# GRAPHICS PROCESSING UNITS WITH PYTHON

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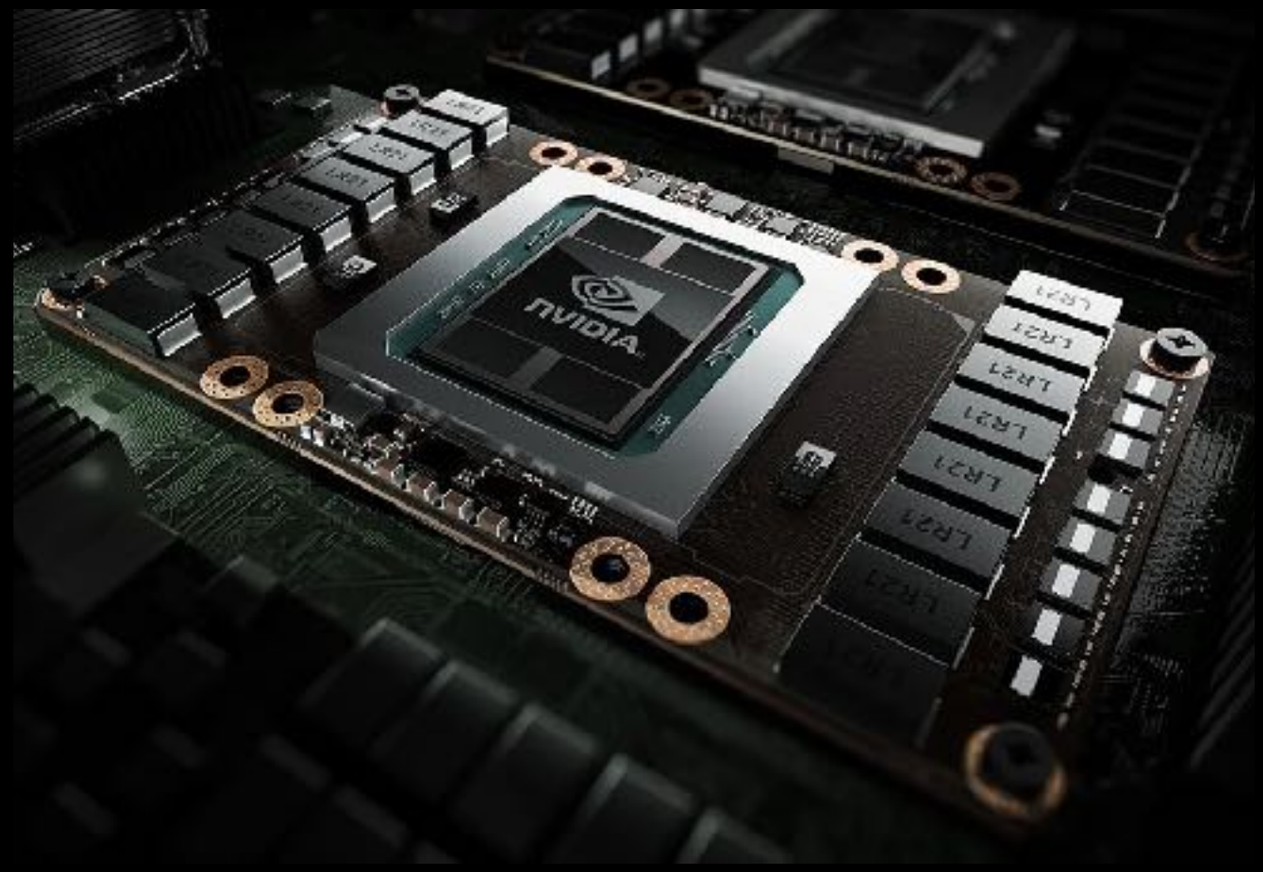
# CO-PROCESSORS, INCLUDING GPUS

## *Graphics Processing Unit (GPU) - Overview*

- designed for fast graphics processing
- graphics are a form of arithmetic
- have gradually evolved a design that is also useful for non-graphics computing
- Are not standalone, work alongside CPU (host) - coprocessor

