GPU Programming

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Agenda

- Computation
- Memory
- Synchronization
- Functions
- Support
- Streams
- Topics
- Case Study Graphs

Hello World.

```
#include <stdio.h>
int main() {
    printf("Hello World.\n");
    return 0;
}
```

Compile: nvcc hello.cu

Run: a.out

GPU Hello World.

```
#include <stdio.h>
                       #include <cuda.h>
                         global__ void dkernel() {
                         printf("Hello World.\n");
         Kernel
                       int main() {
                      → dkernel<<<1, 1>>>();
Kernel Launch -
                         return 0;
                      Compile: nvcc hello.cu
                      Run: ./a.out
                      - No output. --
```

GPU Hello World.

```
#include <stdio.h>
 #include <cuda.h>
   global___ void dkernel() {
   printf("Hello World.\n");
 int main() {
   dkernel<<<1, 1>>>();
   cudaDeviceSynchronize();
   return 0;
Compile: nvcc hello.cu
Run: ./a.out
Hello World.
```

Takeaway

CPU function and GPU kernel run asynchronously.

Homework

- Find out where nvcc is.
- Find out the CUDA version.
- Find out where deviceQuery is.

GPU Hello World in Parallel.

```
#include <stdio.h>
 #include <cuda.h>
   _global___ void dkernel() {
   printf("Hello World.\n");
 int main() {
   dkernel<<<1, 32>>>();
   cudaDeviceSynchronize();
   return 0;
Compile: nvcc hello.cu
Run: ./a.out
Hello World.
Hello World.
```

Parallel Programming Concepts

- Process: a.out, notepad, chrome
- Thread: light-weight process
- Operating system: Windows, Android, Linux
 - OS is a software, but it manages the hardware.
- Hardware
 - Cache, memory
 - Cores
- Core
 - Threads run on cores.
 - A thread may jump from one core to another.

Classwork

 Write a CUDA code corresponding to the following sequential C code.

```
#include <stdio.h>
#define N 100
int main() {
  int i
  for (i = 0; i < N; ++i)
     printf("%d\n", i * i);
  return 0;
```

```
#include <stdio.h>
#include <cuda.h>
#define N 100
  global void fun() {
     printf("%d\n", threadIdx.x);
int main() {
     fun<<<1, N>>>();
     cudaDeviceSynchronize();
     return 0;
```

Classwork

 Write a CUDA code corresponding to the following sequential C code.

```
#include <stdio.h>
#define N 100
int main() {
   int a[N], i;
   for (i = 0; i < N; ++i)
      a[i] = i * i;
   return 0;
}</pre>
```

Takeaway

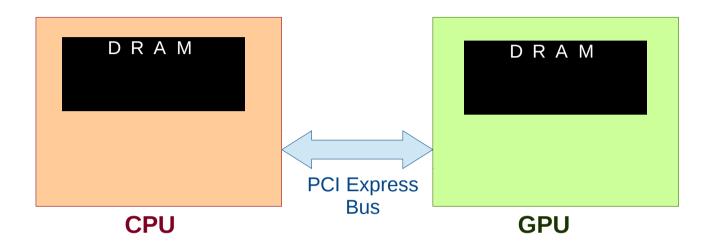
No cudaDeviceSynchronize required.

```
#include <stdio.h>
#include <cuda.h>
#define N 100
  global___ void fun(int *a) {
     a[threadIdx.x] = threadIdx.x * threadIdx.x;
int main() {
     int a[N], *da;
     int i:
     cudaMalloc(&da, N * sizeof(int));
     fun<<<1, N>>>(da);
     cudaMemcpy(a, da, N * sizeof(int),
                   cudaMemcpyDeviceToHost);
     for (i = 0; i < N; ++i)
          printf("%d\n", a[i]);
     return 0;
```

GPU Hello World with a Global.

