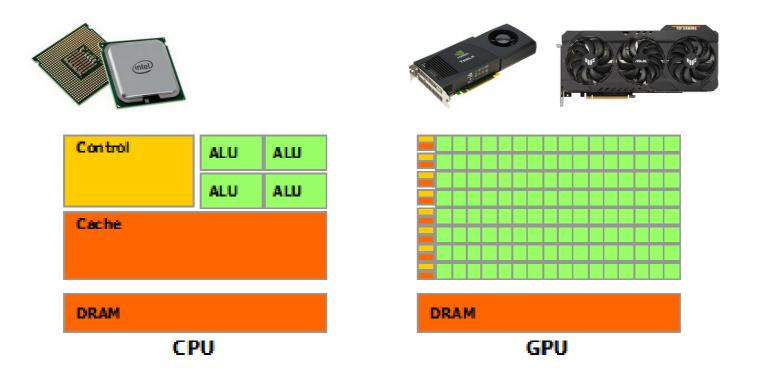
Computación Concurrente, Paralela y Distribuida *Leandro Rodríguez Liñares – David Olivieri* Curso 2024/25

Tema 11: Introducción a Nvidia CUDA



CUDA (or Compute Unified Device Architecture) is a parallel computing platform and application programming interface (API) that allows software to use certain types of graphics processing units (GPUs) for general purpose processing, an approach called general-purpose computing on GPUs (GPGPU). CUDA is a software layer that gives direct access to the GPU's virtual instruction set and parallel computational elements, for the execution of compute kernels.

Tema 11: NVidia CUDA 2/34



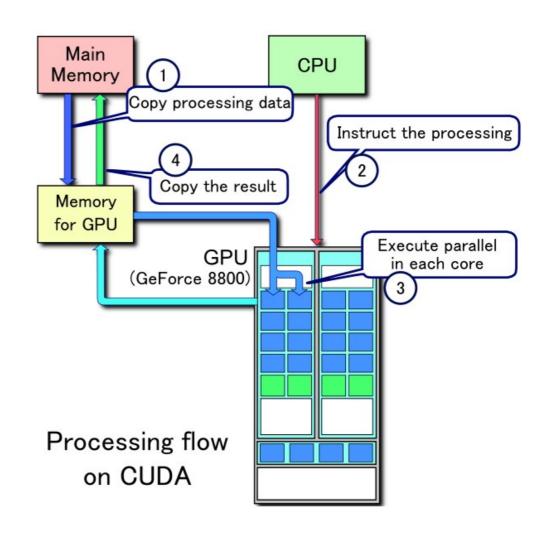
GPUs: herramientas con alta paralelización, multihilo, con numerosos núcleos, con altísima capacidad de cálculo y con alto ancho de banda de acceso a los datos.

GPUs: especializadas en computación intensiva y altamente paralela (necesario para renderizado de gráficos): memorias caché reducidas y poca capacidad de control de flujo.

Tema 11: NVidia CUDA 3/34

NVidia CUDA usa un modelo de programación basado en *offloading*:

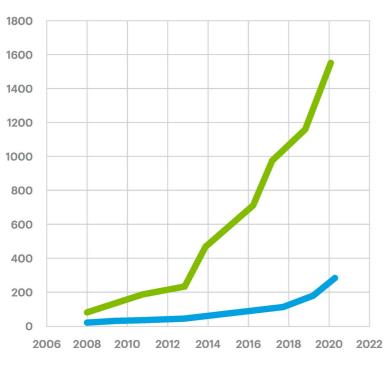
- Los datos se copian de la memoria principal a la memoria de la GPU
- 2) La CPU ordena el procesamiento en la GPU
- 3) La GPU procesa los datos de acuerdo a las órdenes de la CPU
- 4) Los resultados se copian de la memoria de la GPU a la memoria principal



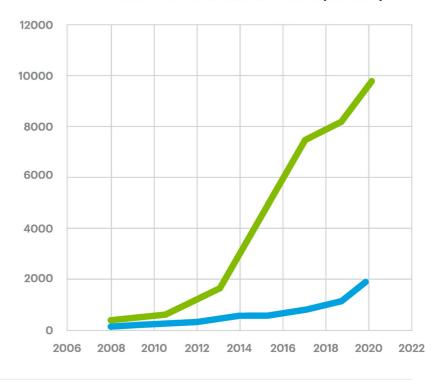
Tema 11: NVidia CUDA 4/34

¿Porqué CUDA?

PEAK MEMORY BANDWIDTH (GB/s)



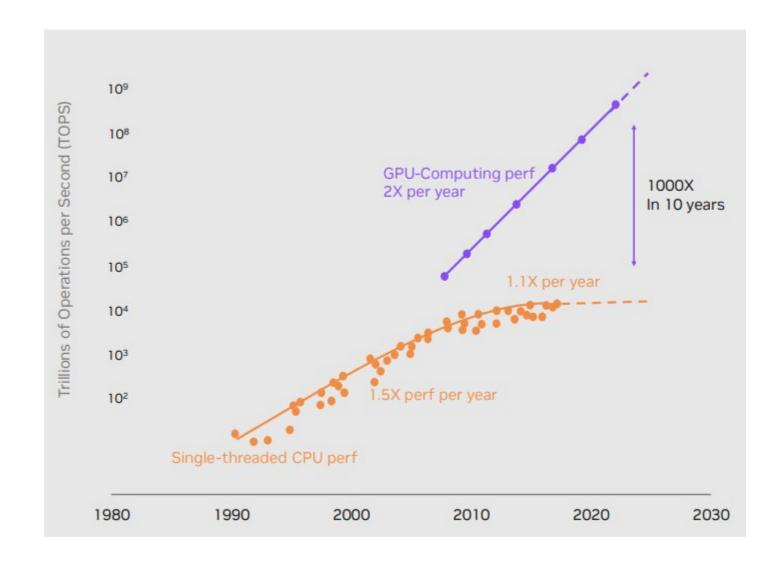
PEAK DOUBLE PRECISION FLOPS (GFLOPs)



