Lecture 5: libraries and tools

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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
  - hyperbolic functions and their inverses
  - error functions and their inverses
  - Bessel and Gamma functions
  - 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
  - includes matrix-vector and matrix-matrix product
  - it is possible to call cuBLAS routines from user kernels – device API
  - some support for a single routine call to do a “batch” of smaller matrix-matrix multiplications
  - also support for using CUDA streams to do a large number of small tasks concurrently
  - `simpleCUBLAS` example in Practical 5 – taken from NVIDIA sample codes

CUDA libraries

cuBLAS is a set of routines to be called by user host code:

- helper routines:
  - memory allocation
  - data copying from CPU to GPU, and vice versa
  - error reporting
- compute routines:
  - matrix-matrix and matrix-vector product
  - Warning! Some calls are asynchronous, i.e. the call starts the operation but the host code then continues before it has completed

cuBLASxt extends cuBLAS to multiple GPUs

CUDA libraries

- cuFFT
  - 1D, 2D, 3D Fast Fourier Transform
  - has most variations found in FFTW and elsewhere
  - like cuBLAS, routines called by user host code:
    - helper routines include "plan" construction
    - 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 Practical 5 – taken from NVIDIA sample codes

CUDA libraries

- cuTENSOR
  - tensor linear algebra library
  - makes extensive use of new Tensor Cores
- 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
  - note: batched tridiagonal solver is in cuBLAS not cuSPARSE

CUDA libraries

- cuRAND
  - random number generation
  - XORWOW, `mrg32k3a`, Mersenne Twister and `Philox_4x32_10` pseudo-random generators
  - Sobol quasi-random generator (with optional scrambling)
  - uniform, Normal, log-Normal, Poisson outputs
  - also device level routines for RNG within kernels
- cuSOLVER:
  - key LAPACK dense solvers, 3 – 6x faster than MKL
  - sparse direct solvers, 2–14x faster than CPU
  - latest version uses iterative refinement with low-precision Tensor Core operations

CUDA libraries

- CUB
  - collection of basic building blocks (e.g. sort, scan, reduction) at three levels: device, thread block, warp
  - available from `github.com/NVIDIA/cub`
- CUTLASS (CUDA Templates for Linear Algebra Subroutines)
  - collection of CUDA C++ template abstractions for implementing matrix-multiplication (GEMM)
  - available from `github.com/NVIDIA/cutlass`
- AmgX
  - library for algebraic multigrid
  - available from `developer.nvidia.com/amgx`

CUDA Libraries

- NCCL
  - NVIDIA Collective Communications Library
  - multi-GPU over both PCIe and NVlink
  - multi-node over NVIDIA/Mellanox NICs
- cuDNN
  - library for Deep Neural Networks
- 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 Libraries

- Thrust
  - high-level C++ template library with an interface based on the C++ Standard Template Library (STL)
  - very different philosophy to other libraries; users write standard C++ code (no CUDA) but get the benefits of GPU parallelisation
  - also supports x86 execution
  - relies on C++ object-oriented programming; certain objects exist on the GPU, and operations involving them are implicitly performed on the GPU
  - I've not used it, but for some applications it can be very powerful – e.g. lots of built-in functions for operations like sort and scan
  - also simplifies memory management and data movement

CUDA Libraries

- Kokkos
  - another high-level C++ template library
  - developed in the US DoE Labs, so considerable investment in both capabilities and on-going software maintenance
  - again I've not used it, but possibly worth investigating
  - for more information see
    `https://github.com/kokkos/kokkos/wiki`
    `https://trilinos.org/packages/kokkos/`

Useful header files

- `dbldbl.h` available from
  `https://gist.github.com/seibert/5914108`
  Header file for double-double arithmetic for quad-precision (developed by NVIDIA, but published independently under the terms of the BSD license)
- `cuComplex.h` part of the standard CUDA distribution
  Header file for complex arithmetic – defines a class and overloaded arithmetic operations.
- `helper_math.h` available with NVIDIA sample codes
  Defines operator-overloading operations for CUDA intrinsic vector datatypes such as `float4`

Other libraries

- MAGMA
  - a new LAPACK for GPUs – higher level numerical linear algebra, layered on top of CUBLAS
  - open source – freely available from `https://icl.utk.edu/magma/`
  - developed by Jack Dongarra, Jim Demmel and others

Other libraries

- ArrayFire from Accelereyes:
  - was commercial software, but now open source
  - supports both CUDA and OpenCL execution
  - C, C++ and Fortran interfaces
  - wide range of functionality including linear algebra, image and signal processing, random number generation, sorting
  - `www.accelereyes.com/products/arrayfire`

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

The 7 dwarfs

- Phil Colella, senior researcher at Lawrence Berkeley National Laboratory, talked about “7 dwarfs” of numerical computation in 2004
- expanded to 13 by a group of UC Berkeley professors in a 2006 report: “A View from Berkeley”
  `www.eecs.berkeley.edu/Pubs/TechRpts/2006/EECS-2006-183.pdf`
- key algorithmic kernels in many scientific computing applications
- very helpful to focus attention on HPC challenges and development of libraries and problem-solving environments/frameworks.

