Introduction to CUDA

1. Our first GPU Program
   - running Newton's method in complex arithmetic
   - examining the CUDA Compute Capability
2. CUDA Program Structure
   - steps to write code for the GPU
   - code to compute complex roots
   - the kernel function and main program
   - a scalable programming model
3. using CUDA.jl
   - vector addition with thread organization

MCS 572 Lecture 18
Introduction to Supercomputing
Jan Verschelde, 7 October 2024

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computing complex square roots

To compute $\sqrt{c}$ for $c \in \mathbb{C}$,
we apply Newton's method on $x^2 - c = 0$:

$$x_0 := c, \quad x_{k+1} := x_k - \frac{x_k^2 - c}{2x_k}, \quad k = 0, 1, \ldots$$

Five iterations suffice to obtain an accurate value for $\sqrt{c}$.

Suitable on GPU?

- Finding roots is relevant for scientific computing.
- Data parallelism: compute for many different c's.

Application: complex root finder for polynomials in one variable.

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CUDA Compute Capability

The compute capability of an NVIDIA GPU

- is represented by a version number in the format x.y,
- identifies the features supported by the hardware.

What does it mean for the programmer? Some examples:

1.3 : double-precision floating-point operations
2.0 : synchronizing threads
3.5 : dynamic parallelism
5.3 : half-precision floating-point operations
6.0 : atomic addition operation on 64-bit floats
8.0 : tensor cores supporting double float precision

The compute capability is not the same as the CUDA version.

checking the card with deviceQuery on pascal

```
$ /usr/local/cuda/samples/1_Utilities/deviceQuery/deviceQuery
/usr/local/cuda/samples/1_Utilities/deviceQuery/deviceQuery Starting...

 CUDA Device Query (Runtime API) version (CUDART static linking)

Detected 2 CUDA Capable device(s)

Device 0: "Tesla P100-PCIE-16GB"
  CUDA Driver Version / Runtime Version          11.0 / 8.0
  CUDA Capability Major/Minor version number:    6.0
  Total amount of global memory:                 16276 MBytes (17066885120 bytes)
  (56) Multiprocessors, ( 64) CUDA Cores/MP:     3584 CUDA Cores
  GPU Max Clock rate:                            405 MHz (0.41 GHz)
  Memory Clock rate:                             715 Mhz
  Memory Bus Width:                              4096-bit
  L2 Cache Size:                                 4194304 bytes
  Maximum Texture Dimension Size (x,y,z)         1D=(131072), 2D=(131072, 65536), 3D=(16384, 16384, 16384)
  Maximum Layered 1D Texture Size, (num) layers  1D=(32768), 2048 layers
  Maximum Layered 2D Texture Size, (num) layers  2D=(32768, 32768), 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 2 copy engine(s)
  Run time limit on kernels:                     No
  Integrated GPU sharing Host Memory:            No
  Support host page-locked memory mapping:       Yes
  Alignment requirement for Surfaces:            Yes
  Device has ECC support:                        Enabled
  Device supports Unified Addressing (UVA):      Yes
  Device PCI Domain ID / Bus ID / location ID:   0 / 2 / 0
  Compute Mode:
     < Default (multiple host threads can use ::cudaSetDevice() with device simultaneously) >
```

running bandwidthTest on pascal

```
$ /usr/local/cuda/samples/1_Utilities/bandwidthTest/bandwidthTest
[CUDA Bandwidth Test] - Starting...
Running on...

 Device 0: Tesla P100-PCIE-16GB
 Quick Mode

 Host to Device Bandwidth, 1 Device(s)
 PINNED Memory Transfers
   Transfer Size (Bytes) Bandwidth(MB/s)
   33554432 11530.1

 Device to Host Bandwidth, 1 Device(s)
 PINNED Memory Transfers
   Transfer Size (Bytes) Bandwidth(MB/s)
   33554432 12848.3

 Device to Device Bandwidth, 1 Device(s)
 PINNED Memory Transfers
   Transfer Size (Bytes) Bandwidth(MB/s)
   33554432 444598.8

Result = PASS

$
```

