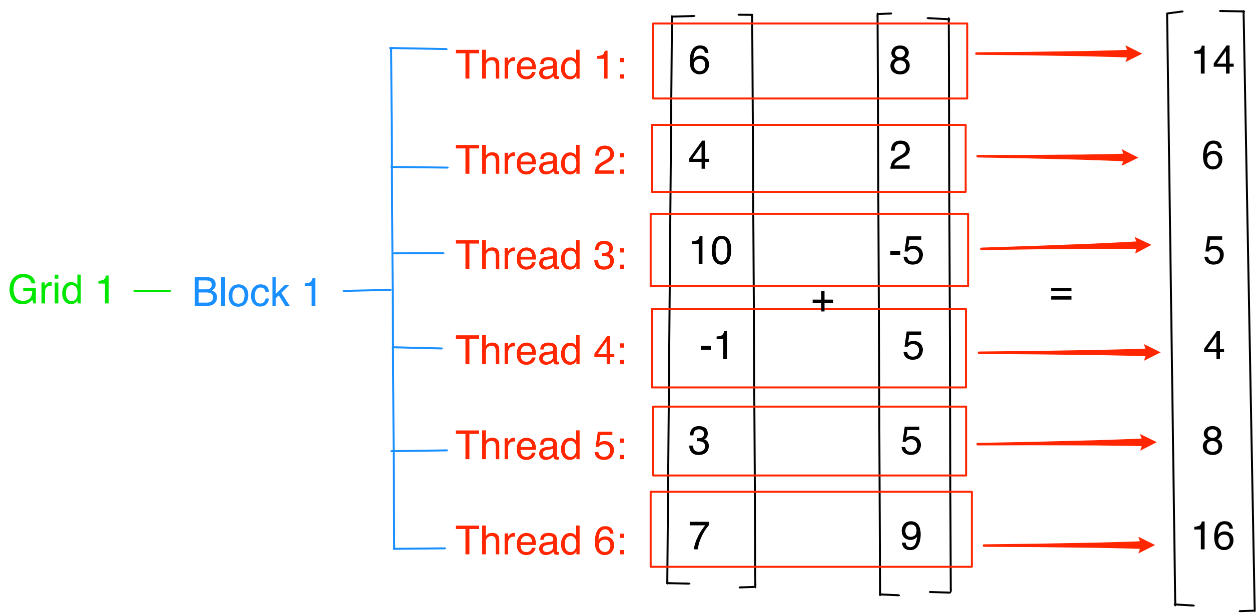
Say I have two vectors:

$$a = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} \quad b = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

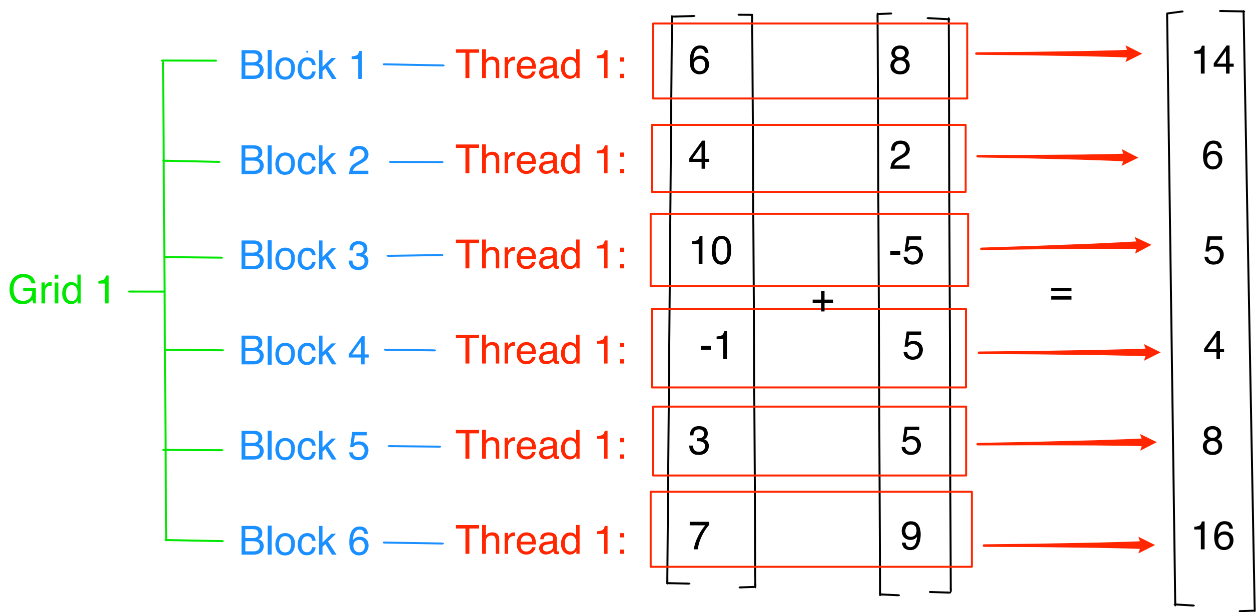
I compute their sum, $c = a + b$, by:

$$c = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix} = \begin{bmatrix} a_1 + b_1 \\ a_2 + b_2 \\ \vdots \\ a_n + b_n \end{bmatrix}$$

