programming GPUs in Python and Julia

1. Graphics Processing Units
   - introduction to general purpose GPUs
   - data parallelism
2. PyOpenCL
   - parallel programming of heterogeneous systems
   - matrix matrix multiplication
3. PyCUDA
   - about PyCUDA
   - matrix matrix multiplication
4. CUDA.jl
   - about CUDA.jl
   - a first kernel

MCS 507 Lecture 14
Mathematical, Statistical and Scientific Software
Jan Verschelde, 22 September 2023

GPU Acceleration in Python and Julia

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A Bifurcation in Moore's Law?

by Nick Trefethen SIAM News September 2023

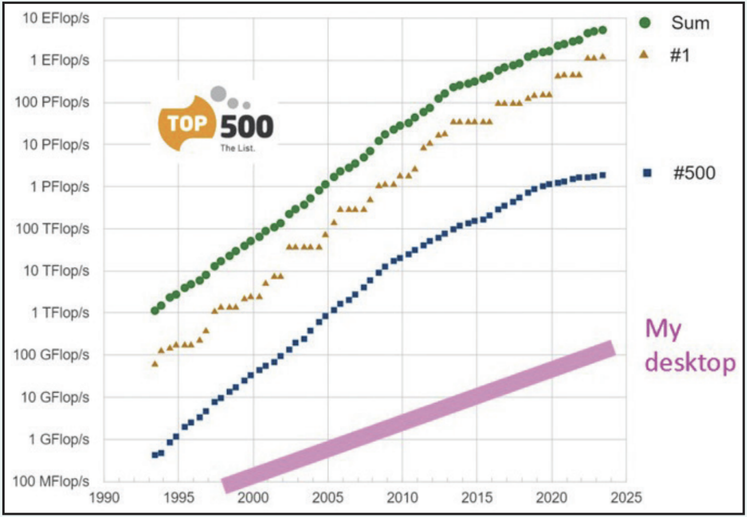

Figure 1. *Performance development from 1990 to the present day. Figure adapted from the TOP500 project: https://www.top500.org/statistics/perfdevel.*

general purpose graphics processing units

Thanks to the industrial success of video game development graphics processors became faster than general CPUs.

General Purpose Graphic Processing Units (GPGPUs) are available, capable of double floating point calculations.

Accelerations by a factor of 10 with one GPGPU are not uncommon.

Comparing electric power consumption is advantageous for GPGPUs.

Thanks to the popularity of the PC market, millions of GPUs are available – every PC has a GPU. This is the first time that massively parallel computing is feasible with a mass-market product.

Example: Actual clinical applications on magnetic resonance imaging (MRI) use some combination of PC and special hardware accelerators.

kepler versus pascal versus volta

NVIDIA Tesla K20 “Kepler” C-class Accelerator

- 2,496 CUDA cores, 2,496 = 13 SM $\times$ 192 cores/SM
- 5GB Memory at 208 GB/sec peak bandwidth
- peak performance: 1.17 TFLOPS double precision

NVIDIA Tesla P100 16GB “Pascal” Accelerator

- 3,586 CUDA cores, 3,586 = 56 SM $\times$ 64 cores/SM
- 16GB Memory at 720GB/sec peak bandwidth
- peak performance: 5.3 TFLOPS double precision

NVIDIA Tesla V100 32GB “Volta” Accelerator

- 5,120 CUDA cores, 640 Tensor cores
- 32GB Memory at 870GB/sec peak bandwidth
- peak performance: 7.9 TFLOPS double precision

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the programming model

Programming model: Single Instruction Multiple Data (SIMD).

- Data parallelism: blocks of threads read from memory, execute the same instruction(s), write to memory.
- Massively parallel: need 10,000 threads for full occupancy.

The code that runs on the GPU is defined in a function, the kernel.

A kernel launch

- creates a grid of blocks, and
- each block has one or more threads.

The organization of the grids and blocks can be 1D, 2D, or 3D.