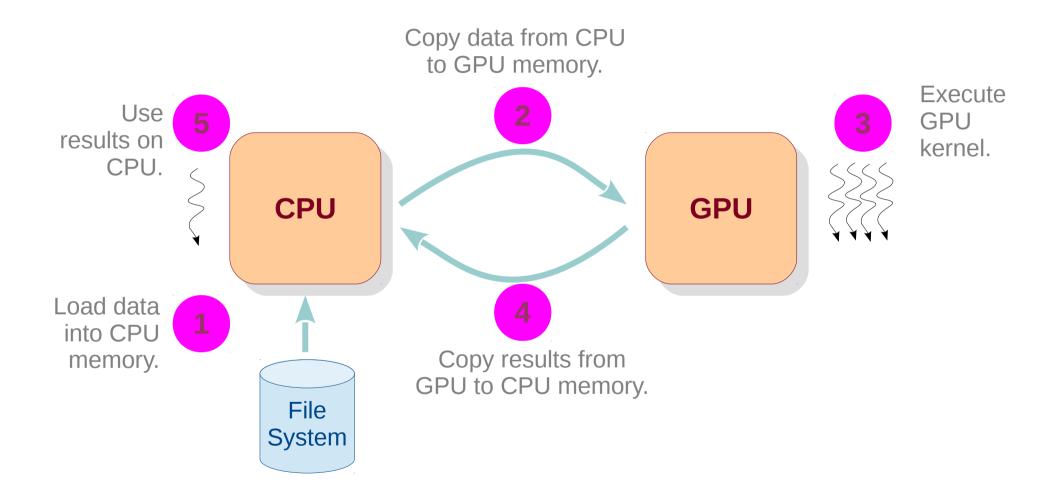
```
#include <stdio.h>
#include <cuda.h>
                                                  Takeaway
const char *msg = "Hello World.\n";
   global___ void dkernel() {
   printf(msg);
                                             CPU and GPU
                                             memories are
                                             separate
int main() {
                                             (for discrete GPUs).
   dkernel<<<1, 32>>>();
   cudaDeviceSynchronize();
   return 0;
Compile: nvcc hello.cu
error: identifier "msg" is undefined in device code
```

Separate Memories



- CPU and its associated (discrete) GPUs have separate physical memory (RAM).
- A variable in CPU memory cannot be accessed directly in a GPU kernel.
- A programmer needs to maintain copies of variables.
- It is programmer's responsibility to keep them in sync.

Typical CUDA Program Flow



Typical CUDA Program Flow

- Load data into CPU memory.
 - fread / rand
- Copy data from CPU to GPU memory.
 - cudaMemcpy(..., cudaMemcpyHostToDevice)
- 3 Call GPU kernel.
 - mykernel<<<x, y>>>(...)
- Copy results from GPU to CPU memory.
 - cudaMemcpy(..., cudaMemcpyDeviceToHost)
- Use results on CPU.

Typical CUDA Program Flow

- Copy data from CPU to GPU memory.
 - cudaMemcpy(..., cudaMemcpyHostToDevice)

This means we need two copies of the same variable – one on CPU another on GPU.

```
e.g., int *cpuarr, *gpuarr;

Matrix cpumat, gpumat;

Graph cpug, gpug;
```

CPU-GPU Communication

```
#include <stdio.h>
#include <cuda.h>
__global___ void dkernel(char *arr, int arrlen) {
    unsigned id = threadIdx.x;
    if (id < arrlen) {
        ++arr[id];
    }
}</pre>
```

Classwork

- 1. Write a CUDA program to initialize an array of size 32 to all zeros in parallel.
- 2. Change the array size to 1024.
- 3. Create another kernel that adds *i* to *array[i]*.
- 4. Change the array size to 8000.
- 5. Check if answer to problem 3 still works.

Homework $(z = x^2 + y^3)$

- Read a sequence of integers from a file.
- Square each number.
- Read another sequence of integers from another file.
- Cube each number.
- Sum the two sequences element-wise, store in the third sequence.
- Print the computed sequence.

Thread Organization

- A kernel is launched as a grid of threads.
- A grid is a 3D array of thread-blocks (gridDim.x, gridDim.y and gridDim.z).
 - Thus, each block has blockIdx.x, .y, .z.
- A thread-block is a 3D array of threads (blockDim.x, .y, .z).
 - Thus, each thread has threadIdx.x, .y, .z.

Grids, Blocks, Threads

Each thread uses IDs to decide what data to work on.