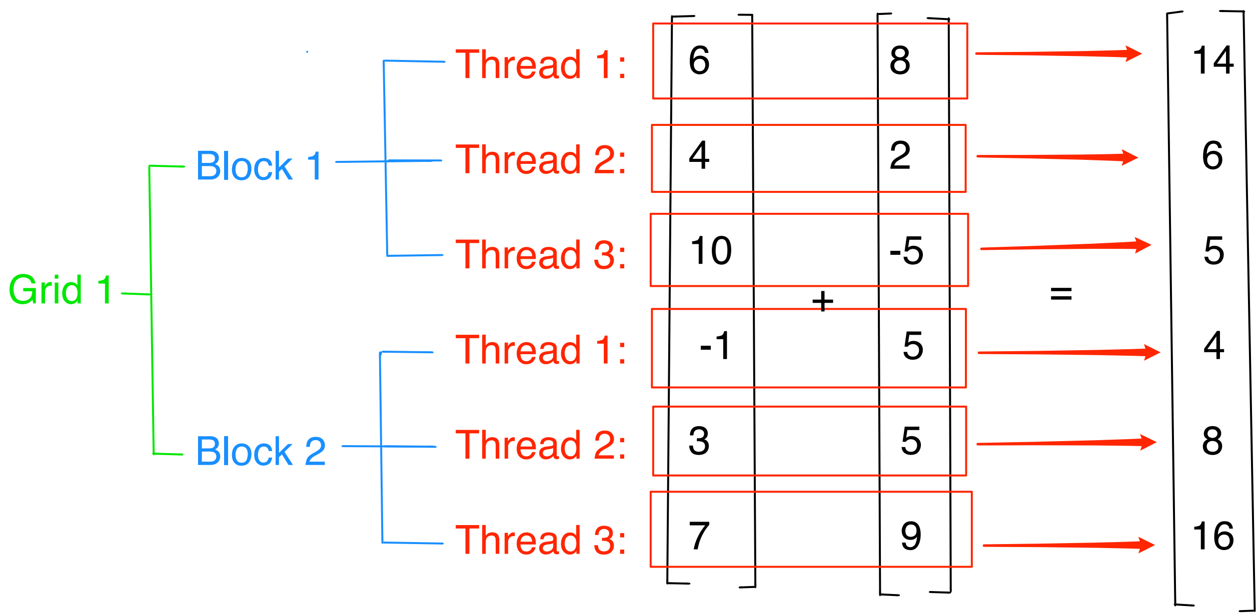
PARALLELIZING VECTOR ADDITION: METHOD 1 OF 3



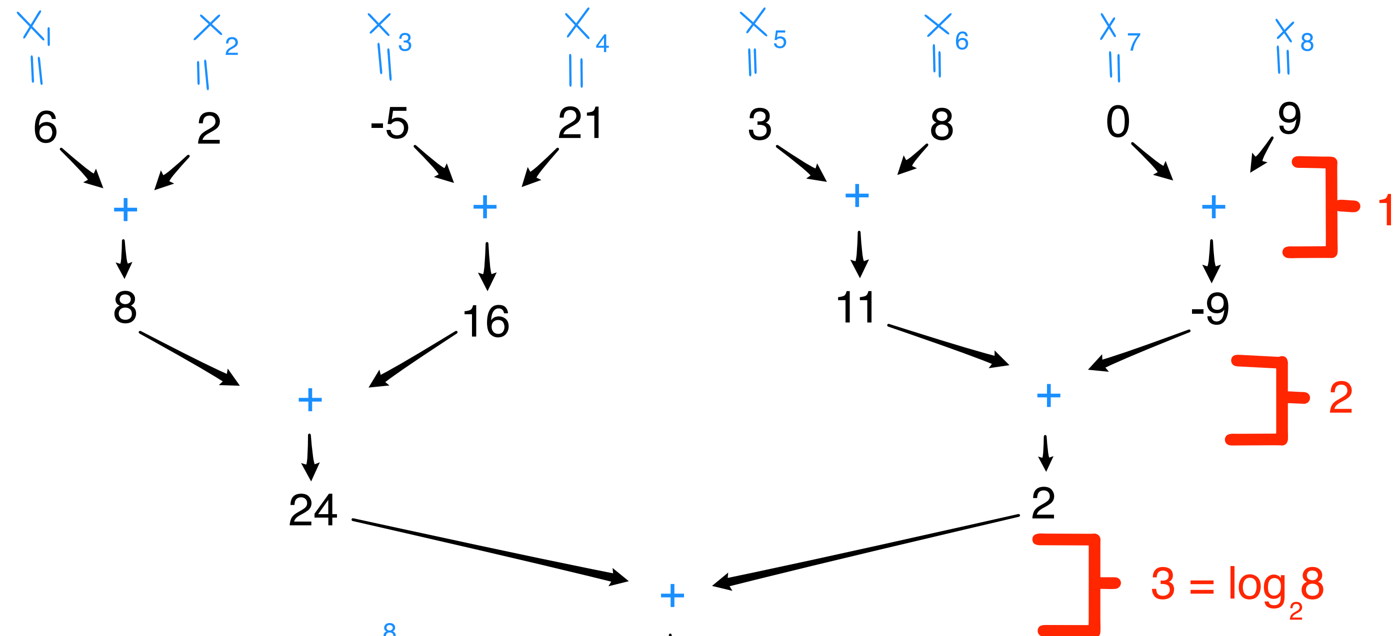
PARALLELIZING VECTOR ADDITION: METHOD 2 OF 3



PARALLELIZING VECTOR ADDITION: METHOD 3 OF 3



2. THE PAIRWISE (CASCADING) SUM



$$\sum_{i=1}^{8} x_i = 26$$

A RIGOROUS DESCRIPTION

Suppose you have a vector $X_0 = (x_{(0,1)}, x_{(0,2)}, \ldots, x_{(0,n)})$, where $n = 2^m$ for some $m > 0$.