During the running of the kernel:

- Threads in the same block are executed simultaneously.
- Blocks are scheduled by the streaming multiprocessors.

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OpenCL: Open Computing Language

OpenCL, the Open Computing Language, is the open standard for parallel programming of heterogeneous system.

OpenCL is maintained by the Khronos Group — a not for profit industry consortium creating open standards for the authoring and acceleration of parallel computing, graphics, dynamic media, computer vision and sensor processing on a wide variety of platforms and devices — with home page at `www.khronos.org`.

Another related standard is OpenGL (`www.opengl.org`), the open standard for high performance graphics.

B.R. Gaster, L. Howes, D.R. Kaeli, P. Mistry, D. Schaa: *Heterogeneous Computing with OpenCL.* Revised OpenCL 1.2 Edition. Elsevier 2013.

about OpenCL

The development of OpenCL was initiated by Apple.

Many aspects of OpenCL are familiar to a CUDA programmer because of similarities with data parallelism and complex memory hierarchies.

OpenCL offers a more complex platform and device management model to reflect its support for multiplatform and multivendor portability.

OpenCL implementations exist for AMD ATI and NVIDIA GPUs as well as x86 CPUs.

The code in this lecture ran on an Intel Iris Graphics 6100, the graphics card of a MacBook Pro.

The current version for python3 is installed on pascal.math.uic.edu.

about PyOpenCL

A. Klöckner, N. Pinto, Y. Lee, B. Catanzaro, P. Ivanov, and A. Fasih: **PyCUDA and PyOpenCL: A scripting-based approach to GPU run-time code generation.** *Parallel Computing*, 38(3):157–174, 2012.

Same benefits of PyOpenCL as PyCUDA:

- takes care of a lot of “boiler plate” code;
- focus on the kernel, with numpy typing.

Instead of a programming model tied to a single hardware vendor’s products, open standards enable portable software frameworks for heterogeneous platforms.

a sanity check on the installation

PyOpenCL can be installed with pip, just do

```
$ pip3 install pyopencl
```

Then we launch python:

```
$ python3
>>> import pyopencl
>>> from pyopencl.tools import get_test_platforms_and_devices
>>> get_test_platforms_and_devices()
[(<pyopencl.Platform 'NVIDIA CUDA' at 0x21dd450>, \
[<pyopencl.Device 'Tesla P100-PCIE-16GB' on 'NVIDIA CUDA' \
at 0x219cd00>, \
<pyopencl.Device 'Quadro K420' on 'NVIDIA CUDA' at 0x220df10>]
>>>
```

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data parallelism

Many applications process large amounts of data.

Data parallelism refers to the property where many arithmetic operations can be safely performed on the data simultaneously.

Consider the multiplication of matrices A and B: $C = A \cdot B$, with

$$A = [a_{i,j}] \in \mathbb{R}^{n \times m}, \quad B = [b_{i,j}] \in \mathbb{R}^{m \times p}, \quad C = [c_{i,j}] \in \mathbb{R}^{n \times p}.$$

$c_{i,j}$ is the inner product of the ith row of A with the jth column of B:

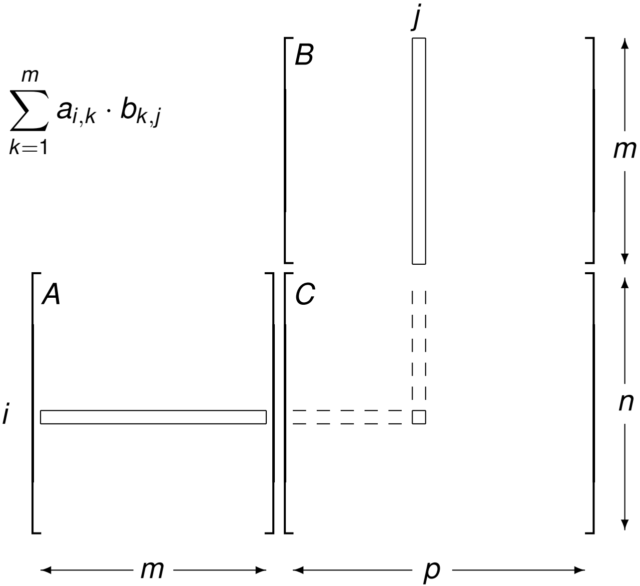
$$c_{i,j} = \sum_{k=1}^{m} a_{i,k} \cdot b_{k,j}.$$

All $c_{i,j}$'s can be computed independently from each other.

