N-WAYS GPU BOOTCAMP

A QUICK GUIDE TO CUPY

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A QUICK GUIDE TO CUPY

What to expect?

- What is CuPy?
- Features of CuPy
- Installation Guide
- CuPy Fundamentals
- CUDA Kernels
- Summary

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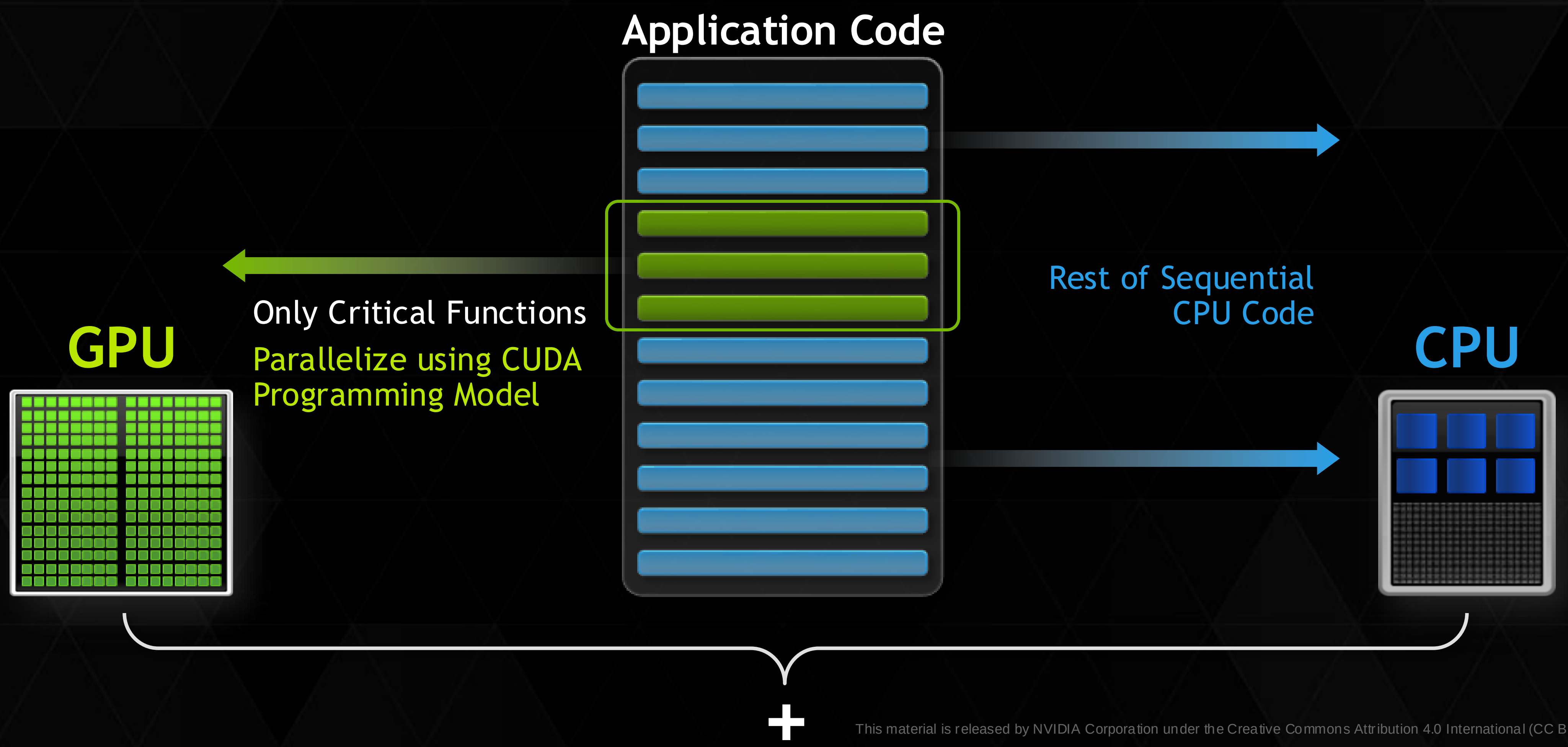
GPU COMPUTING



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CUDA ARCHITECTURE PROGRAMMING MODEL

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CUDA KERNELS

- Parallel portion of application: execute as a kernel
  - Entire GPU executes kernel, many threads
- CUDA threads:
  - Lightweight
  - Fast switching
  - Tens of thousands execute simultaneously

CPU	Host	Executes functions
GPU	Device	Executes kernels

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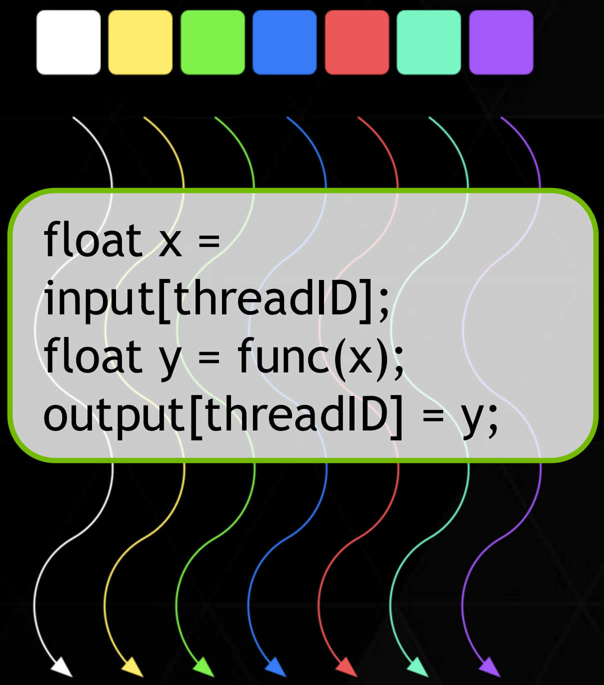
CUDA KERNELS: PARALLEL THREADS

- A kernel is a function executed on the GPU
  - Array of threads, in parallel
- All threads execute the same code, can take different paths
  - Each thread has an ID
  - Select input/output data
  - Control decisions



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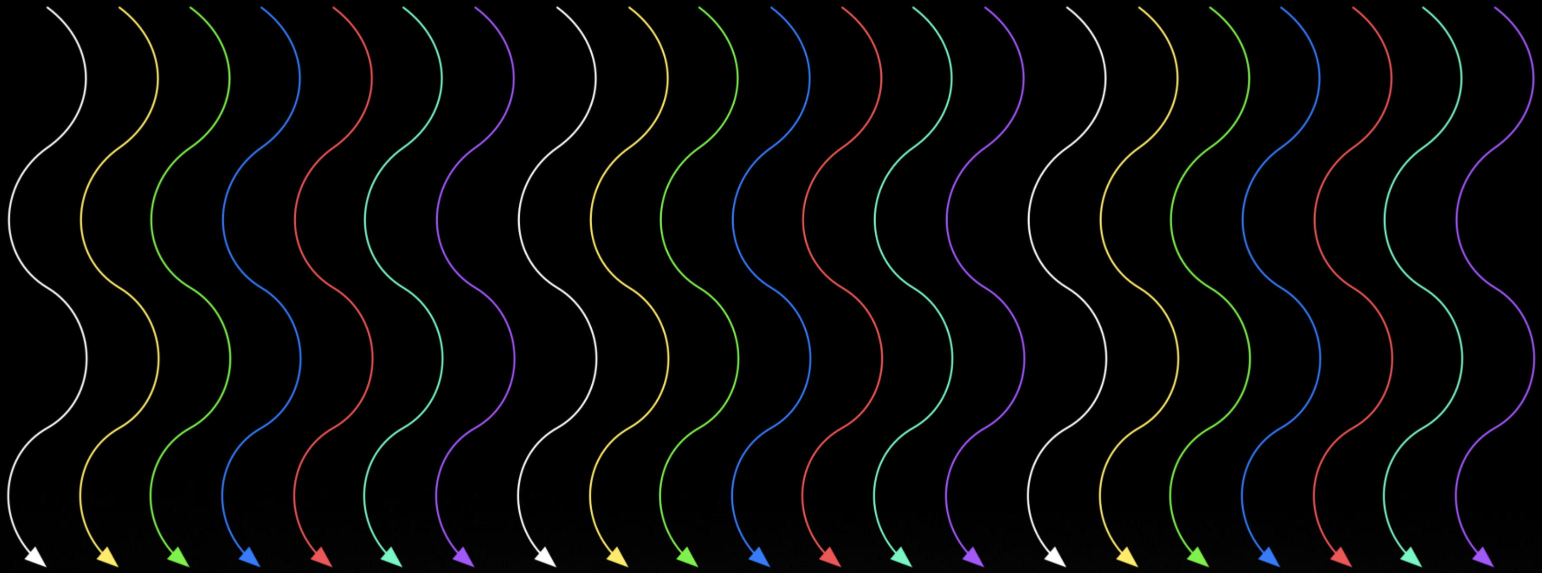
CUDA KERNELS: SUBDIVIDE INTO BLOCKS