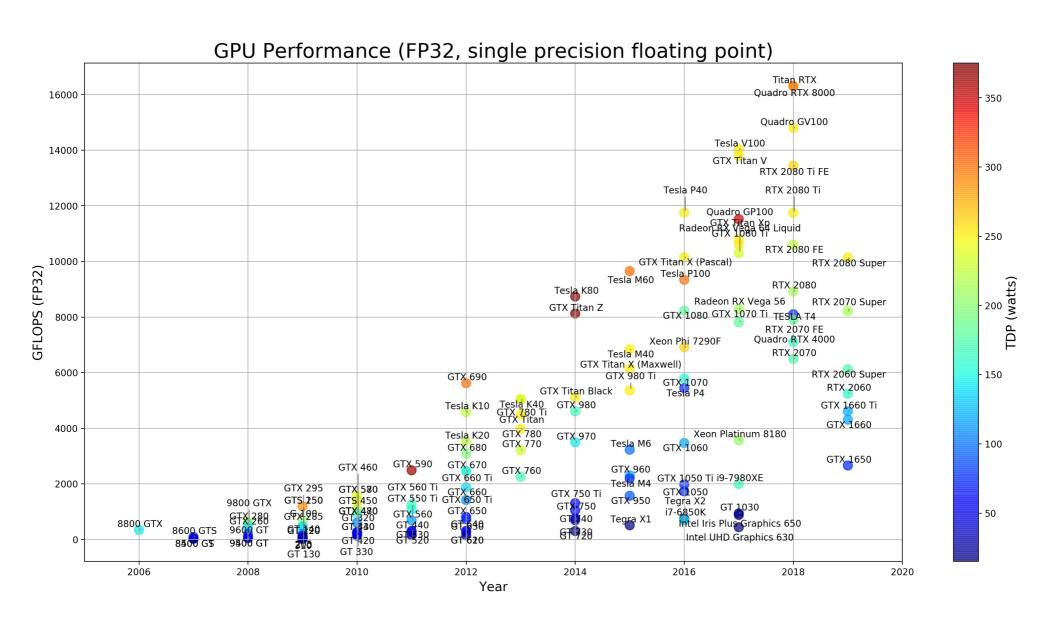
CPU

Figure 2. Comparison of evolution of memory bandwidth (left) and double precision flops (right) on GPU and CPU

Tema 11: NVidia CUDA 5/34



Tema 11: NVidia CUDA 6/34



Tema 11: NVidia CUDA 7/34

Noviembre 2024



| Rank | System | Cores | Rmax (PFlop/s) | Rpeak (PFlop/s) | Power (kW) |
|------|--|------------|-------------------|--------------------|---------------|
| 1 | El Capitan - HPE Cray EX255a, AMD 4th Gen EPYC 24C 1.8GHz, AMD Instinct MI300A, Slingshot-11, TOSS, HPE DOE/NNSA/LLNL United States | 11,039,616 | 1,742.00 | 2,746.38 | 29,581 |
| 2 | Frontier - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE Cray OS, HPE D0E/SC/Oak Ridge National Laboratory United States | 9,066,176 | 1,353.00 | 2,055.72 | 24,607 |
| 3 | Aurora - HPE Cray EX - Intel Exascale Compute Blade, Xeon CPU Max 9470 52C 2.4GHz, Intel Data Center GPU Max, Slingshot-11, Intel DOE/SC/Argonne National Laboratory United States | 9,264,128 | 1,012.00 | 1,980.01 | 38,698 |
| 4 | Eagle - Microsoft NDv5, Xeon Platinum 8480C 48C 2GHz, NVIDIA H100, NVIDIA Infiniband NDR, Microsoft Azure Microsoft Azure United States | 2,073,600 | 561.20 | 846.84 | |
| 5 | HPC6 - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, RHEL 8.9, HPE Eni S.p.A. Italy | 3,143,520 | 477.90 | 606.97 | 8,461 |
| 6 | Supercomputer Fugaku - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan | 7,630,848 | 442.01 | 537.21 | 29,899 |

Tema 11: NVidia CUDA 8/34

| Alps - HPE Cray EX254n, NVIDIA Grace 72C 3.1GHz, NVIDIA GH200 Superchip, Slingshot-11, HPE Cray OS, HPE Swiss National Supercomputing Centre (CSCS) Switzerland | 2,121,600 | 434.90 | 574.84 | 7,124 |
|--|--|--|--|--|
| LUMI - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland | 2,752,704 | 379.70 | 531.51 | 7,107 |
| Leonardo - BullSequana XH2000, Xeon Platinum 8358 32C 2.6GHz, NVIDIA A100 SXM4 64 GB, Quad-rail NVIDIA HDR100 Infiniband, EVIDEN EuroHPC/CINECA Italy | 1,824,768 | 241.20 | 306.31 | 7,494 |
| Tuolumne - HPE Cray EX255a, AMD 4th Gen EPYC 24C 1.8GHz, AMD Instinct MI300A, Slingshot-11, TOSS, HPE DOE/NNSA/LLNL United States | 1,161,216 | 208.10 | 288.88 | 3,387 |
| MareNostrum 5 ACC - BullSequana XH3000, Xeon Platinum 8460Y+ 32C 2.3GHz, NVIDIA H100 64GB, Infiniband NDR, EVIDEN EuroHPC/BSC Spain | 663,040 | 175.30 | 249.44 | 4,159 |
| | GH200 Superchip, Slingshot-11, HPE Cray OS, HPE Swiss National Supercomputing Centre (CSCS) Switzerland LUMI - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland Leonardo - BullSequana XH2000, Xeon Platinum 8358 32C 2.6GHz, NVIDIA A100 SXM4 64 GB, Quad-rail NVIDIA HDR100 Infiniband, EVIDEN EuroHPC/CINECA Italy Tuolumne - HPE Cray EX255a, AMD 4th Gen EPYC 24C 1.8GHz, AMD Instinct MI300A, Slingshot-11, TOSS, HPE DOE/NNSA/LLNL United States MareNostrum 5 ACC - BullSequana XH3000, Xeon Platinum 8460Y+ 32C 2.3GHz, NVIDIA H100 64GB, Infiniband NDR, EVIDEN EuroHPC/BSC | GH200 Superchip, Slingshot-11, HPE Cray OS, HPE Swiss National Supercomputing Centre (CSCS) Switzerland LUMI - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland Leonardo - BullSequana XH2000, Xeon Platinum 8358 32C 2.6GHz, NVIDIA A100 SXM4 64 GB, Quad-rail NVIDIA HDR100 Infiniband, EVIDEN EuroHPC/CINECA Italy Tuolumne - HPE Cray EX255a, AMD 4th Gen EPYC 24C 1.8GHz, AMD Instinct MI300A, Slingshot-11, TOSS, HPE D0E/NNSA/LLNL United States MareNostrum 5 ACC - BullSequana XH3000, Xeon Platinum 8460Y+ 32C 2.3GHz, NVIDIA H100 64GB, Infiniband NDR, EVIDEN EuroHPC/BSC | GH200 Superchip, Slingshot-11, HPE Cray OS, HPE Swiss National Supercomputing Centre (CSCS) Switzerland LUMI - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland Leonardo - BullSequana XH2000, Xeon Platinum 8358 32C 2.6GHz, NVIDIA A100 SXM4 64 GB, Quad-rail NVIDIA HDR100 Infiniband, EVIDEN EuroHPC/CINECA Italy Tuolumne - HPE Cray EX255a, AMD 4th Gen EPYC 24C 1.8GHz, AMD Instinct MI300A, Slingshot-11, TOSS, HPE DOE/NNSA/LLNL United States MareNostrum 5 ACC - BullSequana XH3000, Xeon Platinum 8460Y+ 32C 2.3GHz, NVIDIA H100 64GB, Infiniband NDR, EVIDEN EuroHPC/BSC | GH200 Superchip, Slingshot-11, HPE Cray OS, HPE Swiss National Supercomputing Centre (CSCS) Switzerland LUMI - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland Leonardo - BullSequana XH2000, Xeon Platinum 8358 32C 2.6GHz, NVIDIA A100 SXM4 64 GB, Quad-rail NVIDIA HDR100 Infiniband, EVIDEN EuroHPC/CINECA Italy Tuolumne - HPE Cray EX255a, AMD 4th Gen EPYC 24C 1.8GHz, AMD Instinct MI300A, Slingshot-11, TOSS, HPE DOE/NNSA/LLNL United States MareNostrum 5 ACC - BullSequana XH3000, Xeon Platinum 8460Y+ 32C 2.3GHz, NVIDIA H100 64GB, Infiniband NDR, EVIDEN EuroHPC/BSC |