For $n = m = p = 1,000$ we have 1,000,000 inner products.

data parallelism in matrix multiplication

$$c_{i,j} = \sum_{k=1}^{m} a_{i,k} \cdot b_{k,j}$$



matrix matrix multiplication

Our running example will be the multiplication of two matrices:

```
$ python matmatmulocl.py
matrix A:
[[ 0.  0.  1.  1.]
 [ 1.  1.  1.  1.]
 [ 1.  1.  1.  1.]]
matrix B:
[[ 1.  1.  0.  1.  1.]
 [ 1.  1.  1.  0.  1.]
 [ 0.  0.  1.  0.  1.]
 [ 1.  0.  1.  0.  1.]]
multiplied A*B:
[[ 1.  0.  2.  0.  2.]
 [ 3.  2.  3.  1.  4.]
 [ 3.  2.  3.  1.  4.]]
$
```

the script matmatmulocl.py

```
import pyopencl as cl
import numpy as np

import os
os.environ['PYOPENCL_COMPILER_OUTPUT'] = '1'
# context: 0 for Apple, 1 for the graphics card
os.environ['PYOPENCL_CTX'] = '0:1'

(n, m, p) = (3, 4, 5)

a = np.random.randint(2, size=(n*m))
b = np.random.randint(2, size=(m*p))
c = np.zeros((n*p), dtype=np.float32)

a = a.astype(np.float32)
b = b.astype(np.float32)
```

context, queue, and buffers

```
ctx = cl.create_some_context()
queue = cl.CommandQueue(ctx)

mf = cl.mem_flags
a_buf = cl.Buffer\
   (ctx, mf.READ_ONLY | mf.COPY_HOST_PTR, hostbuf=a)
b_buf = cl.Buffer\
   (ctx, mf.READ_ONLY | mf.COPY_HOST_PTR, hostbuf=b)
c_buf = cl.Buffer(ctx, mf.WRITE_ONLY, c.nbytes)
```

defining the kernel

```
prg = cl.Program(ctx, """
    __kernel void multiply(ushort n,
    ushort m, ushort p, __global float *a,
    __global float *b, __global float *c)
    {
      int gid = get_global_id(0);
      c[gid] = 0.0f;
      int rowC = gid/p;
      int colC = gid%p;
      __global float *pA = &a[rowC*m];
      __global float *pB = &b[colC];
      for(int k=0; k<m; k++)
      {
         pB = &b[colC+k*p];
         c[gid] += (*(pA++))*(*pB);
      }
    }
    """).build()
```

executing the program

```
prg.multiply(queue, c.shape, None,
             np.uint16(n), np.uint16(m), np.uint16(p),
             a_buf, b_buf, c_buf)

a_mul_b = np.empty_like(c)
cl.enqueue_copy(queue, a_mul_b, c_buf)
# Python 3 version of print statements
print("matrix A:")
print(a.reshape(n, m))
print("matrix B:")
print(b.reshape(m, p))
print("multiplied A*B:")
print(a_mul_b.reshape(n, p))
```

running the NVIDIA OpenCL SDK

```
$ python matmatmulsdk.py
GPU push+compute+pull total [s]: 0.0844735622406
GPU push [s]: 0.00011818313599
GPU pull [s]: 0.0014328956604
GPU compute (host-timed) [s]: 0.0829288482666
GPU compute (event-timed) [s]:  0.08261928

GFlops/s: 24.6958693242

GPU==CPU: True

CPU time (s) 0.0495228767395

GPU speedup (with transfer):  0.586252969875
GPU speedup (without transfer):  0.59717309205
$
```