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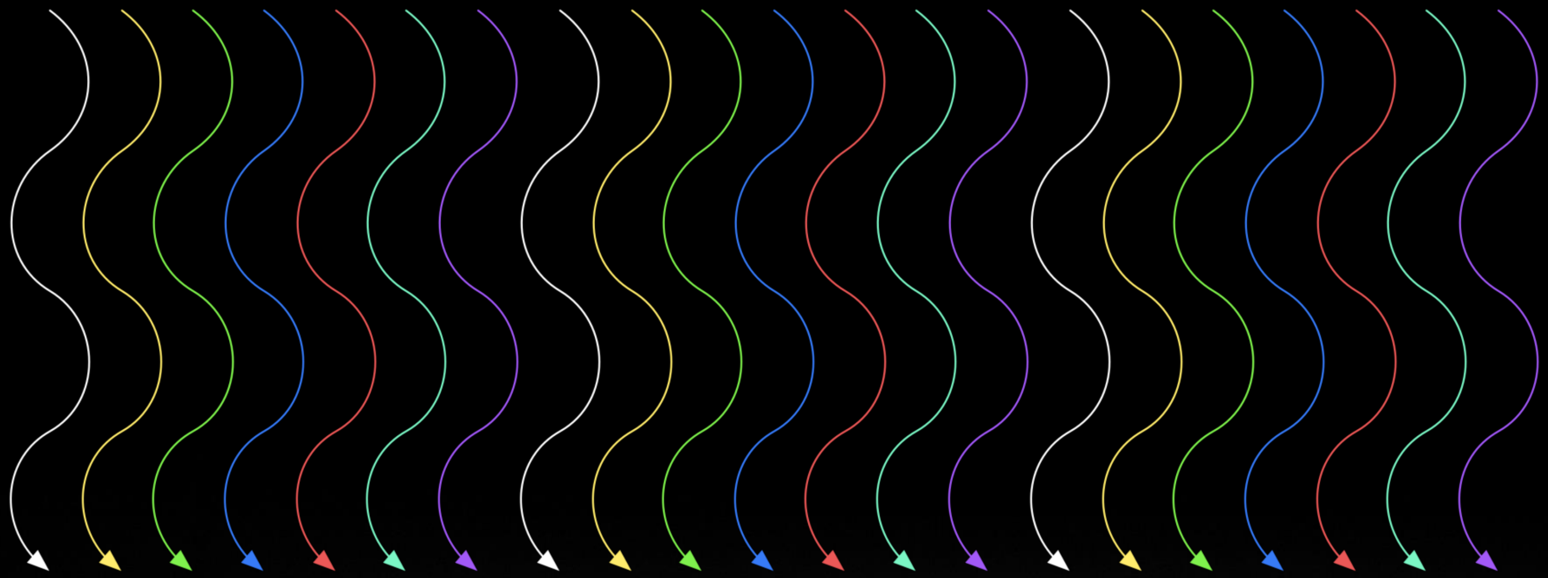
CUDA KERNELS: SUBDIVIDE INTO BLOCKS



- Threads are grouped into blocks

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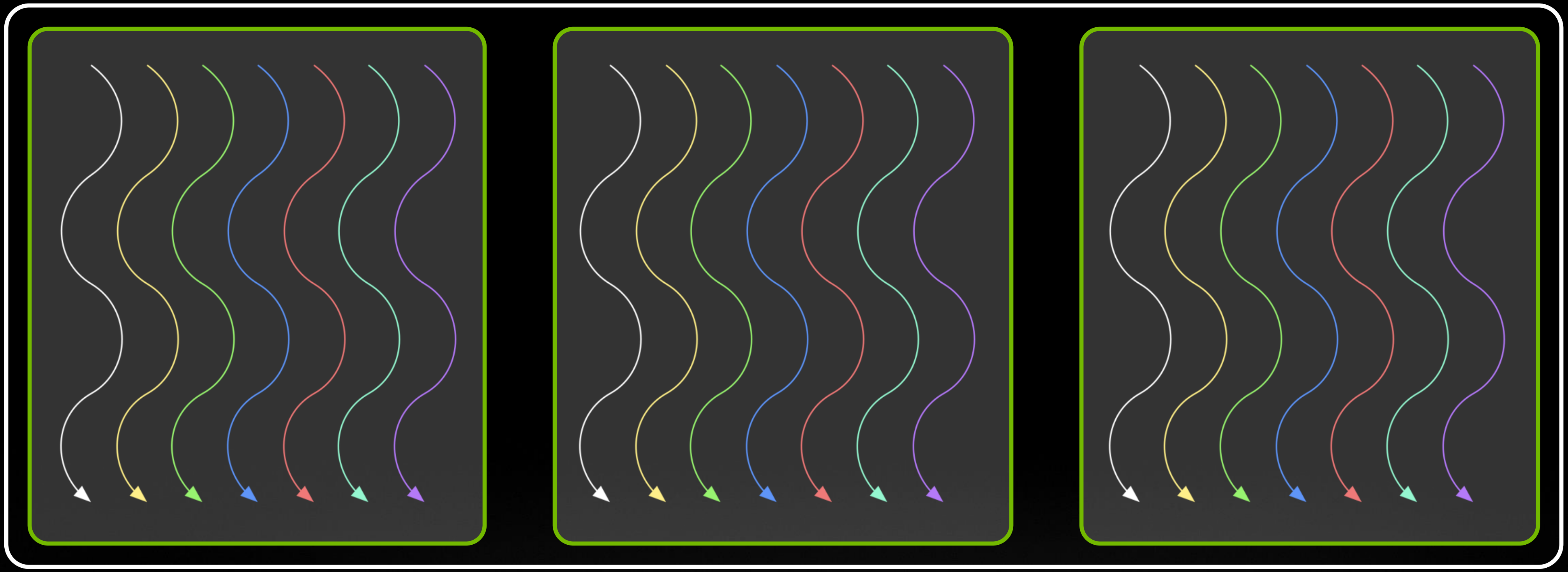
CUDA KERNELS: SUBDIVIDE INTO BLOCKS



- Threads are grouped into blocks
- Blocks are grouped into a grid

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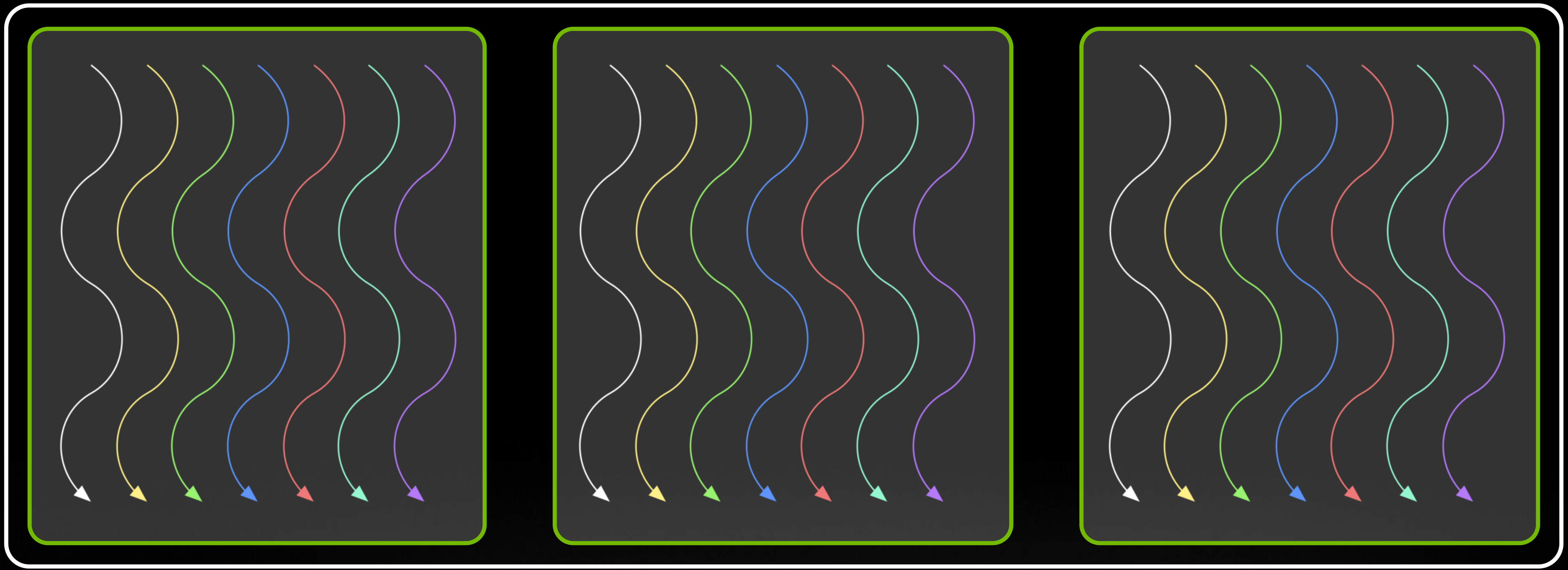
CUDA KERNELS: SUBDIVIDE INTO BLOCKS



- Threads are grouped into blocks
- Blocks are grouped into a grid
- A kernel is executed as a grid of blocks of threads

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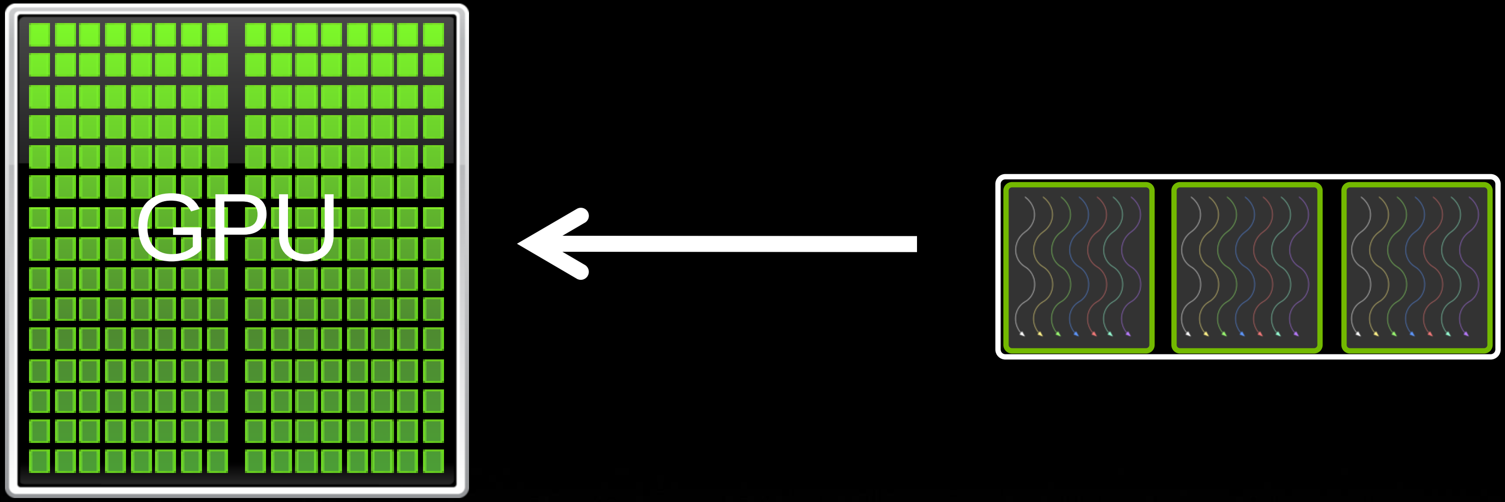
CUDA KERNELS: SUBDIVIDE INTO BLOCKS