Compute $\sum_{i=1}^{n} x_{(0,i)}$ in the following way:

1. Create a new vector:
   $X_1 = (\underbrace{x_{(0,1)} + x_{(0,2)}}_{x_{(1,1)}},\ \underbrace{x_{(0,3)} + x_{(0,4)}}_{x_{(1,2)}},\ \ldots, \underbrace{x_{(0,n-1)} + x_{(0,n)}}_{x_{(1,n/2)}})$
2. Create another new vector:
   $X_2 = (\underbrace{x_{(1,1)} + x_{(1,2)}}_{x_{(2,1)}},\ \underbrace{x_{(1,3)} + x_{(1,4)}}_{x_{(2,2)}},\ \ldots, \underbrace{x_{(1,n/2-1)} + x_{(1,n/2)}}_{x_{(2,n/4)}})$
3. Continue this process until you get a singleton vector:
   $X_m = (\underbrace{x_{(m-1,1)},\ x_{(m-1,2)}}_{x_{(m,1)}})$

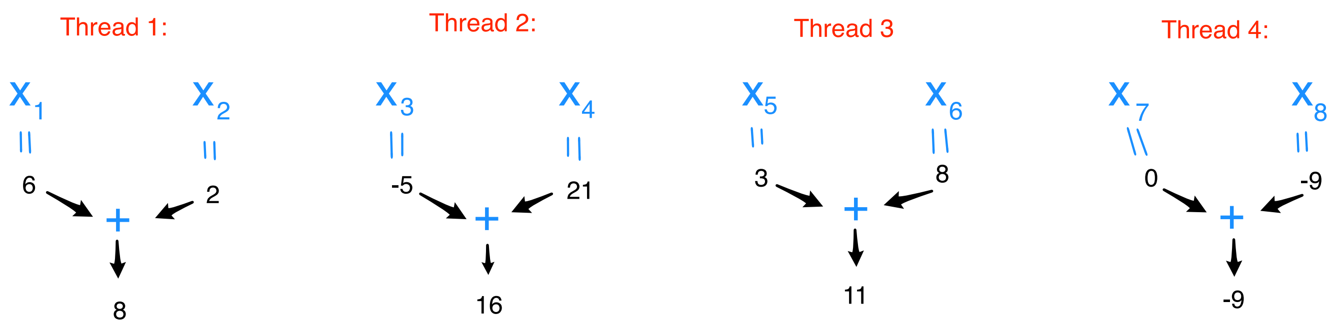
Notice: $\sum_{i=1}^{n} x_{(0,i)} = x_{(m,1)}$

PARALLELIZING THE PAIRWISE SUM

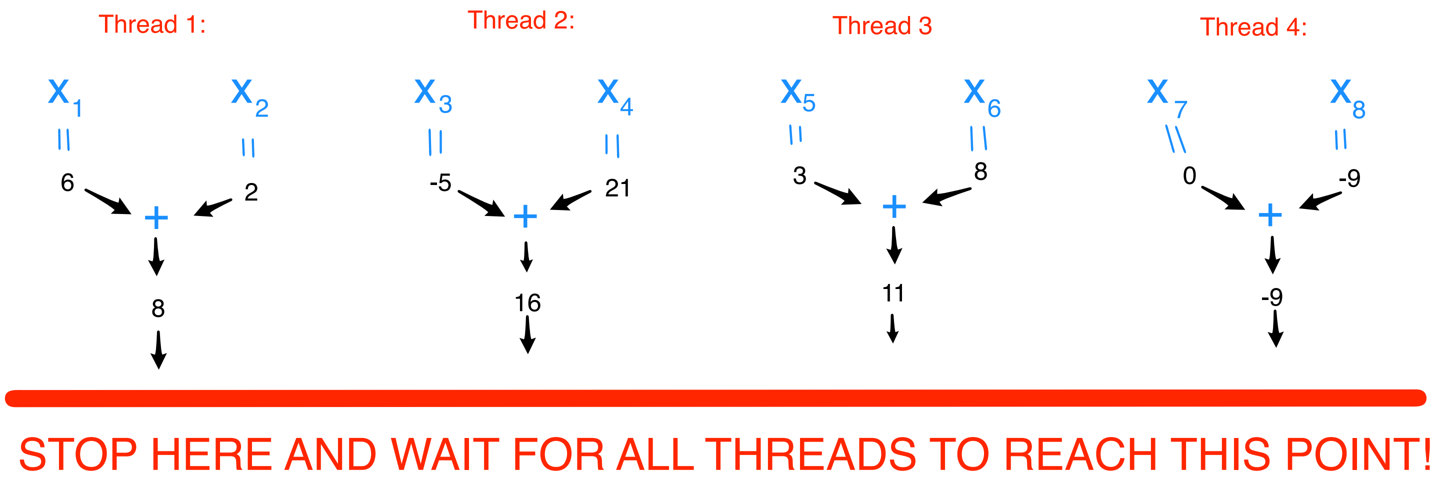
Spawn one grid with a single block and $n = 2^m$ threads. For each iteration $i = 1, 2, \cdots, m$, do the following:

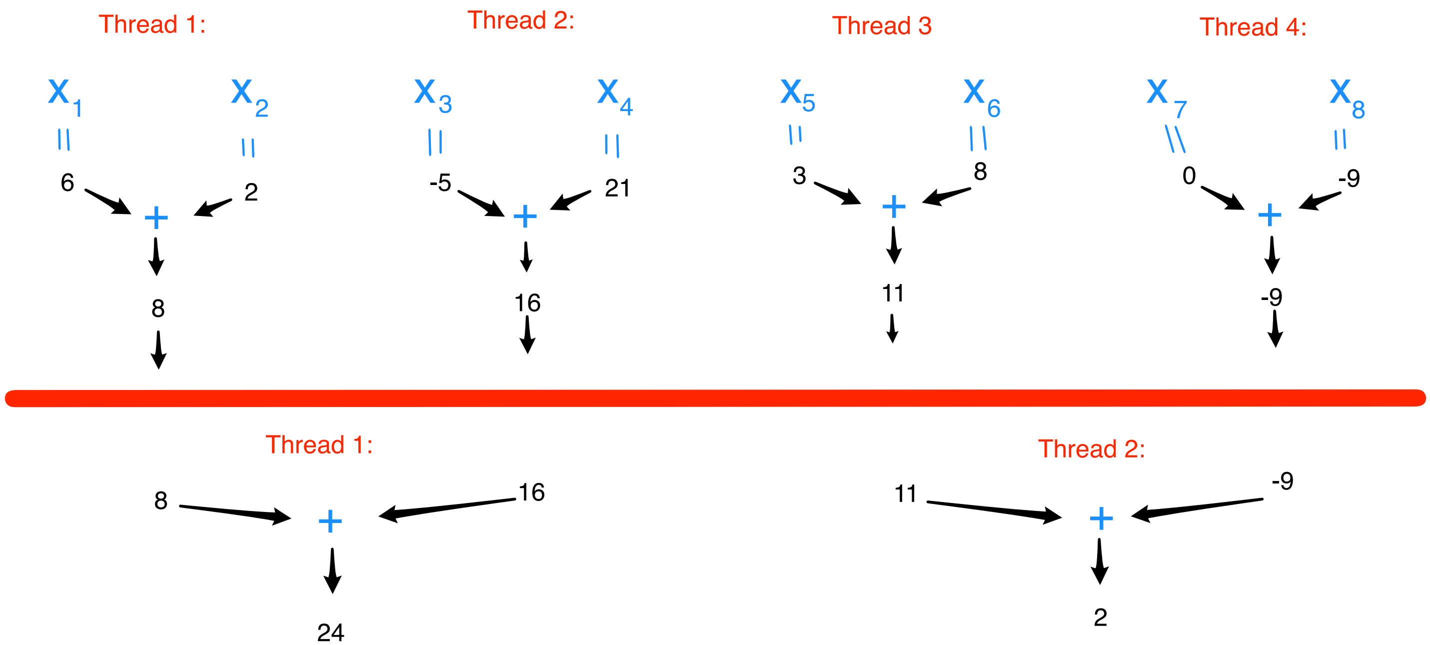
1. Assign thread j to compute:
$$x_{(i,j)} = x_{(i-1,\ 2j-1)} + x_{(i-1,\ 2j)}$$
for $j = 1, 2, \cdots, \frac{n}{2^i}$.
2. Wait until all the above $\frac{n}{2^i}$ threads have completed step 1.
3. Set $i = i + 1$ and repeat.