• Block ID: 1D, 2D, or 3D

Thread ID: 1D, 2D, or 3D

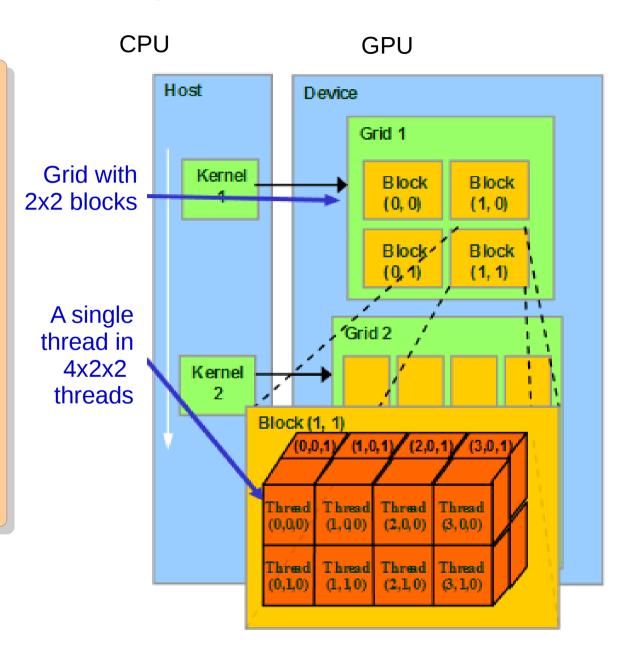
Simplifies memory addressing when processing multi-dimensional data

- Image processing
- Solving PDEs on volumes

• ...

Typical configuration:

- 1-5 blocks per SM
- 128-1024 threads per block.
- Total 2K-100K threads.
- You can launch a kernel with millions of threads.



Accessing Dimensions

```
#include <stdio.h>
                                                       How many times the kernel printf
#include <cuda.h>
                                                       gets executed when the if
  global___ void dkernel() {
                                                       condition is changed to
     if (threadIdx.x == 0 \&\& blockIdx.x == 0 \&\&
                                                       if (threadIdx.x == 0)?
        threadIdx.y == 0 \&\& blockIdx.y == 0 \&\&
        threadIdx.z == 0 \&\& blockIdx.z == 0) {
          printf("%d %d %d %d %d %d.\n", gridDim.x, gridDim.y, gridDim.z,
                                              blockDim.x, blockDim.y, blockDim.z);
                                      Number of threads launched = 2 * 3 * 4 * 5 * 6 * 7.
int main() {
                                      Number of threads in a thread-block = 5 * 6 * 7.
     dim3 grid(2, 3, 4);
                                      Number of thread-blocks in the grid = 2 * 3 * 4.
     dim3 block(5, 6, 7);
     dkernel<<<grid, block>>>();
                                      ThreadId in x dimension is in [0..5).
                                      BlockId in y dimension is in [0..3).
     cudaThreadSynchronize();
     return 0;
```

```
#include <stdio.h>
#include <cuda.h>
  global___ void dkernel(unsigned *matrix) {
     unsigned id = threadIdx.x * blockDim.y + threadIdx.y;
     matrix[id] = id;
#define N
#define M
int main() {
     dim3 block(N, M, 1);
     unsigned *matrix, *hmatrix;
     cudaMalloc(&matrix, N * M * sizeof(unsigned));
     hmatrix = (unsigned *)malloc(N * M * sizeof(unsigned));
     dkernel<<<1, block>>>(matrix);
     cudaMemcpy(hmatrix, matrix, N * M * sizeof(unsigned), cudaMemcpyDeviceToHost);
     for (unsigned ii = 0; ii < N; ++ii) {
          for (unsigned jj = 0; jj < M; ++jj) {
               printf("%2d ", hmatrix[ii * M + jj]);
          printf("\n");
     return 0;
```

Write the kernel to initialize the matrix to unique ids.