- Threads are grouped into blocks
- Blocks are grouped into a grid
- A kernel is executed as a grid of blocks of threads

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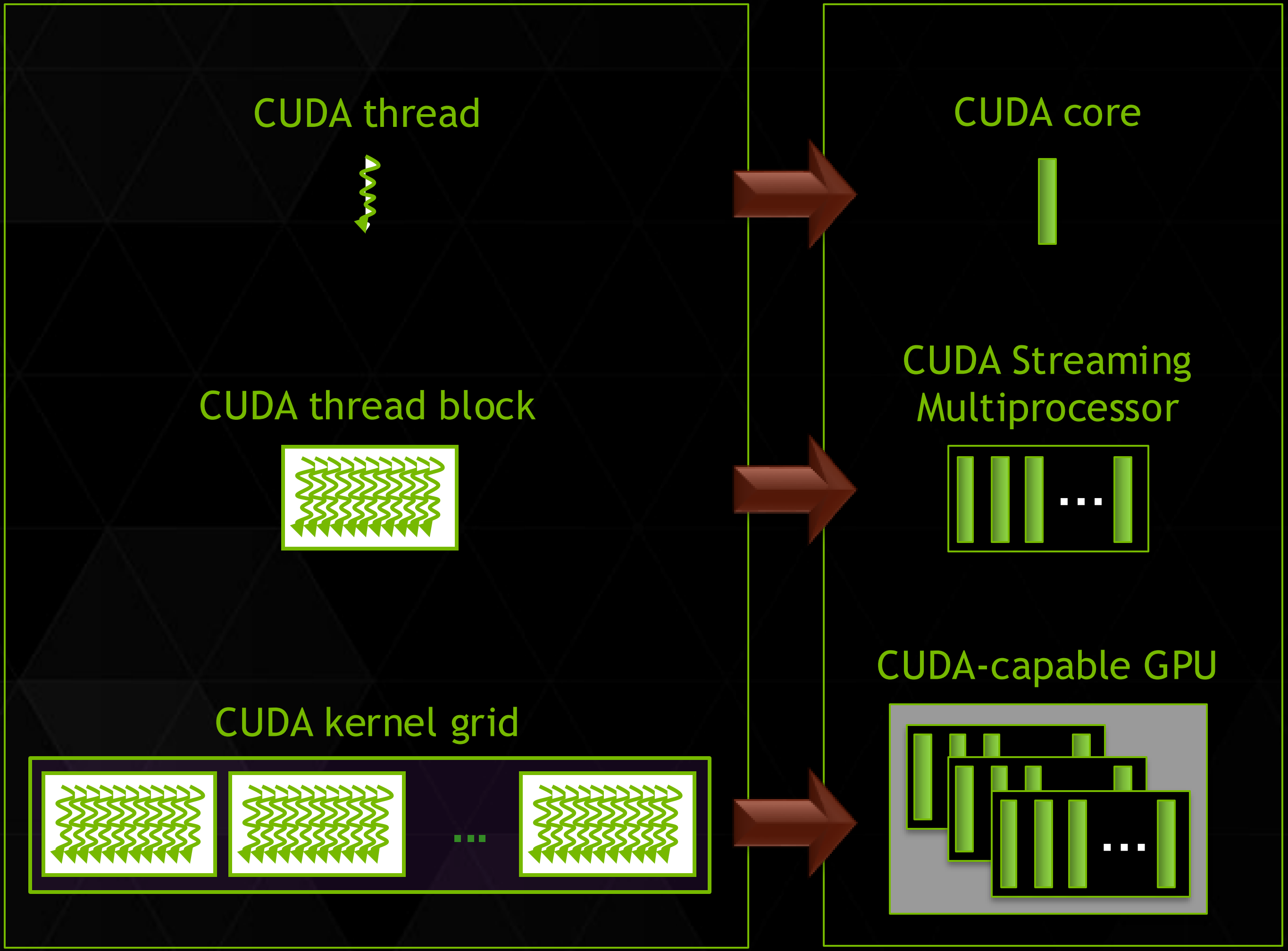
KERNEL EXECUTION



- Each thread is executed by a core
- Each block is executed by one SM and does not migrate
- Several concurrent blocks can reside on one SM depending on the blocks' memory requirements and the SM's memory resources
- Each kernel is executed on one device
- Multiple kernels can execute on a device at one time

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COMMUNICATION WITHIN A BLOCK

- Threads may need to cooperate
  - Memory accesses
  - Share results
- Cooperate using shared memory
  - Accessible by all threads within a block
- Restriction to “within a block” permits scalability
  - Fast communication between N threads is not feasible when N large

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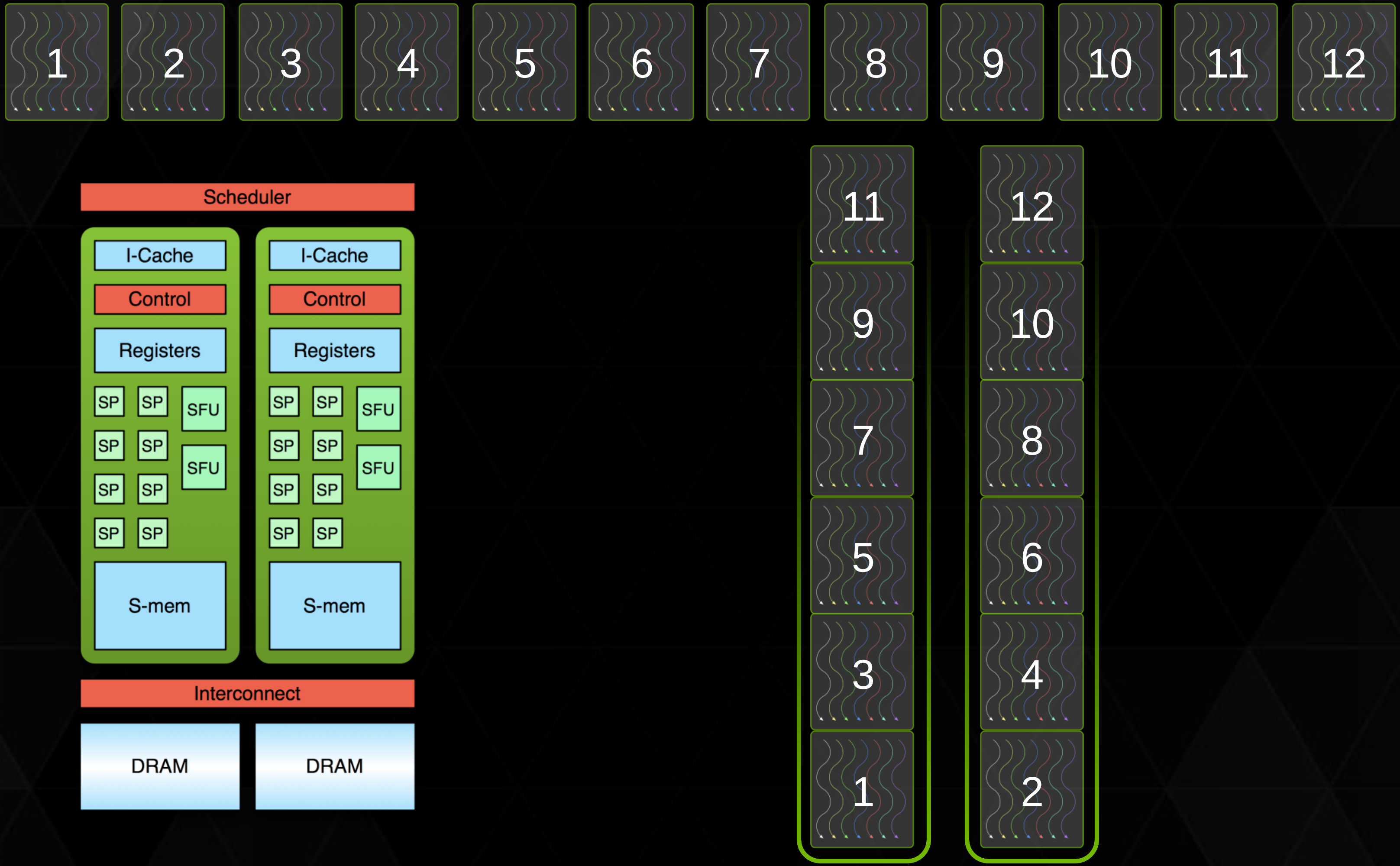
TRANSPARENT SCALABILITY