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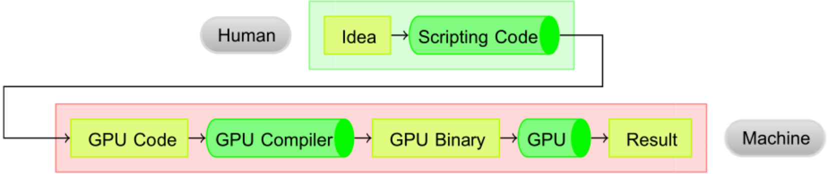
about PyCUDA

A. Klöckner, N. Pinto, Y. Lee, B. Catanzaro, P. Ivanov, and A. Fasih: **PyCUDA and PyOpenCL: A scripting-based approach to GPU run-time code generation.** *Parallel Computing*, 38(3):157–174, 2012.

The operating principle of GPU code generation:



PyCUDA is installed on `pascal.math.uic.edu`.

checking the installation on `pascal`

```
$ python
>>> import pycuda
>>> import pycuda.autoinit
>>> from pycuda.tools import make_default_context
>>> c = make_default_context()
>>> d = c.get_device()
>>> d.name()
'Tesla P100-PCIE-16GB'
>>>
```

checking the installation on a windows laptop

```
> pytthon
Python 3.10.10 | packaged by Anaconda, Inc.  |
(main, Mar 21 2023, 18:39:17)
[MSC v.1916 64 bit (AMD64)] on win32
>>> import pycuda
>>> import pycuda.autoinit
>>> from pycuda.tools import make_default_context
>>> c = make_default_context()
>>> d = c.get_device()
>>> d.name()
'NVIDIA GeForce RTX 4080 Laptop GPU'
>>>
```

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running the script

We multipy an n-by-m matrix with an m-by-p matrix with a two dimensional grid of $n \times p$ threads. For testing we use 0/1 matrices.

```
$ python matmatmul.py
matrix A:
[[ 0.   0.   1.   0.]
 [ 0.   0.   1.   1.]
 [ 0.   1.   1.   0.]]
matrix B:
[[ 1.   1.   0.   1.   1.]
 [ 1.   0.   1.   0.   0.]
 [ 0.   0.   1.   1.   0.]
 [ 0.   0.   1.   1.   0.]]
multiplied A*B:
[[ 0.   0.   1.   1.   0.]
 [ 0.   0.   2.   2.   0.]
 [ 1.   0.   2.   1.   0.]]
$
```

headers and type declarations

```
import pycuda.driver as cuda
import pycuda.autoinit
from pycuda.compiler import SourceModule
import numpy

(n, m, p) = (3, 4, 5)

n = numpy.int32(n)
m = numpy.int32(m)
p = numpy.int32(p)

# a = numpy.random.randn(n, m)
# b = numpy.random.randn(m, p)
a = numpy.random.randint(2, size=(n, m))
b = numpy.random.randint(2, size=(m, p))
c = numpy.zeros((n, p), dtype=numpy.float32)
```

allocation and copy from host to device

```
a_gpu = cuda.mem_alloc(a.size * a.dtype.itemsize)
b_gpu = cuda.mem_alloc(b.size * b.dtype.itemsize)
c_gpu = cuda.mem_alloc(c.size * c.dtype.itemsize)

cuda.memcpy_htod(a_gpu, a)
cuda.memcpy_htod(b_gpu, b)
```

definition of the kernel

```
mod = SourceModule("""
    __global__ void multiply
      ( int n, int m, int p,
        float *a, float *b, float *c )
    {
        int idx = p*threadIdx.x + threadIdx.y;

        c[idx] = 0.0;
        for(int k=0; k<m; k++)
           c[idx] += a[m*threadIdx.x+k]
                    *b[threadIdx.y+k*p];
    }
    """)
```

launching the kernel

```
func = mod.get_function("multiply")
func(n, m, p, a_gpu, b_gpu, c_gpu, \
     block=(numpy.int(n), numpy.int(p), 1), \
     grid=(1, 1), shared=0)

cuda.memcpy_dtoh(c, c_gpu)

print("matrix A:")
print(a)
print("matrix B:")
print(b)
print("multiplied A*B:")
print(c)
```