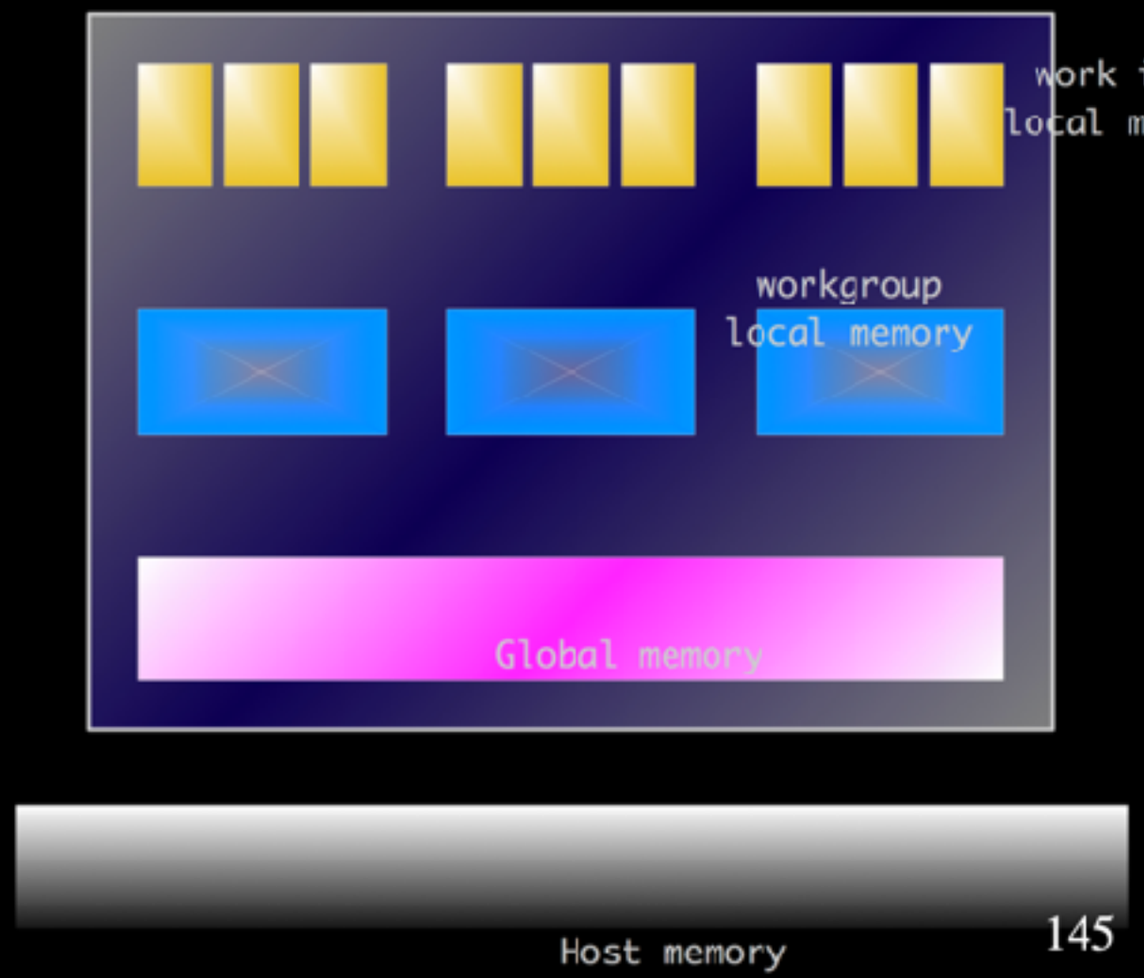



*NVIDIA Ampere A100 Tensor Core GPU is the world's most powerful accelerator for deep learning, machine learning, high-performance computing, and graphics.*

# CO-PROCESSORS, INCLUDING GPUS

## *GPUs - Memory Management*

- In *GPUs*, the solution is to support many more threads with fast switching between them.
- Because of this, memory management is key in GPU computing. Smaller caches!




