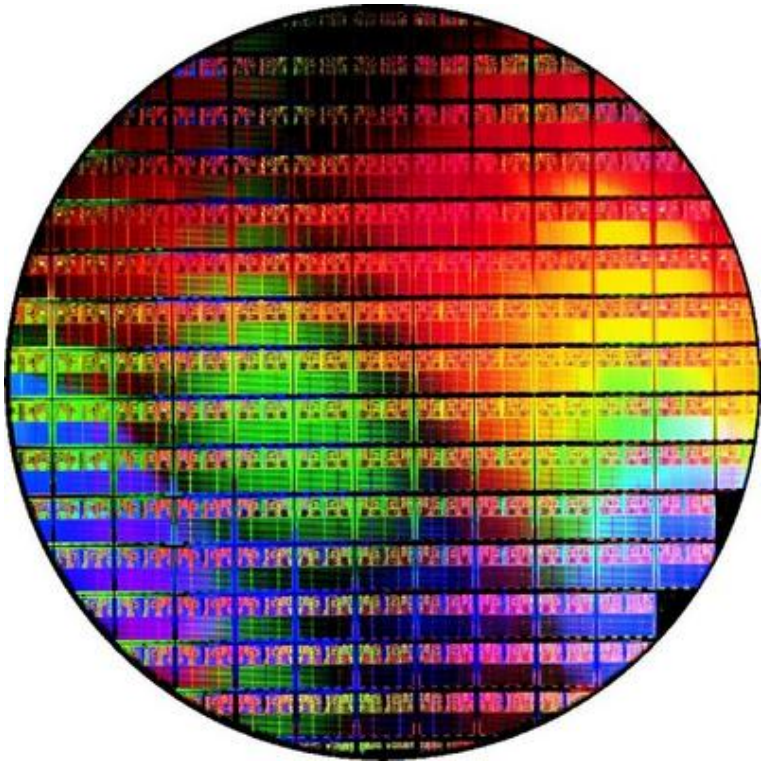
nclab
Public Computing



GPU Computing with PyCUDA

www.nclab.com

Contents

1 GPU, CUDA, and PyCUDA

Graphical Processing Unit (GPU) computing belongs to the newest trends in Computational Science worldwide. The reason for its attractivity is mainly the high computing power of modern graphics cards. For example, the Nvidia Tesla C2070 GPU computing processor shown in Fig. 1 has 448 cores and 6 GB of memory, with peak performance of 1030 and 515 GFlops in single and double precision arithmetic, respectively.

Figure 1: Nvidia Tesla C2070.

These cards are still quite expensive – the card shown in Fig. 1 costs around $2,000 as of March 2012. Therefore, GPU computing may not be easily accessible to all who would like to experiment with it. This was the main reason why we decided to include GPU programming in NCLab.

Compute Unified Device Architecture (CUDA) is a parallel computing architecture developed by Nvidia for graphics processing. CUDA is the computing engine in Nvidia GPUs that is accessible to software developers through variants of industry standard programming languages.

CUDA bindings are available in many high-level languages including Fortran, Haskell, Lua, Ruby, Python and others. We are specifically interested in Python bindings (PyCUDA) since Python is the main programming language of NCLab. PyCUDA was written by Andreas Klöckner (Courant Institute of Mathematical Sciences, New York University).

2 PyCUDA in NCLab

In order to make the most of this tutorial, we invite the reader to create an account in NCLab and log in. More instructions on how to do this are given at the beginning of the introductory tutorial "Meet Your New Graphing Calculator" that is available in PDF via a link on NCLab home page `http://nclab.com`.

After login, you will see a desktop with several icons on it, as shown in Fig. 2.