2024

8 MareNostrum 5 ACC - BullSequana XH3000, Xeon 680,960 138.20 265.57 2,560
Platinum 8460Y+ 40C 2.3GHz, NVIDIA H100 64GB,
Infiniband NDR200, EVIDEN
EuroHPC/BSC
Spain

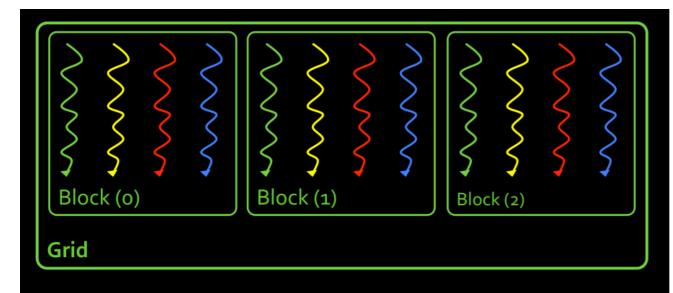
2023

88 MareNostrum - Lenovo SD530, Xeon Platinum 8160 24C 153,216 6.47 10.30 1,632 2.1GHz, Intel Omni-Path, Lenovo Barcelona Supercomputing Center Spain

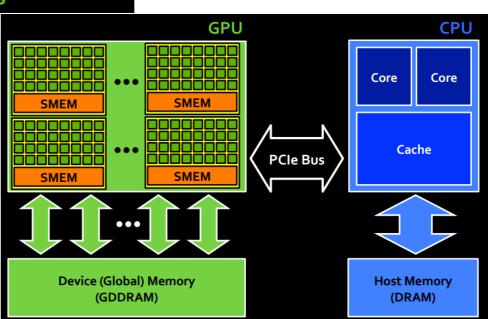
2022

Тета 11: N

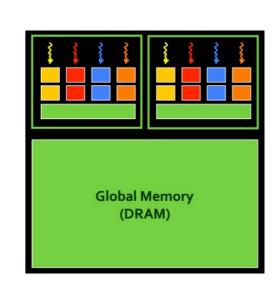
9/34



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



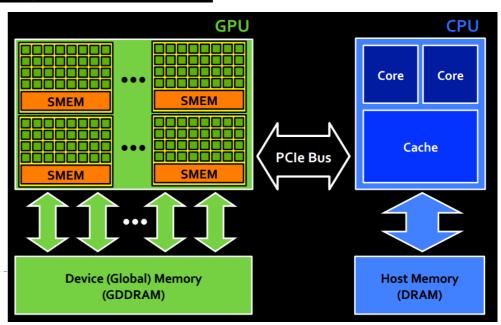
- A thread executes on a single streaming processor
 - Allows use of familiar scalar code within kernel
- A block executes on a single streaming multiprocessor
 - Threads and blocks do not migrate to different SMs
 - All threads within block execute in concurrently, in parallel
- A streaming multiprocessor may execute multiple blocks
 - Must be able to satisfy aggregate register and memory demands
- A grid executes on a single device (GPU)
 - Blocks from the same grid may execute concurrently or serially*
 - Blocks from multiple grids may execute concurrently
 - A device can execute multiple kernels concurrently



En la GPU tenemos varios tipos de memoria:

- Memoria global
- Memoria compartida
- Registros
- Memoria local
- Memoria de constantes
- Memoria de texturas





Memoria Global

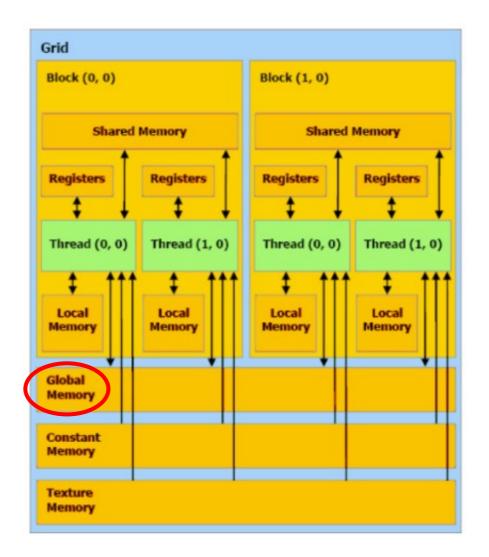
- Es la memoria "principal" de la GPU. Todos los hilos pueden acceder a ella
- La memoria permanece reservada mientras se ejecuta el kernel que la reservó o se libera explícitamente
- Reserva:

m = cuda.device_array(n, dtype=np.float32)

Liberación:

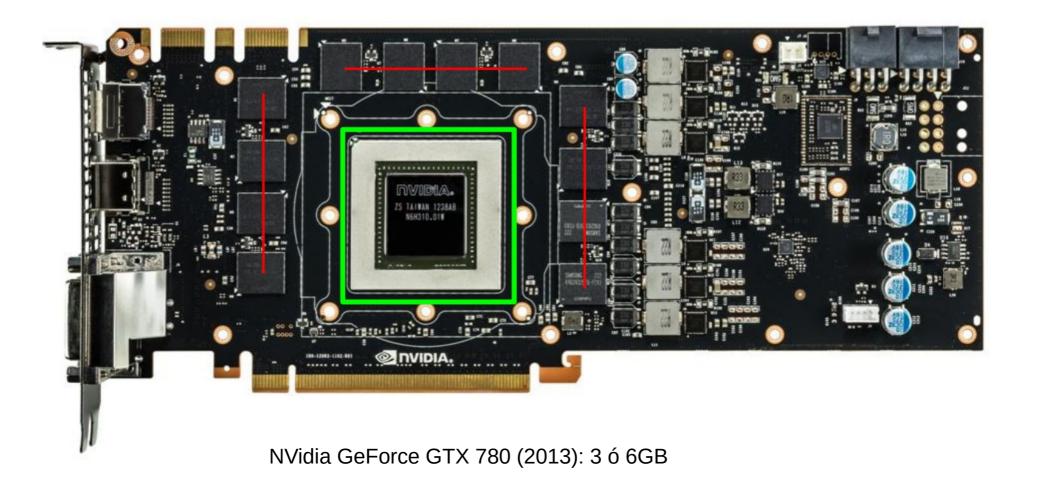
m.close()