*Memory structure of a GPU.*

# CO-PROCESSORS, INCLUDING GPUS

## *GPUs - GPUs versus CPUs*

### *CPUs:*

- Data exist on the CPU - somewhere.
- Peak performance = more cores. More flexible cache.
- Single stream of potentially very different instructions.
- Perform well on a single or few threads.

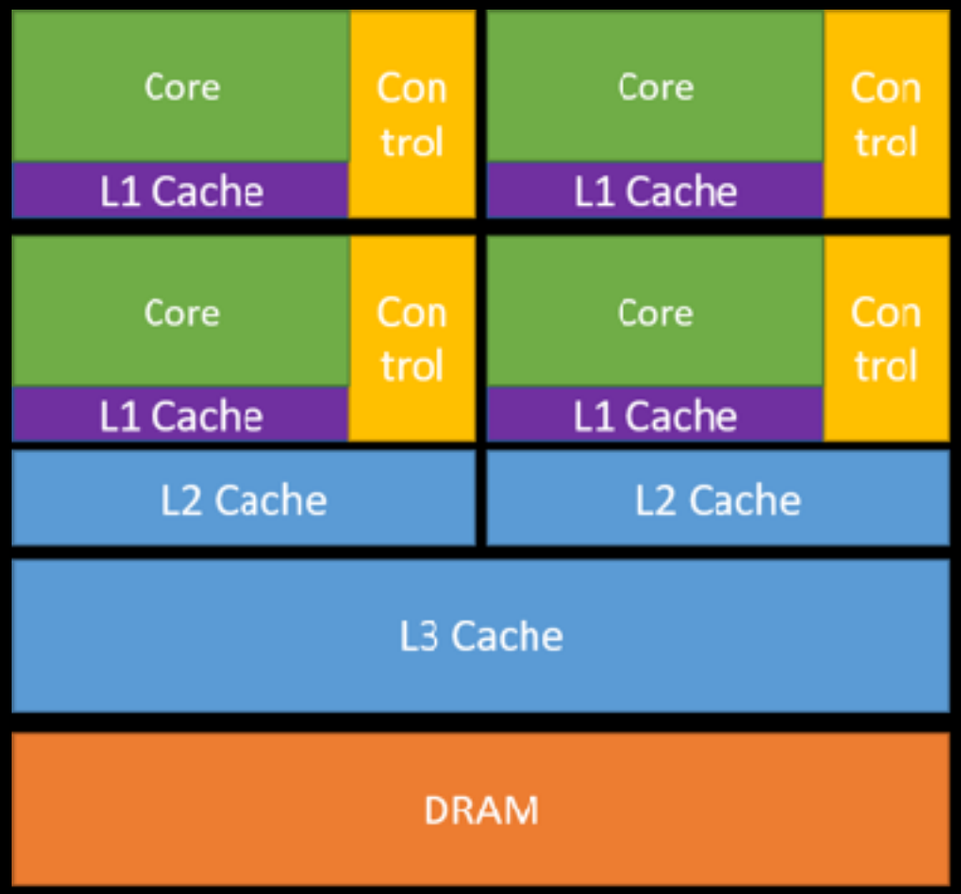
### *GPUs:*

- GPUs are co-processors, meaning they require data to be transferred.
- Limited cache size, datatype (size) limited. Smaller datatypes = higher peak performance.
- Poor performance on “traditional codes”
- Designed to perform well on *many* threads.