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TRANSPARENT SCALABILITY

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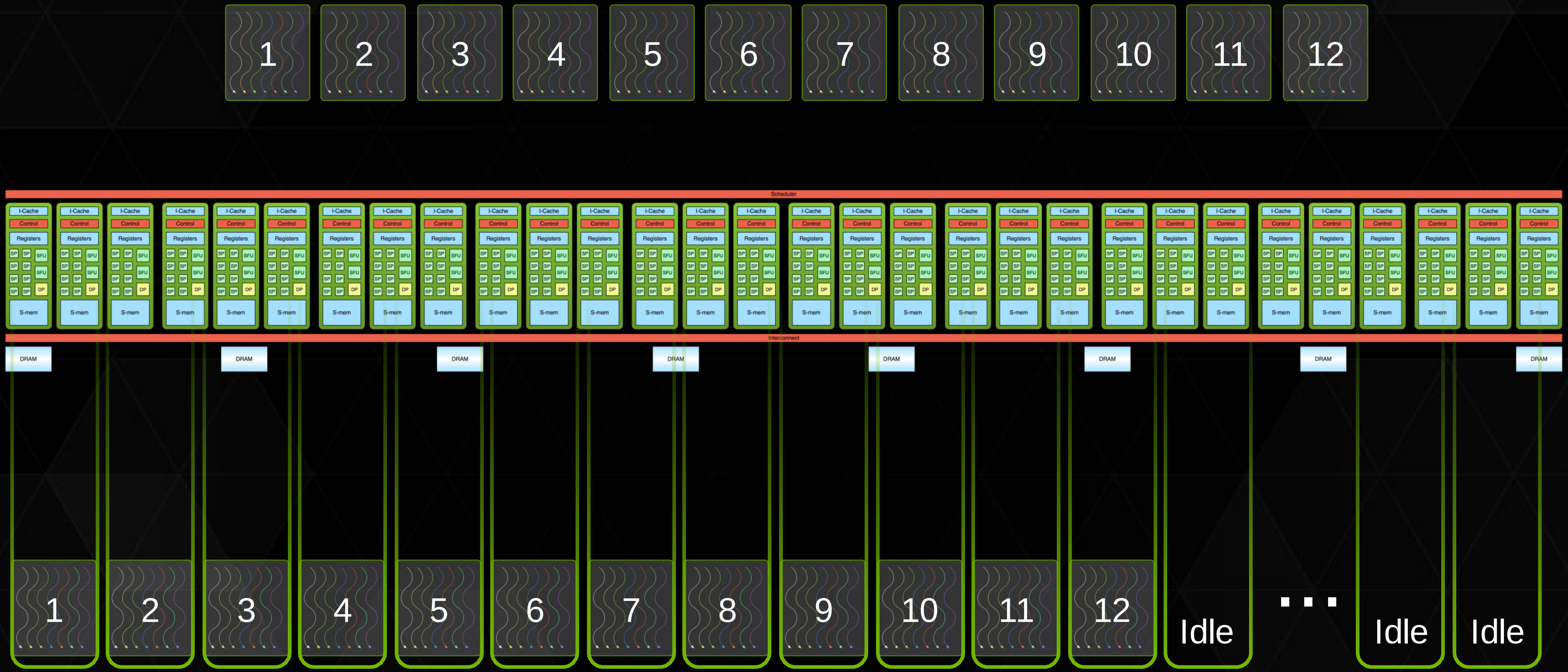
TRANSPARENT SCALABILITY –



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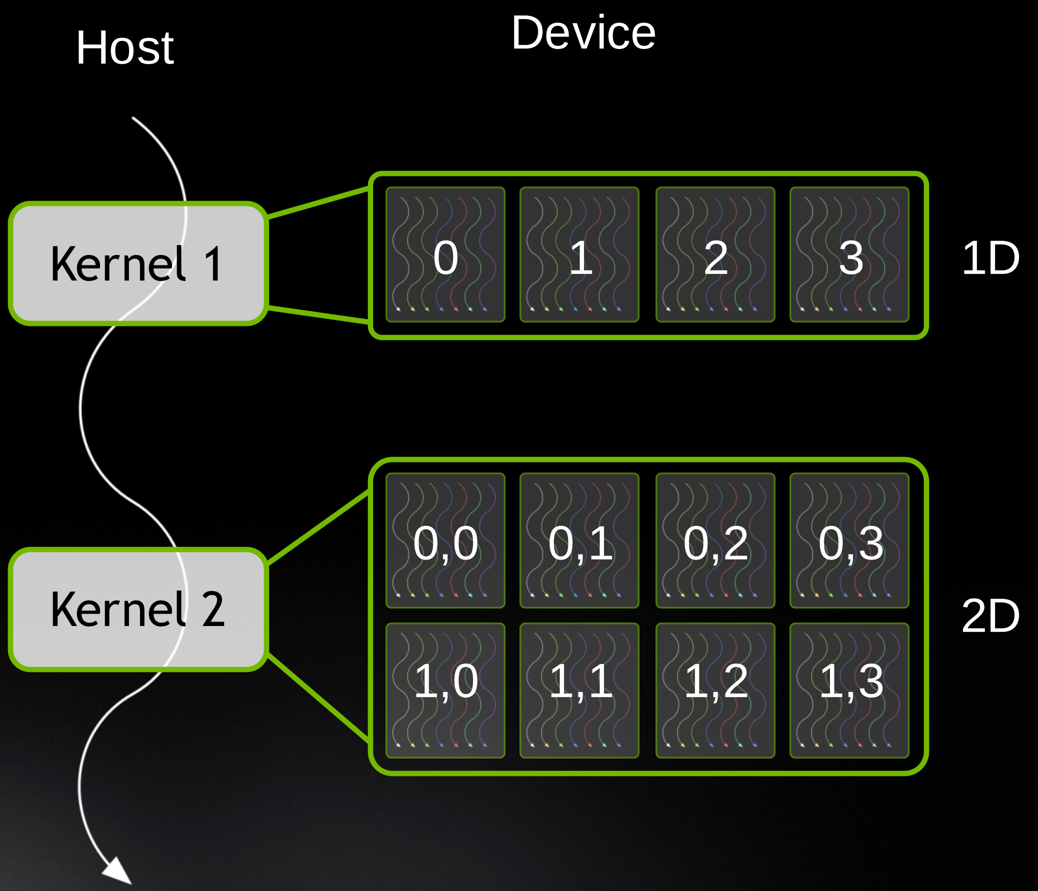
CUDA PROGRAMMING MODEL - SUMMARY

- A kernel executes as a grid of thread blocks
- A block is a batch of threads
  - Communicate through shared memory
- Each block has a block ID
- Each thread has a thread ID



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CUDA ARCHITECTURE MEMORY MODEL

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GPU ARCHITECTURE

Two Main components

Global memory

Analogous to RAM in a CPU server

Accessible by both GPU and CPU

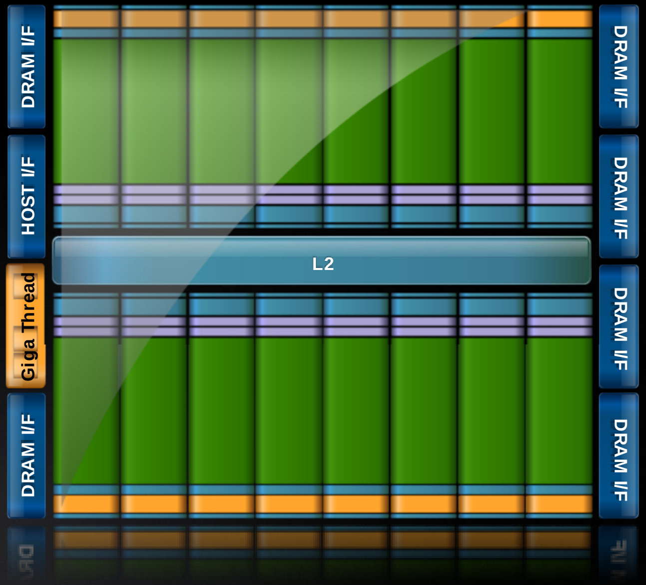
48GB with bandwidth currently up to 1 TB/s

Streaming Multiprocessors (SMs)

SMs perform the actual computations

Each SM has its own:

Control units, registers, execution pipelines, caches



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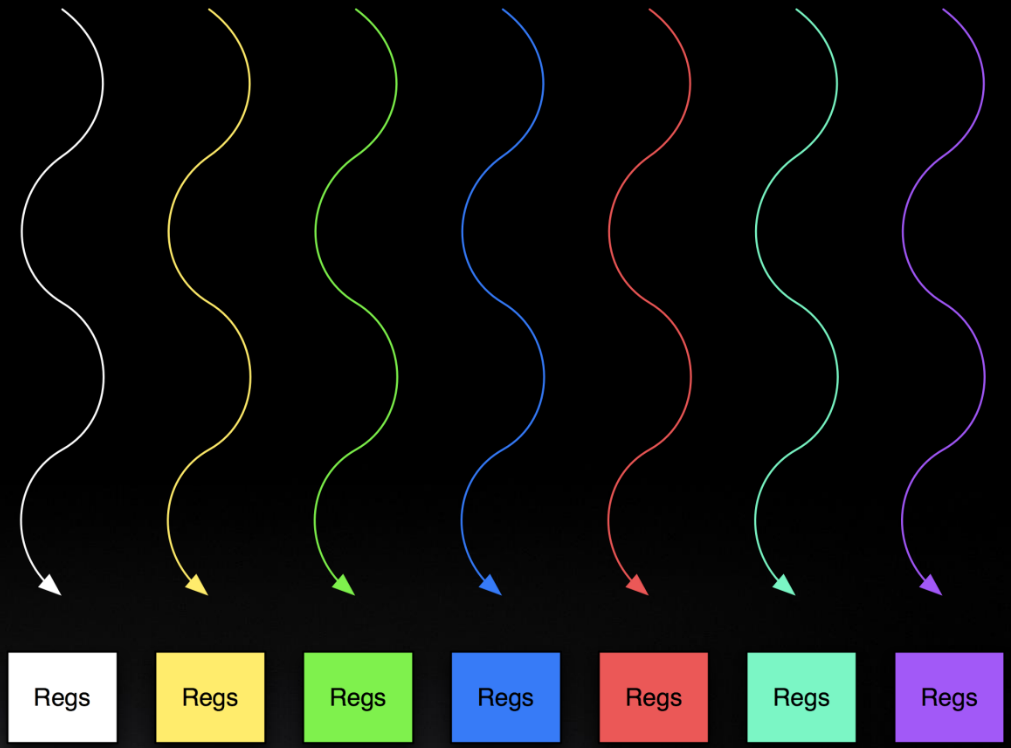
MEMORY HIERARCHY