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about CUDA.jl

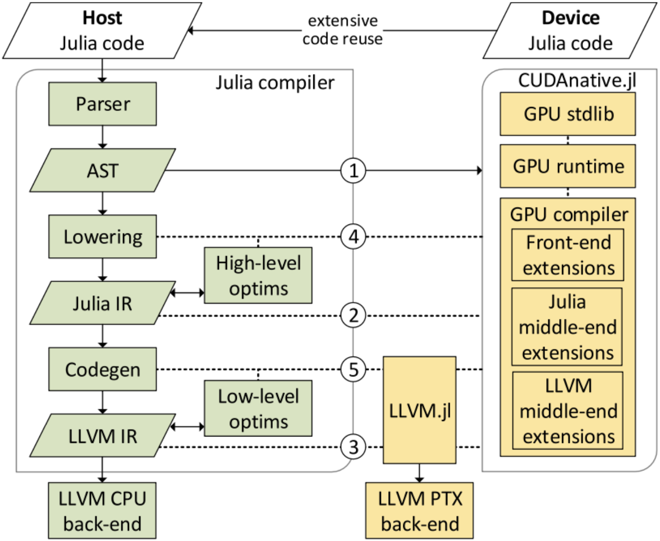
T. Besard, C. Foket, and B. De Sutter:
Effective Extensible Programming: Unleashing Julia on GPUs.
IEEE Transactions on Parallel and Distributed Systems,
Vol. 30, No. 4, pages 827–841, 2019.

Installation:

1. Verify that the computer has an NVIDIA GPU
   and that the CUDA Software Development Kit is installed.
2. Type `using CUDA` to install in Julia.
3. Type `]` to get the `pkg>` prompt and type `test CUDA`.
4. Be patient.

`https://juliagpu.org` is the site of JuliaGPU, the organization to unify the many packages for programming GPUs in Julia.

the compilation process for Julia GPU code



From Besard et al., 2019.

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a first kernel

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

```
using CUDA
using Test

function gpu_add1!(y, x)
    for i = 1:length(y)
        @inbounds y[i] += x[i]
    end
    return nothing
end

N = 2^20              # adding one million Float32 numbers
x_d = CUDA.fill(1.0f0, N) # stored on GPU filled with 1.0
y_d = CUDA.fill(2.0f0, N) # stored on GPU filled with 2.0

fill!(y_d, 2)
@cuda gpu_add1!(y_d, x_d)
result = (@test all(Array(y_d) .== 3.0f0))
println(result)
```

running at the command prompt

The code on the previous slide is saved in `gpuadd.jl`.

Type `julia gpuadd.jl` at the command prompt.

`Test Passed` is the result.

vendor agnostic GPU computing

The following is copied from the github page.

KernelAbstractions (KA) is a package that enables you

- to write GPU-like kernels
- targetting different execution backends.

KA is intended to be a minimal and performant library that explores ways to write heterogeneous code.

Currently, the following backends are supported:

- NVIDIA CUDA
- AMD ROCm
- Intel oneAPI
- Apple Metal

Summary and Exercises

We can accelerate our computations in Python.

Exercises :

1. Investigate the capabilities of the graphics card on your computer. Install PyOpenCL and/or PyCUDA, depending on the type of GPU.
2. Examine the possibilities to extend the code for matrix multiplication to work with 3-dimensional matrices.
3. Compare the theoretical peak performance on the CPU and GPU on your computer.
4. For sufficiently large enough dimension of the matrices, compare the performance of the matrix matrix multiplication on the CPU and GPU on your computer.