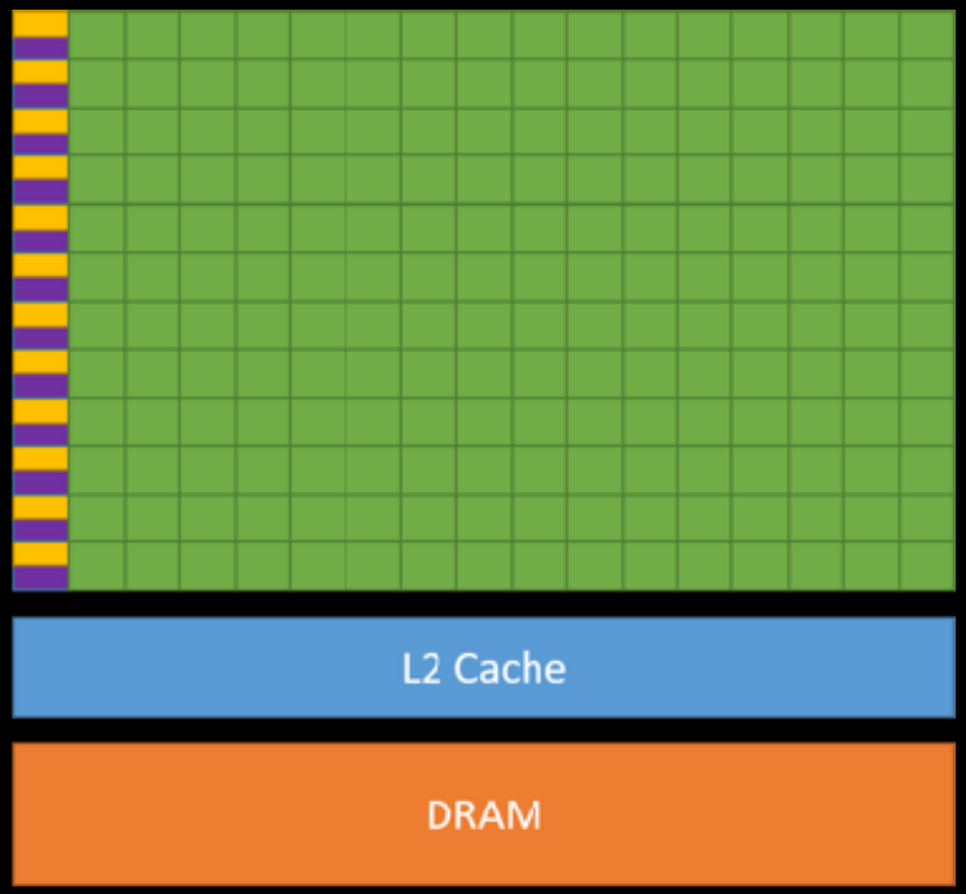
# CO-PROCESSORS, INCLUDING GPUS

## *GPUs - GPUs versus CPUs*

### *CPU:*




### *GPU:*

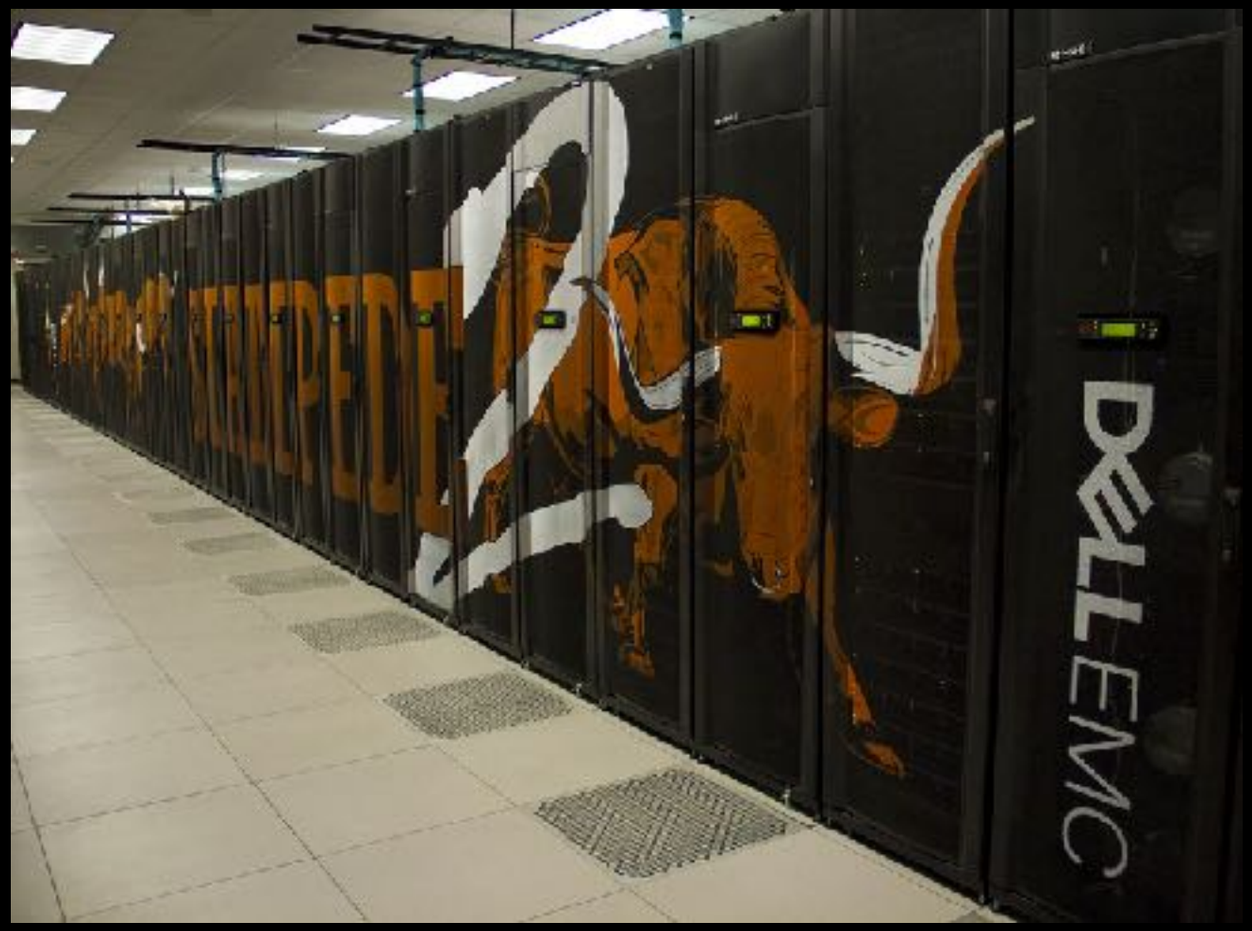



*Schematic diagram of CPU and GPU.*

# CO-PROCESSORS, INCLUDING GPUS

## *GPUs - Expected benefits*

- Very good at doing **data parallel** computing
- CUDA provides a tool for writing code for the GPU
- Requires computation to have “enough data parallelism”.
- Other co-processors exist!




*Stampede 2 at Texas Advanced Computing Center. Uses Intel Knights Landing many-core processors as stand alone processors.*

## CO-PROCESSORS, INCLUDING GPUS

Your target architecture can determine your approach

# UTILIZING MODERN GPUS

## *CUDA Programming Model*

- CUDA®: A General-Purpose Parallel Computing Platform and Programming Model
- Comes with a software environment that allows developers to use C++ as a high-level programming language
- Automatic scalability to newer GPUs

# UTILIZING MODERN GPUS

## *CUDA Programming Model - CUDA Kernels*

- Functions, called *kernels*, that, when called, are executed N times in parallel by N different *CUDA threads*

