CUDA Libraries & OpenCL

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Contents

Objectives

- Know the existing CUDA libraries
  - Math, Vision, Helpers,
  - Scope and lifetime
- OpenCL
  - CUDA equivalents of OpenCL functions
- Thrust C++ template library
  - Common data types & functions

CUDA Libraries

- Originally, NVIDIA planned to provide only one or two maths libraries, but over time these have steadily increased
- CUDA math library all of the standard math functions you would expect (i.e. very similar to what you would get from Intel)
  - various exponential and log functions
  - trigonometric functions and their inverses
  - error functions and their inverses
  - vector norms and reciprocals (esp. for graphics)
  - mainly single and double precision; a few in half precision
  - …

CUDA Libraries

cuBLAS

- Basic linear algebra subroutines for dense matrices various exponential and log functions
- Includes matrix-vector and matrix-matrix product
- It is possible to call cuBLAS routines from user kernels
- Support for using CUDA streams to do a large number of small tasks concurrently
- cuBLAS is a set of routines to be called by user host code:
  - memory allocation
  - Data copying CPU-GPU
  - Error reporting
  - Matrix-matrix product
  - Matrix-vector product
- simpleCUBLAS example in SDK is a good example code to start using it

CUDA Libraries

cuFFT

- Fast Fourier Transform
- 1D, 2D, 3D
- Similar to FFTW and other CPU libraries
- Like cuBLAS, it is a set of routines called by user host code:
  - Compute routines perform 1D, 2D, 3D FFTs
  - It supports doing a “batch” of independent transforms, e.g. applying 1D transform to a 3D dataset
  - simpleCUFFT example in SDK

CUDA Libraries

cuSPARSE

- Various routines to work with sparse matrices
- Includes sparse matrix-vector and matrix-matrix products
- Could be used for iterative solution
- also has solution of sparse triangular system

cuRAND

- Random number generation
- XORWOW, mrg32k3a, Mersenne Twister and Philox 4x32 10 pseudo-random generators
- Uniform, Normal, log-Normal, Poisson outputs
- Sobol quasi-random generator (with optimal scrambling)

CUDA Libraries

CUB

– Provides a collection of basic building blocks at three levels: device, thread block, warp
– Functions include sort, scan, reduction
– Thrust uses CUB for CUDA version of key algorithms

cuDNN

– library for Deep Neural Networks
– Used by most DL libraries: Tensorflow, Caffee, Torch, …

nvGraph

– Page Rank, Single Source Shortest Path, Single Source Widest Path

NPP (NVIDIA Performance Primitives)

– library for imaging and video processing
– Includes functions for filtering, JPEG decoding, etc.

CUDA Video Decoder API

CUDA Libraries

NVIDIA maintains webpages with links to a variety of CUDA libraries:
http://developer.nvidia.com/gpu-accelerated-libraries
and other tools:
http://developer.nvidia.com/tools-ecosystem

Applications

Libraries	Compiler Directives	Programming Languages
Easy to use Most Performance	Easy to use Portable code	Most Performance Most Flexibility

Tools

Other languages:

- Fortran: PGI (Portland Group) CUDA FORTRAN compiler with natural FORTRAN equivalent to CUDA C;
- MATLAB: can call kernels directly, or use OOP like Thrust to define MATLAB objects which live on the GPU
- Mathematica: similar to MATLAB
- Python: http://mathema.tician.de/software/pycuda
- C#
- R: http://www.fuzzyl.com/products/gpu-analytics/
- Java
- …

Tools

OpenACC

- Like Thrust, aims to hide CUDA programming by doing everything in the top-level CPU code;
- Programmer takes standard C/C++/Fortran code and inserts pragmas saying what can be done in parallel and where data should be located
- https://www.openacc.org/
- Similar to OpenMP pragmas

OpenMP 4.0:

- strongly pushed by Intel to accommodate Xeon Phi and unify things, in some sense
- http://on-demand.gputechconf.com/gtc/2016/presentation/s6510-jeff-larkin-targeting-gpus-openmp.pdf

OpenCL

- Cross platform for parallel computing on heterogeneous devices
- Ensure proper execution but not max performance on different devices
- There are OpenCL implementations for NVIDIA, AMD GPUs, x86 CPUs, and other devices (FPGAs).
- Support for multiple devices from different manufacturers