- Thread
  - Registers



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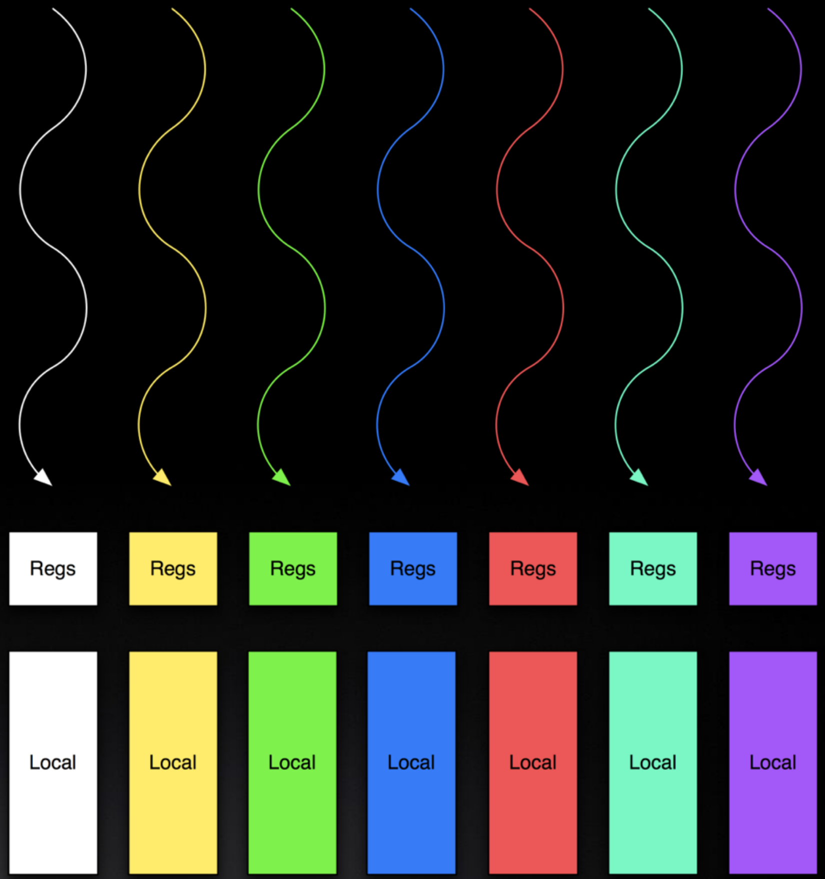
MEMORY HIERARCHY

- Thread
  - Registers
- Thread
  - Local memory



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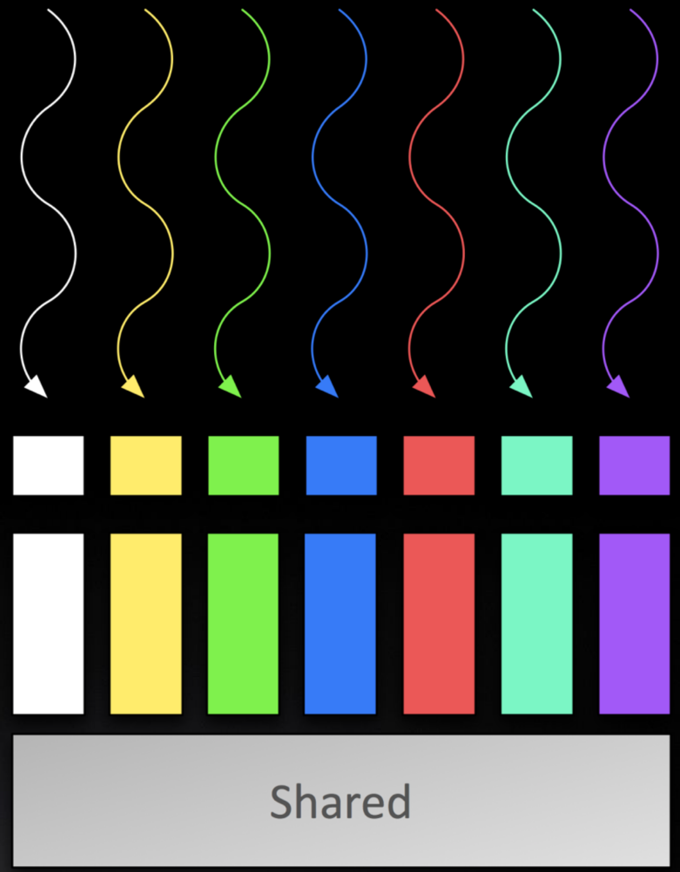
MEMORY HIERARCHY

- Thread
  - Registers
- Thread
  - Local memory
- Block of threads
  - Shared memory



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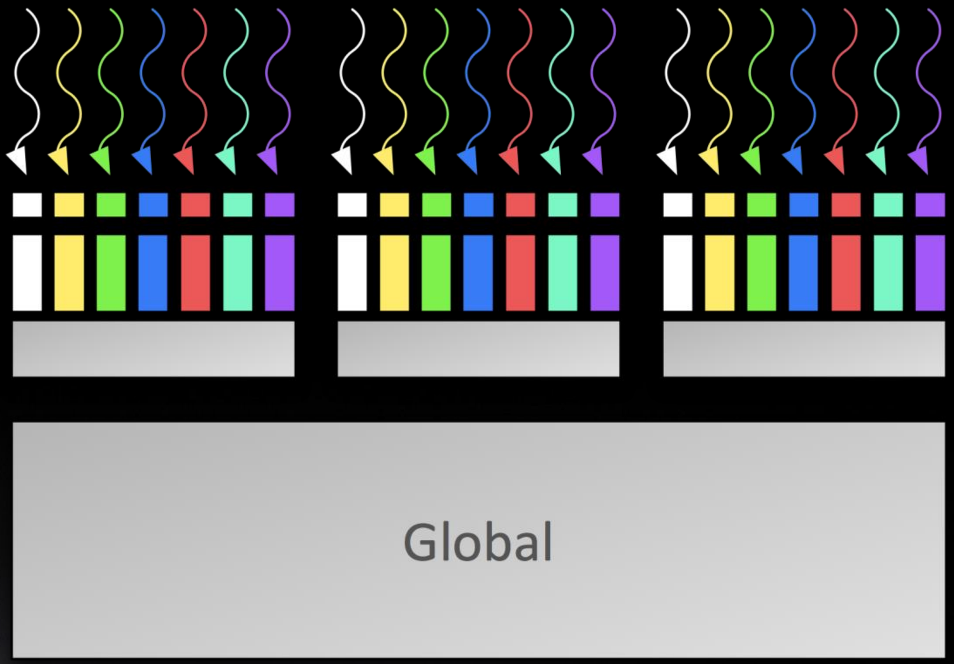
MEMORY HIERARCHY

- Thread
  - Registers
- Thread
  - Local memory
- Block of threads
  - Shared memory
- All blocks
  - Global memory



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WHAT IS CUPY?

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OVERVIEW OF CUPY

- **CuPy** is an implementation of NumPy-compatible multi-dimensional array on CUDA
- **CuPy** consists of :

✓ cupy.ndarray

✓ the core multi-dimensional array class

✓ many functions

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OVERVIEW OF CUPY

- **CuPy** supports a subset of numpy.ndarray interface which include:

✓ Basic & advance indexing, and Broadcasting

✓ Data types (int32, float32, uint64, complex64,...)

✓ Array manipulation routine (reshape)

✓ Linear Algebra functions (dot, matmul, etc)

✓ Reduction along axis (max, sum, argmax, etc)

For more details on broadcasting visit

(https://numpy.org/doc/stable/user/basics.broadcasting.html)

```
>>> import numpy as np
>>> X = np.array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
#Basic indexing and slicing
>>> X[5:]
array([5, 6, 7, 8, 9])
>>> X[1:7:2]
array([1, 3, 5])

#Advance indexing
>>> X = np.array([[1, 2],[3, 4],[5, 6]])
>>> X[[0, 1, 2], [0, 1, 0]]
array([1, 4, 5])

#reduction and Linear Algebra function
>>> max(X)
9.0
>>> B = np.array([1,2,3,4], dtype=np.float32)
>>> C = np.array([5,6,7,8], dtype=np.float32)
>>> np.matmul(B, C)
70.0
#data type and array manipulation routine
>>> A =1j*np.arange(9, dtype=np.complex64).reshape(3,3)
[[0.+0.j 0.+1.j 0.+2.j]
 [0.+3.j 0.+4.j 0.+5.j]
 [0.+6.j 0.+7.j 0.+8.j]]
```


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FEATURES OF CUPY

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FEATURES OF CUPY

- Features of CuPy includes:

✓ User-define elementwise CUDA kernels

✓ User-define reduction CUDA kernels

✓ Fusing CUDA kernels to optimize user-define calculation

✓ Customizable memory allocator and memory pool

✓ cuDNN utilities

- These features are developed to support performance.

- **CuPy uses on-the-fly kernel synthesis**: when a kernel call is required, it compiles a kernel code optimized for the shapes and dtypes of given arguments, sends it to the GPU device, and executes the kernel.

- **CuPy** also caches the kernel code sent to GPU device within the process, which reduces the kernel transfer time on further calls.

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INSTALLATION GUIDE

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REQUIREMENTS

- **Recommended Linux distributions are Centos and Ubuntu**

✓ NVIDIA CUDA GPU with the Compute Capability 3.0 or larger

✓ CUDA Toolkit: v9.0 - v11.2

✓ Python: v3.5.1+ - v3.9.0+

- **Python Dependencies**

✓ NumPy/SciPy-compatible API in CuPy v8 is based on NumPy 1.19 and SciPy 1.5.

1. Wheels (precompiled binary package)

CUDA	Command
v9.0	`$ pip install cupy-cuda90`
v9.2	`$ pip install cupy-cuda92`
v10.0	`$ pip install cupy-cuda100`
v10.1	`$ pip install cupy-cuda101`
v10.2	`$ pip install cupy-cuda102`
v11.0	`$ pip install cupy-cuda110`
v11.1	`$ pip install cupy-cuda111`

2. Conda-Forge

✓ $ conda install -c conda-forge cupy

- **To install CuPy with the cuTENSOR support enabled, you can do:**

✓ $ conda install -c conda-forge cupy cutensor cudatoolkit=10.2

3. CuPy inside Docker

You can pull CuPy Docker images from:

https://hub.docker.com/r/cupy/cupy/.