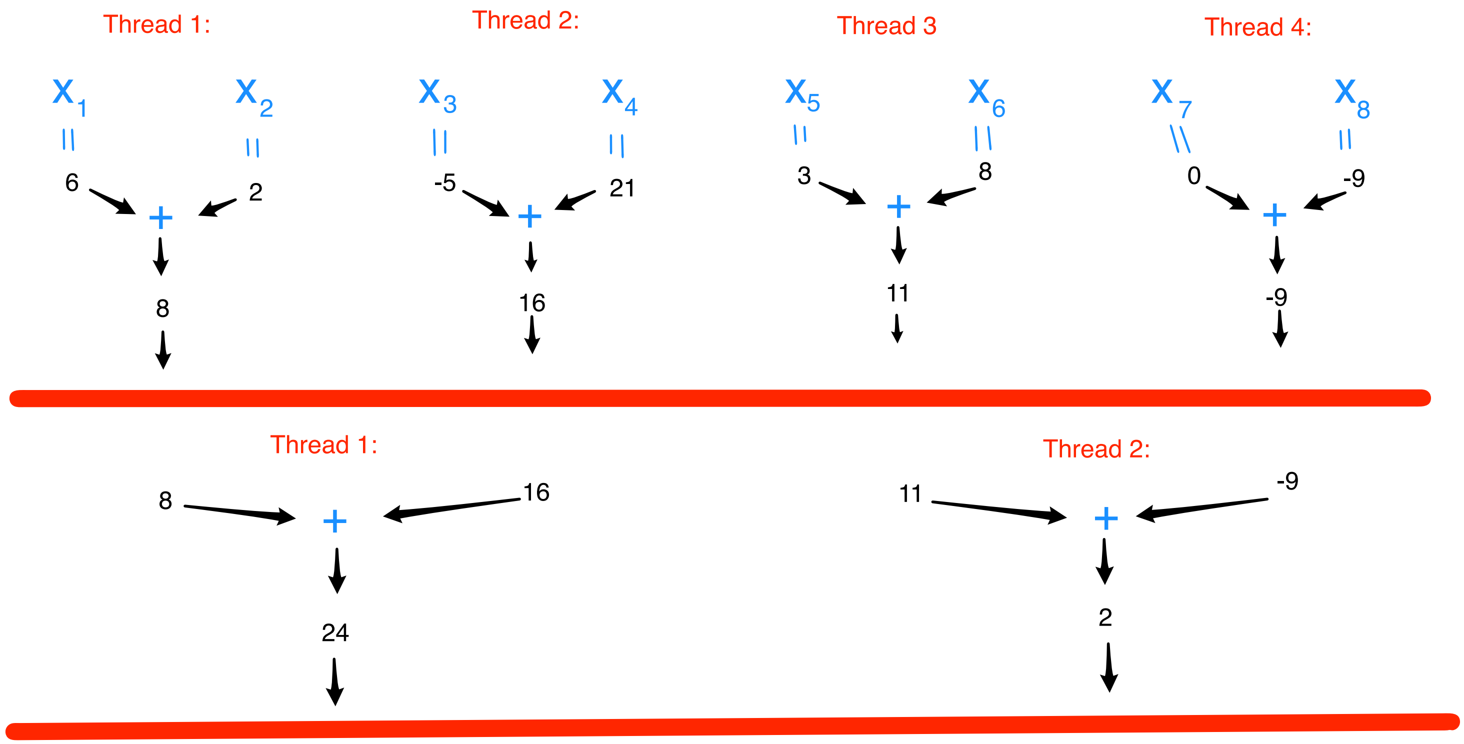
EXAMPLE



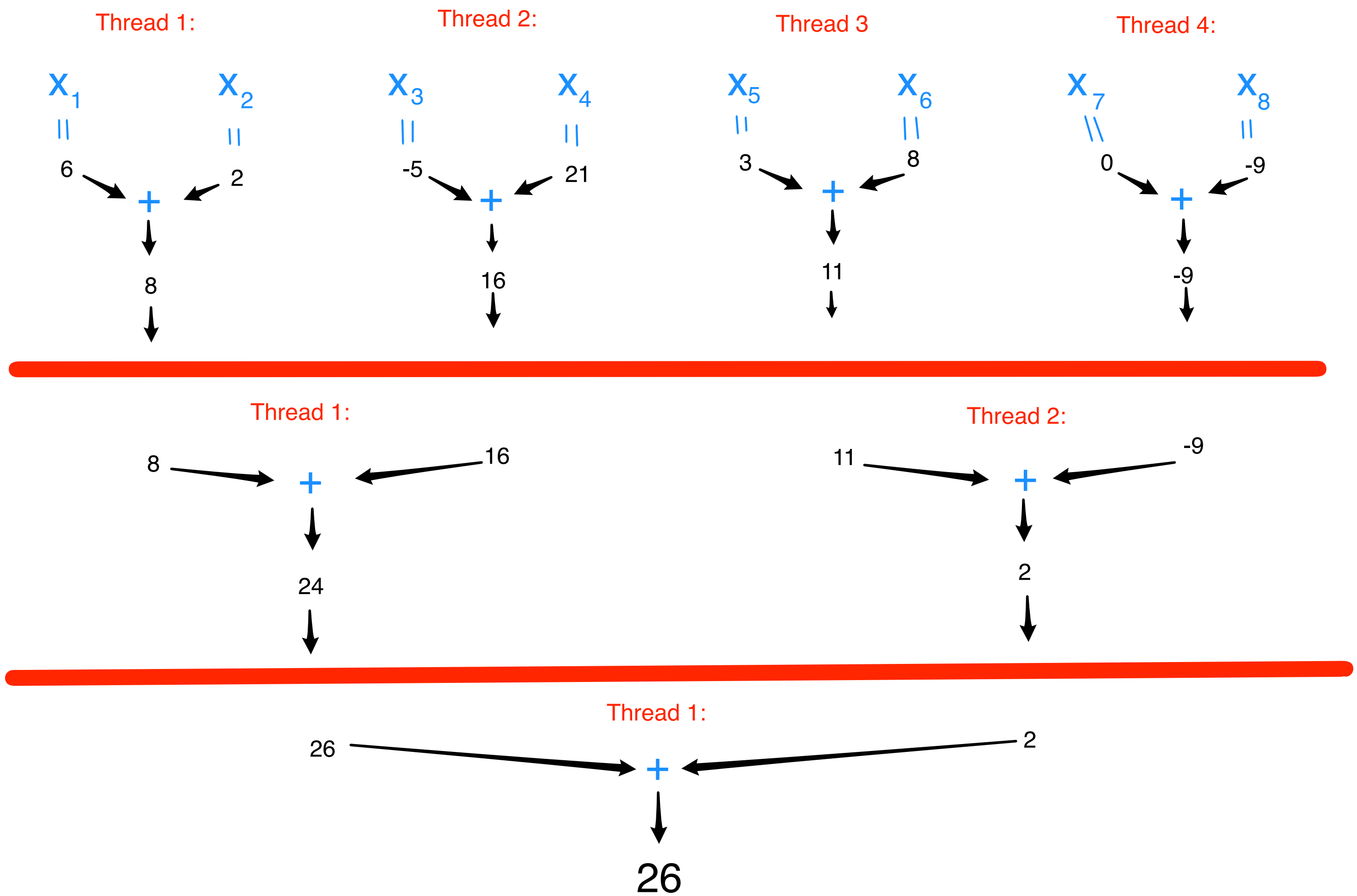
Thread 1:
x1
6
2
x2
+
8
Thread 2:
x3
x4
-5
21
+
16
Thread 3
x5
x6
3
8
+
11
Thread 4:
x7
x8
0
-9
+
-9


Thread 1:
Thread 2:
Thread 3
Thread 4:
x1
x2
x3
x4
x5
x6
x7
x8
6
2
-5
21
3
8
0
-9
+
8
16
11
-9
STOP HERE AND WAIT FOR ALL THREADS TO REACH THIS POINT!