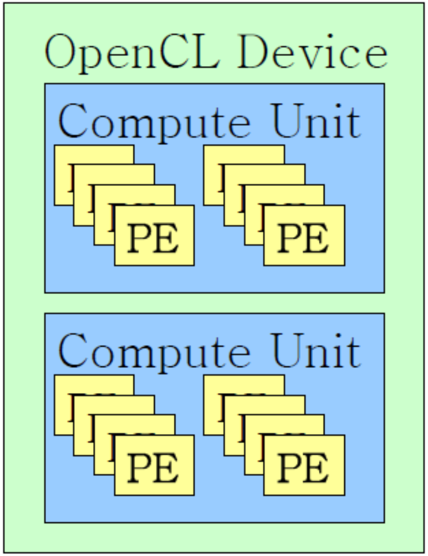
OpenCL

- OpenCV – CUDA concepts

OpenCL Parallelism Concept	CUDA Equivalent
kernel	kernel
host program	host program
NDRange (index space)	grid
work item	thread
work group	block

OpenCL

- OpenCL Hardware abstraction
  - Handles multi-core CPUs, GPUs, and other accelerators as devices
  - Each device contains one or more 'Computing Units'. (SMs)
  - Each 'Computing Unit' contains one or more SIMD processing elements



OpenCL

– OpenCL – CUDA - Memories

OpenCL Memory Types	CUDA Equivalent
global memory	global memory
constant memory	constant memory
local memory	shared memory
private memory	registers

OpenCL

- The code running on accelerator devices is analogous to CUDA kernels

- ```
  __kernel void vadd(__global const float *a,
  __global const float *b, __global float
  *result){
     int id = get_global_id(0);
     result[id] = a[id] + b[id];
  }
  ```

- As in CUDA, each OpenCL work unit gets its own indexes

3DPERCEPTIONLAB
  ```

OpenCL

– List of OpenCL - CUDA dimensions and indexes

OpenCL API Call	Explanation	CUDA Equivalent
get_global_id(0);	global index of the work item in the x dimension	blockIdx.x×blockDim.x+ threadIdx.x
get_local_id(0)	local index of the work item within the work group in the x dimension	threadIdx.x
get_global_size(0);	size of NDRange in the x dimension	gridDim.x × blockDim.x
get_local_size(0);	Size of each work group in the x dimension	blockDim.x

OpenCL

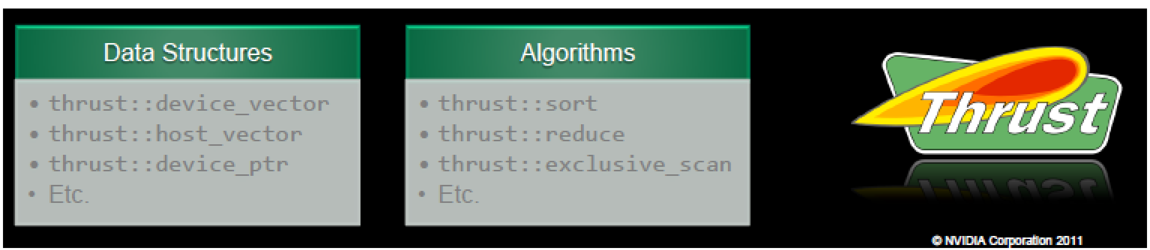
- Conclusions
  - OpenCL intrinsically evolves slower than CUDA
  - Although OpenCL is correct in terms of execution, the performance of one kernel is not guaranteed on different devices
  - Application programming in OpenCL requires more testing than in the CUDA Runtime API
  - In the future it should become the standard for GPU programming

Thrust

- Thrust is a C++ template library for CUDA based on the Standard Template Library (STL)
- Minimal programming effort through a high-level interface that is fully interoperable with CUDA C

```
int main(void)
{
  // generate random data on the host
  thrust::host_vector<int> h_vec(100);
  thrust::generate(h_vec.begin(), h_vec.end(), rand);

