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

MCS 572 Lecture 30
Introduction to Supercomputing
Jan Verschelde, 31 October 2016

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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

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

checking the card with deviceQuery on kepler

```
$ /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 3 CUDA Capable device(s)

Device 0: "Tesla K20c"
  CUDA Driver Version / Runtime Version          6.0 / 5.5
  CUDA Capability Major/Minor version number:    3.5
  Total amount of global memory:                 4800 MBytes (5032706048 bytes)
  (13) Multiprocessors, (192) CUDA Cores/MP:     2496 CUDA Cores
  GPU Clock rate:                                706 MHz (0.71 GHz)
  Memory Clock rate:                             2600 Mhz
  Memory Bus Width:                              320-bit
  L2 Cache Size:                                 1310720 bytes
  Maximum Texture Dimension Size (x,y,z)         1D=(65536), 2D=(65536, 65536), 3D=(4096, 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 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 Bus ID / PCI location ID:           4 / 0
  Compute Mode:
     < Default (multiple host threads can use ::cudaSetDevice() with device simultaneously) >
```

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          8.0 / 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 kepler

```
$ /usr/local/cuda/samples/1_Utilities/bandwidthTest/bandwidthTest

[CUDA Bandwidth Test] - Starting...
Running on...

 Device 0: Tesla K20c
 Quick Mode

 Host to Device Bandwidth, 1 Device(s)
 PINNED Memory Transfers
   Transfer Size (Bytes) Bandwidth(MB/s)
   33554432 5819.5

 Device to Host Bandwidth, 1 Device(s)
 PINNED Memory Transfers
   Transfer Size (Bytes) Bandwidth(MB/s)
   33554432 6415.8

 Device to Device Bandwidth, 1 Device(s)
 PINNED Memory Transfers
   Transfer Size (Bytes) Bandwidth(MB/s)
   33554432 143248.0

Result = PASS
```

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

$
```

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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`.

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*.

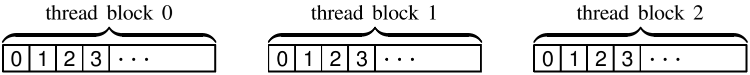
CUDA extensions to C function declarations:

	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`

Then if the `makefile` contains

```
runCudaComplexSqrt:
        nvcc -o /tmp/run_cmpsqrt -arch=sm_13 \
                runCudaComplexSqrt.cu
```

typing `make runCudaComplexSqrt` does

```
nvcc -o /tmp/run_cmpsqrt -arch=sm_13 runCudaComplexSqrt.cu
```

The `-arch=sm_13` is needed for `double` arithmetic, for the K20C.

The option `-arch=sm_13` is no longer recognized on the new P100.

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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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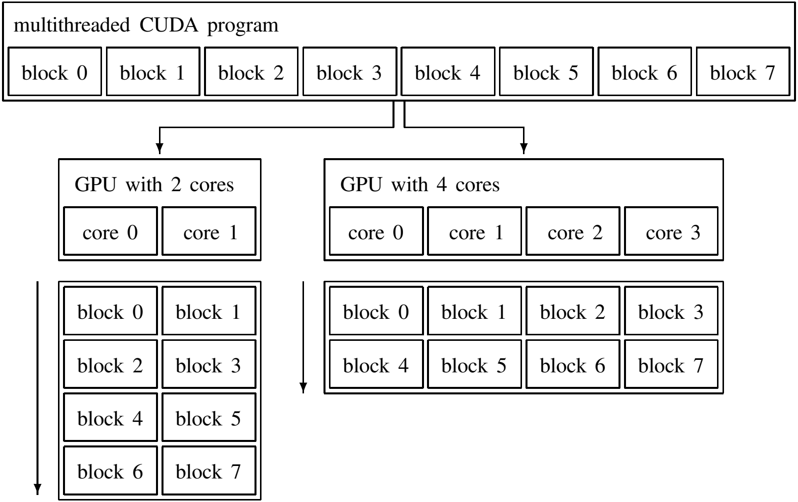
a scalable programming model



running the code on kepler

A test on the correctness:

```
$ /tmp/run_cmpsqrt 1 1 1 1
testing number 0
        x = 5.3682227446949737e-01  -8.4369535119816541e-01
  sqrt(x) = 8.7659063264145631e-01  -4.8123680528950746e-01
sqrt(x)^2 = 5.3682227446949726e-01  -8.4369535119816530e-01
```

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

```
$ time /tmp/run_cmpsqrt 64000 32 10000 1
testing number 50325
        x = 7.9510606509728776e-01  -6.0647039931517477e-01
  sqrt(x) = 9.4739275517002119e-01  -3.2007337822967424e-01
sqrt(x)^2 = 7.9510606509728765e-01  -6.0647039931517477e-01

real    0m1.618s
user    0m0.526s
sys     0m0.841s
$
```

changing #threads in a block

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

real    0m17.345s
user    0m9.829s
sys     0m7.303s

$ time /tmp/run_cmpsqrt 128000 64 100000 0

real    0m10.502s
user    0m5.711s
sys     0m4.497s

$ time /tmp/run_cmpsqrt 128000 128 100000 0

real    0m9.295s
user    0m5.231s
sys     0m3.865s
```

running the code on pascal

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

real    0m2.516s
user    0m1.250s
sys     0m1.236s

$ time /tmp/run_cmpsqrt 128000 64 100000 0

real    0m2.521s
user    0m1.245s
sys     0m1.234s

$ time /tmp/run_cmpsqrt 128000 128 100000 0

real    0m2.496s
user    0m1.288s
sys     0m1.195s
```

summary and references

In five steps we wrote our first complete CUDA program.

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 nvdia.com.

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

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?