2.1 Cloning Displayed Projects

All examples that we are going to work with in the following are also available as Displayed Projects. This means that you can clone them by launching the File Manager, going to the *Project* menu, and clicking on

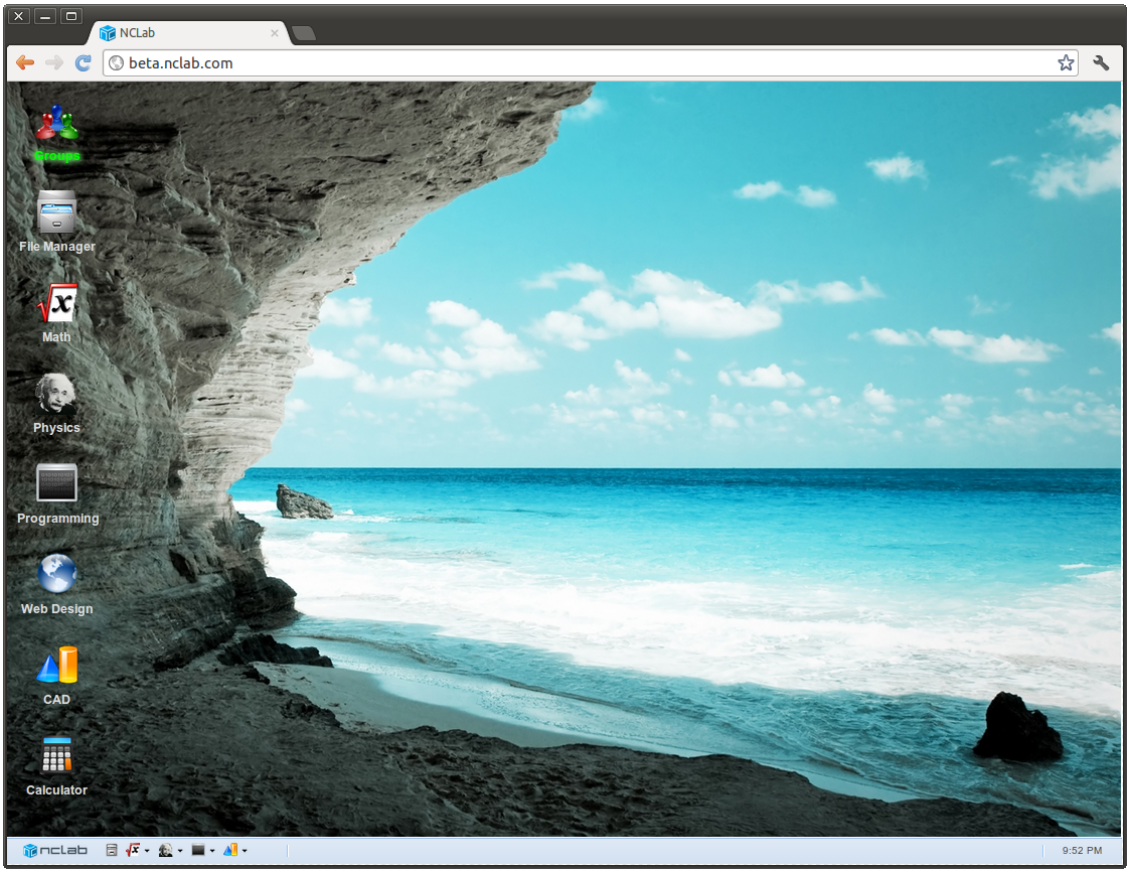


Figure 2: NCLab desktop after login.

Clone. This will launch a window with many displayed projects from various areas of programming, math and computing. Look for projects whose names start with "PyCUDA - Tutorial". After you locate a project that you would like to clone, click on it, and then click on the button *Clone* at the bottom of the window. This will create exact copy of that project in your account, and you can open it by clicking on it in the File Manager. You can change the project in any way you like, the changes will not affect the original Displayed Project.

2.2 Launching a new PyCUDA project

Alternatively, you can start by launching an empty PyCUDA project through *Programming* → *PyCUDA*, as shown in Fig. 3.