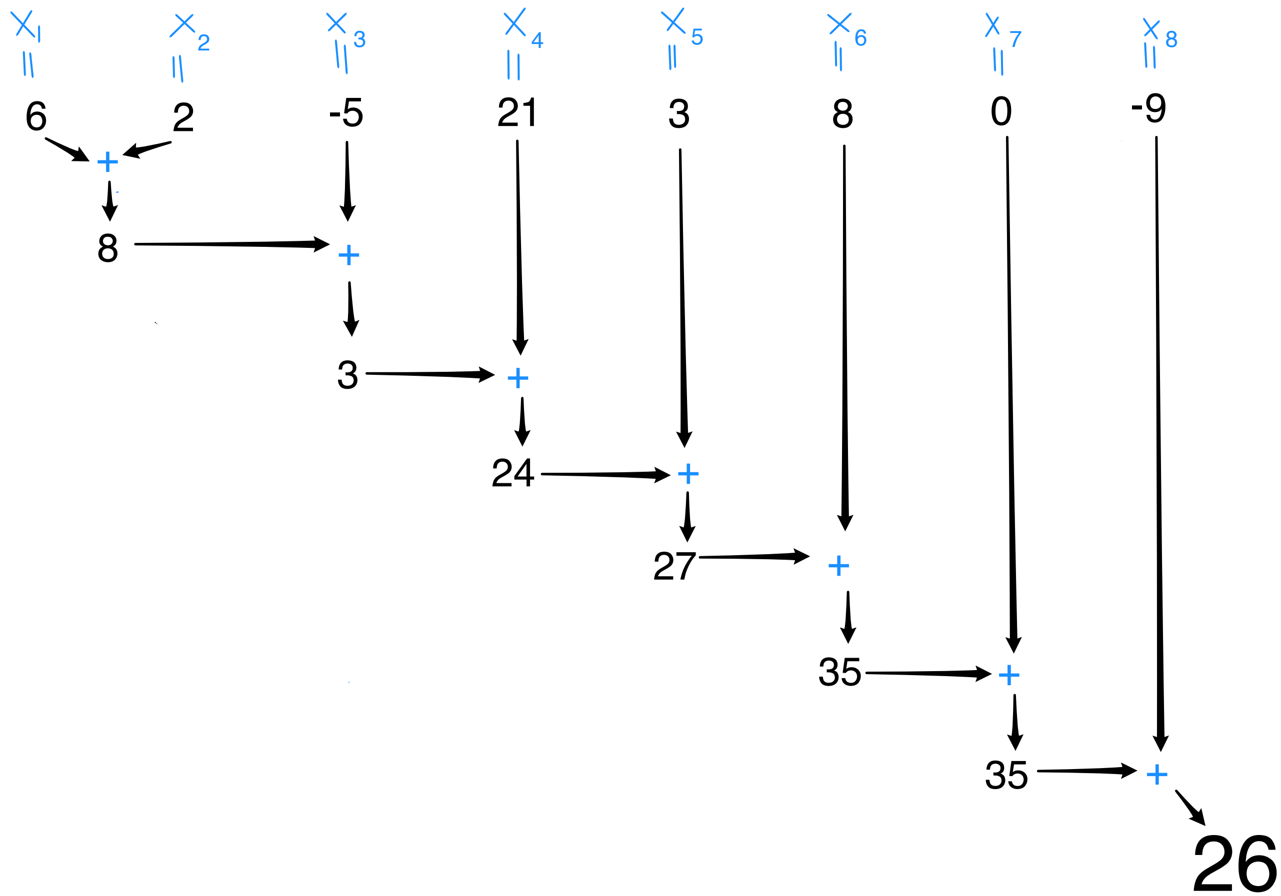

Thread 1:
Thread 2:
Thread 3
Thread 4:
X1
X2
X3
X4
X5
X6
X7
X8
6
2
-5
21
3
8
0
-9
8
16
11
-9
Thread 1:
Thread 2:
8
16
24
11
-9
2



STOP AND WAIT FOR THREADS 1 AND 2 TO REACH THIS POINT!


Thread 1:
Thread 2:
Thread 3
Thread 4:
X1
X2
X3
X4
X5
X6
X7
X8
6
2
-5
21
3
8
0
-9
+
8
16
11
-9
Thread 1:
Thread 2:
8
16
11
-9
24
2
Thread 1:
26
2
26

COMPARE TO THE SEQUENTIAL VERSION



The pairwise sum requires only $\log_2(n)$ sequential steps, whereas the sequential sum requires $n - 1$ steps.

AN ASIDE: SYNCHRONIZING THREADS

Synchronization: Waiting for all parallel tasks to reach a checkpoint before allowing any of those tasks to proceed beyond that checkpoint.

NOTE:

- Threads from the same block can be synchronized easily.
- In general, do not try to synchronize threads from different blocks. It's possible, but extremely inefficient.

3. MATRIX MULTIPLICATION

Consider an $m \times n$ matrix, $A = (a_{ij})$, and an $n \times p$ matrix, $B = (b_{ij})$. Compute $A \cdot B$:

1. Break apart A into its rows: $A = \begin{bmatrix} a_{1\cdot} \\ a_{2\cdot} \\ \vdots \\ a_{m\cdot} \end{bmatrix}$, where each $a_{i\cdot} = \begin{bmatrix} a_{i1} & a_{i2} & \cdots & a_{in} \end{bmatrix}$

2. Break apart B into its columns: $B = \begin{bmatrix} b_{\cdot 1} & b_{\cdot 2} & \cdots & b_{\cdot p} \end{bmatrix}$, where each $b_{\cdot j} = \begin{bmatrix} b_{1j} \\ b_{2j} \\ \vdots \\ b_{nj} \end{bmatrix}$

3. Compute $C = A \cdot B$ elementwise, using the usual matrix multiplication rules to find each $a_i \cdot b_j$:

$$C = A \cdot B = \begin{bmatrix} (a_{1\cdot} \cdot b_{\cdot 1}) & (a_{1\cdot} \cdot b_{\cdot 2}) & \cdots & (a_{1\cdot} \cdot b_{\cdot p}) \\ (a_{2\cdot} \cdot b_{\cdot 1}) & (a_{2\cdot} \cdot b_{\cdot 2}) & & (a_{2\cdot} \cdot b_{\cdot p}) \\ \vdots & & \ddots & \vdots \\ (a_{m\cdot} \cdot b_{\cdot 1}) & (a_{m\cdot} \cdot b_{\cdot 2}) & \cdots & (a_{m\cdot} \cdot b_{\cdot p}) \end{bmatrix}$$

i.e.:

$$C_{(i,j)} = a_{i\cdot} \cdot b_{\cdot j}$$

PARALLELIZING MATRIX MULTIPLICATION

Spawn one grid with $m \cdot p$ blocks. Assign block (i, j) to compute $C_{(i,j)} = a_{i\cdot} \cdot b_{\cdot j}$ using the following steps:

1. Spawn n threads.
2. Tell the k'th thread to compute $c_{ijk} = a_{ik} b_{kj}$.
3. Synchronize the n threads to make sure we have finished calculating all of $c_{ij1}, c_{ij2}, \ldots, c_{ijn}$ before proceeding.
4. Compute $C_{(i,j)} = \sum_{k=1}^{n} c_{ijk}$ as a pairwise sum.