The 7 dwarfs

- dense linear algebra
- sparse linear algebra
- spectral methods
- N-body methods
- structured grids
- unstructured grids
- Monte Carlo

Dense linear algebra

- cuBLAS
- cuSOLVER
- CUTLASS
- MAGMA
- ArrayFire

Sparse linear algebra

- iterative solvers:
  - some available in PetSc
  - others can be implemented using sparse matrix-vector multiplication from cuSPARSE
  - NVIDIA has AmgX, an algebraic multigrid library
- direct solvers:
  - NVIDIA's cuSOLVER
  - SuperLU and STRUMPACK:

    `https://www.exascaleproject.org/wp-content/uploads/2022/06/LiSherrySparseBofSlides.pdf`

Spectral methods

- cuFFT
  - library provided / maintained by NVIDIA
- nothing else needed?

N-body methods

- OpenMM
  - `http://openmm.org/`
  - open source package to support molecular modelling, developed at Stanford
- Fast multipole methods:
  - ExaFMM by Yokota and Barba:
    `http://www.bu.edu/exafmm/`
    `https://lorenabarba.com/figshare/exafmm-10-years-7-re-writes-the-tortuous-progress-of-computational-research/`
  - FMM2D by Holm, Engblom, Goude, Holmgren:
    `http://user.it.uu.se/~stefane/freeware`
  - software by Takahashi, Cecka, Fong, Darve:
    `onlinelibrary.wiley.com/doi/10.1002/nme.3240/pdf`

Structured grids

- lots of people have developed one-off applications
- no great need for a library for single block codes (though possible improvements from "tiling"?)
- multi-block codes could benefit from a general-purpose library, mainly for MPI communication
- Oxford OPS project has developed a high-level open-source framework for multi-block codes, using GPUs for code execution and MPI for distributed-memory message-passing

  all implementation details are hidden from "users", so they don't have to know about GPU/MPI programming

Unstructured grids

In addition to GPU implementations of specific codes there are projects to create high-level solutions which others can use for their application codes:

- Alonso, Darve and others (Stanford)
- Oxford / Imperial College project developed OP2, a general-purpose open-source framework based on a previous framework built on MPI

  See `https://op-dsl.github.io/` for both OPS and OP2

Monte Carlo

- NVIDIA cuRAND library
- some use examples among NVIDIA sample codes
- Accelereyes ArrayFire library
- nothing else needed except for more output distributions?

Tools

Debugging using NVIDIA Compute Sanitizer:

- `compute-sanitizer --tool memcheck`
  detects array out-of-bounds errors, and mis-aligned device memory accesses
- `compute-sanitizer --tool racecheck`
  checks for shared memory race conditions:
  - Write-After-Write (WAW): two threads write data to the same memory location but the order is uncertain
  - Read-After-Write (RAW), Write-After-Read (WAR): one thread writes & one reads, with uncertain order
- `compute-sanitizer --tool initcheck`
  detects reading of uninitialised device memory
- `compute-sanitizer --tool synccheck`
  detects incorrect use of `__syncthreads` and related intrinsics

Tools

Other languages:

- CUDA Fortran: available from NVIDIA
- Python:
  `https://developer.nvidia.com/cuda-python`
  `https://numba.pydata.org/`
- MATLAB: can call kernels directly, or use OOP like Thrust to define MATLAB objects which live on the GPU
  `https://www.mathworks.com/solutions/gpu-computing.html`
- Mathematica: similar to MATLAB?
  `https://reference.wolfram.com/language/CUDALink/tutorial/Overview.html`
- R:
  `https://developer.nvidia.com/blog/accelerate-r-applications-cuda/`
  `http://www.r-tutor.com/gpu-computing`

Tools

OpenACC ("More Science, Less Programming"):

- 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/`

OpenMP 5.0 is similar but newer:

- strongly pushed by Intel to accommodate Xeon Phi and unify things, in some sense
- `https://www.openmp.org/wp-content/uploads/20210924-OpenMP-update-for-DOE.pdf`

Tools

Integrated Development Environments (IDE):

- Nsight Visual Studio edition – NVIDIA plug-in for Microsoft Visual Studio
  `developer.nvidia.com/nsight-visual-studio-edition`
- Nsight Eclipse edition – IDE for Linux systems (now distributed as plug-ins for standard Eclipse)
  `developer.nvidia.com/nsight-eclipse-edition`
- these come with editor, debugger, profiler integration

Tools

NVIDIA Nsight Compute CLI profiler `ncu`:

- standalone software for Linux and Windows systems
- uses hardware counters to collect a lot of useful information
- I think only 1 SM is instrumented – implicitly assumes the others are behaving similarly
- lots of things can be measured, but a limited number of counters, so it runs the application multiple times if necessary to get full info
- see practical 3 for an example of its use
- can also visualise output using `ncu-ui`
  `https://docs.nvidia.com/nsight-compute/NsightCompute/index.html`

Tools

GPU Direct:

- webpage:
  `https://developer.nvidia.com/gpudirect`
- software support for direct data transfers from one GPU to another
- works across PCIe within a single machine
- works across PCIe-connected network adapters between different systems
- includes capabilities to work with cameras and other video input devices (e.g. for self-driving cars)
- very important in applications which might otherwise be limited by PCIe bandwidth

Summary

- active work on all of the dwarfs
- in most cases, significant effort to develop general purpose libraries or frameworks, to enable users to get the benefits without being CUDA experts
- too much going on for one person (e.g. me) to keep track of it all
- NVIDIA maintains a webpage with links to CUDA tools/libraries:
  `developer.nvidia.com/cuda-tools-ecosystem`
- the existence of this ecosystem is part of why I think CUDA will remain more used than OpenCL for HPC