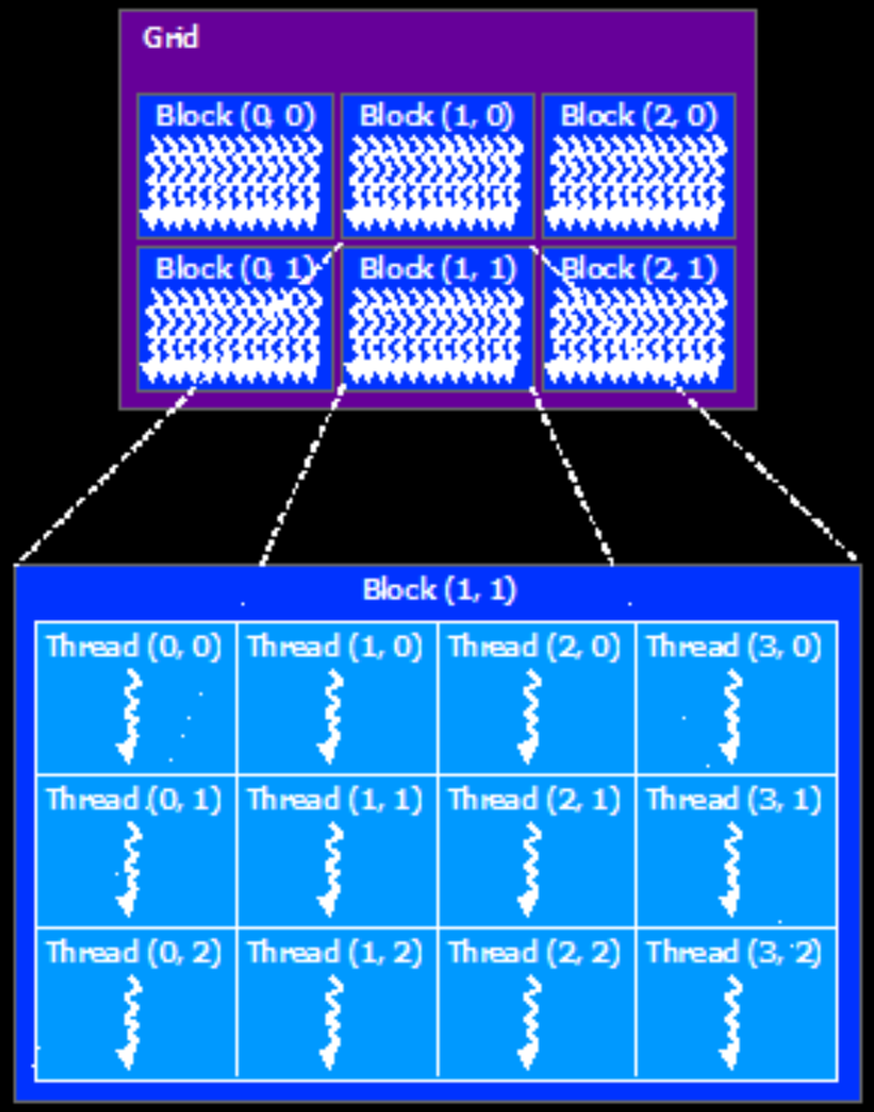
```
// Kernel definition
__global__ void VecAdd(float* A, float* B, float* C)
{
    int i = threadIdx.x;
    C[i] = A[i] + B[i];
}

int main()
{
    ...
    // Kernel invocation with N threads
    VecAdd<<<1, N>>>(A, B, C);
    ...
}
```

# UTILIZING MODERN GPUS

## *CUDA Programming Model - Grids and Thread Blocks*

- Kernels can be executed by individual **threads** or multiple equally-shaped thread blocks.
- **Blocks** are a collection of threads.
- A **Grid** is a collection of **Block**s.