- La mayoría de la memoria de las GPUs es memoria global
- La latencia en torno a 300 ns para GPUs Kepler GTX 700 (la latencia de la memoria principal de la CPU ≥ 100 ns)
- Potencialmente 150 veces más lenta que la memoria compartida o los registros
- Tamaño: hasta 48-64 GBs



https://en.wikipedia.org/wiki/List_of_Nvidia_graphics_processing_units

Tema 11: NVidia CUDA 12/34



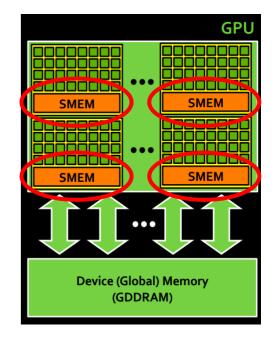
Las líneas rojas marcan la memoria global

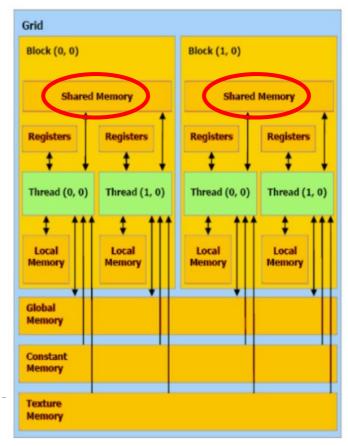
Tema 11: NVidia CUDA 13/34

Memoria Compartida

- Memoria muy rápida localizada en los SMs
- Mismo hardware que el caché L1
- Declarada estáticamente <u>en el kernel</u>:
 sm = cuda.shared.array(128, dtype=numba.float32)
- Declarada dinámicamente en host y kernel:
 kernel[grid_dim, block_dim, numBytesShMem](args)
- Latencia en torno a 5 ns
- Tamaño: 48 128 kiB. Reparto entre caché L1 y memoria compartida es configurable

https://en.wikipedia.org/wiki/List_of_Nvidia_graphics_processing_units





Memoria para constantes (constant memory)

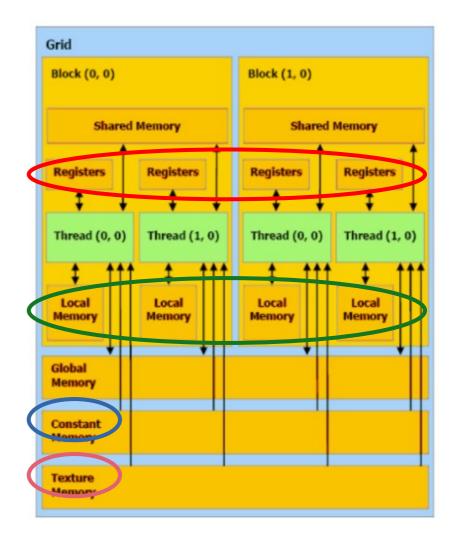
- Memoria que es utilizada desde el host
- Visible (read-only) para todos los hilos del kernel
- Tamaño constante: 64 KB
- Uso típico: almacenar constantes

Registros

- Variables locales de los threads
- Hasta 128K / 32 bits cada uno

Memoria local

• Si se acaban los registros, se reserva un espacio en memoria global



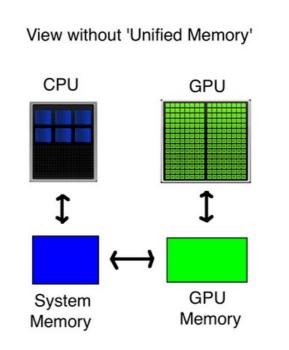
Texture memory

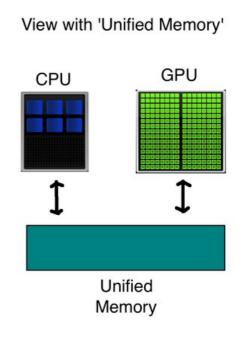
• Parte de la memoria global. Se obtiene localidad espacial mediante cachés. Ideal para imágenes. Es de acceso read-only desde el kernel

Tema 11: NVidia CUDA 15/34

Memoria unificada

- Unifica las memorias de GPU y CPU en un espacio único
- Bajas prestaciones
- Compute capability ≥ 3.0





| Feature support (unlisted features are supported for all compute capabilities) | | Compute capability (version) | | | | | | | | | | | |
|--|----|------------------------------|-----|-----|-----|--------|--------|--------|--------|--------|-----|-----|-----|
| | | 1.2, 1.3 | 2.x | 3.0 | 3.2 | 3.5, 3 | .7, 5. | x, 6.> | κ, 7.0 | 0, 7.2 | 7.5 | 8.x | 9.0 |
| Warp vote functions (all(),any()) | No | | Yes | | | | | | | | | | |
| Warp vote functions (ballot()) Memory fence functions (threadfence_system()) | | | | | | | | | | | | | |
| | | | | | | | | | | | | | |
| Synchronization functions (syncthreads_count(),syncthreads_and(),syncthreads_or()) | No | | | Yes | | | | | | | | | |
| Surface functions | | | | | | | | | | | | | |
| 3D grid of thread blocks | | | | | | | | | | | | | |
| Warp shuffle functions | No | | Yes | | | | | | | | | | |
| nified memory programming | | NU | | ies | | | | | | | | | |
| Funnel shift | | No | | Yes | | | | | | | | | |
| Dynamic parallelism | No | | | Yes | | | | | | | | | |

Tema 11: NVidia CUDA 16/34

```
Device 0: "GeForce GT 720"
 CUDA Driver Version / Runtime Version
                                                 7.0 / 7.0
 CUDA Capability Major/Minor version number:
                                                 3.5
 Total amount of global memory:
                                                 2047 MBytes (2146762752 bytes)
  ( 1) Multiprocessors, (192) CUDA Cores/MP:
                                                 192 CUDA Cores
 GPU Max Clock rate:
                                                 797 MHz (0.80 GHz)
 Memory Clock rate:
                                                 900 Mhz
 Memory Bus Width:
                                                 64-bit
 L2 Cache Size:
                                                 524288 bytes
 Maximum Texture Dimension Size (x,y,z)
                                                 1D=(65536), 2D=(65536, 65536), 3D=(4096, 65536)
4096, 4096)
 Maximum Layered 1D Texture Size, (num) layers 1D=(16384), 2048 layers
 Maximum Layered 2D Texture Size, (num) layers 2D=(16384, 16384), 2048 layers
 Total amount of constant memory:
                                                 65536 bytes
 Total amount of shared memory per block:
                                                 49152 bytes
 Total number of registers available per block: 65536
 Warp size:
                                                 32
 Maximum number of threads per multiprocessor: 2048
 Maximum number of threads per block:
                                                 1024
 Max dimension size of a thread block (x,y,z): (1024, 1024, 64)
 Max dimension size of a grid size (x,y,z): (2147483647, 65535, 65535)
 Maximum memory pitch:
                                                 2147483647 bytes
 Texture alignment:
                                                 512 bytes
 Concurrent copy and kernel execution:
                                                 Yes with 1 copy engine(s)
 Run time limit on kernels:
                                                 Yes
 Integrated GPU sharing Host Memory:
                                                 No
 Support host page-locked memory mapping:
                                                 Yes
 Alignment requirement for Surfaces:
                                                 Yes
 Device has ECC support:
                                                 Disabled
 Device supports Unified Addressing (UVA):
                                                 Yes
 Device PCI Domain ID / Bus ID / location ID:
                                                 0 / 1 / 0
 Compute Mode:
     < Default (multiple host threads can use ::cudaSetDevice() with device simultaneously) >
deviceQuery, CUDA Driver = CUDART, CUDA Driver Version = 7.0, CUDA Runtime Version = 7.0,
NumDevs = 1, Device0 = GeForce GT 720
Result = PASS
```