What is the output of this program?

```
$ a.out
 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 25 26 27 28 29
```

Write the kernel to initialize the matrix to unique ids.

```
#include <stdio.h>
#include <cuda.h>
  global void dkernel(unsigned *matrix) {
     unsigned id = blockldx.x * blockDim.x + threadIdx.x;
     matrix[id] = id;
#define N
              5
#define M
int main() {
     unsigned *matrix, *hmatrix;
     cudaMalloc(&matrix, N * M * sizeof(unsigned));
     hmatrix = (unsigned *)malloc(N * M * sizeof(unsigned));
     dkernel<<<N, M>>>(matrix);
     cudaMemcpy(hmatrix, matrix, N * M * sizeof(unsigned), cudaMemcpyDeviceToHost);
     for (unsigned ii = 0; ii < N; ++ii) {
          for (unsigned jj = 0; jj < M; ++jj) {
               printf("%2d ", hmatrix[ii * M + ji]);
          printf("\n");
  return 0;
```

Takeaway

One can perform computation on a multi-dimensional data using a onedimensional block.

If I want the launch configuration to be <<2, X>>>, what is X? The rest of the code should be intact.

Launch Configuration for Huge Data

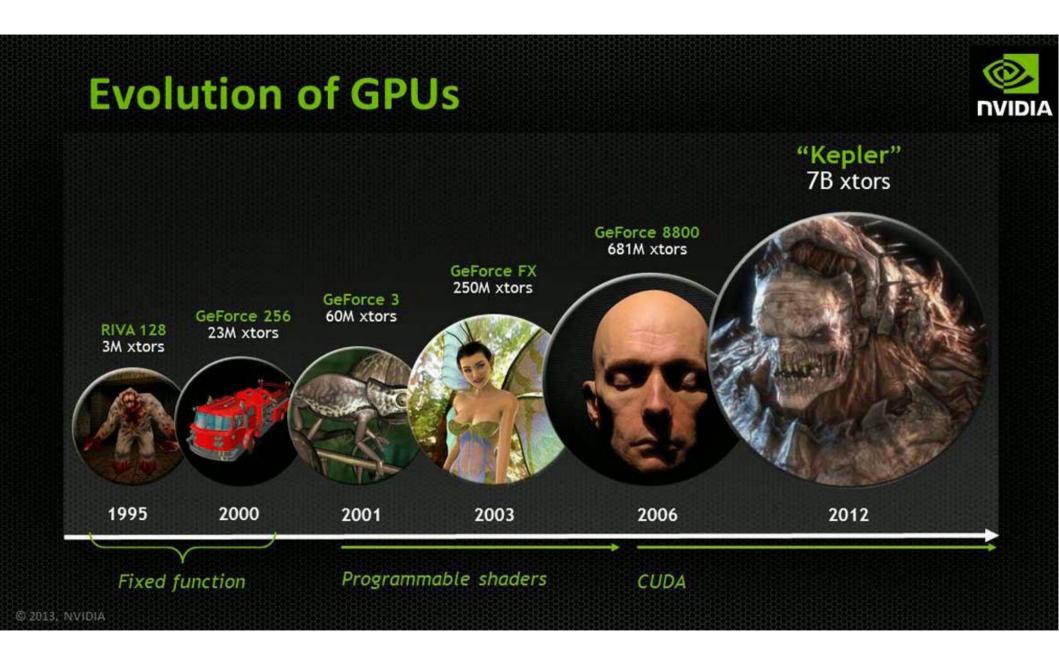
```
#include <stdio.h>
#include <cuda.h>
  global void dkernel(unsigned *vector) {
     unsigned id = blockIdx.x * blockDim.x + threadIdx.x;
                                                            Access out-of-bounds
    vector[id] = id; ◀-
#define BLOCKSIZE
                        1024
int main(int nn, char *str[]) {
                                                               Find two issues
    unsigned N = atoi(str[1]);
                                                               with this code.
     unsigned *vector, *hvector;
     cudaMalloc(&vector, N * sizeof(unsigned));
     hvector = (unsigned *)malloc(N * sizeof(unsigned));
     unsigned nblocks = ceil(N / BLOCKSIZE); <
                                                            Needs floating-point
     printf("nblocks = %d\n", nblocks);
                                                             division
     dkernel<<<nbl/>hocks, BLOCKSIZE>>>(vector);
     cudaMemcpy(hvector, vector, N * sizeof(unsigned), cudaMemcpyDeviceToHost);
    for (unsigned ii = 0; ii < N; ++ii) {
         printf("%4d ", hvector[ii]);
     return 0;
```