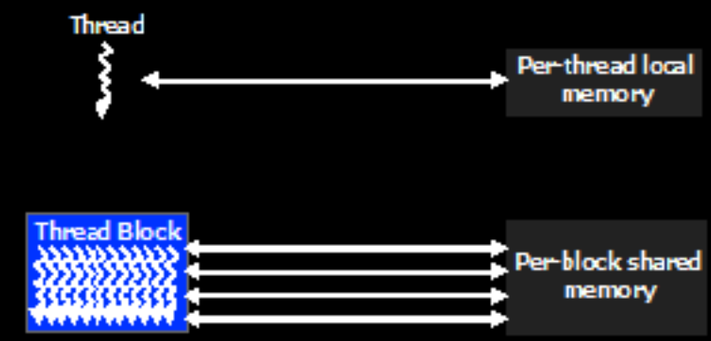


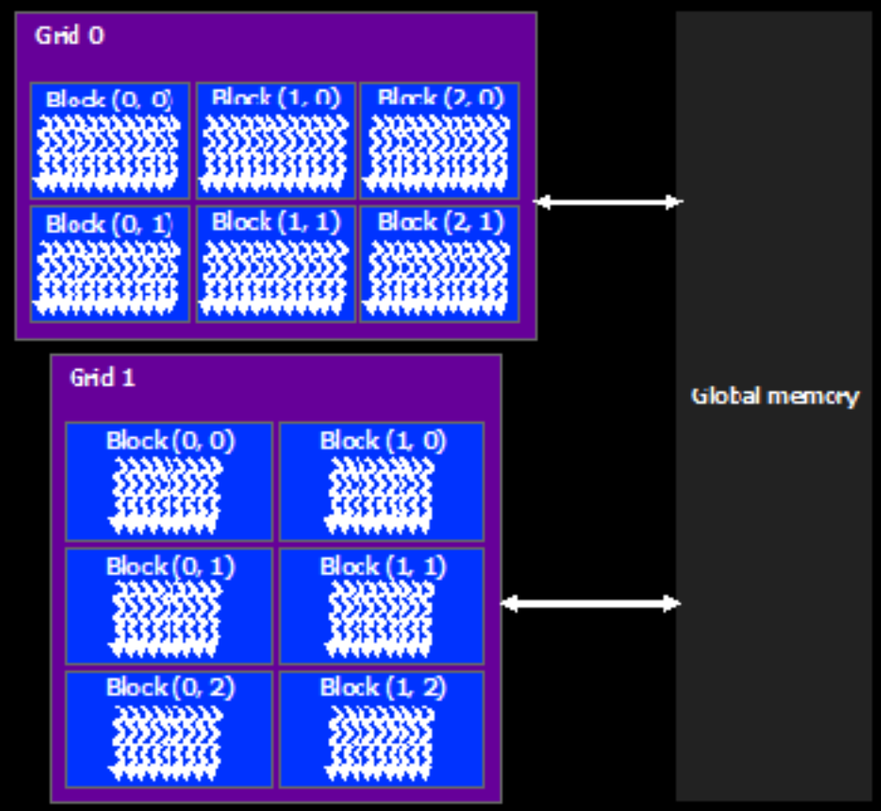

*Schematic diagram of Thread Blocks*

# UTILIZING MODERN GPUS

## *CUDA Programming Model - Memory Hierarchy*

- Threads have access to local memory.
- Blocks can share memory among threads
- Grids have access to global memory.
- Programs designed with memory hierarchy in mind.



# UTILIZING MODERN GPUS

## *CUDA Programming Model - Heterogeneous Computing*

- CUDA model assumes GPUs operate as co-processors.
- Requires explicit management of data to and from **device.**
- CUDA Programming interface has many options including in Python!