Tema 11: NVidia CUDA 17/34

```
Device 0: "NVIDIA T400 4GB"
 CUDA Driver Version / Runtime Version
                                                 12.0 / 12.1
 CUDA Capability Major/Minor version number:
                                                 7.5
 Total amount of global memory:
                                                 3901 MBytes (4090494976 bytes)
  ( 6) Multiprocessors x (192) CUDA Cores/MP:
                                                 1152 CUDA Cores
 GPU Clock rate:
                                                 1425 MHz (1.42 GHz)
 Memory Clock rate:
                                                 5001 Mhz
 Memory Bus Width:
                                                 64-bit
 L2 Cache Size:
                                                 524288 bytes
 Max Texture Dimension Size (x, y, z)
                                                 1D=(131072), 2D=(131072,65536),
3D=(16384, 16384, 16384)
 Max Layered Texture Size (dim) x layers
                                                 1D=(32768) x 2048, 2D=(32768,32768) x 2048
 Total amount of constant memory:
                                                 65536 bytes
 Total amount of shared memory per block:
                                                 49152 bytes
 Total number of registers available per block: 65536
                                                 32
 Warp size:
 Maximum number of threads per multiprocessor:
                                                 1024
 Maximum number of threads per block:
                                                 1024
 Maximum sizes of each dimension of a block:
                                                 1024 x 1024 x 64
 Maximum sizes of each dimension of a grid:
                                                 2147483647 x 65535 x 65535
 Maximum memory pitch:
                                                 2147483647 bytes
 Texture alignment:
                                                 512 bytes
 Concurrent copy and kernel execution:
                                                 Yes with 3 copy engine(s)
 Run time limit on kernels:
                                                 Yes
 Integrated GPU sharing Host Memory:
                                                 No
 Support host page-locked memory mapping:
                                                 Yes
 Alignment requirement for Surfaces:
                                                 Yes
 Device has ECC support:
                                                 Disabled
 Device supports Unified Addressing (UVA):
                                                 Yes
 Device PCI Bus ID / PCI location ID:
                                                 1 / 0
 Compute Mode:
    < Default (multiple host threads can use ::cudaSetDevice() with device simultaneously) >
deviceQuery, CUDA Driver = CUDART, CUDA Driver Version = 12.0, CUDA Runtime Version = 12.1,
NumDevs = 1, Device0 = NVIDIA T400 4GB
```

Tema 11: NVidia CUDA 18/34

```
Detected 2 CUDA Capable device(s)
Device 0: "GeForce GTX 1080 Ti"
  CUDA Driver Version / Runtime Version
                                                 10.1 / 10.1
  CUDA Capability Major/Minor version number:
                                                  6.1
  Total amount of global memory:
                                                 11178 MBytes (11721506816 bytes)
  (28) Multiprocessors x (192) CUDA Cores/MP:
                                                 5376 CUDA Cores
  GPU Clock rate:
                                                 1633 MHz (1.63 GHz)
  Memory Clock rate:
                                                 5505 Mhz
  Memory Bus Width:
                                                 352-bit
  L2 Cache Size:
                                                 2883584 bytes
  Max Texture Dimension Size (x, y, z)
                                                 1D=(131072), 2D=(131072,65536),
3D=(16384,16384,16384)
  Max Layered Texture Size (dim) x layers
                                                 1D=(32768) x 2048, 2D=(32768,32768) x 2048
  Total amount of constant memory:
                                                  65536 bytes
  Total amount of shared memory per block:
                                                 49152 bytes
  Total number of registers available per block: 65536
  Warp size:
                                                  32
  Maximum number of threads per multiprocessor:
                                                 2048
  Maximum number of threads per block:
                                                 1024
  Maximum sizes of each dimension of a block:
                                                 1024 x 1024 x 64
  Maximum sizes of each dimension of a grid:
                                                 2147483647 x 65535 x 65535
  Maximum memory pitch:
                                                 2147483647 bytes
  Texture alignment:
                                                 512 bytes
  Concurrent copy and kernel execution:
                                                 Yes with 2 copy engine(s)
  Run time limit on kernels:
                                                  Nο
  Integrated GPU sharing Host Memory:
                                                  No
  Support host page-locked memory mapping:
                                                 Yes
  Alignment requirement for Surfaces:
                                                 Yes
  Device has ECC support:
                                                 Disabled
  Device supports Unified Addressing (UVA):
                                                 Yes
  Device PCI Bus ID / PCI location ID:
                                                 23 / 0
  Compute Mode:
     < Default (multiple host threads can use ::cudaSetDevice() with device simultaneously) >
```

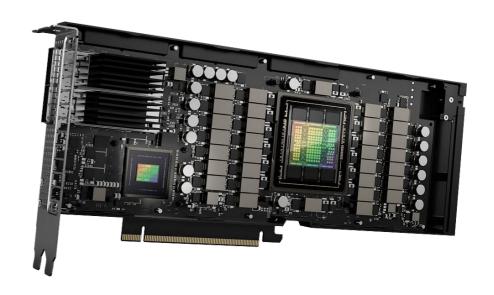
Tema 11: NVidia CUDA 19/34

```
Detected 1 CUDA Capable device(s)
Device 0: "NVIDIA RTX A6000"
  CUDA Driver Version / Runtime Version
                                                 12.2 / 12.1
  CUDA Capability Major/Minor version number:
                                                  8.6
  Total amount of global memory:
                                                 48669 MBytes (51032686592 bytes)
  (84) Multiprocessors x (192) CUDA Cores/MP:
                                                 16128 CUDA Cores
  GPU Clock rate:
                                                 1800 MHz (1.80 GHz)
  Memory Clock rate:
                                                 8001 Mhz
  Memory Bus Width:
                                                 384-bit
  L2 Cache Size:
                                                 6291456 bytes
  Max Texture Dimension Size (x, y, z)
                                                 1D=(131072), 2D=(131072,65536),
3D=(16384, 16384, 16384)
  Max Layered Texture Size (dim) x layers
                                                 1D=(32768) x 2048, 2D=(32768,32768) x 2048
  Total amount of constant memory:
                                                 65536 bytes
  Total amount of shared memory per block:
                                                 49152 bytes
  Total number of registers available per block: 65536
  Warp size:
                                                  32
  Maximum number of threads per multiprocessor:
                                                 1536
  Maximum number of threads per block:
                                                 1024
  Maximum sizes of each dimension of a block:
                                                 1024 x 1024 x 64
  Maximum sizes of each dimension of a grid:
                                                 2147483647 x 65535 x 65535
  Maximum memory pitch:
                                                 2147483647 bytes
  Texture alignment:
                                                 512 bytes
  Concurrent copy and kernel execution:
                                                 Yes with 2 copy engine(s)
  Run time limit on kernels:
                                                  Yes
  Integrated GPU sharing Host Memory:
                                                  No
  Support host page-locked memory mapping:
                                                 Yes
  Alignment requirement for Surfaces:
                                                 Yes
  Device has ECC support:
                                                 Disabled
  Device supports Unified Addressing (UVA):
                                                 Yes
  Device PCI Bus ID / PCI location ID:
                                                 1 / 0
  Compute Mode:
     < Default (multiple host threads can use ::cudaSetDevice() with device simultaneously) >
```