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REQUIREMENTS & ARCHITECTURE

4. Full RAPIDS Package

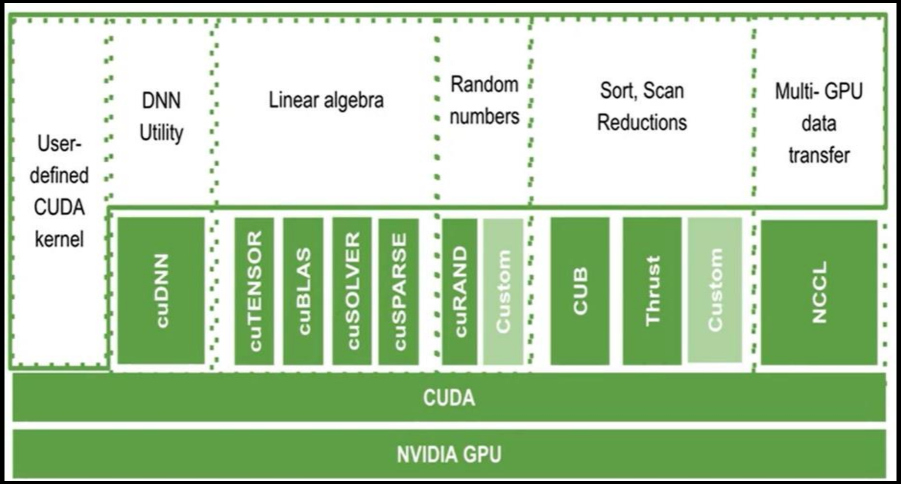
	Preferred		Advanced				
METHOD	Conda	Docker + Examples	Docker + Dev Env	Source			
RELEASE	Stable (0.18)		Nightly (0.19a)				
TYPE	RAPIDS and BlazingSQL		RAPIDS Core (w/o BlazingSQL)				
PACKAGES	All Packages	cuDF	cuML	cuGraph	cuSignal	cuSpatial	cuxfilter
LINUX	Ubuntu 16.04	Ubuntu 18.04	Ubuntu 20.04	CentOS 7	CentOS 8	RHEL 7&8	
PYTHON	Python 3.7		Python 3.8				
CUDA	CUDA 10.1.2	CUDA 10.2	CUDA 11.0				

NOTE: Ubuntu 16.04/18.04/20.04 & CentOS 7/8 use the same `conda create` commands.

COMMAND

```
conda create -n rapids-0.18 -c rapidsai -c nvidia -c conda-forge \
    -c defaults rapids-blazing=0.18 python=3.7 cudatoolkit=10.1
```

CuPy Architecture



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CUPY FUNDAMENTALS

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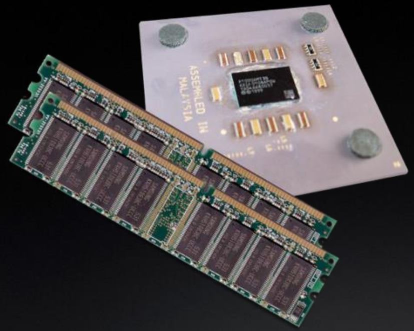
TERMINOLOGY

- *Host* – The CPU and its memory (host memory)
- *Device* – The GPU and its memory (device memory)
- *Kernel* - A GPU function launched by the host and executed on the device.

Host



Device

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CUPY.NDARRAY

- CuPy is a GPU array backend that implements a subset of NumPy interface

CuPy	NumPy

`import cupy as cp`
 	
`X_gpu = cp.array([1, 2, 3, 4, 5])`
	`import numpy as np`
	
	`x = np.array([1, 2, 3, 4, 5])`

Current device (GPU ID: 0)

```
import cupy as cp

gpu_0 = cp.array([1, 2, 3, 4, 5])

# Switch device
cp.cuda.Device(1).use()
gpu_1 = cp.array([1, 2, 3, 4])
```

Switch GPU temporarily

```
import numpy as np
import cupy as cp

with cp.cuda.Device(1):
      gpu_1 = cp.array([1, 2, 3, 4])

# back to device id 0
gpu0 = cp.array([1, 2, 3, 4, 5])
```


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DATA TRANSFER

Host →Device using **cupy.asarray**.

```
import cupy as cp
import numpy as np

X = np.array([1, 2, 3, 4, 5])
x_gpu = cp.asarray(x)
print(x_gpu)
Output:[1 2 3 4 5]
```

Device →Host using **cupy.asnumpy** or **cupy.ndarray.get()**

```
import cupy as cp
import numpy as np

X_gpu = cp.array([1, 2, 3, 4, 5])
# copy to Host
x_cpu = cp.asnumpy(x_gpu)
print(x_cpu)
[1 2 3 4 5]

#alternative option
x_cpu_alt = x_gpu.get()
x_cpu_alt
Output:[1 2 3 4 5]
```

Devices(GPU to GPU)

```
import cupy as cp
with cp.cuda.Device(0):
    x_gpu_0 = cp.ndarray([ 2, 3, 3])
x_gpu_0
[[[0. 0. 0.]
  [0. 0. 0.]
  [0. 0. 0.]]

 [[0. 0. 0.]
  [0. 0. 0.]
  [0. 0. 0.]]]

with cp.cuda.Device(1):
    x_gpu_1 = cp.asarray(x_gpu_0)
x_gpu_1
[[[0. 0. 0.]
  [0. 0. 0.]
  [0. 0. 0.]]

 [[0. 0. 0.]
  [0. 0. 0.]
  [0. 0. 0.]]]
```


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GPU & CPU AGNOSTIC CODE

- Using **cupy.get_array_module()**

```
>>> import cupy as cp
>>> import numpy as np
>>>
>>> #example: log(1 + exp(x))
>>> x_cpu = np.array([1, 2, 3, 4, 5])
>>> x_gpu = cp.get_array_module(x_cpu)
>>> result = x_gpu.maximum(0, x_cpu)+ x_gpu.log1p(x_gpu.exp(-abs(x_cpu))
>>> result
Output: [1.31326169 2.12692801 3.04858735 4.01814993 5.00671535]
>>>
>>>
>>> #An explicit conversion to host
>>> x_gpu = cp.array([6, 7, 8, 9, 10])
>>> result = cp.asnumpy(x_gpu) + x_cpu
>>> result
Output: [ 7  9 11 13 15]
>>> #An explicit conversion to device
>>> result = x_gpu + cp.asarray(x_cpu)
>>> result
Output: [ 7  9 11 13 15]
>>>
```


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HOW MUCH FASTER IS CUPY THAN NUMPY ?

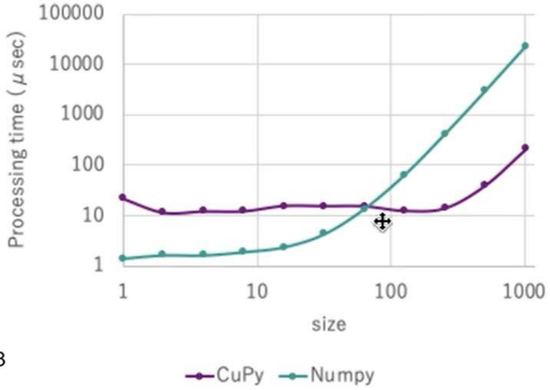
Dot product

```python
a = xp.ones((size, size), 'f')
b = xp.ones((size, size), 'f')

def f():
  xp.dot(a, b)
```

For a rough estimation, if the array size is larger than L1 cache of your CPU, CuPy gets faster than NumPy.

Try on Google Colab! http://bit.ly/cupywest2018



Add Function

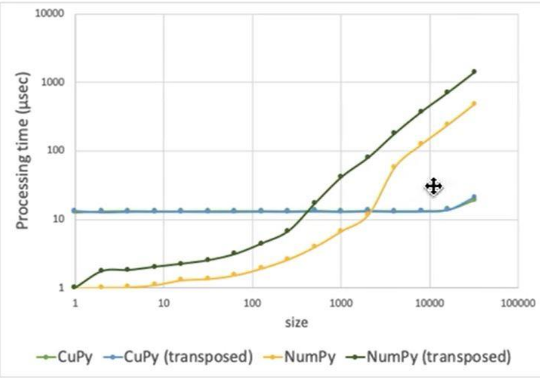
```python
a = xp.ones((size, 32), 'f')
b = xp.ones((size, 32), 'f')

def f():
  a + b
```

```python
# Transpose
a = xp.ones((32, size), 'f').T
b = xp.ones((size, 32), 'f')

def f():
  a + b
```

Xeon Gold 6154 CPU @ 3.00GHz
Tesla V100-PCIE-16GB



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CUDA KERNELS

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CUPY CUDA KERNELS

- **CUDA Kernels can be defined in Cupy as follows:**

✓ Elementwise Kernels

✓ Reduction Kernels

✓ Raw Kernels

✓ Kernel Fusion

- These kernels are user-defined based.

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ELEMENTWISE KERNEL

- The **ElementwiseKernel** class is used to define this type of kernel.
- This kernel consists of four parts which includes:

✓ a list of input argument

✓ a list of output argument

✓ a loop body code

✓ a kernel name

- Variable name starting with underscore “_” , “n”, and “i” are regarded as reserved keywords.