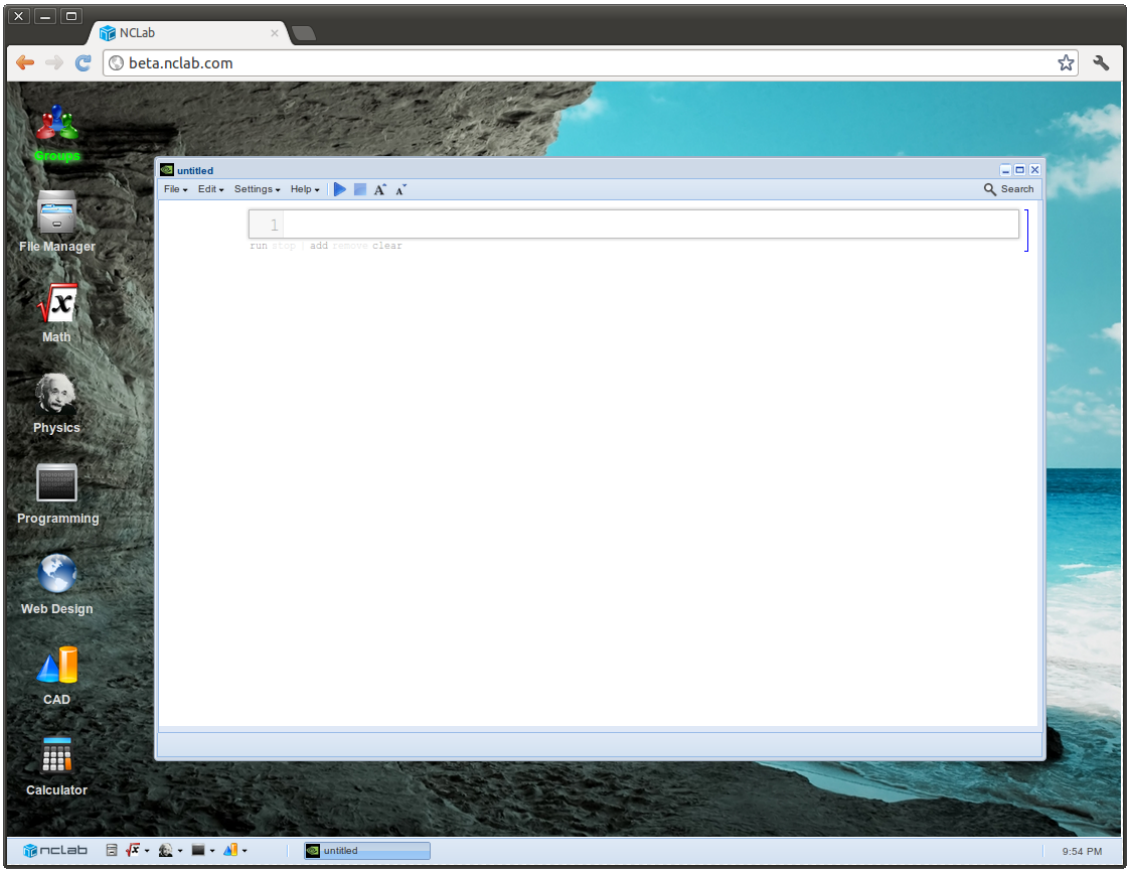


Figure 3: Launching a new PyCUDA project.

3 Hello World!

Let us demonstrate the PyCUDA workflow on a very simple example that generates a 4x4 random array on the CPU, sends it to the GPU where all entries are doubled in parallel, and then the result is sent back to the CPU and displayed.

3.1 Import and initialize PyCUDA

Either clone the displayed project "PyCUDA - Tutorial - 01" or type the following code into a newly opened PyCUDA project:

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

Here, `pycuda.autoinit` serves for automatic initialization, context creation, and cleanup. The `SourceModule` is where a (usually short) C-like code for the GPU is to be written. More about this will be said in a moment.