Launch Configuration for Large Size

```
#include <stdio.h>
#include <cuda.h>
  global void dkernel(unsigned *vector, unsigned vectorsize) {
     unsigned id = blockIdx.x * blockDim.x + threadIdx.x;
     if (id < vectorsize) vector[id] = id;</pre>
#define BLOCKSIZE
                         1024
int main(int nn, char *str[]) {
     unsigned N = atoi(str[1]);
     unsigned *vector, *hvector;
     cudaMalloc(&vector, N * sizeof(unsigned));
     hvector = (unsigned *)malloc(N * sizeof(unsigned));
     unsigned nblocks = ceil((float)N / BLOCKSIZE);
     printf("nblocks = %d\n", nblocks);
     dkernel<<<nbl/>blocks, BLOCKSIZE>>>(vector, N);
     cudaMemcpy(hvector, vector, N * sizeof(unsigned),
cudaMemcpyDeviceToHost);
     for (unsigned ii = 0; ii < N; ++ii) {
          printf("%4d ", hvector[ii]);
     return 0;
```

Classwork

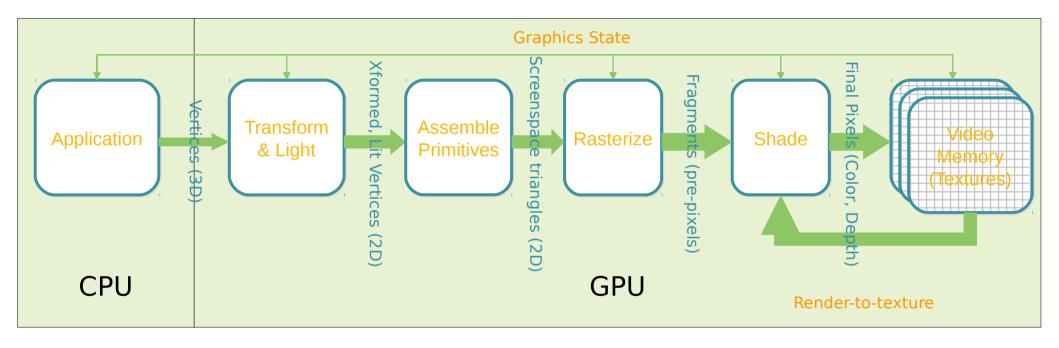
- Read several points as (x, y) coordinates from input.
- For each pair of points, compute euclidean distance sqrt((x2 - x1)² + (y2 - y1)²) in parallel.
- Print the maximum distance.



GPGPU: General Purpose Graphics Processing Unit

Earlier GPGPU Programming

GPGPU = General Purpose Graphics Processing Units.



- Applications: Protein Folding, Stock Options Pricing, SQL Queries, MRI Reconstruction.
- Required intimate knowledge of graphics API and GPU architecture.
- Program complexity: Problems expressed in terms of vertex coordinates, textures and shaders programs.
- Random memory reads/writes not supported.
- Lack of double precision support.

GPU Vendors

- NVIDIA
- AMD
- Intel
- QualComm
- ARM
- Broadcom
- Matrox Graphics
- Vivante
- Samsung

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GPU Languages

- CUDA (compute unified device language)
 - Proprietary, NVIDIA specific
- OpenCL (open computing language)
 - Universal, works across all computing devices
- OpenACC (open accelerator)
 - Universal, works across all accelerators
- There are also interfaces:
 - Python → CUDA
 - Javascript → OpenCL
 - LLVM → PTX

Two Configurations

Feature	K80	P100
# of SMX Units	26 (13 per GPU)	56
# of CUDA Cores	4992 (2496 per GPU)	3584
Memory Clock	2500 MHz	715 MHz
GPU Base Clock	560 MHz	1329 MHz
GPU Boost Support	Yes – Dynamic	Yes – Dynamic
Architecture features	Dynamic Parallelism, Hyper-Q	
Compute Capability	3.7	6.0
Onboard GDDR5 Memory	24 GB	12 GB

top500.org

- Listing of most powerful machines.
 - Ranked by performance (FLOPS)
- As of November 2019
 - Rank 1: Summit from USA (over 2.4 million cores)
 - Rank 2: Sierra from USA (over 1.5 million cores)
 - Rank 3: TaihuLight from China (over 10 million cores)
 - Rank 4: Tianhe-2A from China (3 million cores)
 - Rank 5: Frontera from USA (0.4 million cores)

Homework: What is India's rank? Where is this computer? How many cores?