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ELEMENTWISE KERNEL

- Example : z = x*w + b

```
import cupy as cp                                          Data type
input_list = 'float32 x , float32 w, float32 b'  ←        Input argument list
output_list = 'float32 z' ←                               Output argument list
code_body  = 'z =  (x * w) + b' ←                          A loop body code
# elementwisekernel class defined
dnnLayerNode = cp.ElementwiseKernel(input_list, output_list, code_body,'dnnLayerNode')
x = cp.arange(9, dtype=cp.float32).reshape(3,3)
w = cp.arange(9, dtype=cp.float32).reshape(3,3)
b = cp.array([-0.5], dtype=cp.float32)
z = cp.empty((3,3), dtype=cp.float32)
# kernel call with argument passing
dnnLayerNode(x,w,b,z)
print(z)
#output
[[-0.5  0.5  3.5]
 [ 8.5 15.5 24.5]
 [35.5 48.5 63.5]]
```


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ELEMENTWISE KERNEL: GENERIC-TYPE KERNELS

- Example : z = x*w + b

Generic type placeholder

```
import cupy as cp
input_list = 'T x , T w, T b'
output_list = 'T z'
code_body  = 'z =  (x * w) + b'
# elementwisekernel class defined
dnnLayerNode = cp.ElementwiseKernel(input_list, output_list, code_body,'dnnLayerNode')
x = cp.arange(9, dtype=cp.float32).reshape(3,3)
w = cp.arange(9, dtype=cp.float32).reshape(3,3)
b = cp.array([-0.5], dtype=cp.float32)
z = cp.empty((3,3), dtype=cp.float32)
# kernel call with argument passing
dnnLayerNode(x,w,b,z)
print(z)
#output
[[-0.5  0.5  3.5]
 [ 8.5 15.5 24.5]
 [35.5 48.5 63.5]]
```

Multiple generic placeholder

```
import cupy as cp
input_list =  'T x , W w,   B b'
output_list = 'T z'
..............................
..............................
..............................
#output
..............................
..............................
```

Different types of placeholder

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REDUCTION KERNEL

- Reduction kernel is implemented through the **ReductionKernel** class.

- In order to implement this kernel class, the following parts must be defined:

✓ Identity value: to initialize reduction value.

✓ Mapping expression: Used for the pre-processing of each element to be reduced.

✓ Reduction expression: It is an operator to reduce the multiple mapped values. The special variables **a** and **b** are used for its operands.

✓ Post mapping expression: It is used to transform the resulting reduced values. The special variable **a** is used as its input. Output should be written to the output parameter.

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REDUCTION KERNEL

Example: $z = \sum_{i=1} x_i \, w_i + b$

```
import cupy as cp
dnnLayer = cp.ReductionKernel(
      'T x, T w, T bias’, ← input params. The bias represents b from the above equation.
      'T z’, ← output params
      'x * w’, ← map
      'a + b’, ← reduce
      'z = a + bias’, ← post-reduction map
      '0’, ← identity value
      'dnnLayer’ ← kernel name
         )
x = cp.arange(10, dtype=cp.float32).reshape(2,5)
w = cp.arange(10, dtype=cp.float32).reshape(2,5)
bias = -0.1
z = dnnLayer(x,w,bias) ← kernel call
print(z)
#output
284.9
```

inputs

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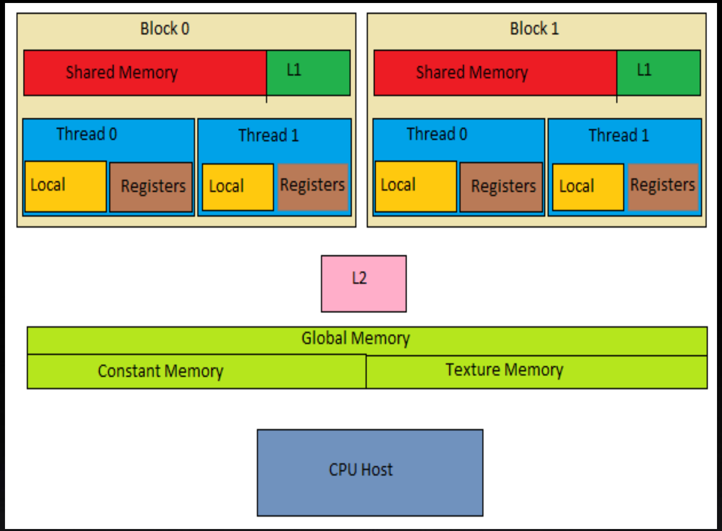
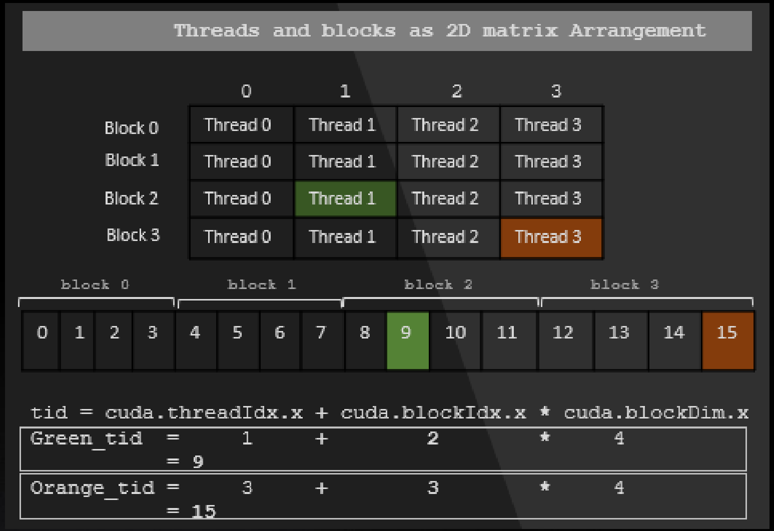
RAW KERNEL

- Raw kernels enable the direct use of kernels from CUDA source, and it is defined through the ***RawKernel*** class.

- *The **RawKernel*** object allows you to call the kernel with **CUDA's cuLaunchKernel interface**. In other words, you have control over:





✓ grid size

✓ block size

✓ shared memory size

✓ and stream.

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RAW KERNEL EXAMPLE

```
import cupy as cp
add_kernel = cp.RawKernel(r'''
extern "C" __global__
void add_func(const float* x1, const float* x2, float* y) {
int tid = blockDim.x * blockIdx.x + threadIdx.x;
y[tid] = x1[tid] + x2[tid];
}
''', 'add_func')
N = 100
shape = (10, 10)
x1 = cp.arange(N, dtype=cp.float32).reshape(shape)
x2 = cp.arange(N, dtype=cp.float32).reshape(shape)
y  = cp.zeros((shape), dtype=cp.float32)
add_kernel((10,), (10,), (x1, x2, y))
```

grid size   block size   arguments

```
#output
[[  0.   2.   4.   6.   8.  10.  12.  14.  16.  18.]
 [ 20.  22.  24.  26.  28.  30.  32.  34.  36.  38.]
 [ 40.  42.  44.  46.  48.  50.  52.  54.  56.  58.]
 [ 60.  62.  64.  66.  68.  70.  72.  74.  76.  78.]
 [ 80.  82.  84.  86.  88.  90.  92.  94.  96.  98.]
 [100. 102. 104. 106. 108. 110. 112. 114. 116. 118.]
 [120. 122. 124. 126. 128. 130. 132. 134. 136. 138.]
 [140. 142. 144. 146. 148. 150. 152. 154. 156. 158.]
 [160. 162. 164. 166. 168. 170. 172. 174. 176. 178.]
 [180. 182. 184. 186. 188. 190. 192. 194. 196. 198.]]
```

```
This also yield the same output:
add_kernel((1,), (100,), (x1, x2, y))
```


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RAW MODULES

- The **RawModule** class is used to defining a large raw CUDA C source or loading an existing CUDA binary.
- It is initialized by a CUDA C source code having several kernels (functions) such that needed kernels are retrieved by calling the ***get_function()*** method.

```
import cupy as cp
loaded_from_source = r'''
extern "C" {
__global__ void sum(const float* A, const float* B, float* C, int N)
 {
    int tid = blockDim.x * blockIdx.x + threadIdx.x;
    if(tid < N)
    {
      C[tid] = A[tid] + B[tid];
    }
 }
 __global__ void multiply(const float* A, const float* B, float* C, int N)
 {
    int tid = blockDim.x * blockIdx.x + threadIdx.x;
    if(tid < N)
    {
        C[tid] = A[tid] * B[tid];
    }
 }
}'''
```


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EXAMPLE OF RAW MODULE

```
import cupy as cp
loaded_from_source = r'''
extern "C" {
__global__ void sum_ker(const float* a, const float* b, float* c, int N)
 {
    int tid = blockDim.x * blockIdx.x + threadIdx.x;
    if(tid < N)
    {
      c[tid] = a[tid] + b[tid];
    }
 }
 __global__ void multiply_ker(const float* a, const float* b, float* c, int N )
 {
    int tid = blockDim.x * blockIdx.x + threadIdx.x;
    if(tid < N)
    {
        c[tid] = c[tid] * b[tid];
    }
 }
}'''
```

```
ker_sum((1,),(25,), (a, b, c))
print(y)
#output1
[[ 1.  2.  3.  4.  5.]
 [ 6.  7.  8.  9. 10.]
 [11. 12. 13. 14. 15.]
 [16. 17. 18. 19. 20.]
 [21. 22. 23. 24. 25.]]
```

```
ker_times((5,),(5,),(a, b, c))
print(y)
#output2
[[ 0.  1.  2.  3.  4.]
 [ 5.  6.  7.  8.  9.]
 [10. 11. 12. 13. 14.]
 [15. 16. 17. 18. 19.]
 [20. 21. 22. 23. 24.]]
```

```
Module    = cp.RawModule(code = load_raw_module)   ← Loading raw module
ker_sum   = module.get_function('sum_ker')         ← Accessing the sum_ker kernel
ker_times = module.get_function('multiply_ker')    ← Accessing the multiple_ker
```

```
a  = cp.arange(25,  dtype=cp.float32).reshape(5,5)
b  = cp.ones((5,5), dtype=cp.float32)
c   = cp.zeros((5,5),dtype=cp.float32)
```
← Creating arguments (input and output parameters)

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KERNEL FUSION

- **Kernel fusion** is a decorator that fuses functions. It can be used to define an **elementwise** or **reduction** kernels easily.

```python
import cupy as cp

@cp.fuse(kernel_name='dnnlayerNode')
def dnnlayerNode(x, w, bias):
    return  (x * w) + bias


x = cp.arange(9, dtype=cp.float32).reshape(3,3)
w = cp.arange(9, dtype=cp.float32).reshape(3,3)
bias = cp.array([-0.5], dtype=cp.float32)
z = dnnlayerNode(x, w, bias)
print(z)
#output
[[-0.5   0.5   3.5]
 [ 8.5  15.5  24.5]
 [35.5  48.5  63.5]]
```

decorator

Function scope

```python
import cupy as cp

@cp.fuse
def sumlayer(x, w):
     return cp.sum(x * w, axis = -1)

x = cp.arange(10, dtype=cp.float32)
w = cp.arange(10, dtype=cp.float32)
z = sumLayer(x,w)
print(z)
#output
285.0
```