3.2 Generate your data

Numpy arrays (large matrices) are the most frequently used data type to be transferred to a GPU. So, let us import Numpy and generate a 4x4 random array:

```
import numpy
a = numpy.random.randn(4, 4)
```

3.3 Convert your data to single precision if needed

The array created in Step 2 contains double precision numbers and the GPU units in NCLab can process them (in general, older units cannot). However, if accuracy does not matter so much and we want this job done faster, we can convert the double precision numbers into single precision anyway:

```
a = a.astype(numpy.float32)
```

3.4 Transfer your data to GPU

First we need to allocate memory on the device using the CUDA driver:

```
a_gpu = cuda.mem_alloc(a.nbytes)
```

Then we can transfer the Numpy array to the device:

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

Notably, the array `a_gpu` is one-dimensional and on the device we need to handle it as such.

3.5 Compile your parallel C code and load it on the GPU

To keep the Hello World example simple, let us write a program that just doubles each entry of the (now one-dimensional) array:

```
mod = SourceModule("""
  __global__ void doublify(float *a)
  {
    int idx = threadIdx.x + threadIdx.y * 4;
    a[idx] *= 2;
  }
  """)
```

The thing that makes this code interesting is that *it only gets executed once* – in 16 different threads. Both the variables `threadIdx.x` and `threadIdx.y` contain indices between 0 and 3, and the pair is different for each thread.

3.6 Call your function

The code from Step 5 is compiled with the `nvcc` compiler automatically. If there are no errors, we can obtain a pointer to the compiled function:

```
func = mod.get_function("doublify")
```

Then we can call it with `a_gpu` as the argument, and the block size of 4x4:

```
func(a_gpu, block = (4, 4, 1))
```

3.7 Fetch your results from the GPU

To fetch the result, first we create an empty array of the same dimensions as the original array `a`:

```
a_doubled = numpy.empty_like(a)
```

Last, we get the result from the GPU:

```
cuda.memcpy_dtoh(a_doubled, a_gpu)
```

This is it! Now you can start writing your own applications.

4 Useful Simplifications

4.1 Using the driver's InOut() function

The creation of the auxiliary array `a_gpu` can be avoided if we do not mind overwriting the original array `a`:

```
func(cuda.InOut(a), block=(4, 4, 1))
```

4.2 Using GPUArray

The above code becomes much simpler and shorter using `pycuda.gpuarray`:

```
import pycuda.gpuarray as gpuarray
import pycuda.driver as cuda
import pycuda.autoinit
import numpy

a_gpu = gpuarray.to_gpu(numpy.random.randn(4, 4))
print "a_gpu ="
print a_gpu

a_doubled = (2*a_gpu).get()
print
print "a_doubled ="
print a_doubled
```

In the rest of the tutorial we will go through diverse examples where you will be able to catch some additional tips and tricks for your specific applications of interest.

5 Examples

All following examples can be cloned via the Project → Clone menu. We do not copy the codes here as they are well commented, but an overview of interesting features of each example is given.

5.1 Obtain GPU Card Parameters

This example shows how to obtain the number of GPU units found in your hardware, and their types and parameters.

5.2 Using GPU to Generate Random Data

This example show how to generate random numbers on the GPU using the `curandom` module, and also how to print them nicely using Matplotlib.

5.3 Fill GPU with Zeros

This example shows how to determine the size of free and total memory on the GPU via `cuda.mem_get_info()`, and how to fill the free memory with zeros.

5.4 Doubling an Array

This is a repetition, in a more concise form, of the Introductory Course from Section 3.

5.5 Linear Combination (with ElementwiseKernel)

Evaluating involved expressions on GPUArray instances can be somewhat inefficient, because a new temporary is created for each intermediate result. The functionality in the module pycuda.elementwise contains tools to help generate kernels that evaluate multi-stage expressions on one or several operands in a single pass. Usage:

```
class pycuda.elementwise.ElementwiseKernel(arguments, operation,
      name="kernel", keep=False, options=[], preamble="")
```

This generates a kernel that takes a number of scalar or vector arguments and performs the scalar operation on each entry of its arguments, if that argument is a vector.