checking the card with deviceQuery on ampere

```
$ /usr/local/cuda/samples/bin/x86_64/linux/release/deviceQuery
/usr/local/cuda/samples/bin/x86_64/linux/release/deviceQuery Starting...

 CUDA Device Query (Runtime API) version (CUDART static linking)

Detected 1 CUDA Capable device(s)

Device 0: "NVIDIA A100 80GB PCIe"
  CUDA Driver Version / Runtime Version          12.4 / 12.4
  CUDA Capability Major/Minor version number:    8.0
  Total amount of global memory:                 81038 MBytes (84974239744 bytes)
  (108) Multiprocessors, (064) CUDA Cores/MP:    6912 CUDA Cores
  GPU Max Clock rate:                            1410 MHz (1.41 GHz)
  Memory Clock rate:                             1512 Mhz
  Memory Bus Width:                              5120-bit
  L2 Cache Size:                                 41943040 bytes
  Maximum Texture Dimension Size (x,y,z)         1D=(131072), 2D=(131072, 65536), 3D=(16384, 16384, 16384)
  Maximum Layered 1D Texture Size, (num) layers  1D=(32768), 2048 layers
  Maximum Layered 2D Texture Size, (num) layers  2D=(32768, 32768), 2048 layers
  Total amount of constant memory:               65536 bytes
  Total amount of shared memory per block:       49152 bytes
  Total shared memory per multiprocessor:        167936 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 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:                        Enabled
  Device supports Unified Addressing (UVA):      Yes
  Device supports Managed Memory:                Yes
  Device supports Compute Preemption:            Yes
  Supports Cooperative Kernel Launch:            Yes
  Supports MultiDevice Co-op Kernel Launch:      Yes
  Device PCI Domain ID / Bus ID / location ID:   0 / 202 / 0
  Compute Mode:
     < Default (multiple host threads can use ::cudaSetDevice() with device
simultaneously) >

deviceQuery, CUDA Driver = CUDART, CUDA Driver Version = 12.4, CUDA Runtime
Version = 12.4, NumDevs = 1
Result = PASS
```

running bandwidthTest on ampere

```
$ /usr/local/cuda/samples/bin/x86_64/linux/release/bandwidthTest
[CUDA Bandwidth Test] - Starting...
Running on...

 Device 0: NVIDIA A100 80GB PCIe
 Quick Mode

 Host to Device Bandwidth, 1 Device(s)
 PINNED Memory Transfers
   Transfer Size (Bytes)        Bandwidth(GB/s)
   32000000                     25.2

 Device to Host Bandwidth, 1 Device(s)
 PINNED Memory Transfers
   Transfer Size (Bytes)        Bandwidth(GB/s)
   32000000                     26.3

 Device to Device Bandwidth, 1 Device(s)
 PINNED Memory Transfers
   Transfer Size (Bytes)        Bandwidth(GB/s)
   32000000                     1313.8

Result = PASS

$
```

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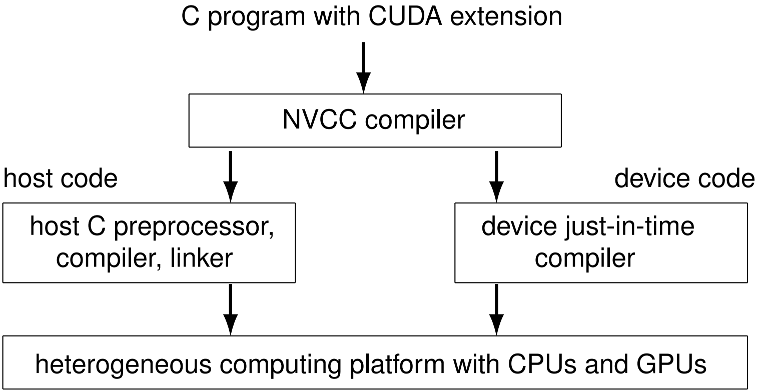
steps to write code for the GPU

Five steps to get GPU code running:

1. C and C++ functions are labeled with CUDA keywords `__device__`, `__global__`, or `__host__`.
2. Determine the data for each thread to work on.
3. Transferring data from/to host (CPU) to/from the device (GPU).
4. Statements to launch data-parallel functions, called *kernels*.
5. Compilation with `nvcc`.

the NVCC compilation process



step 1: CUDA extensions to functions

Three keywords before a function declaration:

`__host__` : The function will run on the host (CPU).

`__device__` : The function will run on the device (GPU).