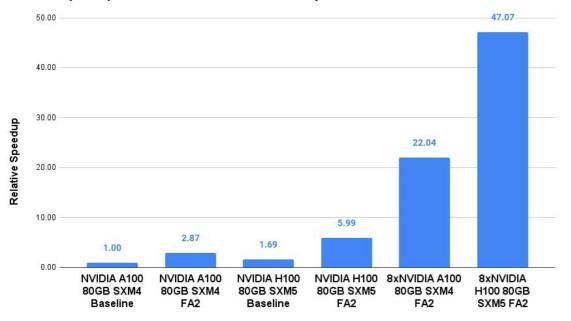
Tema 11: NVidia CUDA 20/34

Arquitectura NVidia Hopper

- Incluye *tensor cores*
- Diseñadas específicamente para deep learning
- Precio ≥ 25000 euros



Relative Speedup Over NVIDIA A100 + Baseline Implementation

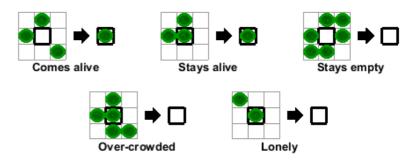


- NVidia H100 vs A100
- Precio A100 ≥ 5000 euros

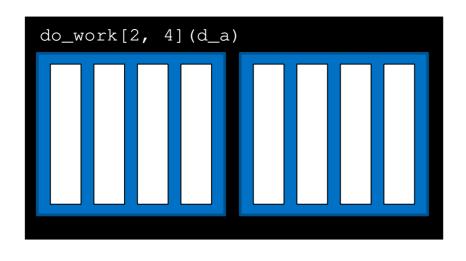
Tema 11: NVidia CUDA 21/34

¿Porqué hay que implementar Kernels en CUDA?

- Ufuncs muy útiles, pero limitados a casos en que es la misma operación a todos los elementos de una estructura
- Normalmente hay que acceder a más de un elemento para hacer cálculos



Los kernel lanzan hilos (*threads*) agrupados en bloques (*blocks*). El conjunto de bloques forma un *grid*. Todos los bloques poseen el mismo número de hilos



gridDim.x is the number of blocks in
the grid, in this case 2

blockIdx.x is the index of the current block within the grid

blockDim. x describes the number of threads in a block. In this case **4**

Inside a kernel **threadIdx.x** describes the index of the thread within a block

Tema 11: NVidia CUDA

Primer kernel CUDA

```
from numba import cuda
import numpy as np
# Kernels decorados con `@cuda.jit` no devuelven valores
# No es necesaria signatura de tipos
@cuda.jit
def add kernel(x, y, out):
    idx = cuda.grid(1)
        # 1 = grid unidimensional
        \# cuda.grid(1) = cuda.threadIdx.x + cuda.blockIdx.x*cuda.blockDim.x
                                                                                Mejores
    out[idx] = x[idx] + y[idx]
                                                                                prestaciones
n = 4096
h x = np.arange(n).astype(np.float32)
                                     # [1.0 ... 1.0]
h y = np.ones like(h x)
d x = cuda.to device(h x)
                                                                         128*32=4096
d y = cuda.to device(h y)
d out = cuda.device array like(d x)
# Necesitamos un hilo para cada elemento (409)
threads per block = 128
blocks per grid = 32
add kernel[blocks per grid, threads per block] (d x, d y, d out)
cuda.synchronize() # Esto sería innecesario
print(d out.copy to host().astype(np.int16)) # Resultado: [1...4096]
              3 ... 4094 4095 4096]
/home/leandro/anaconda3/envs/tftorch/lib/python3.11/site-packages/numba/cuda/
ikely result in GPU under-utilization due to low occupancy.
  warn(NumbaPerformanceWarning(msg))
```

Tema 11: NVidia CUDA 23/34

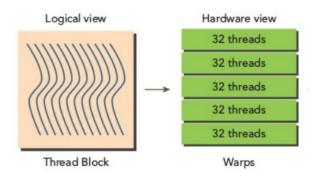
Ejercicio 1: crear un kernel a partir de una función

Partiendo del código suministrado, modificarlo para realizar el cálculo en la GPU

```
import numpy as np
n = 16384
def h square(a):
   return a**2
# TODO: implementar un kernel d square()
a = np.arange(n, dtype=np.float32)
# TODO: crear vector d a y copiar al kernel
# TODO: crear vector en GPU para obtener la salida
# TODO: modificar estos valores e invocar kernel
blocks = 0
threads = 0
# TODO: Launch as a kernel with an appropriate execution configuration
out = h square(a)
out aux = a**2
np.testing.assert almost equal(out, out aux)
# TODO: reemplazar out aux con lo obtenido en el kernel (usar .copy to host())
        %timeit h square(h a)
        %timeit d square[blocks,threads](d a,d out)
                          er loop (mean \pm std. dev. of 7 runs, 10,000 loops each)
                           per loop (mean \pm std. dev. of 7 runs, 10,000 loops each)
```

Tema 11: NVidia CUDA 24/34

Rendimiento de los kernel CUDA



Notas sobre la ejecución de kernels CUDA:

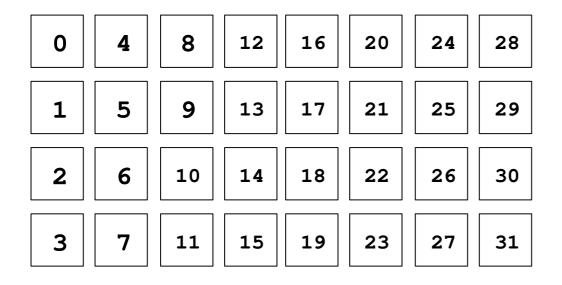
- En la ejecución, cada bloque se asigna a un SM, con potencialmente muchos bloques asignados a cada SM
- Los hilos de un bloque se dividen en grupos de 32 llamados <u>warps</u>. Los warps se ejecutan en paralelo
- CUDA gestiona de manera automática los cambios de los warps en ejecución. No hay latencia apreciable entre cambios de warp
- Un kernel debe estar compuesto de un número de warps suficiente (configurando el número de bloques)
- El tamaño de un grid vendrá dado por el problema y la compute capability de la GPU. Algunas ideas:
 - Tamaño de bloque múltiplo de 32 (hilos/warp): típicamente entre 128 y 512 hilos/bloque
 - Tamaño de grid que ocupe eficientemente la GPU. Típicamente nº de bloques 2x-4x el nº de SMs de la GPU
 - Si el tamaño de los datos es muy grande, en vez de aumentar mucho el número de bloques, hacer kernels que procesen más datos. Ejecutar bloques tiene latencia

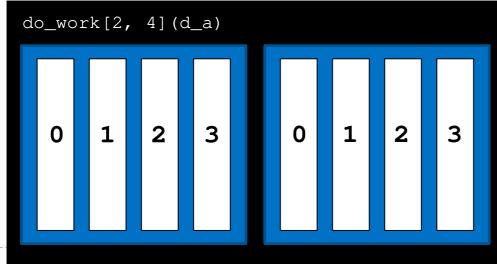
Tema 11: NVidia CUDA 25/34

Uso de stride en Kernels CUDA

A menudo el conjunto de datos es muy grande:

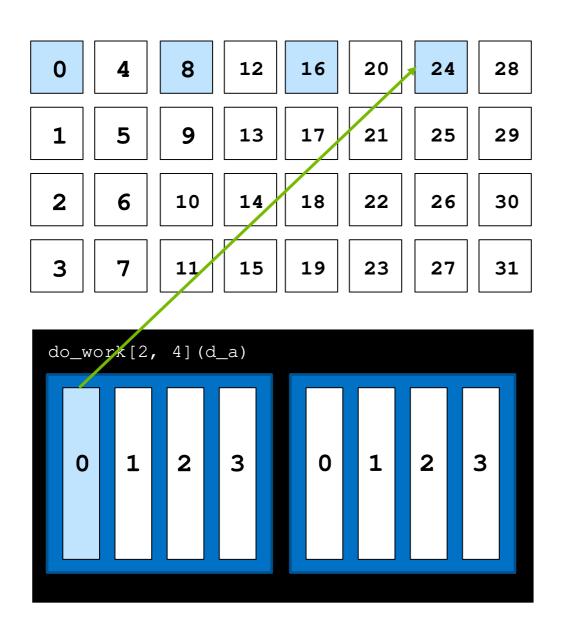
- No es conveniente aumentar el número de bloques en exceso
- Mejor que cada hilo procese más de un elemento: uso de **stride**





Ejemplo

- 2 bloques
- 4 hilos/bloque
- 32 elementos a procesar



One way to address this programmatically is with a grid-stride loop

In a grid-stride loop, the thread's first element is calculated as usual, with cuda.grid()

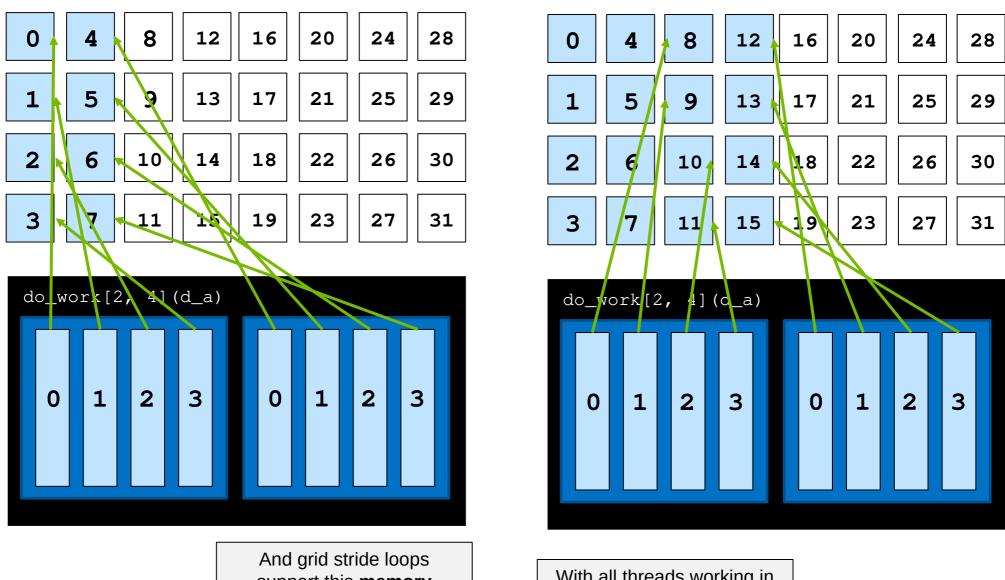
The thread then strides forward by the total number of threads in the grid (blockDim.x * gridDim.x), in this case 8

Numba provides another convenience function for this common calculation:

cuda.gridsize(),
returning the number of threads in the grid

The thread continues in this way until its data index is greater than the number of data elements

Tema 11: NVidia CUDA 27/34



support this memory
coalescing because
threads executing in parallel
will access adjacent data
elements

With all threads working in this way, all elements are covered with the performance advantage of memory coalescing

Tema 11: NVidia CUDA 28/34

Sin stride:

Con stride: from numba import cuda

```
from numba import cuda
                                                                  import numpy as np
import numpy as np
                                                                  @cuda.jit
@cuda.jit
                                                                  def add kernel(x, y, out):
def add kernel(x, y, out):
                                                                       start = cuda.grid(1)
    idx = cuda.grid(1)
                                                                      stride = cuda.gridsize(1)
    out[idx] = x[idx] + y[idx]
                                                                      for i in range(start, x.shape[0], stride):
                                                                          out[i] = x[i] + y[i]
n = 4096
h x = np.arange(n).astype(np.float32)
h y = np.ones like(h x)
                                                                  n = 125000
                                                                  h x = np.arange(n).astype(np.float32)
d x = cuda.to device(h x)
                                                                  h y = np.ones like(h x)
d y = cuda.to device(h y)
d out = cuda.device array like(d x)
                                                                  d x = cuda.to device(h x)
                                                                  d y = cuda.to device(h y)
threads per block = 128
                                                                  d out = cuda.device array like(d x)
blocks per grid = 32
                                                                  threads per block = 128
add kernel[blocks per grid, threads per block](d x, d y, d out)
                                                                  blocks per grid = 56
d out.copy to host().astype(np.int16)
                                                                  add kernel[blocks per grid, threads per block](d x, d y, d out)
/home/leandro/anaconda3/envs/tftorch/lib/python3.11/site-package
                                                                  d out.copy to host().astype(np.float16)
ikely result in GPU under-utilization due to low occupancy.
  warn(NumbaPerformanceWarning(msg))
                                                                  /home/leandro/anaconda3/envs/tftorch/lib/python3.11/site-package
arrav([
                      3, ..., 4094, 4095, 4096], dtype=int16)
                                                                   ikely result in GPU under-utilization due to low occupancy.
                                                                    warn(NumbaPerformanceWarning(msg))
                                                                  /tmp/ipykernel 6055/1658409643.py:24: RuntimeWarning: overflow €
                                                                    d out.copy to host().astype(np.float16)
                                                                  array([ 1., 2., 3., ..., inf, inf, inf], dtype=float16)
```