The first argument `arguments` of `ElementwiseKernel()` is specified as a string formatted as a C argument list. The second argument `operation` is specified as a C assignment statement, without a semicolon. Vectors in `operation` should be indexed by the variable i. The argument `name` specifies the name under which the kernel is compiled, `keep` and `options` are passed unmodified to `pycuda.compiler.SourceModule`.

The argument `preamble` specifies some source code that is included before the elementwise kernel specification. You may use this to include other files and/or define functions that are used by operation.

5.6 Multiplying Two Real Arrays (without ElementwiseKernel)

This example shows standard multiplication of two randomly generated arrays without employing `ElementwiseKernel`.

5.7 Multiplying Two Complex Arrays (with ElementwiseKernel)

This example shows the multiplication of two complex arrays using `ElementwiseKernel`.

5.8 Matrix Multiplication (Using a Single Block of Threads)

This example multiples two square matrices together using a single block of threads and global memory only. Each thread computes one element of the resulting matrix.

5.9 Matrix Multiplication (Tiled)

This example multiples two square matrices together using multiple blocks and shared memory. Each thread block is assigned a "tile" of the resulting matrix and is responsible for generating the elements in that tile. Each thread in a block computes one element of the tile.

5.10 Using Structs

This example shows how to use structs, doubling two real arrays for illustration.

5.11 Using C++ Templates

This example shows how to use C++ templates in PyCUDA. You can use them but you must allow name mangling to be used for the templates in order to let nvcc compile them.

5.12 Simple Speed Test

Very simple speed testing code. This shows you how to run a loop over sin() using different methods with a note of the time each method takes. For the GPU this uses SourceModule, ElementwiseKernel, GPUArray. For the CPU this uses Numpy.

5.13 Measuring GPU Array Speed

That's what this example does!

5.14 Convolution

This sample implements a separable convolution filter of a 2D signal with a Gaussian kernel.

5.15 Matrix Transpose

Matrix Transpose on a GPU.

5.16 Fast Fourier Transform Using PyFFT

This code does the fast Fourier transform on 2d data of any size. It uses the transpose split method to achieve larger sizes and to use multiprocessing. The number of parts the input image is to be split into, is decided by the user based on the available GPU memory and CPU processing cores.

5.17 Optimized Matrix Multiplication Using Cheetah

PyCuda Optimized Matrix Multiplication Template Meta-programming Example using Cheetah.

5.18 Using Codepy

This example shows how to use Codepy, a C/C++ metaprogramming toolkit for Python developed by Andreas Klöckner. It handles two aspects of native-code metaprogramming: (1) Generating C/C++ source code and (2) Compiling this source code and dynamically loading it into the Python interpreter.

Both capabilities are meant to be used together, but also work on their own. In particular, the code generation facilities work well in conjunction with PyCuda. Dynamic compilation and linking are so far only supported in Linux with the GNU toolchain.

5.19 Using Jinja2 Templates

Jinja2 is a full featured template engine for Python. It has full unicode support and an optional integrated sandboxed execution environment.

5.20 Rotating an Image

This example rotates an image on the GPU, using the Image library.

5.21 Kernel Concurrency Test

Demonstrates concurrent execution of multiple (2) kernels, using PyCuda. To "prove" that both kernels are executing at the same time, simply comment out line 63. This should break concurrency and the runtime should be doubled.

5.22 Select to List

Generate an array of random numbers between 0 and 1. List the indices of those numbers that are greater than a given limit.

5.23 Multiple Threads

Derived from a test case by Chris Heuser. Also see FAQ about PyCUDA and threads.

5.24 Mandelbrot Fractal

This example renders a Mandelbrot fractal using GPU.

5.25 Sparse Solve

Sparse matrix solver on the GPU.

5.26 Sobel Filter

Python port of SobelFilter example in NVIDIA CUDA C SDK. Shows how opengl interoperability works.

5.27 Scalar Multiplication

This is another speed test.