`__global__` : The function is called from the host but runs on the device. This function is called a *kernel*.

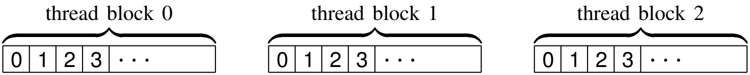
CUDA extensions to C function declarations:

	executed on	callable from
`__device__ double D()`	device	device
`__global__ void K()`	device	host
`__host__ int H()`	host	host

step 2: data for each thread

The grid consists of N blocks, with `blockIdx.x` $\in \{0, N-1\}$.

Within each block, `threadIdx.x` $\in \{0,$ `blockDim.x` $- 1\}$.




```
int threadId = blockIdx.x *
    blockDim.x + threadIdx.x
...
float x = input[threadID]
float y = f(x)
output[threadID] = y
...
```

step 3: allocating and transferring data

```
cudaDoubleComplex *xhost = new cudaDoubleComplex[n];

// we copy n complex numbers to the device
size_t s = n*sizeof(cudaDoubleComplex);
cudaDoubleComplex *xdevice;
cudaMalloc((void**)&xdevice,s);

cudaMemcpy(xdevice,xhost,s,cudaMemcpyHostToDevice);

// allocate memory for the result
cudaDoubleComplex *ydevice;
cudaMalloc((void**)&ydevice,s);

// copy results from device to host
cudaDoubleComplex *yhost = new cudaDoubleComplex[n];

cudaMemcpy(yhost,ydevice,s,cudaMemcpyDeviceToHost);
```

step 4: launching the kernel

The kernel is declared as

```
__global__ void squareRoot
 ( int n, cudaDoubleComplex *x, cudaDoubleComplex *y )
// Applies Newton's method to compute the square root
// of the n numbers in x and places the results in y.
{
   int i = blockIdx.x*blockDim.x + threadIdx.x;
   ...
```

For frequency `f`, dimension `n`, and block size `w`, we do:

```
// invoke the kernel with n/w blocks per grid
// and w threads per block
for(int i=0; i<f; i++)
   squareRoot<<<n/w,w>>>(n,xdevice,ydevice);
```

step 5: compiling with `nvcc`

If the `makefile` contains

```
runCudaComplexSqrt:
        nvcc -ccbin /usr/bin/gcc -o run_cmpsqrt \
                runCudaComplexSqrt.cu
```

typing `make runCudaComplexSqrt` at the command prompt does

```
nvcc -ccbin /usr/bin/gcc -o run_cmpsqrt runCudaComplexSqrt.cu
```

With `-ccbin` we define the location of the C compiler.

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defining complex numbers

```
#ifndef __CUDADOUBLECOMPLEX_CU__
#define __CUDADOUBLECOMPLEX_CU__

#include <cmath>
#include <cstdlib>
#include <iomanip>
#include <vector_types.h>
#include <math_functions.h>

typedef double2 cudaDoubleComplex;
```

We use the `double2` of `vector_types.h` to define complex numbers because `double2` is a native CUDA type allowing for coalesced memory access.

random complex numbers

```
__host__ cudaDoubleComplex randomDoubleComplex()
// Returns a complex number on the unit circle
// with angle uniformly generated in [0,2*pi].
{
   cudaDoubleComplex result;
   int r = rand();
   double u = double(r)/RAND_MAX;
   double angle = 2.0*M_PI*u;
   result.x = cos(angle);
   result.y = sin(angle);
   return result;
}
```

calling sqrt of math_functions.h

```
__device__ double radius ( const cudaDoubleComplex c )
// Returns the radius of the complex number.
{
   double result;
   result = c.x*c.x + c.y*c.y;
   return sqrt(result);
}
```

overloading for output

```
__host__ std::ostream& operator<<
 ( std::ostream& os, const cudaDoubleComplex& c)
// Writes real and imaginary parts of c,
// in scientific notation with precision 16.
{
   os << std::scientific << std::setprecision(16)
      << c.x << "  " << c.y;
   return os;
}
```

defining complex addition

```
__device__ cudaDoubleComplex operator+
 ( const cudaDoubleComplex a, const cudaDoubleComplex b )
// Returns the sum of a and b.
{
   cudaDoubleComplex result;
   result.x = a.x + b.x;
   result.y = a.y + b.y;
   return result;
}
```

The rest of the arithmetical operations are defined in a similar manner.