EXAMPLE

Say I want to compute $A \cdot B$, where:

$$A = \begin{bmatrix} 1 & 2 \\ -1 & 5 \\ 7 & -9 \end{bmatrix} \quad B = \begin{bmatrix} 8 & 8 & 7 \\ 3 & 5 & 2 \end{bmatrix}$$

which I'm setting up as:

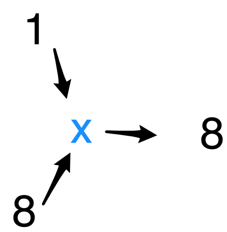
$$C = A \cdot B = \begin{bmatrix} \left(\begin{bmatrix} 1 & 2 \end{bmatrix} \cdot \begin{bmatrix} 8 \\ 3 \end{bmatrix} \right) & \left(\begin{bmatrix} 1 & 2 \end{bmatrix} \cdot \begin{bmatrix} 8 \\ 5 \end{bmatrix} \right) & \left(\begin{bmatrix} 1 & 2 \end{bmatrix} \cdot \begin{bmatrix} 7 \\ 2 \end{bmatrix} \right) \\ \left(\begin{bmatrix} -1 & 5 \end{bmatrix} \cdot \begin{bmatrix} 8 \\ 3 \end{bmatrix} \right) & \left(\begin{bmatrix} -1 & 5 \end{bmatrix} \cdot \begin{bmatrix} 8 \\ 5 \end{bmatrix} \right) & \left(\begin{bmatrix} -1 & 5 \end{bmatrix} \cdot \begin{bmatrix} 7 \\ 2 \end{bmatrix} \right) \\ \left(\begin{bmatrix} 7 & -9 \end{bmatrix} \cdot \begin{bmatrix} 8 \\ 3 \end{bmatrix} \right) & \left(\begin{bmatrix} 7 & -9 \end{bmatrix} \cdot \begin{bmatrix} 8 \\ 5 \end{bmatrix} \right) & \left(\begin{bmatrix} 7 & -9 \end{bmatrix} \cdot \begin{bmatrix} 7 \\ 2 \end{bmatrix} \right) \end{bmatrix}$$

$$
\begin{bmatrix}
\overset{\text{Block (1, 1)}}{\left(\begin{bmatrix} 1 & 2 \end{bmatrix} \cdot \begin{bmatrix} 8 \\ 3 \end{bmatrix} \right)} & \overset{\text{Block (1, 2)}}{\left(\begin{bmatrix} 1 & 2 \end{bmatrix} \cdot \begin{bmatrix} 8 \\ 5 \end{bmatrix} \right)} & \overset{\text{Block (1, 3)}}{\left(\begin{bmatrix} 1 & 2 \end{bmatrix} \cdot \begin{bmatrix} 7 \\ 2 \end{bmatrix} \right)} \\
\overset{\text{Block (2, 1)}}{\left(\begin{bmatrix} -1 & 5 \end{bmatrix} \cdot \begin{bmatrix} 8 \\ 3 \end{bmatrix} \right)} & \overset{\text{Block (2, 2)}}{\left(\begin{bmatrix} -1 & 5 \end{bmatrix} \cdot \begin{bmatrix} 8 \\ 5 \end{bmatrix} \right)} & \overset{\text{Block (2, 3)}}{\left(\begin{bmatrix} -1 & 5 \end{bmatrix} \cdot \begin{bmatrix} 7 \\ 2 \end{bmatrix} \right)} \\
\overset{\text{Block (3,1)}}{\left(\begin{bmatrix} 7 & -9 \end{bmatrix} \cdot \begin{bmatrix} 8 \\ 3 \end{bmatrix} \right)} & \overset{\text{Block (3, 2)}}{\left(\begin{bmatrix} 7 & -9 \end{bmatrix} \cdot \begin{bmatrix} 8 \\ 5 \end{bmatrix} \right)} & \overset{\text{Block (3, 3)}}{\left(\begin{bmatrix} 7 & -9 \end{bmatrix} \cdot \begin{bmatrix} 7 \\ 2 \end{bmatrix} \right)}
\end{bmatrix}
$$

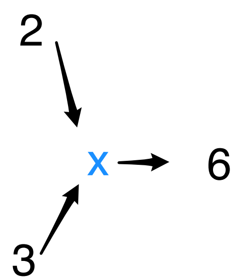
We don't need to synchronize the blocks because we can compute them independently.