Matrix Squaring

```
void squarecpu(unsigned *matrix, unsigned *result,
                  unsigned matrixsize) {
  for (unsigned ii = 0; ii < matrixsize; ++ii) {
  for (unsigned jj = 0; jj < matrixsize; ++jj) {
     for (unsigned kk = 0; kk < matrixsize; ++kk) {
        result[ii * matrixsize + ji] +=
          matrix[ii * matrixsize + kk] * matrix[kk * matrixsize + ii];
```

Matrix Squaring (version 1)

```
square<<<1, N>>>(matrix, result, N); // N = 64
```

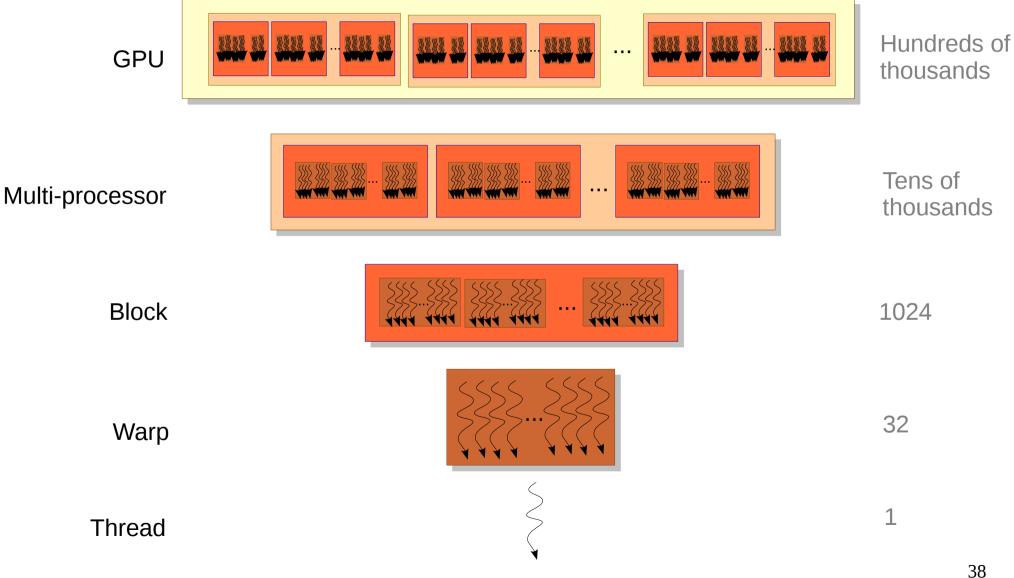
```
global void square(unsigned *matrix,
                       unsigned *result,
                       unsigned matrixsize) {
  unsigned id = blockIdx.x * blockDim.x + threadIdx.x;
  for (unsigned ii = 0; ii < matrixsize; ++ii) {
       for (unsigned kk = 0; kk < matrixsize; ++kk) {
             result[id * matrixsize + jj] +=
                       matrix[id * matrixsize + kk] *
                       matrix[kk * matrixsize + jj];
```

Matrix Squaring (version 2)

```
square<<<N, N>>>(matrix, result, N); // N = 64
```

```
global void square(unsigned *matrix,
                       unsigned *result,
                       unsigned matrixsize) {
  unsigned id = blockIdx.x * blockDim.x + threadIdx.x;
  unsigned ii = id / matrixsize;
                                       Homework: What if you
                                       interchange ii and jj?
  unsigned jj = id % matrixsize;
  for (unsigned kk = 0; kk < matrixsize; ++kk) {
    result[ii * matrixsize + jj] += matrix[ii * matrixsize + kk] *
                                  matrix[kk * matrixsize + jj];
```

GPU Computation Hierarchy



What is a Warp?



Warp

- A set of consecutive threads (currently 32) that execute in SIMD fashion.
- SIMD == Single Instruction Multiple Data
- Warp-threads are fully synchronized. There is an implicit barrier after each step / instruction.
- Memory coalescing is closely related to warps.