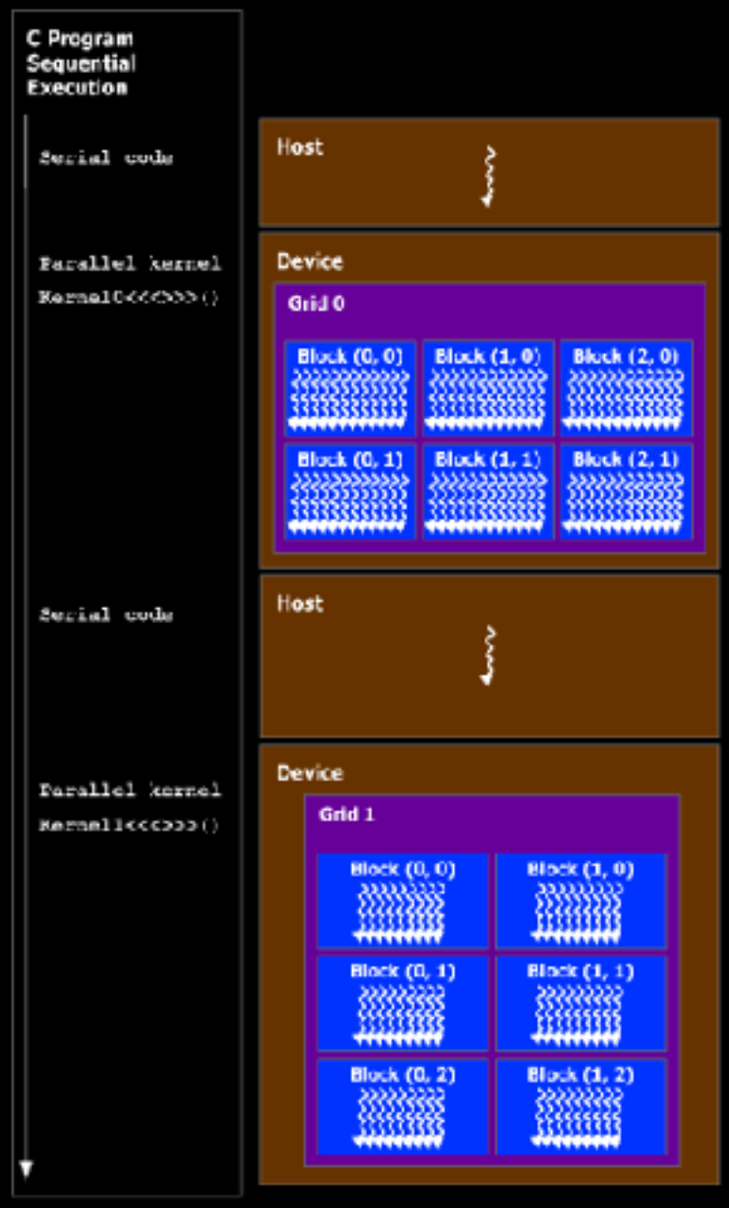



*Diagram showing Heterogeneous Programming.*

# UTILIZING MODERN GPUS

Tools leveraging the CUDA programming model in Python exist!

# PARALLEL COMPUTING WITH GPUS

*Numba makes Python code fast (on GPUs too)*

Numba

*Kernel declaration:*

```
@cuda.jit
def increment_by_one(an_array):
    """
    Increment all array elements by one.
    """
    # code elided here; read further for different implementations
```

# PARALLEL COMPUTING WITH GPUS

*Numba makes Python code fast (on GPUs too)*


*Kernel invocation:*

```
threadsperblock = 32
blockspergrid = (an_array.size + (threadsperblock - 1)) // threadsperblock
increment_by_one[blockspergrid, threadsperblock](an_array)
```

- Depends on array size, requires some knowledge of available threads

# PARALLEL COMPUTING WITH GPUS

*Numba makes Python code fast (on GPUs too)*


*Choosing the block size:*

- On the software side, the block size determines how many threads share a given area of shared memory.
- On the hardware side, the block size must be large enough for full occupation of execution units.
- Code will typically run but not be maximally efficient tools for measuring efficiency and block size.

# PARALLEL COMPUTING WITH GPUS

*Numba makes Python code fast (on GPUs too)*

Numba

*Thread positioning:*

```python
@cuda.jit
def increment_by_one(an_array):
    # Thread id in a 1D block
    tx = cuda.threadIdx.x
    # Block id in a 1D grid
    ty = cuda.blockIdx.x
    # Block width, i.e. number of threads per block
    bw = cuda.blockDim.x
    # Compute flattened index inside the array
    pos = tx + ty * bw
    if pos < an_array.size:  # Check array boundaries
        an_array[pos] += 1
```

- Tools for determining thread positioning.

# PARALLEL COMPUTING WITH GPUS

## *cuDF - GPU DataFrames*

RAPIDS

- cuDF is a Python GPU DataFrame library (built on the Apache Arrow columnar memory format) for loading, joining, aggregating, filtering, and otherwise manipulating data
- cuDF also provides a **pandas**-like API
- Accelerate their workflows without going into the details of CUDA programming

# PARALLEL COMPUTING WITH GPUS

## *cuDF - GPU DataFrames*

RAPIDS

## *When to use what:*

- workflow is fast enough on a single GPU or your data comfortably fits in memory on a single GPU, you would want to use **cuDF**

- want to distribute your workflow across multiple GPUs, have more data than you can fit in memory on a single GPU, or want to analyze data spread across many files at once, you would want to use **Dask-cuDF**.

*Specific examples at https://docs.rapids.ai/api*

# PARALLEL COMPUTING WITH GPUS

The best approach will likely be a combination of different tools.