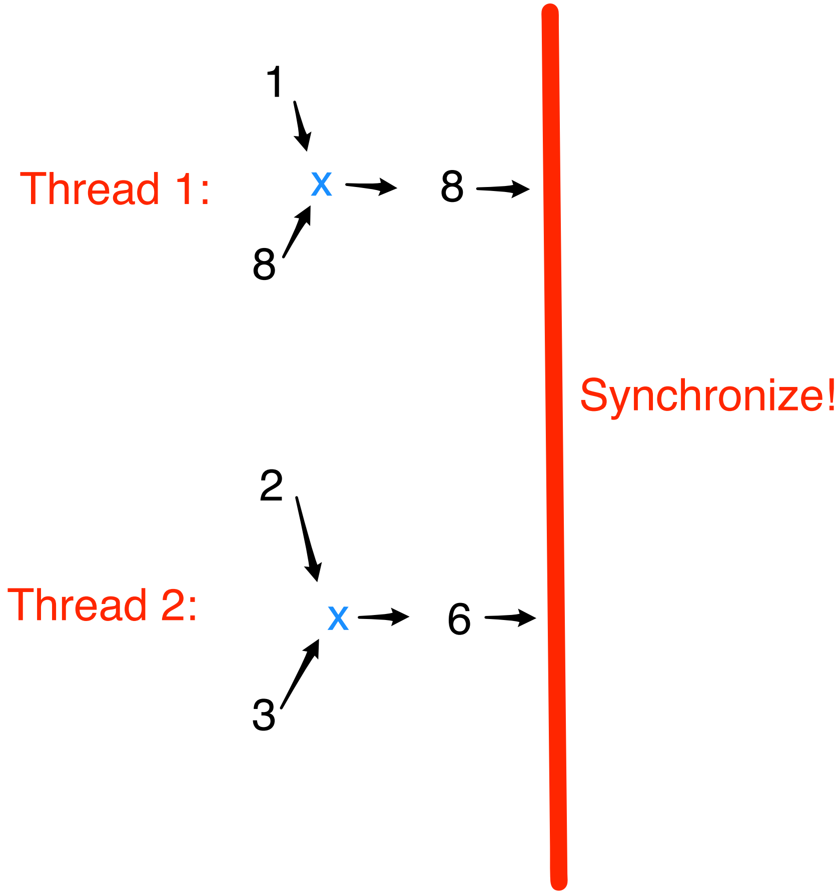
Consider Block (1,1), which computes $\begin{bmatrix} 1 & 2 \end{bmatrix} \cdot \begin{bmatrix} 8 \\ 3 \end{bmatrix}$:

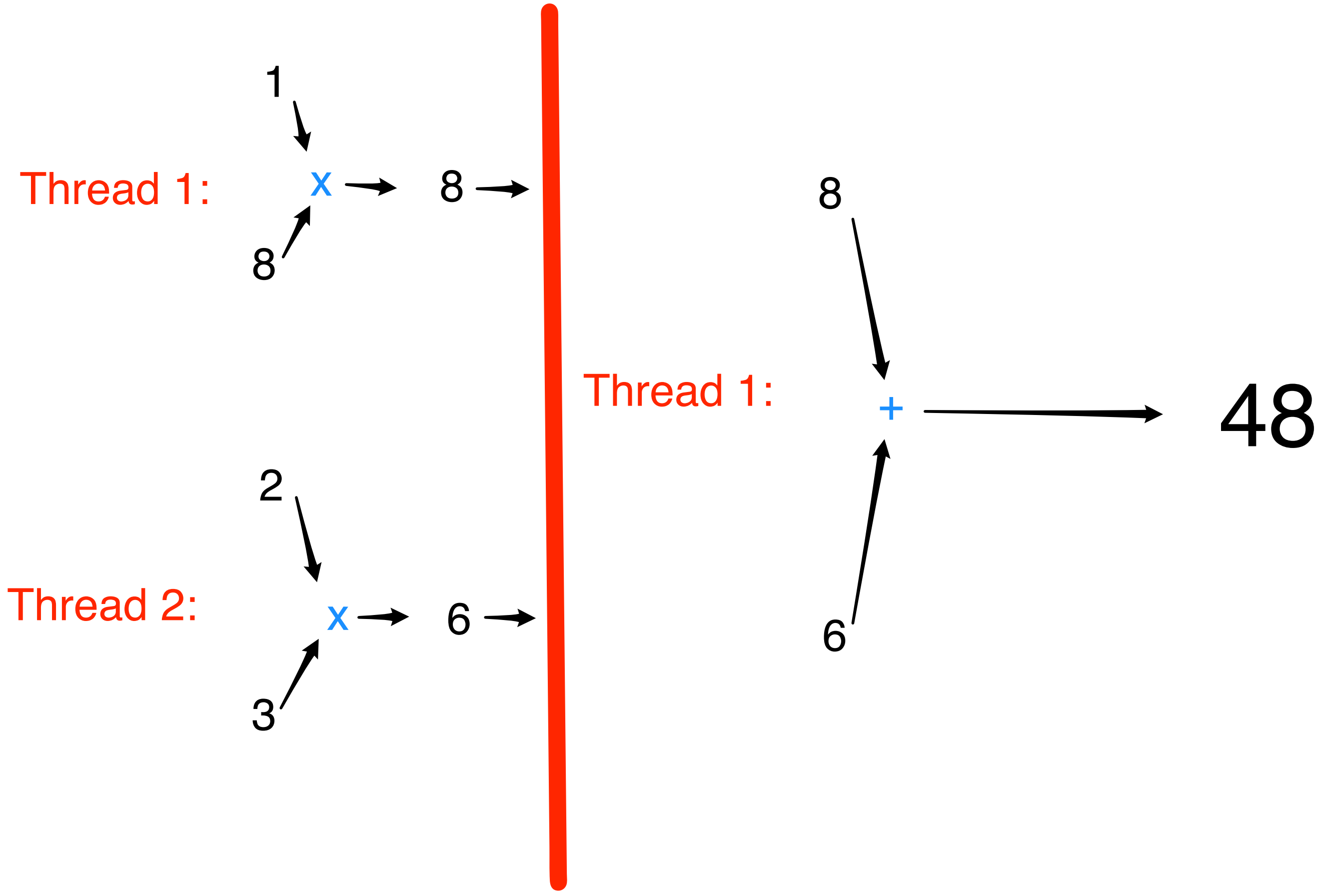
Thread 1:



Thread 2:




1
Thread 1:
x
8
8
Synchronize!
2
Thread 2:
x
6
3


Thread 1:
1
x
8
8
Thread 2:
2
x
6
3
6
Thread 1:
8
+
48
6

LECTURE SERIES MATERIALS

These lecture slides, a tentative syllabus for the series, and code are available at:

https://github.com/wlandau/gpu.

REFERENCES

Lay, David C. *L*inear Algebra and Its Applications. 3rd Ed. Addison Wesley, 2006.

J. Sanders and E. Kandrot. *CUDA by Example*. Addison-Wesley, 2010.