All definitions related to complex numbers are stored in the file `cudaDoubleComplex.cu`.

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the kernel function

```
#include "cudaDoubleComplex.cu"

__global__ void squareRoot
 ( int n, cudaDoubleComplex *x, cudaDoubleComplex *y )
// Applies Newton's method to compute the square root
// of the n numbers in x and places the results in y.
{
   int i = blockIdx.x*blockDim.x + threadIdx.x;
   cudaDoubleComplex inc;
   cudaDoubleComplex c = x[i];
   cudaDoubleComplex r = c;
   for(int j=0; j<5; j++)
   {
      inc = r + r;
      inc = (r*r - c)/inc;
      r = r - inc;
   }
   y[i] = r;
}
```

the main function — command line arguments

```
int main ( int argc, char*argv[] )
{
   if(argc < 5)
   {
      cout << "call with 4 arguments : " << endl;
      cout << "dimension, block size, frequency, and check (0 or 1)"
           << endl;
   }
   else
   {
      int n = atoi(argv[1]); // dimension
      int w = atoi(argv[2]); // block size
      int f = atoi(argv[3]); // frequency
      int t = atoi(argv[4]); // test or not
      // we generate n random complex numbers on the host
      cudaDoubleComplex *xhost = new cudaDoubleComplex[n];
      for(int i=0; i<n; i++) xhost[i] = randomDoubleComplex();
```

The main program generates `n` random complex numbers with radius 1.

transferring data and launching the kernel

```
// copy the n random complex numbers to the device
size_t s = n*sizeof(cudaDoubleComplex);
cudaDoubleComplex *xdevice;
cudaMalloc((void**)&xdevice,s);
cudaMemcpy(xdevice,xhost,s,cudaMemcpyHostToDevice);
// allocate memory for the result
cudaDoubleComplex *ydevice;
cudaMalloc((void**)&ydevice,s);
// invoke the kernel with n/w blocks per grid
// and w threads per block
for(int i=0; i<f; i++)
   squareRoot<<<n/w,w>>>(n,xdevice,ydevice);
// copy results from device to host
cudaDoubleComplex *yhost = new cudaDoubleComplex[n];
cudaMemcpy(yhost,ydevice,s,cudaMemcpyDeviceToHost);
```

testing one random number

```
      if(t == 1) // test the result
      {
         int k = rand() % n;
         cout << "testing number " <<  k << endl;
         cout << "          x = " << xhost[k] << endl;
         cout << "  sqrt(x) = " << yhost[k] << endl;
         cudaDoubleComplex z = Square(yhost[k]);
         cout << "sqrt(x)^2 = " << z << endl;
      }
   }
   return 0;
}
```

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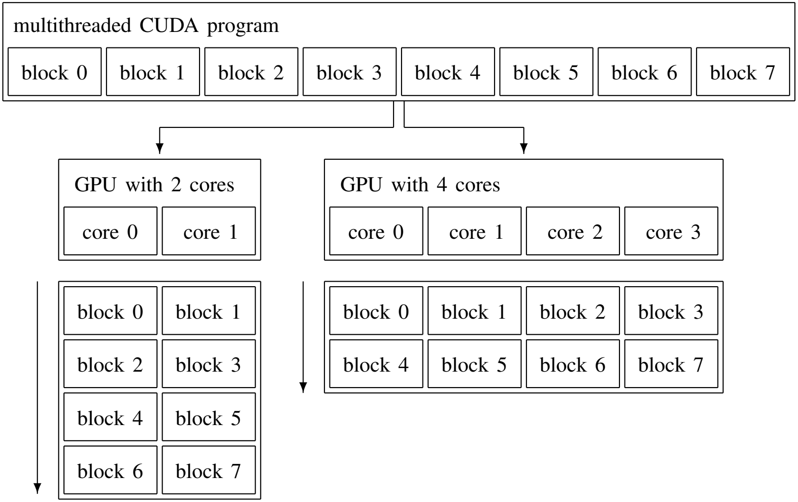
a scalable programming model



running the code on pascal

A test on the correctness:

```
$ ./run_cmpsqrt 1 1 1 1
testing number 0
        x = 5.368222744694973 7e-01  -8.436953511981654 1e-01
  sqrt(x) = 8.765906326414563 1e-01  -4.812368052895074 6e-01
sqrt(x)^2 = 5.368222744694972 6e-01  -8.436953511981653 0e-01
```