  // transfer to device and compute sum
  thrust::device_vector<int> d_vec = h_vec;
  int x = thrust::reduce(d_vec.begin(), d_vec.end(), 0, thrust::plus<int>());
  return 0;
}
```



Thrust

- Data types:
  - Host:
    - thrust::host_vector<int> H(4);
  - Device:
    - thrust::device_vector<int> D(5)

Thrust

- Algorithms:
  - Transformations
    - // fill Z with twos
    - thrust::fill(Z.begin(), Z.end(), 2);
    - // compute Y = X mod 2
    - thrust::transform(X.begin(), X.end(), Z.begin(), Y.begin(), thrust::modulus<int>());
  - Reductions
  - Prefix-Sums
  - Reordering
  - Sorting

Thrust

- Algorithms:
  - Transformations
  - Reductions
    - int sum = thrust::reduce(D.begin(), D.end(), (int) 0, thrust::plus<int>());
  - Prefix-Sums
  - Reordering
  - Sorting

Thrust

- Algorithms:
  - Transformations
  - Reductions
  - Prefix-Sums
    - thrust::inclusive_scan(data, data + 6, data);
    - thrust::exclusive_scan(data, data + 6, data);
  - Reordering
  - Sorting

Thrust

- Algoritmos:
  - Transformations
  - Reductions
  - Prefix-Sums
  - Reordering
    - copy_if : copies only the items that meet the condition
    - partition : sort the elements according to a predicate (true first)
    - remove, remove_if : removes items that do not meet the condition
    - unique: removes consecutive duplicates from a collection
  - Sorting

Thrust

- Algoritmos:
  - Transformations
  - Reductions
  - Prefix-Sums
  - Reordering
  - Sorting
    - thrust::sort(A, A + N);
    - thrust::sort_by_key(keys, keys + N, values);

Thrust

- Iterators: they are useful structures to operate on data and algorithms
  - constant_iterator
    - ```
      thrust::constant_iterator<int> first(10);
      thrust::constant_iterator<int> last = first + 3;

      first[0]   // returns 10
      first[1]   // returns 10
      first[100] // returns 10
      ```
  - counting_iterator
  - transform_iterator
  - permutation_iterator
  - zip_iterator
      ```

Thrust

- Iterators: they are useful structures to operate on data and algorithms
  - constant_iterator
  - counting_iterator
    - ```
      thrust::counting_iterator<int> first(10);
      thrust::counting_iterator<int> last = first + 3;

      first[0]   // returns 10
      first[1]   // returns 11
      first[100] // returns 110
      ```
  - transform_iterator
  - permutation_iterator
  - zip_iterator
      ```

Thrust

- Iterators: they are useful structures to operate on data and algorithms
  - constant_iterator
  - counting_iterator
  - transform_iterator
    - ```
      thrust::device_vector<int> vec(3);
      vec[0] = 10; vec[1] = 20; vec[2] = 30;
      ... first = thrust::make_transform_iterator(vec.begin(), negate<int>());
      ... last  = thrust::make_transform_iterator(vec.end(),   negate<int>());
      first[0]   // returns -10
      first[1]   // returns -20
      first[2]   // returns -30
      ```
  - permutation_iterator
  - zip_iterator
      ```

Thrust

- Iteradores: son estructuras útiles para operar sobre los datos y los algoritmos
  - constant_iterator
  - counting_iterator
  - transform_iterator
  - zip_iterator

```
A[0] = 10;  A[1] = 20;  A[2] = 30;
B[0] = 'x'; B[1] = 'y'; B[2] = 'z';
first = thrust::make_zip_iterator(thrust::make_tuple(A.begin(), B.begin()));
last  = thrust::make_zip_iterator(thrust::make_tuple(A.end(),   B.end()));
first[0]   // returns tuple(10, 'x')
first[1]   // returns tuple(20, 'y')
first[2]   // returns tuple(30, 'z')
// maximum of [first, last)
thrust::maximum< tuple<int,char> > binary_op;
thrust::tuple<int,char> init = first[0];
thrust::reduce(first, last, init, binary_op); // returns tuple(30, 'z')
```

https://github.com/thrust/thrust/wiki/Quick-Start-Guide

```
#include <thrust/host_vector.h>
#include <thrust/device_vector.h>

#include <thrust/copy.h>
#include <thrust/fill.h>
#include <thrust/sequence.h>

#include <iostream>

int main(void)
{
    // initialize all ten integers of a device_vector to 1
    thrust::device_vector<int> D(10, 1);

    // set the first seven elements of a vector to 9
    thrust::fill(D.begin(), D.begin() + 7, 9);

    // initialize a host_vector with the first five elements of D
    thrust::host_vector<int> H(D.begin(), D.begin() + 5);

    // set the elements of H to 0, 1, 2, 3, ...
    thrust::sequence(H.begin(), H.end());

    // copy all of H back to the beginning of D
    thrust::copy(H.begin(), H.end(), D.begin());

    // print D
    for(int i = 0; i < D.size(); i++)
        std::cout << "D[" << i << "] = " << D[i] << std::endl;

    return 0;
}
```

Where To From Here?

- NVIDIA developer blog
  - How to Implement Performance Metrics in CUDA C++
  - How to Query Device Properties and Handle Errors in CUDA C++
  - How to Optimize Data Transfers in CUDA C++
  - How to Overlap Data Transfers in CUDA C++
  - How to Access Global Memory Efficiently in CUDA C++
  - Using Shared Memory in CUDA C++
  - An Efficient Matrix Transpose in CUDA C++
  - Finite Difference Methods in CUDA C++, Part 1
  - Finite Difference Methods in CUDA C++, Part 2

- Online courses on CUDA programming
  - https://www.udacity.com/course/intro-to-parallel-programming--cs344

- Parallel for all blog (Mark Harris, NVIDIA)
  - https://devblogs.nvidia.com/

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Thanks for your attention!

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