Tema 11: NVidia CUDA 29/34

Ejercicio 2: kernel CUDA con stride

En el código proporcionado, implementar el kernel

```
import numpy as np
from math import hypot
from numba import cuda
                                          r = \sqrt{x^2 + y^2} = \sqrt{x^2 \left(1 + \left(\frac{y}{x}\right)\right)}
def cpu hypot(a,b):
     return np.hypot(a,b)
# TODO: implementar esta función
# usando stride
def gpu hypot stride(a, b, c):
     None
# No modificar a partir de aquí
n = 1000000
h = np.random.uniform(-12, 12, n).astype(np.float32)
h b = np.random.uniform(-12, 12, n).astype(np.float32)
d a = cuda.to device(h a)
db = cuda.to device(hb)
d c = cuda.device array like(d b)
blocks = 128
threads per block = 64
qpu hypot stride[blocks, threads per block](d a, d b, d c)
np.testing.assert almost equal(np.hypot(h a, h b), d c.copy to host(), decimal=5)
   %timeit cpu hypot(h a,h b)
   %timeit gpu hypot stride[128, 64](d a, d b, d c)
                      per loop (mean ± std. dev. of 7 runs, 100 loops each)
                     ber loop (mean \pm std. dev. of 7 runs, 10,000 loops each)
```

Tema 11: NVidia CUDA 30/34

Con los hilos en paralelo, es posible que se den *race conditions*. Por ejemplo, un contador global:

- Leemos el valor del contador
- Incrementamos el valor del contador
- Escribimos el contador

Para evitar estos problemas, tenemos operaciones atómicas

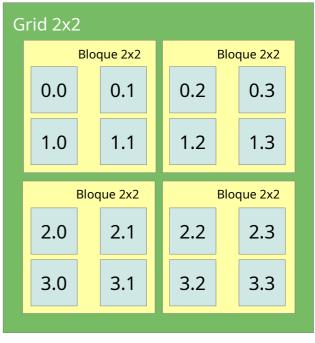
```
import numpy as np
from numba import cuda
@cuda.jit
def thread counter race condition(global counter):
   global counter[0] += 1 # Mal
@cuda.jit
def thread counter safe(global counter):
    cuda.atomic.add(global counter, 0, 1)
# Esto no funciona bien
global counter = cuda.to device(np.array([0], dtype=np.float32))
thread counter race condition[64, 64](global counter)
print('Debería dar %d:' % (64*64), global counter.copy to host().astype(np.int16))
# Esto sí funciona bien
global counter = cuda.to device(np.array([0], dtype=np.float32))
thread counter safe[64, 64](global counter)
print('Debería dar %d:' % (64*64), global counter.copy to host().astype(np.int16))
```

Kernels bidimensionales y tridimensionales

F

Dependiendo de la naturaleza del cálculo y del problema, puede ser interesante tener grids y bloques de más de una dimensión

```
import numpy as np
from numba import cuda
@cuda.jit
def get 2D indices(A):
    x, y = cuda.grid(2) # Obtenemos las dos dimensiones
    # Equivalente a:
    \# x = cuda.blockIdx.x * cuda.blockDim.x + cuda.threadIdx.x
    # y = cuda.blockIdx.y * cuda.blockDim.y + cuda.threadIdx.y
    # Escribimos índice x + '.' + índice y
    A[x][y] = x + y / 10
d A = cuda.device array(shape=(4,4), dtype=np.float32)
    # Matriz 4x4 en la GPU
blocks = (2, 2) # Grid = 2x2 bloques
threads per block = (2, 2) # Bloque = 2x2 threads
get 2D indices[blocks, threads per block](d A)
np.set printoptions(precision=1, floatmode="fixed")
print(d A.copy to host())
/home/leandro/anaconda3/envs/tftorch/lib/python3.11/site-packages/
kely result in GPU under-utilization due to low occupancy.
  warn(NumbaPerformanceWarning(msg))
[[0.0 0.1 0.2 0.3]
 [1.0 1.1 1.2 1.3]
 [2.0 2.1 2.2 2.3]
 [3.0 3.1 3.2 3.3]]
```



Tema 11: NVidia CUDA 32/34

Kernel bidimensional: suma de matrices

```
from numba import cuda
import numpy as np
@cuda.jit # Adjust block size as needed
def add matrices(a, b, c):
    i, j = cuda.grid(2) # Get thread indices in two dimensions (row, column)
    c[i, j] = a[i, j] + b[i, j]
# Example usage
rows = 4096
cols = 4096
h a = np.random.rand(rows, cols).astype(np.float32) # Allocate matrices on CPU
h b = np.random.rand(rows, cols).astype(np.float32)
d a = cuda.to device(h a) # Transfer matrices to GPU
d b = cuda.to device(h b)
d c = cuda.device array like(d b)
threads per block = (32, 32)
blocks = (128, 128)
add matrices[blocks, threads per block] (d a, d b, d c) # Launch kernel with appropriate grid size
h c = d c.copy to host()
np.testing.assert almost equal(h c, h a+h b)
%timeit c aux= (h a + h b)
%timeit add matrices[blocks, threads per block](d a, d b, d c)
19.2 ms ± 11.3 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
11.3 ms \pm 153 \mus per loop (mean \pm std. dev. of 7 runs, 1,000 loops each)
```

Tema 11: NVidia CUDA 33/34

Ejercicio 3: kernel bidimensional para procesar una imagen

```
# Necesitamos skimage
 Instalar con
        conda install scikit-image
import matplotlib.pyplot as plt
from skimage import data, color
import numpy as np
@cuda.jit
def blur(input, output):
    x, y = cuda.grid(2)
    if x>0 and y>0 and x<(input.shape[0]-1) and y<(input.shape[1]-1):
        output[x][y] = 0.25*(input[x-1][y]+input[x+1][y]+input[x][y-1]+input[x][y+1])
    else:
        output[x][y] = input [x][y]
# TODO: definir tamaño de grid y de bloque
num cycles = 100
astronaut = (255.-color.rgb2gray(data.astronaut()))/255.0
print("Image size: ",astronaut.shape)
fig, ax = plt.subplots()
im = ax.imshow(astronaut, cmap='Greys')
# TODO: datos a GPU (duplicar imagen)
# TODO: ejecutar num cycles veces un el kernel blur
# TODO: copiar imagen desenfocada al host
fig, ax = plt.subplots()
im = ax.imshow(astronaut blurred, cmap='Greys')
```

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