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KERNEL FUSION: MERITS & DEMERITS

- **Merits**

✓ Relax the bandwidth bottleneck

✓ Reduce memory consumption

✓ Speedup function calls

- **Demerits**

✓ No support for **cupy.matmul()** and **cupy.reshape()** operations

✓ Support only reduction and element-wise operations

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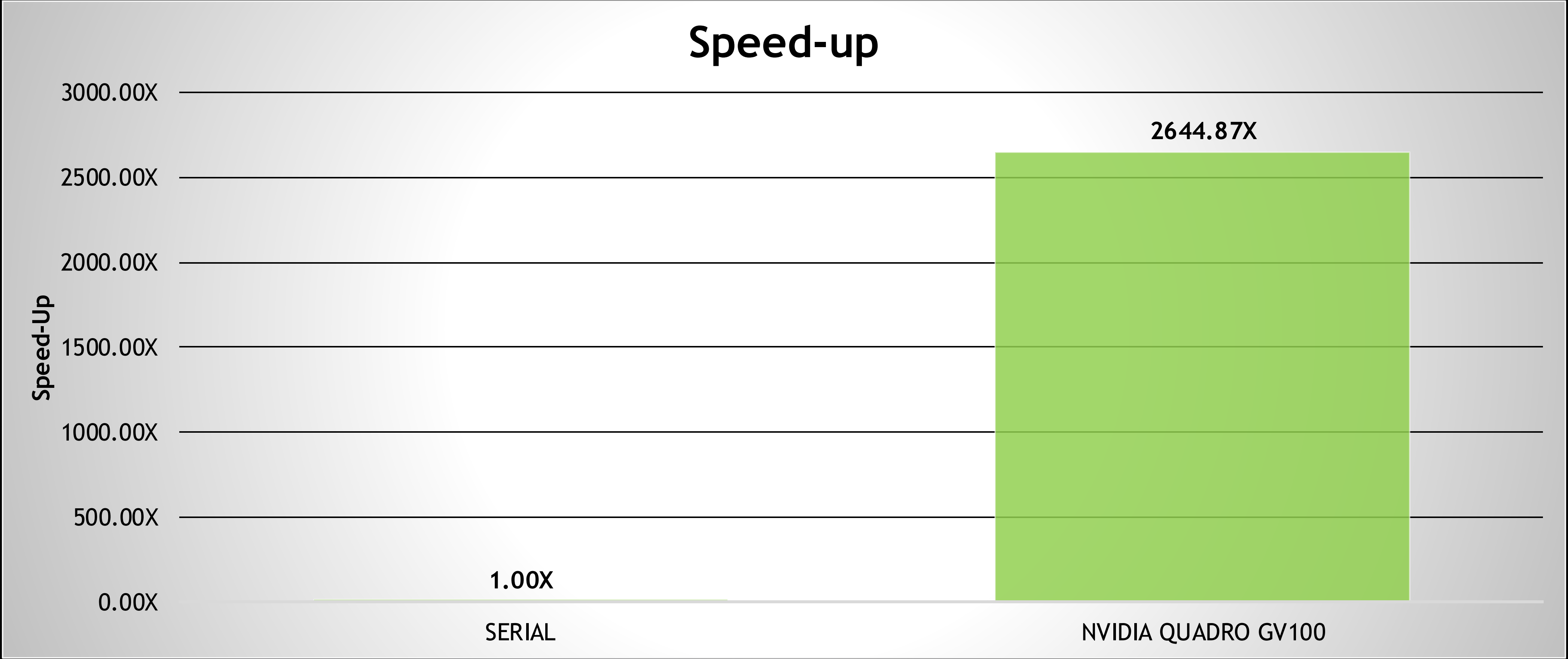
CUPY SPEEDUP



HPC SDK 21.2, NVIDIA Quadro GV100

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SUMMARY

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SUMMARY

- **CuPy** is an implementation of NumPy-compatible multi-dimensional array on **CUDA**

Installation

✓ Wheels (precompiled binary package)

✓ Conda-Forge

✓ CuPy inside Docker

✓ Conda (full RAPIDS package)

Data Movement

✓ Host to Device (CPU →GPU) using cupy.asarray.

✓ Device to Host(GPU→CPU) using cupy.asnumpy or cupy.ndarray.get()

✓ between devices(GPU to GPU), cupy.ndarray is used.

Cupy User-defined Kernels

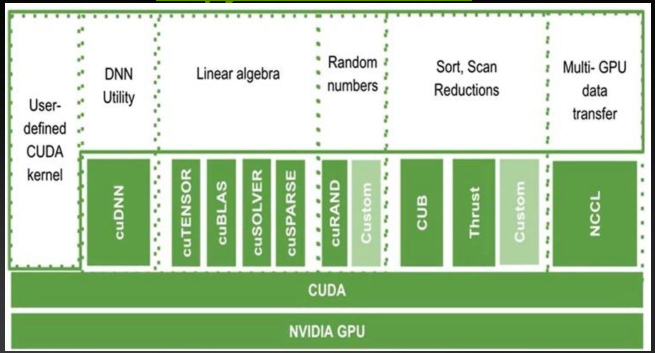
✓ Elementwise Kernels

✓ Reduction Kernels

✓ Raw Kernels

✓ Kernel Fusion

Cupy Architecture



You want to save GPU memory?

```
import cupy as cp
size = 32768
a = cp.ones((size, size)) # 8GB
b = cp.ones((size, size)) # 8GB
cp.dot(a, b)              # 8GB
```

```
Traceback (most recent call last):
  ...
cupy.cuda.memory.OutOfMemoryError: out of memory to
allocate 8589934592 bytes (total 17179869184 bytes)
```

Try Unified Memory! (Supported only on V100)

- Just edit 2 lines to enable **unified memory**

```
import cupy as cp

pool = cp.cuda.MemoryPool(cp.cuda.malloc_managed)
cp.cuda.set_allocator(pool.malloc)

size = 32768
a = cp.ones((size, size)) # 8GB
b = cp.ones((size, size)) # 8GB
cp.dot(a, b)              # 8GB
```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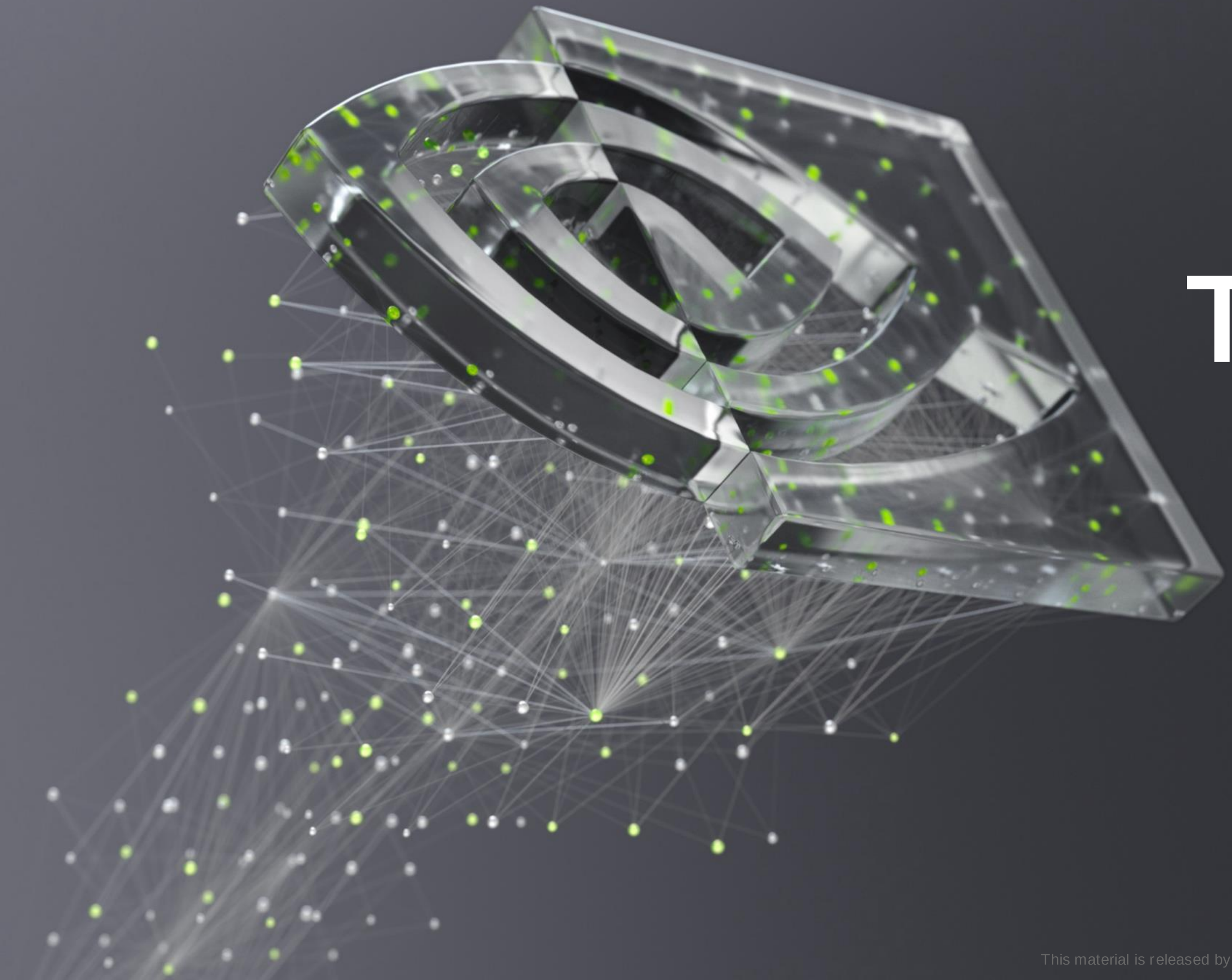

THANK YOU

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