Takeaway

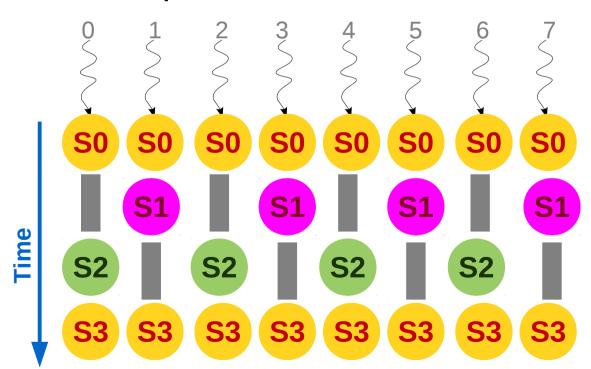
It is a misconception that all threads in a GPU execute in lock-step. Lock-step execution is true for threads only within a warp.

Warp with Conditions

```
global void dkernel(unsigned *vector, unsigned vectorsize)
     unsigned id = blockldx.x * blockDim.x + threadIdx.x; S0
     if (id % 2) vector[id] = id; S1
     else vector[id] = vectorsize * vectorsize; S2
     vector[id]++; S3
                      S0
        S0
             S0
    S0
                 S0
                          S0
                               S0
                                    S0
                                                           NOP
        S1
                                    S1
                 S1
                          S1
Time
    S2
             S2
                      S2
                               S2
                                                                  41
                      S3
```

Warp with Conditions

- When different warp-threads execute different instructions, threads are said to diverge.
- Hardware executes threads satisfying same condition together, ensuring that other threads execute a no-op.
- This adds sequentiality to the execution.
- This problem is termed as thread-divergence.



Degree of Divergence

- DoD for a warp is the number of steps required to complete one instruction for each thread in the warp.
- Without any thread-divergence, DoD = 1.
- For fully divergent code, DoD = 32.
- Classwork: Write a code to achieve DoD = 4.

Thread-Divergence

```
global void dkernel(unsigned *vector, unsigned vectorsize) {
   unsigned id = blockldx.x * blockDim.x + threadldx.x;
   switch (id) {
   case 0: vector[id] = 0;
                                             break;
   case 1: vector[id] = vector[id];
                                             break:
   case 2: vector[id] = vector[id - 2];
                                             break;
   case 3: vector[id] = vector[id + 3];
                                             break;
   case 4: vector[id] = 4 + 4 + vector[id];
                                             break;
   case 5: vector[id] = 5 - vector[id];
                                             break;
   case 6: vector[id] = vector[6];
                                             break;
   case 7: vector[id] = 7 + 7;
                                             break;
   case 8: vector[id] = vector[id] + 8;
                                             break;
   case 9: vector[id] = vector[id] * 9;
                                             break;
```

What is this code's Degree of Divergence?

Thread-Divergence

 Since thread-divergence makes execution sequential, conditions are evil in the kernel codes?

```
if (vectorsize < N) S1; else S2; Condition but no divergence
```

 Then, conditions evaluating to different truth-values are evil?

```
if (id / 32) S1; else S2;
```

Different truth-values but no divergence

Takeaway

Conditions are not bad; they evaluating to different truth-values is also not bad; they evaluating to different truth-values for warp-threads is bad.

Classwork

 Rewrite the following program fragment to remove thread-divergence.

```
// assert(x == y || x == z);
if (x == y) x = z;
else x = y;
```

Classwork

- Find the maximum in a large array as follows:
 - Let the array have N elements.
 - Launch a kernel with N/K threads.
 - Each thread finds the maximum among K elements.
 - The K elements are written to same or different array.
 - The same kernel is launched with K threads to find the final maximum.
- Find an element in parallel.
 - Return its index.

Homework

- Write kernels to encrypt and decrypt messages.
 Assume that the message contains only a..z.
 - *Encrypt*: each character c becomes c+1. z becomes a.
 - Encrypt: each ith character c becomes c+i.
- Parallelize run-length-encoding to compress data.
 - e.g., if input is 000110100010001111011101100001 then the output is 032113134131131. The initial bit is same as input, followed by frequencies of that bit and its negation.
 - For the same input, another compression output is 4271111154213261301. This stores index and frequency.