On 64,000 numbers, 32 threads in a block, doing it 10,000 times:

```
$ time ./run_cmpsqrt 64000 32 10000 1
testing number 50325
        x = 7.951060650972877 6e-01  -6.064703993151747 7e-01
  sqrt(x) = 9.473927551700211 9e-01  -3.200733782296742 4e-01
sqrt(x)^2 = 7.951060650972876 5e-01  -6.064703993151747 7e-01

real    0m0.302s
user    0m0.095s
sys     0m0.207s
$
```

changing #threads in a block

```
$ time ./run_cmpsqrt 128000 32 100000 0

real    0m1.639s
user    0m0.989s
sys     0m0.650s

$ time ./run_cmpsqrt 128000 64 100000 0

real    0m1.640s
user    0m1.001s
sys     0m0.639s

$ time ./run_cmpsqrt 128000 128 100000 0

real    0m1.652s
user    0m0.952s
sys     0m0.700s
```

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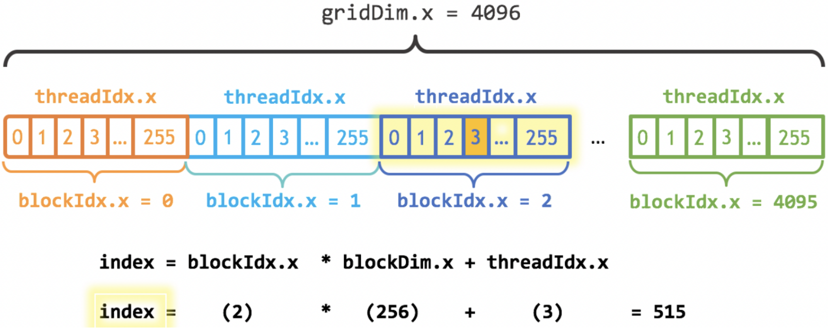
division of the work per thread

From the CUDA.jl tutorial:



Which is taken from the technical blog at
https://developer.nvidia.com/blog/even-easier-introduction-cuda
An Even Easier Introduction to CUDA, by Mark Harris.

copied from the CUDA.jl tutorial

https://cuda.juliagpu.org/stable/tutorials/introduction

```
using CUDA
using Test

function gpu_add3!(y, x)
    index = (blockIdx().x - 1) * blockDim().x
          + threadIdx().x
    stride = gridDim().x * blockDim().x
    for i = index:stride:length(y)
        @inbounds y[i] += x[i]
    end
    return
end
```

launching the kernel with 256 threads per block

```
N = 2^20
x_d = CUDA.fill(1.0f0, N) # N Float32 1.0 on GPU
y_d = CUDA.fill(2.0f0, N) # N Float32 2.0

# run with 256 threads per block

numblocks = ceil(Int, N/256)
@cuda threads=256 blocks=numblocks gpu_add3!(y_d, x_d)
result = (@test all(Array(y_d) .== 3.0f0))

println(result)
```

prints `Test Passed`

summary and references

In five steps we wrote our first complete CUDA program in C.

We started chapter 3 of the textbook by Kirk & Hwu,
covering more of the CUDA Programming Guide.

Available in `/usr/local/cuda/doc` are

- CUDA C Best Practices Guide
- CUDA Programming Guide

Also available online at nvidia.com.

Many examples of CUDA applications are available in
`/usr/local/cuda/samples`.

Julia solves the two languages problem.

exercises

1. Instead of 5 Newton iterations in `runCudaComplexSqrt.cu` use `k` iterations where `k` is entered by the user at the command line. What is the influence of `k` on the timings?
2. Modify the kernel for the complex square root so it takes on input an array of complex coefficients of a polynomial of degree d. Then the root finder applies Newton's method, starting at random points. Test the correctness and experiment to find the rate of success, i.e.: for polynomials of degree d how many random trials are needed to obtain $d/2$ roots of the polynomial?
3. Use the kernel in a python script with PyCUDA.
4. Use CUDA.jl (or Metal.jl, oneAPI.jl, AMDGPU.jl on your GPU) for the square roots example.